A. Bahmani and F. Mueller, “Scalable performance analysis of exascale MPI programs through signature-based clustering algorithms”, *Proceedings of the 28th ACM international conference on Supercomputing*. ACM, Jun. 10, 2014. doi: 10.1145/2597652.2597676.  
  
A. Bahmani and F. Mueller, “ACURDION: An adaptive clustering-based algorithm for tracing large-scale MPI applications”, *2015 IEEE International Conference on Big Data (Big Data)*. IEEE, Oct. 2015. doi: 10.1109/bigdata.2015.7363823.  
  
K. B. Ferreira, K. Pedretti, R. Brightwell, P. G. Bridges, D. Fialaand F. Mueller, “Evaluating operating system vulnerability to memory errors”, *Proceedings of the 2nd International Workshop on Runtime and Operating Systems for Supercomputers*. ACM, Jun. 29, 2012. doi: 10.1145/2318916.2318930.  
  
D. Fiala, “Detection and Correction of Silent Data Corruption for Large-Scale High-Performance Computing”, *2011 IEEE International Symposium on Parallel and Distributed Processing Workshops and Phd Forum*. IEEE, May 2011. doi: 10.1109/ipdps.2011.379.  
  
D. Fiala, K. B. Ferreira, F. Muellerand C. Engelmann, “A Tunable, Software-Based DRAM Error Detection and Correction Library for HPC”, *Euro-Par 2011: Parallel Processing Workshops*. Springer Berlin Heidelberg, pp. 251–261, 2012. doi: 10.1007/978-3-642-29740-3\_29.  
  
D. Fiala, F. Mueller, C. Engelmann, R. Riesen, K. Ferreiraand R. Brightwell, “Detection and correction of silent data corruption for large-scale high-performance computing”, *2012 International Conference for High Performance Computing, Networking, Storage and Analysis*. IEEE, Nov. 2012. doi: 10.1109/sc.2012.49.  
  
A. Rezaei, G. Coviello, C.-H. Li, S. Chakradharand F. Mueller, “Snapify”, *Proceedings of the 23rd international symposium on High-performance parallel and distributed computing*. ACM, Jun. 23, 2014. doi: 10.1145/2600212.2600215.  
  
A. Rezaei and F. Mueller, “Sustained Resilience via Live Process Cloning”, *2013 IEEE International Symposium on Parallel & Distributed Processing, Workshops and Phd Forum*. IEEE, May 2013. doi: 10.1109/ipdpsw.2013.224.  
  
A. Rezaei and F. Mueller, “DINO: Divergent Node Cloning for Sustained Redundancy in HPC”, *2015 IEEE International Conference on Cluster Computing*. IEEE, Sep. 2015. doi: 10.1109/cluster.2015.36.  
  
A. Saini, A. Rezaei, F. Mueller, P. Hargroveand E. Roman, “Affinity-aware checkpoint restart”, *Proceedings of the 15th International Middleware Conference on - Middleware ‘14*. ACM Press, 2014. doi: 10.1145/2663165.2663325.  
  
Y. Zhang and F. Mueller, “CuNesl: Compiling Nested Data-Parallel Languages for SIMT Architectures”, *2012 41st International Conference on Parallel Processing*. IEEE, Sep. 2012. doi: 10.1109/icpp.2012.21.  
  
K. M. Aikens, G. A. Blaisdelland A. S. Lyrintzis, “Analysis of Converging-Diverging Beveled Nozzle Jets Using Large Eddy Simulation with a Wall Model”, *53rd AIAA Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 03, 2015. doi: 10.2514/6.2015-0509.  
  
K. M. Aikens, “Equilibrium Wall Model for Large Eddy Simulations of Jets for Aeroacoustics”, *52nd Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 10, 2014. doi: 10.2514/6.2014-0180.  
  
B. Acun, P. Millerand L. V. Kale, “Variation Among Processors Under Turbo Boost in HPC Systems”, *Proceedings of the 2016 International Conference on Supercomputing*. ACM, Jun. 2016. doi: 10.1145/2925426.2926289.  
  
J. Choi, D. F. Richards, L. V. Kaleand A. Bhatele, “End-to-end performance modeling of distributed GPU applications”, *Proceedings of the 34th ACM International Conference on Supercomputing*. ACM, Jun. 29, 2020. doi: 10.1145/3392717.3392737.  
  
N. Jain, “OpenAtom: Scalable Ab-Initio Molecular Dynamics with Diverse Capabilities”, *Lecture Notes in Computer Science*. Springer International Publishing, pp. 139–158, 2016. doi: 10.1007/978-3-319-41321-1\_8.  
  
E. Meneses, X. Ni, G. Zheng, C. L. Mendesand L. V. Kale, “Using Migratable Objects to Enhance Fault Tolerance Schemes in Supercomputers”, *IEEE Transactions on Parallel and Distributed Systems*, vol. 26, no. 7. Institute of Electrical and Electronics Engineers (IEEE), pp. 2061–2074, Jul. 01, 2015. doi: 10.1109/tpds.2014.2342228.  
  
P. Cicotti and L. Carrington, “ADAMANT: Tools to Capture, Analyze, and Manage Data Movement”, *Procedia Computer Science*, vol. 80. Elsevier BV, pp. 450–460, 2016. doi: 10.1016/j.procs.2016.05.323.  
  
A. Humphrey, Q. Meng, M. Berzinsand T. Harman, “Radiation modeling using the Uintah heterogeneous CPU/GPU runtime system”, *Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment: Bridging from the eXtreme to the campus and beyond*. ACM, Jul. 16, 2012. doi: 10.1145/2335755.2335791.  
  
F. Gygi and I. Duchemin, “Efficient Computation of Hartree–Fock Exchange Using Recursive Subspace Bisection”, *Journal of Chemical Theory and Computation*, vol. 9, no. 1. American Chemical Society (ACS), pp. 582–587, Dec. 24, 2012. doi: 10.1021/ct3007088.  
  
Q. Wan, L. Spanu, G. A. Galliand F. Gygi, “Raman Spectra of Liquid Water from *Ab Initio* Molecular Dynamics: Vibrational Signatures of Charge Fluctuations in the Hydrogen Bond Network”, *Journal of Chemical Theory and Computation*, vol. 9, no. 9. American Chemical Society (ACS), pp. 4124–4130, Aug. 08, 2013. doi: 10.1021/ct4005307.  
  
Q. Wan, L. Spanu, F. Gygiand G. Galli, “Electronic Structure of Aqueous Sulfuric Acid from First-Principles Simulations with Hybrid Functionals”, *The Journal of Physical Chemistry Letters*, vol. 5, no. 15. American Chemical Society (ACS), pp. 2562–2567, Jul. 15, 2014. doi: 10.1021/jz501168p.  
  
M. Zhu, G. Wangand T. Oyana, “Parallel spatiotemporal autocorrelation and visualization system for large-scale remotely sensed images”, *The Journal of Supercomputing*, vol. 59, no. 1. Springer Science and Business Media LLC, pp. 83–103, Mar. 18, 2010. doi: 10.1007/s11227-010-0420-4.  
  
H. I. Sirikumara, J. Bohorquez-Ballenand T. Jayasekera, “Ge cages at the SiC/graphene interface: A first principles calculation”, *Journal of Crystal Growth*, vol. 393. Elsevier BV, pp. 145–149, May 2014. doi: 10.1016/j.jcrysgro.2013.11.051.  
  
K. Maheshwari, “Job and data clustering for aggregate use of multiple production cyberinfrastructures”, *Proceedings of the fifth international workshop on Data-Intensive Distributed Computing Date*. ACM, Jun. 19, 2012. doi: 10.1145/2286996.2287000.  
  
A. Amritkar, D. Tafti, R. Liu, R. Kufrinand B. Chapman, “OpenMP parallelism for fluid and fluid-particulate systems”, *Parallel Computing*, vol. 38, no. 9. Elsevier BV, pp. 501–517, Sep. 2012. doi: 10.1016/j.parco.2012.05.005.  
  
A. Amritkar, D. Tafti, R. Liu, R. Kufrinand B. Chapman, “OpenMP parallelism for fluid and fluid-particulate systems”, *Parallel Computing*, vol. 38, no. 9. Elsevier BV, pp. 501–517, Sep. 2012. doi: 10.1016/j.parco.2012.05.005.  
  
Z. Bai and X. Zhong, “New very high-order upwind multi-layer compact (MLC) schemes with spectral-like resolution for flow simulations”, *Journal of Computational Physics*, vol. 378. Elsevier BV, pp. 63–109, Feb. 2019. doi: 10.1016/j.jcp.2018.10.049.  
  
Z. Bai and X. Zhong, “Very High-Order Upwind Multi-Layer Compact (MLC) Schemes with Spectral-Like Resolution II: Two-Dimensional Case”, *AIAA Scitech 2019 Forum*. American Institute of Aeronautics and Astronautics, Jan. 06, 2019. doi: 10.2514/6.2019-1398.  
  
C. L. Haley and X. Zhong, “Direct Numerical Simulation of Hypersonic Flow over a Blunt Cone with Axisymmetric Isolated Roughness”, *47th AIAA Fluid Dynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 02, 2017. doi: 10.2514/6.2017-4514.  
  
C. L. Haley and X. Zhong, “Mode F/S Wave Packet Interference And Acoustic-like Emissions in a Mach 8 Flow Over a Cone”, *AIAA Scitech 2020 Forum*. American Institute of Aeronautics and Astronautics, Jan. 05, 2020. doi: 10.2514/6.2020-1579.  
  
S. He and X. Zhong, “Hypersonic Boundary Layer Receptivity over a Blunt Cone to Freestream Pulse Disturbances”, *AIAA Scitech 2020 Forum*. American Institute of Aeronautics and Astronautics, Jan. 05, 2020. doi: 10.2514/6.2020-2057.  
  
C. P. Knisely and X. Zhong, “An Investigation of Sound Radiation by Supersonic Unstable Modes in Hypersonic Boundary Layers”, *47th AIAA Fluid Dynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 02, 2017. doi: 10.2514/6.2017-4516.  
  
C. P. Knisely and X. Zhong, “The Supersonic Mode and the Role of Wall Temperature in Hypersonic Boundary Layers with Thermochemical Nonequilibrium Effects”, *2018 Fluid Dynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 24, 2018. doi: 10.2514/6.2018-3218.  
  
C. P. Knisely and X. Zhong, “Supersonic Modes in Hot-Wall Hypersonic Boundary Layers with Thermochemical Nonequilibrium Effects”, *2018 AIAA Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 07, 2018. doi: 10.2514/6.2018-2085.  
  
C. P. Knisely and X. Zhong, “Significant Supersonic Modes and the Wall Temperature Effect in Hypersonic Boundary Layers”, *AIAA Journal*, vol. 57, no. 4. American Institute of Aeronautics and Astronautics (AIAA), pp. 1552–1566, Apr. 2019. doi: 10.2514/1.j057775.  
  
J. T. Gerig, “Toward a Molecular Dynamics Force Field for Simulations of 40% Trifluoroethanol–Water”, *The Journal of Physical Chemistry B*, vol. 118, no. 6. American Chemical Society (ACS), pp. 1471–1480, Feb. 03, 2014. doi: 10.1021/jp408879g.  
  
Y. Chen, M. Jo, M. Mohamedand R. Xu, “Monte Carlo analysis of dynamic characteristics and high-frequency noise performances of nanoscale double-gate MOSFETs”, *International Journal of Numerical Modelling: Electronic Networks, Devices and Fields*, vol. 27, no. 1. Wiley, pp. 10–21, Mar. 04, 2013. doi: 10.1002/jnm.1886.  
  
N. Hendinejad and Q. K. Timerghazin, “Biological control of*S*-nitrosothiol reactivity: potential role of sigma-hole interactions”, *Physical Chemistry Chemical Physics*, vol. 22, no. 12. Royal Society of Chemistry (RSC), pp. 6595–6605, 2020. doi: 10.1039/c9cp06377c.  
  
V. Hosseininasab, A. C. McQuilken, A. (Gus) . Bakhoda, J. A. Bertke, Q. K. Timerghazinand T. H. Warren, “Lewis Acid Coordination Redirects S‐Nitrosothiol Signaling Output”, *Angewandte Chemie International Edition*, vol. 59, no. 27. Wiley, pp. 10854–10858, Apr. 17, 2020. doi: 10.1002/anie.202001450.  
  
S. Mirzaei, M. V. Ivanovand Q. K. Timerghazin, “Improving Performance of the SMD Solvation Model: Bondi Radii Improve Predicted Aqueous Solvation Free Energies of Ions and p*K*a Values of Thiols”, *The Journal of Physical Chemistry A*, vol. 123, no. 44. American Chemical Society (ACS), pp. 9498–9504, Jul. 18, 2019. doi: 10.1021/acs.jpca.9b02340.  
  
S. Mirzaei, D. Wang, S. V. Lindeman, Q. K. Timerghazinand R. Rathore, “Redox-Induced Molecular Actuators: The Case of Oxy-Alternate Bridged Cyclotetraveratrylene”, *Organic Letters*, vol. 21, no. 19. American Chemical Society (ACS), pp. 7987–7991, Sep. 25, 2019. doi: 10.1021/acs.orglett.9b02971.  
  
H. Vach, L. V. Ivanova, Q. K. Timerghazin, F. Jardaliand H.-L. T. Le, “A deeper insight into strain for the sila-bi[6]prismane ( Si18H12) cluster with its endohedrally trapped silicon atom, Si19H12”, *Journal of Computational Chemistry*, vol. 36, no. 28. Wiley, pp. 2089–2094, Jul. 24, 2015. doi: 10.1002/jcc.24009.  
  
H. Vach, L. V. Ivanova, Q. K. Timerghazin, F. Jardaliand H.-L. T. Le, “Metallic-like bonding in plasma-born silicon nanocrystals for nanoscale bandgap engineering”, *Nanoscale*, vol. 8, no. 42. Royal Society of Chemistry (RSC), pp. 18062–18069, 2016. doi: 10.1039/c6nr04349f.  
  
J. J. Whang, A. Lenharth, I. S. Dhillonand K. Pingali, “Scalable Data-Driven PageRank: Algorithms, System Issues, and Lessons Learned”, *Lecture Notes in Computer Science*. Springer Berlin Heidelberg, pp. 438–450, 2015. doi: 10.1007/978-3-662-48096-0\_34.  
  
A. Lenharth and K. Pingali, “Scaling Runtimes for Irregular Algorithms to Large-Scale NUMA Systems”, *Computer*, vol. 48, no. 8. Institute of Electrical and Electronics Engineers (IEEE), pp. 35–44, Aug. 2015. doi: 10.1109/mc.2015.229.  
  
I. Neft, M. Scungio, N. Culverand S. Singh, “Simulations of aerosol filtration by vegetation: Validation of existing models with available lab data and application to near-roadway scenario”, *Aerosol Science and Technology*, vol. 50, no. 9. Informa UK Limited, pp. 937–946, Jun. 28, 2016. doi: 10.1080/02786826.2016.1206653.  
  
A. Kumar and S. Balasubramanian, “Sparse representation based background subtraction in videos”, *2015 Fifth National Conference on Computer Vision, Pattern Recognition, Image Processing and Graphics (NCVPRIPG)*. IEEE, Dec. 2015. doi: 10.1109/ncvpripg.2015.7489942.  
  
K. P. Grogan and M. Ihme, “Weak and strong ignition of hydrogen/oxygen mixtures in shock-tube systems”, *Proceedings of the Combustion Institute*, vol. 35, no. 2. Elsevier BV, pp. 2181–2189, 2015. doi: 10.1016/j.proci.2014.07.074.  
  
Y. C. See and M. Ihme, “Large eddy simulation of a partially-premixed gas turbine model combustor”, *Proceedings of the Combustion Institute*, vol. 35, no. 2. Elsevier BV, pp. 1225–1234, 2015. doi: 10.1016/j.proci.2014.08.006.  
  
A. Vié, B. Franzelli, Y. Gao, T. Lu, H. Wangand M. Ihme, “Analysis of segregation and bifurcation in turbulent spray flames: A 3D counterflow configuration”, *Proceedings of the Combustion Institute*, vol. 35, no. 2. Elsevier BV, pp. 1675–1683, 2015. doi: 10.1016/j.proci.2014.06.083.  
  
H. Wu and M. Ihme, “Effects of flow-field and mixture inhomogeneities on the ignition dynamics in continuous flow reactors”, *Combustion and Flame*, vol. 161, no. 9. Elsevier BV, pp. 2317–2326, Sep. 2014. doi: 10.1016/j.combustflame.2014.02.007.  
  
G. Ruan and B. Plale, “Horme: Random Access Big Data Analytics”, *2016 IEEE International Conference on Cluster Computing (CLUSTER)*. IEEE, Sep. 2016. doi: 10.1109/cluster.2016.27.  
  
C. J. Azevedo, “Early CNS neurodegeneration in radiologically isolated syndrome”, *Neurology - Neuroimmunology Neuroinflammation*, vol. 2, no. 3. Ovid Technologies (Wolters Kluwer Health), p. e102, Apr. 09, 2015. doi: 10.1212/nxi.0000000000000102.  
  
G. Andrade, R. Ferreira, G. Teodoro, L. Rocha, J. H. Saltzand T. Kurc, “Efficient Execution of Microscopy Image Analysis on CPU, GPU, and MIC Equipped Cluster Systems”, *2014 IEEE 26th International Symposium on Computer Architecture and High Performance Computing*. IEEE, Oct. 2014. doi: 10.1109/sbac-pad.2014.15.  
  
W. Barreiros, G. Teodoro, T. Kurc, J. Kong, A. C. M. A. Meloand J. Saltz, “Parallel and Efficient Sensitivity Analysis of Microscopy Image Segmentation Workflows in Hybrid Systems”, *2017 IEEE International Conference on Cluster Computing (CLUSTER)*. IEEE, Sep. 2017. doi: 10.1109/cluster.2017.28.  
  
J. Gomes, A. C. M. A. de Melo, J. Kong, T. Kurc, J. H. Saltzand G. Teodoro, “Cooperative and out-of-core execution of the irregular wavefront propagation pattern on hybrid machines with Intel®Xeon Phi™”, *Concurrency and Computation: Practice and Experience*, vol. 30, no. 14. Wiley, p. e4425, Jan. 24, 2018. doi: 10.1002/cpe.4425.  
  
J. M. Gomes, G. Teodoro, A. De Melo, J. Kong, T. Kurcand J. H. Saltz, “Efficient Irregular Wavefront Propagation Algorithms on Intel(R) Xeon Phi(TM)”, *2015 27th International Symposium on Computer Architecture and High Performance Computing (SBAC-PAD)*. IEEE, Oct. 2015. doi: 10.1109/sbac-pad.2015.13.  
  
T. Kurc, “Scalable analysis of Big pathology image data cohorts using efficient methods and high-performance computing strategies”, *BMC Bioinformatics*, vol. 16, no. 1. Springer Science and Business Media LLC, Dec. 2015. doi: 10.1186/s12859-015-0831-6.  
  
A. Lucchesi, A. C. Drummondand G. Teodoro, “High-performance IP lookup using Intel Xeon Phi: a Bloom filters based approach”, *Journal of Internet Services and Applications*, vol. 9, no. 1. Sociedade Brasileira de Computacao - SB, Feb. 19, 2018. doi: 10.1186/s13174-017-0075-y.  
  
G. Teodoro, T. Kurc, G. Andrade, J. Kong, R. Ferreiraand J. Saltz, “Application performance analysis and efficient execution on systems with multi-core CPUs, GPUs and MICs: a case study with microscopy image analysis”, *The International Journal of High Performance Computing Applications*, vol. 31, no. 1. SAGE Publications, pp. 32–51, Jul. 27, 2016. doi: 10.1177/1094342015594519.  
  
G. Teodoro, “Algorithm sensitivity analysis and parameter tuning for tissue image segmentation pipelines”, *Bioinformatics*. Oxford University Press (OUP), p. btw749, Jan. 05, 2017. doi: 10.1093/bioinformatics/btw749.  
  
G. Teodoro, “Region templates: Data representation and management for high-throughput image analysis”, *Parallel Computing*, vol. 40, no. 10. Elsevier BV, pp. 589–610, Dec. 2014. doi: 10.1016/j.parco.2014.09.003.  
  
J. Saltz, “Spatial Organization and Molecular Correlation of Tumor-Infiltrating Lymphocytes Using Deep Learning on Pathology Images”, *Cell Reports*, vol. 23, no. 1. Elsevier BV, pp. 181–193.e7, Apr. 2018. doi: 10.1016/j.celrep.2018.03.086.  
  
C. P. Stone, A. T. Alfermanand K. E. Niemeyer, “Accelerating finite-rate chemical kinetics with coprocessors: Comparing vectorization methods on GPUs, MICs, and CPUs”, *Computer Physics Communications*, vol. 226. Elsevier BV, pp. 18–29, May 2018. doi: 10.1016/j.cpc.2018.01.015.  
  
D. M. Rogers, “Efficient Primitives for Standard Tensor Linear Algebra”, *Proceedings of the XSEDE16 Conference on Diversity, Big Data, and Science at Scale*. ACM, Jul. 17, 2016. doi: 10.1145/2949550.2949580.  
  
H. Goel, S. Ling, B. N. Ellis, A. Taconi, B. Slaterand N. Rai, “Predicting vapor liquid equilibria using density functional theory: A case study of argon”, *The Journal of Chemical Physics*, vol. 148, no. 22. AIP Publishing, p. 224501, Jun. 14, 2018. doi: 10.1063/1.5025726.  
  
H. Goel, Z. W. Windom, C. L. Butlerand N. Rai, “Phase Equilibria and Condensed Phase Properties of Fluorinated Alkanes via First Principles Simulations”, *ChemistrySelect*, vol. 2, no. 36. Wiley, pp. 11969–11976, Dec. 21, 2017. doi: 10.1002/slct.201701972.  
  
X. Guo, M. Daveand M. Sayeed, “HPCmatlab: A Framework for Fast Prototyping of Parallel Applications in Matlab”, *Procedia Computer Science*, vol. 80. Elsevier BV, pp. 1461–1472, 2016. doi: 10.1016/j.procs.2016.05.467.  
  
S. V. Moore and S. R. Dunlop, “A Flipped Classroom Approach to Teaching Concurrency and Parallelism”, *2016 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*. IEEE, May 2016. doi: 10.1109/ipdpsw.2016.161.  
  
W. K. Umayanganie Munipala and S. V. Moore, “An evaluation framework for scientific programming productivity”, *Proceedings of the International Workshop on Software Engineering for Science*. ACM, May 14, 2016. doi: 10.1145/2897676.2897682.  
  
N. Acer and M. Turgut, “Measurements of the Insula Volume Using MRI”, *Island of Reil (Insula) in the Human Brain*. Springer International Publishing, pp. 101–111, 2018. doi: 10.1007/978-3-319-75468-0\_10.  
  
K. Akazawa, “Automated Generation of Radiologic Descriptions on Brain Volume Changes From T1-Weighted MR Images: Initial Assessment of Feasibility”, *Frontiers in Neurology*, vol. 10. Frontiers Media SA, Jan. 24, 2019. doi: 10.3389/fneur.2019.00007.  
  
K. H. Alm, “Medial temporal lobe white matter pathway variability is associated with individual differences in episodic memory in cognitively normal older adults”, *Neurobiology of Aging*, vol. 87. Elsevier BV, pp. 78–88, Mar. 2020. doi: 10.1016/j.neurobiolaging.2019.11.011.  
  
H. Arai, Y. Chayama, H. Iyatomiand K. Oishi, “Significant Dimension Reduction of 3D Brain MRI using 3D Convolutional Autoencoders”, *2018 40th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC)*. IEEE, Jul. 2018. doi: 10.1109/embc.2018.8513469.  
  
A. Branch, “An optimized tissue clearing protocol for rat brain labeling, imaging, and high throughput analysis”, *[]*. Cold Spring Harbor Laboratory, May 17, 2019. doi: 10.1101/639674.  
  
R. F. Casseb, B. M. de Campos, A. R. M. Martinez, G. Castellanoand M. C. França Junior, “Selective sensory deafferentation induces structural and functional brain plasticity”, *NeuroImage: Clinical*, vol. 21. Elsevier BV, p. 101633, 2019. doi: 10.1016/j.nicl.2018.101633.  
  
J. B. De Vis, “Arterial-spin-labeling (ASL) perfusion MRI predicts cognitive function in elderly individuals: A 4-year longitudinal study”, *Journal of Magnetic Resonance Imaging*, vol. 48, no. 2. Wiley, pp. 449–458, Jan. 02, 2018. doi: 10.1002/jmri.25938.  
  
S. B. Dhir, K. S. Kutten, M. Li, A. V. Faria, L. Younesand J. T. Ratnanather, “Visualising the topography of the acoustic radiation in clinical diffusion tensor imaging scans”, *Neuroradiology*, vol. 62, no. 9. Springer Science and Business Media LLC, pp. 1157–1167, May 19, 2020. doi: 10.1007/s00234-020-02436-6.  
  
I. Faber, “SPG11 mutations cause widespread white matter and basal ganglia abnormalities, but restricted cortical damage”, *NeuroImage: Clinical*, vol. 19. Elsevier BV, pp. 848–857, 2018. doi: 10.1016/j.nicl.2018.05.031.  
  
A. V. Faria, “Relationship between neuropsychological behavior and brain white matter in first-episode psychosis”, *Schizophrenia Research*, vol. 208. Elsevier BV, pp. 49–54, Jun. 2019. doi: 10.1016/j.schres.2019.04.010.  
  
A. V. Faria, A. Meyer, R. Friedman, D. C. Tippettand A. E. Hillis, “Baseline MRI associates with later naming status in primary progressive aphasia”, *Brain and Language*, vol. 201. Elsevier BV, p. 104723, Feb. 2020. doi: 10.1016/j.bandl.2019.104723.  
  
S. Hannoun, R. Tutunji, M. El Homsi, S. Saaybiand R. Hourani, “Automatic Thalamus Segmentation on Unenhanced 3D T1 Weighted Images: Comparison of Publicly Available Segmentation Methods in a Pediatric Population”, *Neuroinformatics*, vol. 17, no. 3. Springer Science and Business Media LLC, pp. 443–450, Dec. 14, 2018. doi: 10.1007/s12021-018-9408-7.  
  
A. Hiraiwa, “Brain Development of Children With Single Ventricle Physiology or Transposition of the Great Arteries: A Longitudinal Observation Study”, *Seminars in Thoracic and Cardiovascular Surgery*, vol. 32, no. 4. Elsevier BV, pp. 936–944, 2020. doi: 10.1053/j.semtcvs.2019.06.013.  
  
S. Jain, “Computational Anatomy Gateway”, *Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment*. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616553.  
  
S. Kulason, “Cortical thickness atrophy in the transentorhinal cortex in mild cognitive impairment”, *NeuroImage: Clinical*, vol. 21. Elsevier BV, p. 101617, 2019. doi: 10.1016/j.nicl.2018.101617.  
  
B. C. Lee, D. J. Tward, P. P. Mitraand M. I. Miller, “On variational solutions for whole brain serial-section histology using a Sobolev prior in the computational anatomy random orbit model”, *PLOS Computational Biology*, vol. 14, no. 12. Public Library of Science (PLoS), p. e1006610, Dec. 26, 2018. doi: 10.1371/journal.pcbi.1006610.  
  
C.-F. Liu, “Using deep Siamese neural networks for detection of brain asymmetries associated with Alzheimer’s Disease and Mild Cognitive Impairment”, *Magnetic Resonance Imaging*, vol. 64. Elsevier BV, pp. 190–199, Dec. 2019. doi: 10.1016/j.mri.2019.07.003.  
  
G. Liu, “Regional Shape Abnormalities in Thalamus and Verbal Memory Impairment After Subcortical Infarction”, *Neurorehabilitation and Neural Repair*, vol. 33, no. 6. SAGE Publications, pp. 476–485, May 12, 2019. doi: 10.1177/1545968319846121.  
  
Y. Li, “ASL-MRICloud: An online tool for the processing of ASL MRI data”, *NMR in Biomedicine*, vol. 32, no. 2. Wiley, p. e4051, Dec. 26, 2018. doi: 10.1002/nbm.4051.  
  
C. R. Martins Junior, “Structural signature in SCA1: clinical correlates, determinants and natural history”, *Journal of Neurology*, vol. 265, no. 12. Springer Science and Business Media LLC, pp. 2949–2959, Oct. 15, 2018. doi: 10.1007/s00415-018-9087-1.  
  
M. I. Miller, S. Arguillère, D. J. Twardand L. Younes, “Computational anatomy and diffeomorphometry: A dynamical systems model of neuroanatomy in the soft condensed matter continuum”, *WIREs Systems Biology and Medicine*, vol. 10, no. 6. Wiley, Jun. 04, 2018. doi: 10.1002/wsbm.1425.  
  
S. Mori, “MRICloud: Delivering High-Throughput MRI Neuroinformatics as Cloud-Based Software as a Service”, *Computing in Science & Engineering*, vol. 18, no. 5. Institute of Electrical and Electronics Engineers (IEEE), pp. 21–35, Sep. 2016. doi: 10.1109/mcse.2016.93.  
  
M. A. Nowrangi, “The association of neuropsychiatric symptoms with regional brain volumes from patients in a tertiary multi-disciplinary memory clinic”, *International Psychogeriatrics*, vol. 33, no. 3. Cambridge University Press (CUP), pp. 233–244, Feb. 28, 2020. doi: 10.1017/s1041610220000113.  
  
K. Oishi, L. Changand H. Huang, “Baby brain atlases”, *NeuroImage*, vol. 185. Elsevier BV, pp. 865–880, Jan. 2019. doi: 10.1016/j.neuroimage.2018.04.003.  
  
K. Oishi, J. Chotiyanonta, D. Wu, M. I. Miller, S. Moriand K. Oishi, “Developmental trajectories of the human embryologic brain regions”, *Neuroscience Letters*, vol. 708. Elsevier BV, p. 134342, Aug. 2019. doi: 10.1016/j.neulet.2019.134342.  
  
Y. Otsuka, “A Multi‐Atlas Label Fusion Tool for Neonatal Brain MRI Parcellation and Quantification”, *Journal of Neuroimaging*. Wiley, Apr. 29, 2019. doi: 10.1111/jon.12623.  
  
T. J. R. Rezende, “Test–retest reproducibility of a multi‐atlas automated segmentation tool on multimodality brain MRI”, *Brain and Behavior*, vol. 9, no. 10. Wiley, Sep. 04, 2019. doi: 10.1002/brb3.1363.  
  
T. J. R. Rezende, “Structural signature of SCA3: From presymptomatic to late disease stages”, *Annals of Neurology*, vol. 84, no. 3. Wiley, pp. 401–408, Sep. 2018. doi: 10.1002/ana.25297.  
  
D. Tward, “Diffeomorphic Registration With Intensity Transformation and Missing Data: Application to 3D Digital Pathology of Alzheimer’s Disease”, *Frontiers in Neuroscience*, vol. 14. Frontiers Media SA, Feb. 11, 2020. doi: 10.3389/fnins.2020.00052.  
  
D. Tward, X. Li, B. Huo, B. Lee, M. I. Millerand P. P. Mitra, “Solving the *where* problem in neuroanatomy: a generative framework with learned mappings to register multimodal, incomplete data into a reference brain”, *[]*. Cold Spring Harbor Laboratory, Mar. 23, 2020. doi: 10.1101/2020.03.22.002618.  
  
D. Tward and M. Miller, “EM-LDDMM for 3D to 2D registration”, *[]*. Cold Spring Harbor Laboratory, Apr. 10, 2019. doi: 10.1101/604405.  
  
D. J. Tward, P. P. Mitraand M. I. Miller, “Estimating diffeomorphic mappings between templates and noisy data: Variance bounds on the estimated canonical volume form”, *Quarterly of Applied Mathematics*, vol. 77, no. 2. American Mathematical Society (AMS), pp. 467–488, Nov. 20, 2018. doi: 10.1090/qam/1527.  
  
C. Ye, T. Ma, D. Wu, C. Ceritoglu, M. I. Millerand S. Mori, “Atlas pre-selection strategies to enhance the efficiency and accuracy of multi-atlas brain segmentation tools”, *PLOS ONE*, vol. 13, no. 7. Public Library of Science (PLoS), p. e0200294, Jul. 27, 2018. doi: 10.1371/journal.pone.0200294.  
  
H. Zhang, “Age-specific optimization of T1-weighted brain MRI throughout infancy”, *NeuroImage*, vol. 199. Elsevier BV, pp. 387–395, Oct. 2019. doi: 10.1016/j.neuroimage.2019.05.075.  
  
X. Zhang, “Linear Registration of Brain MRI Using Knowledge-Based Multiple Intermediator Libraries”, *Frontiers in Neuroscience*, vol. 13. Frontiers Media SA, Sep. 11, 2019. doi: 10.3389/fnins.2019.00909.  
  
L. Zou, Y. Song, X. Zhou, J. Chuand X. Tang, “Regional morphometric abnormalities and clinical relevance in Wilson’s disease”, *Movement Disorders*, vol. 34, no. 4. Wiley, pp. 545–554, Feb. 28, 2019. doi: 10.1002/mds.27641.  
  
X. Li, “Multi-atlas tool for automated segmentation of brain gray matter nuclei and quantification of their magnetic susceptibility”, *NeuroImage*, vol. 191. Elsevier BV, pp. 337–349, May 2019. doi: 10.1016/j.neuroimage.2019.02.016.  
  
R. Sakamoto, “Cloud-Based Brain Magnetic Resonance Image Segmentation and Parcellation System for Individualized Prediction of Cognitive Worsening”, *Journal of Healthcare Engineering*, vol. 2019. Hindawi Limited, pp. 1–10, Jan. 29, 2019. doi: 10.1155/2019/9507193.  
  
D. J. Tward, “Diffeomorphic registration with intensity transformation and missing data: Application to 3D digital pathology of Alzheimer’s disease”, *[]*. Cold Spring Harbor Laboratory, Dec. 11, 2018. doi: 10.1101/494005.  
  
D. Tward, A. Kolasny, F. Khan, J. Troncosoand M. Miller, “Expanding the Computational Anatomy Gateway from clinical imaging to basic neuroscience research”, *Proceedings of the Practice and Experience in Advanced Research Computing on Rise of the Machines (learning)*. ACM, Jul. 28, 2019. doi: 10.1145/3332186.3332217.  
  
D. Wang, D. J. Foran, X. Qiand M. Parashar, “HetroCV: Auto-tuning Framework and Runtime for Image Processing and Computer Vision Applications on Heterogeneous Platform”, *2015 44th International Conference on Parallel Processing Workshops*. IEEE, Sep. 2015. doi: 10.1109/icppw.2015.21.  
  
M. Safari and M. R. H. Sheikhi, “Large eddy simulation-based analysis of entropy generation in a turbulent nonpremixed flame”, *Energy*, vol. 78. Elsevier BV, pp. 451–457, Dec. 2014. doi: 10.1016/j.energy.2014.10.032.  
  
W. La Cava, K. Danai, L. Spector, P. Fleming, A. Wrightand M. Lackner, “Automatic identification of wind turbine models using evolutionary multiobjective optimization”, *Renewable Energy*, vol. 87. Elsevier BV, pp. 892–902, Mar. 2016. doi: 10.1016/j.renene.2015.09.068.  
  
H. Shah, “Parallel Techniques for Navier-Stokes Solver based on 4th Order Modified Runge-Kutta Scheme with TVD”, *22nd AIAA Computational Fluid Dynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 18, 2015. doi: 10.2514/6.2015-3054.  
  
H. Subramoni, “Designing Non-blocking Personalized Collectives with Near Perfect Overlap for RDMA-Enabled Clusters”, *Lecture Notes in Computer Science*. Springer International Publishing, pp. 434–453, 2015. doi: 10.1007/978-3-319-20119-1\_31.  
  
V. Arias, D. Bochkovand F. Gibou, “Poisson equations in irregular domains with Robin boundary conditions — Solver with second-order accurate gradients”, *Journal of Computational Physics*, vol. 365. Elsevier BV, pp. 1–6, Jul. 2018. doi: 10.1016/j.jcp.2018.03.022.  
  
D. Bochkov and F. Gibou, “Solving Poisson-type equations with Robin boundary conditions on piecewise smooth interfaces”, *Journal of Computational Physics*, vol. 376. Elsevier BV, pp. 1156–1198, Jan. 2019. doi: 10.1016/j.jcp.2018.10.020.  
  
C. Cleret de Langavant, A. Guittet, M. Theillard, F. Temprano-Coletoand F. Gibou, “Level-set simulations of soluble surfactant driven flows”, *Journal of Computational Physics*, vol. 348. Elsevier BV, pp. 271–297, Nov. 2017. doi: 10.1016/j.jcp.2017.07.003.  
  
R. Egan and F. Gibou, “Geometric discretization of the multidimensional Dirac delta distribution – Application to the Poisson equation with singular source terms”, *Journal of Computational Physics*, vol. 346. Elsevier BV, pp. 71–90, Oct. 2017. doi: 10.1016/j.jcp.2017.06.003.  
  
R. Egan and F. Gibou, “Fast and scalable algorithms for constructing Solvent-Excluded Surfaces of large biomolecules”, *Journal of Computational Physics*, vol. 374. Elsevier BV, pp. 91–120, Dec. 2018. doi: 10.1016/j.jcp.2018.07.035.  
  
F. Gibou, R. Fedkiwand S. Osher, “A review of level-set methods and some recent applications”, *Journal of Computational Physics*, vol. 353. Elsevier BV, pp. 82–109, Jan. 2018. doi: 10.1016/j.jcp.2017.10.006.  
  
F. Gibou, D. Hydeand R. Fedkiw, “Sharp interface approaches and deep learning techniques for multiphase flows”, *Journal of Computational Physics*, vol. 380. Elsevier BV, pp. 442–463, Mar. 2019. doi: 10.1016/j.jcp.2018.05.031.  
  
A. Guittet, C. Poignardand F. Gibou, “A Voronoi Interface approach to cell aggregate electropermeabilization”, *Journal of Computational Physics*, vol. 332. Elsevier BV, pp. 143–159, Mar. 2017. doi: 10.1016/j.jcp.2016.11.048.  
  
P. Mistani, “The island dynamics model on parallel quadtree grids”, *Journal of Computational Physics*, vol. 361. Elsevier BV, pp. 150–166, May 2018. doi: 10.1016/j.jcp.2018.01.054.  
  
P. Mistani, A. Guittet, C. Poignardand F. Gibou, “A parallel Voronoi-based approach for mesoscale simulations of cell aggregate electropermeabilization”, *Journal of Computational Physics*, vol. 380. Elsevier BV, pp. 48–64, Mar. 2019. doi: 10.1016/j.jcp.2018.12.009.  
  
G. Ouaknin, N. Laachi, K. Delaney, G. H. Fredricksonand F. Gibou, “Self-consistent field theory simulations of polymers on arbitrary domains”, *Journal of Computational Physics*, vol. 327. Elsevier BV, pp. 168–185, Dec. 2016. doi: 10.1016/j.jcp.2016.09.021.  
  
G. Y. Ouaknin, N. Laachi, K. Delaney, G. H. Fredricksonand F. Gibou, “Level-set strategy for inverse DSA-lithography”, *Journal of Computational Physics*, vol. 375. Elsevier BV, pp. 1159–1178, Dec. 2018. doi: 10.1016/j.jcp.2018.09.021.  
  
G. Ouaknin, N. Laachi, D. Bochkov, K. Delaney, G. H. Fredricksonand F. Gibou, “Functional level-set derivative for a polymer self consistent field theory Hamiltonian”, *Journal of Computational Physics*, vol. 345. Elsevier BV, pp. 207–223, Sep. 2017. doi: 10.1016/j.jcp.2017.05.037.  
  
T. K. Chafin, M. R. Douglas, B. T. Martinand M. E. Douglas, “Hybridization drives genetic erosion in sympatric desert fishes of western North America”, *Heredity*, vol. 123, no. 6. Springer Science and Business Media LLC, pp. 759–773, Aug. 20, 2019. doi: 10.1038/s41437-019-0259-2.  
  
J. R. Boes, M. C. Groenenboom, J. A. Keithand J. R. Kitchin, “Neural network and ReaxFF comparison for Au properties”, *International Journal of Quantum Chemistry*, vol. 116, no. 13. Wiley, pp. 979–987, Mar. 02, 2016. doi: 10.1002/qua.25115.  
  
G. P. Junor, E. A. Romero, X. Chen, R. Jazzarand G. Bertrand, “Readily Available Primary Aminoboranes as Powerful Reagents for Aldimine Synthesis”, *Angewandte Chemie*, vol. 131, no. 9. Wiley, pp. 2901–2904, Feb. 06, 2019. doi: 10.1002/ange.201814081.  
  
G. P. Junor, E. A. Romero, X. Chen, R. Jazzarand G. Bertrand, “Readily Available Primary Aminoboranes as Powerful Reagents for Aldimine Synthesis”, *Angewandte Chemie International Edition*, vol. 58, no. 9. Wiley, pp. 2875–2878, Feb. 06, 2019. doi: 10.1002/anie.201814081.  
  
J. M. Karp, E. Erylimazand D. Cowburn, “Correlation of chemical shifts predicted by molecular dynamics simulations for partially disordered proteins”, *Journal of Biomolecular NMR*, vol. 61, no. 1. Springer Science and Business Media LLC, pp. 35–45, Nov. 22, 2014. doi: 10.1007/s10858-014-9879-2.  
  
G. M. Magnotti and C. L. Genzale, “A Novel Approach to Assess Diesel Spray Models using Joint Visible and X-Ray Liquid Extinction Measurements”, *SAE International Journal of Fuels and Lubricants*, vol. 8, no. 1. SAE International, pp. 167–178, Apr. 14, 2015. doi: 10.4271/2015-01-0941.  
  
G. M. Magnotti and C. L. Genzale, “A NOVEL SPRAY MODEL VALIDATION METHODOLOGY USING LIQUID-PHASE EXTINCTION MEASUREMENTS”, *Atomization and Sprays*, vol. 25, no. 5. Begell House, pp. 397–424, 2015. doi: 10.1615/atomizspr.2014010377.  
  
D. Ojika, D. Acosta, A. Gordon-Ross, A. Carnesand S. Gleyzer, “Accelerating High-energy Physics Exploration with Deep Learning”, *Proceedings of the Practice and Experience in Advanced Research Computing 2017 on Sustainability, Success and Impact*. ACM, Jul. 09, 2017. doi: 10.1145/3093338.3093340.  
  
J. J. Wang, “Automated data processing architecture for the Gemini Planet Imager Exoplanet Survey”, *Journal of Astronomical Telescopes, Instruments, and Systems*, vol. 4, no. 1. SPIE-Intl Soc Optical Eng, p. 1, Jan. 18, 2018. doi: 10.1117/1.jatis.4.1.018002.  
  
J. P. Howard, II, “Phonetic Algorithms in R”, *The Journal of Open Source Software*, vol. 3, no. 22. The Open Journal, p. 480, Feb. 14, 2018. doi: 10.21105/joss.00480.  
  
J. Howard, K. Haynesand Ahood, *k3jph/phonics-in-r: Phonics v1.3.10*. Zenodo, 2021. doi: 10.5281/ZENODO.1041982.  
  
Z. Wang, W.-J. Huand A. H. Nevidomskyy, “Spin Ferroquadrupolar Order in the Nematic Phase of FeSe”, *Physical Review Letters*, vol. 116, no. 24. American Physical Society (APS), Jun. 17, 2016. doi: 10.1103/physrevlett.116.247203.  
  
W. M. Botello-Smith, “Polymodal allosteric regulation of Type 1 Serine/Threonine Kinase Receptors via a conserved electrostatic lock”, *PLOS Computational Biology*, vol. 13, no. 8. Public Library of Science (PLoS), p. e1005711, Aug. 21, 2017. doi: 10.1371/journal.pcbi.1005711.  
  
P. Dickens, C. Dufourand J. Fastook, “Adding embedded simulation to the parallel ice sheet model”, *2015 Winter Simulation Conference (WSC)*. IEEE, Dec. 2015. doi: 10.1109/wsc.2015.7408475.  
  
P. M. Dickens, C. Dufourand J. Fastook, “The Scalability of Embedded Structured Grids and Unstructured Grids in Large Scale Ice Sheet Modeling on Distributed Memory Parallel Computers”, *2018 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*. IEEE, May 2018. doi: 10.1109/ipdpsw.2018.00152.  
  
E. Yildirim and D. J. Foran, “Parallel Versus Distributed Data Access for Gigapixel-Resolution Histology Images: Challenges and Opportunities”, *IEEE Journal of Biomedical and Health Informatics*, vol. 21, no. 4. Institute of Electrical and Electronics Engineers (IEEE), pp. 1049–1057, Jul. 2017. doi: 10.1109/jbhi.2016.2580145.  
  
E. Sayyari and S. Mirarab, “Fast Coalescent-Based Computation of Local Branch Support from Quartet Frequencies”, *Molecular Biology and Evolution*, vol. 33, no. 7. Oxford University Press (OUP), pp. 1654–1668, Apr. 15, 2016. doi: 10.1093/molbev/msw079.  
  
M. Balaban, N. Moshiri, U. Mai, X. Jiaand S. Mirarab, “TreeCluster: Clustering biological sequences using phylogenetic trees”, *PLOS ONE*, vol. 14, no. 8. Public Library of Science (PLoS), p. e0221068, Aug. 22, 2019. doi: 10.1371/journal.pone.0221068.  
  
M. Balaban, S. Sarmashghiand S. Mirarab, “APPLES: Scalable Distance-Based Phylogenetic Placement with or without Alignments”, *Systematic Biology*, vol. 69, no. 3. Oxford University Press (OUP), pp. 566–578, Sep. 23, 2019. doi: 10.1093/sysbio/syz063.  
  
P. Houde, E. L. Braun, N. Narula, U. Minjaresand S. Mirarab, “Phylogenetic Signal of Indels and the Neoavian Radiation”, *Diversity*, vol. 11, no. 7. MDPI AG, p. 108, Jul. 06, 2019. doi: 10.3390/d11070108.  
  
N. Moshiri, M. Ragonnet-Cronin, J. O. Wertheimand S. Mirarab, “FAVITES: simultaneous simulation of transmission networks, phylogenetic trees and sequences”, *Bioinformatics*, vol. 35, no. 11. Oxford University Press (OUP), pp. 1852–1861, Nov. 05, 2018. doi: 10.1093/bioinformatics/bty921.  
  
M. Rabiee and S. Mirarab, “INSTRAL: Discordance-Aware Phylogenetic Placement Using Quartet Scores”, *Systematic Biology*, vol. 69, no. 2. Oxford University Press (OUP), pp. 384–391, Aug. 12, 2019. doi: 10.1093/sysbio/syz045.  
  
M. Rabiee, E. Sayyariand S. Mirarab, “Multi-allele species reconstruction using ASTRAL”, *Molecular Phylogenetics and Evolution*, vol. 130. Elsevier BV, pp. 286–296, Jan. 2019. doi: 10.1016/j.ympev.2018.10.033.  
  
S. Sarmashghi, K. Bohmann, M. T. P. Gilbert, V. Bafnaand S. Mirarab, “Skmer: assembly-free and alignment-free sample identification using genome skims”, *Genome Biology*, vol. 20, no. 1. Springer Science and Business Media LLC, Feb. 13, 2019. doi: 10.1186/s13059-019-1632-4.  
  
E. Sayyari, B. Kawasand S. Mirarab, “TADA: phylogenetic augmentation of microbiome samples enhances phenotype classification”, *Bioinformatics*, vol. 35, no. 14. Oxford University Press (OUP), pp. i31–i40, Jul. 2019. doi: 10.1093/bioinformatics/btz394.  
  
J. Yin, C. Zhangand S. Mirarab, “ASTRAL-MP: scaling ASTRAL to very large datasets using randomization and parallelization”, *Bioinformatics*, vol. 35, no. 20. Oxford University Press (OUP), pp. 3961–3969, Mar. 23, 2019. doi: 10.1093/bioinformatics/btz211.  
  
E. Sayyari and S. Mirarab, “Testing for Polytomies in Phylogenetic Species Trees Using Quartet Frequencies”, *Genes*, vol. 9, no. 3. MDPI AG, p. 132, Feb. 28, 2018. doi: 10.3390/genes9030132.  
  
U. Mai and S. Mirarab, “TreeShrink: Efficient Detection of Outlier Tree Leaves”, *Comparative Genomics*. Springer International Publishing, pp. 116–140, 2017. doi: 10.1007/978-3-319-67979-2\_7.  
  
U. Mai and S. Mirarab, “TreeShrink: fast and accurate detection of outlier long branches in collections of phylogenetic trees”, *BMC Genomics*, vol. 19, no. S5. Springer Science and Business Media LLC, May 2018. doi: 10.1186/s12864-018-4620-2.  
  
U. Mai, E. Sayyariand S. Mirarab, “Minimum variance rooting of phylogenetic trees and implications for species tree reconstruction”, *PLOS ONE*, vol. 12, no. 8. Public Library of Science (PLoS), p. e0182238, Aug. 11, 2017. doi: 10.1371/journal.pone.0182238.  
  
S. Mirarab, “Phylogenomics: Constrained gene tree inference”, *Nature Ecology & Evolution*, vol. 1, no. 2. Springer Science and Business Media LLC, Jan. 13, 2017. doi: 10.1038/s41559-016-0056.  
  
N. Moshiri and S. Mirarab, “A Two-State Model of Tree Evolution and Its Applications to Alu Retrotransposition”, *Systematic Biology*, vol. 67, no. 3. Oxford University Press (OUP), pp. 475–489, Nov. 20, 2017. doi: 10.1093/sysbio/syx088.  
  
M. Rabiee and S. Mirarab, “INSTRAL: Discordance-aware Phylogenetic Placement using Quartet Scores”, *[]*. Cold Spring Harbor Laboratory, Oct. 02, 2018. doi: 10.1101/432906.  
  
M. Rabiee, E. Sayyariand S. Mirarab, “Multi-allele species reconstruction using ASTRAL”, *[]*. Cold Spring Harbor Laboratory, Oct. 11, 2018. doi: 10.1101/439489.  
  
S. Sarmashghi, K. Bohmann, M. T. P. Gilbert, V. Bafnaand S. Mirarab, “Assembly-free and alignment-free sample identification using genome skims”, *[]*. Cold Spring Harbor Laboratory, Dec. 08, 2017. doi: 10.1101/230409.  
  
E. Sayyari and S. Mirarab, “Anchoring quartet-based phylogenetic distances and applications to species tree reconstruction”, *BMC Genomics*, vol. 17, no. S10. Springer Science and Business Media LLC, Nov. 2016. doi: 10.1186/s12864-016-3098-z.  
  
E. Sayyari, J. B. Whitfieldand S. Mirarab, “Fragmentary Gene Sequences Negatively Impact Gene Tree and Species Tree Reconstruction”, *Molecular Biology and Evolution*, vol. 34, no. 12. Oxford University Press (OUP), pp. 3279–3291, Oct. 04, 2017. doi: 10.1093/molbev/msx261.  
  
E. Sayyari, J. B. Whitfieldand S. Mirarab, “DiscoVista: Interpretable visualizations of gene tree discordance”, *Molecular Phylogenetics and Evolution*, vol. 122. Elsevier BV, pp. 110–115, May 2018. doi: 10.1016/j.ympev.2018.01.019.  
  
S. Shekhar, S. Rochand S. Mirarab, “Species Tree Estimation Using ASTRAL: How Many Genes Are Enough?”, *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, vol. 15, no. 5. Institute of Electrical and Electronics Engineers (IEEE), pp. 1738–1747, Sep. 01, 2018. doi: 10.1109/tcbb.2017.2757930.  
  
C. Zhang, M. Rabiee, E. Sayyariand S. Mirarab, “ASTRAL-III: polynomial time species tree reconstruction from partially resolved gene trees”, *BMC Bioinformatics*, vol. 19, no. S6. Springer Science and Business Media LLC, May 2018. doi: 10.1186/s12859-018-2129-y.  
  
C. Zhang, E. Sayyariand S. Mirarab, “ASTRAL-III: Increased Scalability and Impacts of Contracting Low Support Branches”, *Comparative Genomics*. Springer International Publishing, pp. 53–75, 2017. doi: 10.1007/978-3-319-67979-2\_4.  
  
K. Cheshmi, S. Kamil, M. M. Stroutand M. M. Dehnavi, “Sympiler”, *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*. ACM, Nov. 12, 2017. doi: 10.1145/3126908.3126936.  
  
C. J. Jones, S. Sudarshan, I. D. Mehtaand B. W. Beck, “Different Applications for CAS in Functional Classification of Protein Interfaces”, *Biophysical Journal*, vol. 112, no. 3. Elsevier BV, p. 489a, Feb. 2017. doi: 10.1016/j.bpj.2016.11.2645.  
  
I. D. Mehta and B. W. Beck, “Protein Energy Network Models to Classify and Predict Functionally Linked Interfaces of Proteins from Functionally Uncorrelated Interfaces”, *Biophysical Journal*, vol. 112, no. 3. Elsevier BV, p. 345a, Feb. 2017. doi: 10.1016/j.bpj.2016.11.1871.  
  
A. Mohan, T. Hacker, G. P. Rodgersand T. Islam, “Batchsubmit: a high-volume batch submission system for earthquake engineering simulation”, *Concurrency and Computation: Practice and Experience*, vol. 26, no. 13. Wiley, pp. 2240–2252, Mar. 05, 2014. doi: 10.1002/cpe.3234.  
  
R. Sarmento, E. Scannapiecoand S. Cohen, “Following the Cosmic Evolution of Pristine Gas. II. The Search for Pop III–bright Galaxies”, *The Astrophysical Journal*, vol. 854, no. 1. American Astronomical Society, p. 75, Feb. 13, 2018. doi: 10.3847/1538-4357/aa989a.  
  
M. M. Javanmard, Z. Ahmad, M. Kong, L.-N. Pouchet, R. Chowdhuryand R. Harrison, “Deriving parametric multi-way recursive divide-and-conquer dynamic programming algorithms using polyhedral compilers”, *Proceedings of the 18th ACM/IEEE International Symposium on Code Generation and Optimization*. ACM, Feb. 22, 2020. doi: 10.1145/3368826.3377916.  
  
J. Abante, N. Ghaffari, C. D. Johnsonand A. Datta, “HiMMe: using genetic patterns as a proxy for genome assembly reliability assessment”, *BMC Genomics*, vol. 18, no. 1. Springer Science and Business Media LLC, Sep. 05, 2017. doi: 10.1186/s12864-017-3965-2.  
  
L. Ingber, “Forecasting with Importance-Sampling and Path-Integrals: Applications to COVID-19”, *[]*. MDPI AG, Oct. 12, 2020. doi: 10.20944/preprints202009.0385.v3.  
  
N. Spellmon, X. Sun, N. Sirinupong, B. Edwards, C. Liand Z. Yang, “Molecular Dynamics Simulation Reveals Correlated Inter-Lobe Motion in Protein Lysine Methyltransferase SMYD2”, *PLOS ONE*, vol. 10, no. 12. Public Library of Science (PLoS), p. e0145758, Dec. 30, 2015. doi: 10.1371/journal.pone.0145758.  
  
N. Spellmon, X. Sun, N. Sirinupong, B. Edwards, C. Liand Z. Yang, “Molecular Dynamics Simulation Reveals Correlated Inter-Lobe Motion in Protein Lysine Methyltransferase SMYD2”, *PLOS ONE*, vol. 10, no. 12. Public Library of Science (PLoS), p. e0145758, Dec. 30, 2015. doi: 10.1371/journal.pone.0145758.  
  
J. Fischer, “Methodologies and practices for adoption of a novel national research environment”, *Proceedings of the Practice and Experience on Advanced Research Computing*. ACM, Jul. 22, 2018. doi: 10.1145/3219104.3219115.  
  
D. Y. Hancock, “Jetstream—Early operations performance, adoption, and impacts”, *Concurrency and Computation: Practice and Experience*. Wiley, Sep. 02, 2018. doi: 10.1002/cpe.4683.  
  
P. Rodriguez, S. Puthanveetil, J. Will, E. Wuerffeland A. Craig, “Extracting, Assimilating, and Sharing the Results of Image Analysis on the FSA/OWI Photography Collection”, *Proceedings of the Practice and Experience in Advanced Research Computing 2017 on Sustainability, Success and Impact*. ACM, Jul. 09, 2017. doi: 10.1145/3093338.3093365.  
  
K. D. Brauss and A. J. Meir, “On a parallel, 3-dimensional, finite element solver for viscous, resistive, stationary magnetohydrodynamics equations: Velocity–current formulation”, *Applied Numerical Mathematics*, vol. 133. Elsevier BV, pp. 130–143, Nov. 2018. doi: 10.1016/j.apnum.2018.01.014.  
  
B. M. Boyd, “Primates, Lice and Bacteria: Speciation and Genome Evolution in the Symbionts of Hominid Lice”, *Molecular Biology and Evolution*, vol. 34, no. 7. Oxford University Press (OUP), pp. 1743–1757, Apr. 14, 2017. doi: 10.1093/molbev/msx117.  
  
S. Shinde, E. Johnsenand K. J. Maki, “Understanding the effect of cube size on the near wake characteristics in a turbulent boundary layer”, *47th AIAA Fluid Dynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 02, 2017. doi: 10.2514/6.2017-3640.  
  
S. Shinde, S. Tandon, K. Makiand E. Johnsen, “Flow separation over a backward-facing ramp with and without a vortex generator”, *46th AIAA Fluid Dynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 10, 2016. doi: 10.2514/6.2016-3795.  
  
S. Tandon, K. J. Makiand E. Johnsen, “Understanding the dependence of turbulent flow modulation on the spacing between adjacent cubes on a backward-facing ramp”, *AIAA Aviation 2019 Forum*. American Institute of Aeronautics and Astronautics, Jun. 15, 2019. doi: 10.2514/6.2019-3633.  
  
S. Tandon, S. Shinde, K. J. Makiand E. Johnsen, “Flow Control Using Passive Vortex Generators”, *47th AIAA Fluid Dynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 02, 2017. doi: 10.2514/6.2017-3318.  
  
S. Tandon, S. Shinde, K. Makiand E. Johnsen, “Near-Wake Flow Modulation by A Cube On A Backward-Facing Ramp”, *2018 Flow Control Conference*. American Institute of Aeronautics and Astronautics, Jun. 24, 2018. doi: 10.2514/6.2018-3526.  
  
B. M. Boyd, “Phylogenomics using Target-restricted Assembly Resolves Intra-generic Relationships of Parasitic Lice (Phthiraptera: *Columbicola* )”, *Systematic Biology*. Oxford University Press (OUP), p. syx027, Jan. 19, 2017. doi: 10.1093/sysbio/syx027.  
  
N.-. phuong D. Nguyen, V. Deshpande, J. Luebeck, P. S. Mischeland V. Bafna, “ViFi: accurate detection of viral integration and mRNA fusion reveals indiscriminate and unregulated transcription in proximal genomic regions in cervical cancer”, *Nucleic Acids Research*, vol. 46, no. 7. Oxford University Press (OUP), pp. 3309–3325, Mar. 20, 2018. doi: 10.1093/nar/gky180.  
  
Y. Kim, J. Misko, C. Qiand B. Sirkeci, “Mobile high-performance computing (HPC) for synthetic aperture radar signal processing”, *Algorithms for Synthetic Aperture Radar Imagery XXV*. SPIE, Apr. 27, 2018. doi: 10.1117/12.2305009.  
  
W. Montlouis, R. Fauconierand M. Ndoye, “Rapidly Moving Target Parameter Estimation Using Phased Array Radars”, *2020 43rd International Conference on Telecommunications and Signal Processing (TSP)*. IEEE, Jul. 2020. doi: 10.1109/tsp49548.2020.9163492.  
  
H. Xu, M. Piccinelli, B. G. Leshnower, A. Lefieux, W. R. Taylorand A. Veneziani, “Coupled Morphological–Hemodynamic Computational Analysis of Type B Aortic Dissection: A Longitudinal Study”, *Annals of Biomedical Engineering*, vol. 46, no. 7. Springer Science and Business Media LLC, pp. 927–939, Mar. 28, 2018. doi: 10.1007/s10439-018-2012-z.  
  
A. Venugopal, T. Quand R. H. Victora, “Nonlinear Parallel-Pumped FMR: Three and Four Magnon Processes”, *IEEE Transactions on Microwave Theory and Techniques*, vol. 68, no. 2. Institute of Electrical and Electronics Engineers (IEEE), pp. 602–610, Feb. 2020. doi: 10.1109/tmtt.2019.2952128.  
  
H. Liu, H. H. Huangand Y. Hu, “iBFS”, *Proceedings of the 2016 International Conference on Management of Data*. ACM, Jun. 14, 2016. doi: 10.1145/2882903.2882959.  
  
N. Nangia, B. E. Griffith, N. A. Patankarand A. P. S. Bhalla, “A robust incompressible Navier-Stokes solver for high density ratio multiphase flows”, *Journal of Computational Physics*, vol. 390. Elsevier BV, pp. 548–594, Aug. 2019. doi: 10.1016/j.jcp.2019.03.042.  
  
N. Nangia, N. A. Patankarand A. P. S. Bhalla, “A DLM immersed boundary method based wave-structure interaction solver for high density ratio multiphase flows”, *Journal of Computational Physics*, vol. 398. Elsevier BV, p. 108804, Dec. 2019. doi: 10.1016/j.jcp.2019.07.004.  
  
B. Vadala-Roth, S. Acharya, N. A. Patankar, S. Rossiand B. E. Griffith, “Stabilization approaches for the hyperelastic immersed boundary method for problems of large-deformation incompressible elasticity”, *Computer Methods in Applied Mechanics and Engineering*, vol. 365. Elsevier BV, p. 112978, Jun. 2020. doi: 10.1016/j.cma.2020.112978.  
  
Y. Fu, F. Li, F. Songand L. Zhu, “Designing a Parallel Memory-Aware Lattice Boltzmann Algorithm on Manycore Systems”, *2018 30th International Symposium on Computer Architecture and High Performance Computing (SBAC-PAD)*. IEEE, Sep. 2018. doi: 10.1109/cahpc.2018.8645909.  
  
F. Li and F. Song, “A Real-Time Machine Learning and Visualization Framework for Scientific Workflows”, *Proceedings of the Practice and Experience in Advanced Research Computing 2017 on Sustainability, Success and Impact*. ACM, Jul. 09, 2017. doi: 10.1145/3093338.3093380.  
  
F. Li and F. Song, “Building a scientific workflow framework to enable real‐time machine learning and visualization”, *Concurrency and Computation: Practice and Experience*, vol. 31, no. 16. Wiley, Jun. 04, 2018. doi: 10.1002/cpe.4703.  
  
V. M. K. Kotteda, V. Kumarand W. Spotz, “Performance of preconditioned iterative solvers in MFiX–Trilinos for fluidized beds”, *The Journal of Supercomputing*, vol. 74, no. 8. Springer Science and Business Media LLC, pp. 4104–4126, May 18, 2018. doi: 10.1007/s11227-018-2415-5.  
  
T. Frolov, “Grain boundary phases in bcc metals”, *Nanoscale*, vol. 10, no. 17. Royal Society of Chemistry (RSC), pp. 8253–8268, 2018. doi: 10.1039/c8nr00271a.  
  
M. Tan, “ROY revisited, again: the eighth solved structure”, *Faraday Discussions*, vol. 211. Royal Society of Chemistry (RSC), pp. 477–491, 2018. doi: 10.1039/c8fd00039e.  
  
P. Wang, “Pressure-induced structural and electronic transitions, metallization, and enhanced visible-light responsiveness in layered rhenium disulphide”, *Physical Review B*, vol. 97, no. 23. American Physical Society (APS), Jun. 07, 2018. doi: 10.1103/physrevb.97.235202.  
  
Q. Zhu, A. Samanta, B. Li, R. E. Ruddand T. Frolov, “Predicting phase behavior of grain boundaries with evolutionary search and machine learning”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Feb. 01, 2018. doi: 10.1038/s41467-018-02937-2.  
  
D. C. Card, “Genomic Basis of Convergent Island Phenotypes in Boa Constrictors”, *Genome Biology and Evolution*, vol. 11, no. 11. Oxford University Press (OUP), pp. 3123–3143, Oct. 23, 2019. doi: 10.1093/gbe/evz226.  
  
A. Brinckman, “Computing environments for reproducibility: Capturing the “Whole Tale””, *Future Generation Computer Systems*, vol. 94. Elsevier BV, pp. 854–867, May 2019. doi: 10.1016/j.future.2017.12.029.  
  
K. Chard, “Implementing Computational Reproducibility in the Whole Tale Environment”, *Proceedings of the 2nd International Workshop on Practical Reproducible Evaluation of Computer Systems*. ACM, Jun. 17, 2019. doi: 10.1145/3322790.3330594.  
  
X. Luo, “HAN: a Hierarchical AutotuNed Collective Communication Framework”, *2020 IEEE International Conference on Cluster Computing (CLUSTER)*. IEEE, Sep. 2020. doi: 10.1109/cluster49012.2020.00013.  
  
Y. Pei, Q. Cao, G. Bosilca, P. Luszczek, V. Eijkhoutand J. Dongarra, “Communication Avoiding 2D Stencil Implementations over PaRSEC Task-Based Runtime”, *2020 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*. IEEE, May 2020. doi: 10.1109/ipdpsw50202.2020.00127.  
  
D. Zhong, Q. Cao, G. Bosilcaand J. Dongarra, “Using Advanced Vector Extensions AVX-512 for MPI Reductions”, *27th European MPI Users’ Group Meeting*. ACM, Sep. 21, 2020. doi: 10.1145/3416315.3416316.  
  
A. Harbuzariu, J. Kim, E. M. Meyer, A. D. Donnenbergand B. W. Tillman, “CD34 affinity pheresis attenuates a surge among circulating progenitor cells following vascular injury”, *Journal of Vascular Surgery*, vol. 59, no. 6. Elsevier BV, pp. 1686–1694, Jun. 2014. doi: 10.1016/j.jvs.2013.05.043.  
  
I. Volvach, J. G. Alzate, Y.-J. Chen, A. J. Smith, D. L. Kenckeand V. Lomakin, “Thermal stability and magnetization switching in perpendicular magnetic tunnel junctions”, *Applied Physics Letters*, vol. 116, no. 19. AIP Publishing, p. 192408, May 11, 2020. doi: 10.1063/5.0005211.  
  
I. de Pater, “Neptune’s global circulation deduced from multi-wavelength observations”, *Icarus*, vol. 237. Elsevier BV, pp. 211–238, Jul. 2014. doi: 10.1016/j.icarus.2014.02.030.  
  
P. Hassanzadeh, P. S. Marcusand P. Le Gal, “The universal aspect ratio of vortices in rotating stratified flows: theory and simulation”, *Journal of Fluid Mechanics*, vol. 706. Cambridge University Press (CUP), pp. 46–57, May 25, 2012. doi: 10.1017/jfm.2012.180.  
  
M. Mahdinia, P. Hassanzadeh, P. S. Marcusand C.-H. Jiang, “Stability of three-dimensional Gaussian vortices in an unbounded, rotating, vertically stratified, Boussinesq flow: linear analysis”, *Journal of Fluid Mechanics*, vol. 824. Cambridge University Press (CUP), pp. 97–134, Jul. 05, 2017. doi: 10.1017/jfm.2017.303.  
  
P. S. Marcus, S. Pei, C.-H. Jiangand J. A. Barranco, “ZOMBIE VORTEX INSTABILITY. II. THRESHOLDS TO TRIGGER INSTABILITY AND THE PROPERTIES OF ZOMBIE TURBULENCE IN THE DEAD ZONES OF PROTOPLANETARY DISKS”, *The Astrophysical Journal*, vol. 833, no. 2. American Astronomical Society, p. 148, Dec. 13, 2016. doi: 10.3847/1538-4357/833/2/148.  
  
P. S. Marcus, S. Pei, C.-H. Jiang, J. A. Barranco, P. Hassanzadehand D. Lecoanet, “ZOMBIE VORTEX INSTABILITY. I. A PURELY HYDRODYNAMIC INSTABILITY TO RESURRECT THE DEAD ZONES OF PROTOPLANETARY DISKS”, *The Astrophysical Journal*, vol. 808, no. 1. American Astronomical Society, p. 87, Jul. 22, 2015. doi: 10.1088/0004-637x/808/1/87.  
  
S. Oh, C.-H. Jiang, C. Jiangand P. S. Marcus, “Finding the optimal shape of the leading-and-trailing car of a high-speed train using design-by-morphing”, *Computational Mechanics*, vol. 62, no. 1. Springer Science and Business Media LLC, pp. 23–45, Oct. 03, 2017. doi: 10.1007/s00466-017-1482-4.  
  
A. A. Simon, “DRAMATIC CHANGE IN JUPITER’S GREAT RED SPOT FROM SPACECRAFT OBSERVATIONS”, *The Astrophysical Journal*, vol. 797, no. 2. American Astronomical Society, p. L31, Dec. 09, 2014. doi: 10.1088/2041-8205/797/2/l31.  
  
L. A. Sromovsky, I. de Pater, P. M. Fry, H. B. Hammeland P. Marcus, “High S/N Keck and Gemini AO imaging of Uranus during 2012–2014: New cloud patterns, increasing activity, and improved wind measurements”, *Icarus*, vol. 258. Elsevier BV, pp. 192–223, Sep. 2015. doi: 10.1016/j.icarus.2015.05.029.  
  
J. Tollefson, “Changes in Jupiter’s Zonal Wind Profile preceding and during the Juno mission”, *Icarus*, vol. 296. Elsevier BV, pp. 163–178, Nov. 2017. doi: 10.1016/j.icarus.2017.06.007.  
  
M. W. Kunz, T. Bogdanović, C. S. Reynoldsand J. M. Stone, “BUOYANCY INSTABILITIES IN A WEAKLY COLLISIONAL INTRACLUSTER MEDIUM”, *The Astrophysical Journal*, vol. 754, no. 2. American Astronomical Society, p. 122, Jul. 17, 2012. doi: 10.1088/0004-637x/754/2/122.  
  
D. S. Balsara and R. Käppeli, “Von Neumann stability analysis of globally divergence-free RKDG schemes for the induction equation using multidimensional Riemann solvers”, *Journal of Computational Physics*, vol. 336. Elsevier BV, pp. 104–127, May 2017. doi: 10.1016/j.jcp.2017.01.056.  
  
D. S. Balsara and J. Kim, “A subluminal relativistic magnetohydrodynamics scheme with ADER-WENO predictor and multidimensional Riemann solver-based corrector”, *Journal of Computational Physics*, vol. 312. Elsevier BV, pp. 357–384, May 2016. doi: 10.1016/j.jcp.2016.02.001.  
  
D. S. Balsara, A. Taflove, S. Garainand G. Montecinos, “Computational electrodynamics in material media with constraint-preservation, multidimensional Riemann solvers and sub-cell resolution – Part I, second-order FVTD schemes”, *Journal of Computational Physics*, vol. 349. Elsevier BV, pp. 604–635, Nov. 2017. doi: 10.1016/j.jcp.2017.07.024.  
  
J. Kim, D. S. Balsara, M. Lyutikovand S. S. Komissarov, “On the linear stability of magnetized jets without current sheets – relativistic case”, *Monthly Notices of the Royal Astronomical Society*, vol. 467, no. 4. Oxford University Press (OUP), pp. 4647–4662, Feb. 17, 2017. doi: 10.1093/mnras/stx409.  
  
J. Kim, D. S. Balsara, M. Lyutikovand S. S. Komissarov, “On the linear stability of sheared and magnetized jets without current sheets – relativistic case”, *Monthly Notices of the Royal Astronomical Society*, vol. 474, no. 3. Oxford University Press (OUP), pp. 3954–3966, Dec. 04, 2017. doi: 10.1093/mnras/stx3065.  
  
J. Kim, S. K. Garain, D. S. Balsaraand S. K. Chakrabarti, “General relativistic numerical simulation of sub-Keplerian transonic accretion flows on to black holes: Schwarzschild space–time”, *Monthly Notices of the Royal Astronomical Society*, vol. 472, no. 1. Oxford University Press (OUP), pp. 542–549, Aug. 04, 2017. doi: 10.1093/mnras/stx1986.  
  
B. Punsly, D. Balsara, J. Kimand S. Garain, “Riemann solvers and Alfven waves in black hole magnetospheres”, *Computational Astrophysics and Cosmology*, vol. 3, no. 1. Springer Science and Business Media LLC, Sep. 13, 2016. doi: 10.1186/s40668-016-0018-1.  
  
K. M. Schoeffler, N. F. Loureiro, R. A. Fonsecaand L. O. Silva, “Magnetic-Field Generation and Amplification in an Expanding Plasma”, *Physical Review Letters*, vol. 112, no. 17. American Physical Society (APS), Apr. 30, 2014. doi: 10.1103/physrevlett.112.175001.  
  
I. Duţan, “Particle-in-cell Simulations of Global Relativistic Jets with Helical Magnetic Fields”, *Proceedings of the International Astronomical Union*, vol. 12, no. S324. Cambridge University Press (CUP), pp. 199–202, Sep. 2016. doi: 10.1017/s1743921316012722.  
  
Y. Mizuno, M. Pohl, J. Niemiec, B. Zhang, K.-I. Nishikawaand P. E. Hardee, “Magnetic field amplification and saturation in turbulence behind a relativistic shock”, *Monthly Notices of the Royal Astronomical Society*, vol. 439, no. 4. Oxford University Press (OUP), pp. 3490–3503, Feb. 27, 2014. doi: 10.1093/mnras/stu196.  
  
K.-I. Nishikawa, “Microscopic Processes in Global Relativistic Jets Containing Helical Magnetic Fields: Dependence on Jet Radius”, *Galaxies*, vol. 5, no. 4. MDPI AG, p. 58, Sep. 26, 2017. doi: 10.3390/galaxies5040058.  
  
K.-I. Nishikawa, “Microscopic Processes in Global Relativistic Jets Containing Helical Magnetic Fields: Dependence on Jet Radius”, *Galaxies*, vol. 5, no. 4. MDPI AG, p. 58, Sep. 26, 2017. doi: 10.3390/galaxies5040058.  
  
K.-I. Nishikawa, “Microscopic Processes in Global Relativistic Jets Containing Helical Magnetic Fields”, *Galaxies*, vol. 4, no. 4. MDPI AG, p. 38, Sep. 29, 2016. doi: 10.3390/galaxies4040038.  
  
K.-I. Nishikawa, “EVOLUTION OF GLOBAL RELATIVISTIC JETS: COLLIMATIONS AND EXPANSION WITH kKHI AND THE WEIBEL INSTABILITY”, *The Astrophysical Journal*, vol. 820, no. 2. American Astronomical Society, p. 94, Mar. 24, 2016. doi: 10.3847/0004-637x/820/2/94.  
  
G. García-Segura, P. M. Rickerand R. E. Taam, “Common Envelope Shaping of Planetary Nebulae”, *The Astrophysical Journal*, vol. 860, no. 1. American Astronomical Society, p. 19, Jun. 07, 2018. doi: 10.3847/1538-4357/aac08c.  
  
K.-C. Pan, P. M. Rickerand R. E. Taam, “IMPACT OF TYPE Ia SUPERNOVA EJECTA ON A HELIUM-STAR BINARY COMPANION”, *The Astrophysical Journal*, vol. 715, no. 1. American Astronomical Society, pp. 78–85, Apr. 23, 2010. doi: 10.1088/0004-637x/715/1/78.  
  
K.-C. Pan, P. M. Rickerand R. E. Taam, “IMPACT OF TYPE Ia SUPERNOVA EJECTA ON BINARY COMPANIONS IN THE SINGLE-DEGENERATE SCENARIO”, *The Astrophysical Journal*, vol. 750, no. 2. American Astronomical Society, p. 151, Apr. 25, 2012. doi: 10.1088/0004-637x/750/2/151.  
  
K.-C. Pan, P. M. Rickerand R. E. Taam, “EVOLUTION OF POST-IMPACT COMPANION STARS IN SN Ia REMNANTS WITHIN THE SINGLE-DEGENERATE SCENARIO”, *The Astrophysical Journal*, vol. 760, no. 1. American Astronomical Society, p. 21, Oct. 30, 2012. doi: 10.1088/0004-637x/760/1/21.  
  
K.-C. Pan, P. M. Rickerand R. E. Taam, “EVOLUTION OF POST-IMPACT REMNANT HELIUM STARS IN TYPE Ia SUPERNOVA REMNANTS WITHIN THE SINGLE-DEGENERATE SCENARIO”, *The Astrophysical Journal*, vol. 773, no. 1. American Astronomical Society, p. 49, Jul. 24, 2013. doi: 10.1088/0004-637x/773/1/49.  
  
K.-C. Pan, P. M. Rickerand R. E. Taam, “SEARCH FOR SURVIVING COMPANIONS IN TYPE Ia SUPERNOVA REMNANTS”, *The Astrophysical Journal*, vol. 792, no. 1. American Astronomical Society, p. 71, Aug. 18, 2014. doi: 10.1088/0004-637x/792/1/71.  
  
P. M. Ricker, K.-C. Pan, R. E. Taam, V. Kologeraand M. van der Sluys, “The Impact of Type Ia Supernova Ejecta on Binary Companions”, *AIP Conference Proceedings*. AIP, 2010. doi: 10.1063/1.3536379.  
  
P. M. Ricker and R. E. Taam, “AN AMR STUDY OF THE COMMON-ENVELOPE PHASE OF BINARY EVOLUTION”, *The Astrophysical Journal*, vol. 746, no. 1. American Astronomical Society, p. 74, Jan. 25, 2012. doi: 10.1088/0004-637x/746/1/74.  
  
P. M. Sutter, H.-Y. K. Yang, P. M. Ricker, G. Foremanand D. Pugmire, “An examination of magnetized outflows from active galactic nuclei in galaxy clusters”, *Monthly Notices of the Royal Astronomical Society*, vol. 419, no. 3. Oxford University Press (OUP), pp. 2293–2314, Nov. 08, 2011. doi: 10.1111/j.1365-2966.2011.19875.x.  
  
R. Vijayaraghavan, J. S. Gallagher IIIand P. M. Ricker, “The dynamical origin of early-type dwarfs in galaxy clusters: a theoretical investigation”, *Monthly Notices of the Royal Astronomical Society*, vol. 447, no. 4. Oxford University Press (OUP), pp. 3623–3638, Jan. 29, 2015. doi: 10.1093/mnras/stu2761.  
  
R. Vijayaraghavan and P. M. Ricker, “Pre-processing and post-processing in group–cluster mergers”, *Monthly Notices of the Royal Astronomical Society*, vol. 435, no. 3. Oxford University Press (OUP), pp. 2713–2735, Sep. 04, 2013. doi: 10.1093/mnras/stt1485.  
  
R. Vijayaraghavan and P. M. Ricker, “Ram pressure stripping of hot coronal gas from group and cluster galaxies and the detectability of surviving X-ray coronae”, *Monthly Notices of the Royal Astronomical Society*, vol. 449, no. 3. Oxford University Press (OUP), pp. 2312–2335, Mar. 31, 2015. doi: 10.1093/mnras/stv476.  
  
R. Vijayaraghavan and P. M. Ricker, “The Co-evolution of a Magnetized Intracluster Medium and Hot Galactic Coronae: Magnetic Field Amplification and Turbulence Generation”, *The Astrophysical Journal*, vol. 841, no. 1. American Astronomical Society, p. 38, May 22, 2017. doi: 10.3847/1538-4357/aa6eac.  
  
M. A. Abramowicz and P. C. Fragile, “Foundations of Black Hole Accretion Disk Theory”, *Living Reviews in Relativity*, vol. 16, no. 1. Springer Science and Business Media LLC, Jan. 14, 2013. doi: 10.12942/lrr-2013-1.  
  
P. Anninos, C. Bryant, P. C. Fragile, A. M. Holgado, C. Lauand D. Nemergut, “CosmosDG: An *hp* -adaptive Discontinuous Galerkin Code for Hyper-resolved Relativistic MHD”, *The Astrophysical Journal Supplement Series*, vol. 231, no. 2. American Astronomical Society, p. 17, Aug. 09, 2017. doi: 10.3847/1538-4365/aa7ff5.  
  
P. Anninos, P. C. Fragile, S. S. Olivier, R. Hoffman, B. Mishraand K. Camarda, “Relativistic Tidal Disruption and Nuclear Ignition of White Dwarf Stars by Intermediate-mass Black Holes”, *The Astrophysical Journal*, vol. 865, no. 1. American Astronomical Society, p. 3, Sep. 17, 2018. doi: 10.3847/1538-4357/aadad9.  
  
P. Anninos, R. D. Hoffman, M. Grewal, M. J. Lavelland P. C. Fragile, “Nuclear Ignition of White Dwarf Stars by Relativistic Encounters with Rotating Intermediate Mass Black Holes”, *The Astrophysical Journal*, vol. 885, no. 2. American Astronomical Society, p. 136, Nov. 08, 2019. doi: 10.3847/1538-4357/ab4ae0.  
  
J. Dexter, E. Agol, P. C. Fragileand J. C. McKinney, “THE SUBMILLIMETER BUMP IN Sgr A\* FROM RELATIVISTIC MHD SIMULATIONS”, *The Astrophysical Journal*, vol. 717, no. 2. American Astronomical Society, pp. 1092–1104, Jun. 22, 2010. doi: 10.1088/0004-637x/717/2/1092.  
  
J. Dexter and P. Chris Fragile, “OBSERVATIONAL SIGNATURES OF TILTED BLACK HOLE ACCRETION DISKS FROM SIMULATIONS”, *The Astrophysical Journal*, vol. 730, no. 1. American Astronomical Society, p. 36, Mar. 01, 2011. doi: 10.1088/0004-637x/730/1/36.  
  
J. Dexter and P. C. Fragile, “Tilted black hole accretion disc models of Sagittarius A*: time-variable millimetre to near-infrared emission”, Monthly Notices of the Royal Astronomical Society, vol. 432, no. 3. Oxford University Press (OUP), pp. 2252–2272, May 08, 2013. doi: 10.1093/mnras/stt583.*  
  
*S. Dibi, S. Drappeau, P. C. Fragile, S. Markoffand J. Dexter, “General relativistic magnetohydrodynamic simulations of accretion on to Sgr A*: how important are radiative losses?”, *Monthly Notices of the Royal Astronomical Society*, vol. 426, no. 3. Oxford University Press (OUP), pp. 1928–1939, Oct. 08, 2012. doi: 10.1111/j.1365-2966.2012.21857.x.  
  
S. Drappeau, S. Dibi, J. Dexter, S. Markoffand P. C. Fragile, “Self-consistent spectra from radiative GRMHD simulations of accretion on to Sgr A*”, Monthly Notices of the Royal Astronomical Society, vol. 431, no. 3. Oxford University Press (OUP), pp. 2872–2884, Mar. 26, 2013. doi: 10.1093/mnras/stt388.*  
  
*P. C. Fragile, P. Anninos, S. Croft, M. Lacyand J. W. L. Witry, “Numerical Simulations of a Jet–Cloud Collision and Starburst: Application to Minkowski’s Object”, The Astrophysical Journal, vol. 850, no. 2. American Astronomical Society, p. 171, Nov. 30, 2017. doi: 10.3847/1538-4357/aa95c6.*  
  
*P. C. Fragile, D. R. Ballantyneand A. Blankenship, “Interactions of type I X-ray bursts with thin accretion disks”, Nature Astronomy, vol. 4, no. 5. Springer Science and Business Media LLC, pp. 541–546, Jan. 06, 2020. doi: 10.1038/s41550-019-0987-5.*  
  
*P. C. Fragile, D. R. Ballantyne, T. J. Maccaroneand J. W. L. Witry, “Simulating the Collapse of a Thick Accretion Disk due to a Type I X-Ray Burst from a Neutron Star”, The Astrophysical Journal, vol. 867, no. 2. American Astronomical Society, p. L28, Nov. 08, 2018. doi: 10.3847/2041-8213/aaeb99.*  
  
*P. C. Fragile, S. M. Etheridge, P. Anninos, B. Mishraand W. Kluźniak, “Relativistic, Viscous, Radiation Hydrodynamic Simulations of Geometrically Thin Disks. I. Thermal and Other Instabilities”, The Astrophysical Journal, vol. 857, no. 1. American Astronomical Society, p. 1, Apr. 06, 2018. doi: 10.3847/1538-4357/aab788.*  
  
*P. C. Fragile, A. Gillespie, T. Monahan, M. Rodriguezand P. Anninos, “NUMERICAL SIMULATIONS OF OPTICALLY THICK ACCRETION ONTO A BLACK HOLE. I. SPHERICAL CASE”, The Astrophysical Journal Supplement Series, vol. 201, no. 2. American Astronomical Society, p. 9, Jun. 15, 2012. doi: 10.1088/0067-0049/201/2/9.*  
  
*P. C. Fragile, D. Nemergut, P. L. Shawand P. Anninos, “Divergence-free magnetohydrodynamics on conformally moving, adaptive meshes using a vector potential method”, Journal of Computational Physics: X, vol. 2. Elsevier BV, p. 100020, Mar. 2019. doi: 10.1016/j.jcpx.2019.100020.*  
  
*P. C. Fragile, A. Olejarand P. Anninos, “NUMERICAL SIMULATIONS OF OPTICALLY THICK ACCRETION ONTO A BLACK HOLE. II. ROTATING FLOW”, The Astrophysical Journal, vol. 796, no. 1. American Astronomical Society, p. 22, Oct. 30, 2014. doi: 10.1088/0004-637x/796/1/22.*  
  
*P. C. Fragile and A. Sądowski, “On the decay of strong magnetization in global disc simulations with toroidal fields”, Monthly Notices of the Royal Astronomical Society, vol. 467, no. 2. Oxford University Press (OUP), pp. 1838–1843, Feb. 01, 2017. doi: 10.1093/mnras/stx274.*  
  
*P. C. Fragile, O. Strauband O. Blaes, “High-frequency and type-C QPOs from oscillating, precessing hot, thick flow”, Monthly Notices of the Royal Astronomical Society, vol. 461, no. 2. Oxford University Press (OUP), pp. 1356–1362, Jun. 20, 2016. doi: 10.1093/mnras/stw1428.*  
  
*A. Generozov, O. Blaes, P. C. Fragileand K. B. Henisey, “PHYSICAL PROPERTIES OF THE INNER SHOCKS IN HOT, TILTED BLACK HOLE ACCRETION FLOWS”, The Astrophysical Journal, vol. 780, no. 1. American Astronomical Society, p. 81, Dec. 13, 2013. doi: 10.1088/0004-637x/780/1/81.*  
  
*K. B. Henisey, O. M. Blaesand P. C. Fragile, “VARIABILITY FROM NON-AXISYMMETRIC FLUCTUATIONS INTERACTING WITH STANDING SHOCKS IN TILTED BLACK HOLE ACCRETION DISKS”, The Astrophysical Journal, vol. 761, no. 1. American Astronomical Society, p. 18, Nov. 20, 2012. doi: 10.1088/0004-637x/761/1/18.*  
  
*B. Mishra, P. C. Fragile, L. C. Johnsonand W. Kluźniak, “Three-dimensional, global, radiative GRMHD simulations of a thermally unstable disc”, Monthly Notices of the Royal Astronomical Society, vol. 463, no. 4. Oxford University Press (OUP), pp. 3437–3448, Sep. 09, 2016. doi: 10.1093/mnras/stw2245.*  
  
*B. Mishra, W. Kluźniakand P. C. Fragile, “Breathing oscillations in a global simulation of a thin accretion disc”, Monthly Notices of the Royal Astronomical Society, vol. 483, no. 4. Oxford University Press (OUP), pp. 4811–4819, Nov. 27, 2018. doi: 10.1093/mnras/sty3124.*  
  
*D. M. Teixeira, P. C. Fragile, V. V. Zhuravlevand P. B. Ivanov, “CONSERVATIVE GRMHD SIMULATIONS OF MODERATELY THIN, TILTED ACCRETION DISKS”, The Astrophysical Journal, vol. 796, no. 2. American Astronomical Society, p. 103, Nov. 12, 2014. doi: 10.1088/0004-637x/796/2/103.*  
  
*M. Wielgus, P. C. Fragile, Z. Wangand J. Wilson, “Local stability of strongly magnetized black hole tori”, Monthly Notices of the Royal Astronomical Society, vol. 447, no. 4. Oxford University Press (OUP), pp. 3593–3601, Jan. 24, 2015. doi: 10.1093/mnras/stu2676.*  
  
*V. V. Zhuravlev, P. B. Ivanov, P. C. Fragileand D. M. Teixeira, “NO EVIDENCE FOR BARDEEN-PETTERSON ALIGNMENT IN GRMHD SIMULATIONS AND SEMI-ANALYTIC MODELS OF MODERATELY THIN, PROGRADE, TILTED ACCRETION DISKS”, The Astrophysical Journal, vol. 796, no. 2. American Astronomical Society, p. 104, Nov. 12, 2014. doi: 10.1088/0004-637x/796/2/104.*  
  
*S. Tang and Q. D. Wang, “Missing-iron problem and Type Ia supernova enrichment of hot gas in galactic spheroids”, Monthly Notices of the Royal Astronomical Society, vol. 408, no. 2. Oxford University Press (OUP), pp. 1011–1019, Jul. 27, 2010. doi: 10.1111/j.1365-2966.2010.17171.x.*  
  
*K.-Y. Lee, G. Mellemaand P. Lundqvist, “Efficient photoheating algorithms in time-dependent photoionization simulations”, Monthly Notices of the Royal Astronomical Society, vol. 455, no. 4. Oxford University Press (OUP), pp. 4406–4425, Dec. 09, 2015. doi: 10.1093/mnras/stv2556.*  
  
*H. Park (박현배), E. Komatsu, P. R. Shapiro, J. Kodaand Y. Mao, “THE IMPACT OF NONLINEAR STRUCTURE FORMATION ON THE POWER SPECTRUM OF TRANSVERSE MOMENTUM FLUCTUATIONS AND THE KINETIC SUNYAEV–ZEL’DOVICH EFFECT”, The Astrophysical Journal, vol. 818, no. 1. American Astronomical Society, p. 37, Feb. 05, 2016. doi: 10.3847/0004-637x/818/1/37.*  
  
*R. E. Taam and P. M. Ricker, “Common envelope evolution”, New Astronomy Reviews, vol. 54, no. 3–6. Elsevier BV, pp. 65–71, Mar. 2010. doi: 10.1016/j.newar.2010.09.027.*  
  
*J. Liu, A. Ortiz-Vazquezand J. C. Hill, “Constraining multiplicative bias in CFHTLenS weak lensing shear data”, Physical Review D, vol. 93, no. 10. American Physical Society (APS), May 09, 2016. doi: 10.1103/physrevd.93.103508.*  
  
*V. F. Calderon and A. A. Berlind, “Prediction of galaxy halo masses in SDSS DR7 via a machine learning approach”, Monthly Notices of the Royal Astronomical Society, vol. 490, no. 2. Oxford University Press (OUP), pp. 2367–2379, Oct. 04, 2019. doi: 10.1093/mnras/stz2775.*  
  
*V. F. Calderon, A. A. Berlindand M. Sinha, “Small- and large-scale galactic conformity in SDSS DR7”, Monthly Notices of the Royal Astronomical Society, vol. 480, no. 2. Oxford University Press (OUP), pp. 2031–2045, Jul. 25, 2018. doi: 10.1093/mnras/sty2000.*  
  
*K. C. Chan and R. Scoccimarro, “Halo sampling, local bias, and loop corrections”, Physical Review D, vol. 86, no. 10. American Physical Society (APS), Nov. 19, 2012. doi: 10.1103/physrevd.86.103519.*  
  
*K. C. Chan, R. Scoccimarroand R. K. Sheth, “Gravity and large-scale nonlocal bias”, Physical Review D, vol. 85, no. 8. American Physical Society (APS), Apr. 05, 2012. doi: 10.1103/physrevd.85.083509.*  
  
*K. C. Chan, R. K. Shethand R. Scoccimarro, “Consistency relations for the Lagrangian halo bias and their implications”, Monthly Notices of the Royal Astronomical Society, vol. 468, no. 2. Oxford University Press (OUP), pp. 2232–2248, Mar. 14, 2017. doi: 10.1093/mnras/stx609.*  
  
*K. C. Chan, R. K. Shethand R. Scoccimarro, “Effective window function for Lagrangian halos”, Physical Review D, vol. 96, no. 10. American Physical Society (APS), Nov. 27, 2017. doi: 10.1103/physrevd.96.103543.*  
  
*M. Crocce, R. Scoccimarroand F. Bernardeau, “MPTbreeze: a fast renormalized perturbative scheme”, Monthly Notices of the Royal Astronomical Society, vol. 427, no. 3. Oxford University Press (OUP), pp. 2537–2551, Nov. 20, 2012. doi: 10.1111/j.1365-2966.2012.22127.x.*  
  
*C. Hahn, F. Beutler, M. Sinha, A. Berlind, S. Hoand D. W. Hogg, “Likelihood non-Gaussianity in large-scale structure analyses”, Monthly Notices of the Royal Astronomical Society, vol. 485, no. 2. Oxford University Press (OUP), pp. 2956–2969, Feb. 26, 2019. doi: 10.1093/mnras/stz558.*  
  
*J. W. Johnson, A. H. Maller, A. A. Berlind, M. Sinhaand J. K. Holley-Bockelmann, “The secondary spin bias of dark matter haloes”, Monthly Notices of the Royal Astronomical Society, vol. 486, no. 1. Oxford University Press (OUP), pp. 1156–1166, Apr. 03, 2019. doi: 10.1093/mnras/stz942.*  
  
*E. A. Kazin, M. R. Blanton, R. Scoccimarro, C. K. McBrideand A. A. Berlind, “REGARDING THE LINE-OF-SIGHT BARYONIC ACOUSTIC FEATURE IN THE SLOAN DIGITAL SKY SURVEY AND BARYON OSCILLATION SPECTROSCOPIC SURVEY LUMINOUS RED GALAXY SAMPLES”, The Astrophysical Journal, vol. 719, no. 2. American Astronomical Society, pp. 1032–1044, Jul. 26, 2010. doi: 10.1088/0004-637x/719/2/1032.*  
  
*E. A. Kazin, “THE BARYONIC ACOUSTIC FEATURE AND LARGE-SCALE CLUSTERING IN THE SLOAN DIGITAL SKY SURVEY LUMINOUS RED GALAXY SAMPLE”, The Astrophysical Journal, vol. 710, no. 2. American Astronomical Society, pp. 1444–1461, Feb. 01, 2010. doi: 10.1088/0004-637x/710/2/1444.*  
  
*M. Manera, “The clustering of galaxies in the SDSS-III Baryon Oscillation Spectroscopic Survey: a large sample of mock galaxy catalogues”, Monthly Notices of the Royal Astronomical Society, vol. 428, no. 2. Oxford University Press (OUP), pp. 1036–1054, Oct. 31, 2012. doi: 10.1093/mnras/sts084.*  
  
*Q. Mao, A. A. Berlind, C. K. McBride, R. J. Scherrer, R. Scoccimarroand M. Manera, “Constraining primordial non-Gaussianity with moments of the large-scale density field”, Monthly Notices of the Royal Astronomical Society, vol. 443, no. 2. Oxford University Press (OUP), pp. 1402–1415, Jul. 21, 2014. doi: 10.1093/mnras/stu1255.*  
  
*Q. Mao, “Cosmic Voids in the SDSS DR12 BOSS Galaxy Sample: the Alcock–Paczyński test”, The Astrophysical Journal, vol. 835, no. 2. American Astronomical Society, p. 160, Jan. 25, 2017. doi: 10.3847/1538-4357/835/2/160.*  
  
*Q. Mao, “A Cosmic Void Catalog of SDSS DR12 BOSS Galaxies”, The Astrophysical Journal, vol. 835, no. 2. American Astronomical Society, p. 161, Jan. 25, 2017. doi: 10.3847/1538-4357/835/2/161.*  
  
*A. N. Salcedo, “Spatial clustering of dark matter haloes: secondary bias, neighbour bias, and the influence of massive neighbours on halo properties”, Monthly Notices of the Royal Astronomical Society, vol. 475, no. 4. Oxford University Press (OUP), pp. 4411–4423, Jan. 15, 2018. doi: 10.1093/mnras/sty109.*  
  
*R. K. Sheth, K. C. Chanand R. Scoccimarro, “Nonlocal Lagrangian bias”, Physical Review D, vol. 87, no. 8. American Physical Society (APS), Apr. 03, 2013. doi: 10.1103/physrevd.87.083002.*  
  
*M. Sinha, A. A. Berlind, C. K. McBride, R. Scoccimarro, J. A. Piscionereand B. D. Wibking, “Towards accurate modelling of galaxy clustering on small scales: testing the standard ΛCDM + halo model”, Monthly Notices of the Royal Astronomical Society, vol. 478, no. 1. Oxford University Press (OUP), pp. 1042–1064, Apr. 19, 2018. doi: 10.1093/mnras/sty967.*  
  
*D. F. Watson, A. A. Berlindand A. R. Zentner, “CONSTRAINING SATELLITE GALAXY STELLAR MASS LOSS AND PREDICTING INTRAHALO LIGHT. I. FRAMEWORK AND RESULTS AT LOW REDSHIFT”, The Astrophysical Journal, vol. 754, no. 2. American Astronomical Society, p. 90, Jul. 11, 2012. doi: 10.1088/0004-637x/754/2/90.*  
  
*R. F. Penna, R. Narayanand A. Sądowski, “General relativistic magnetohydrodynamic simulations of Blandford–Znajek jets and the membrane paradigm”, Monthly Notices of the Royal Astronomical Society, vol. 436, no. 4. Oxford University Press (OUP), pp. 3741–3758, Oct. 26, 2013. doi: 10.1093/mnras/stt1860.*  
  
*A. Sądowski, R. Narayan, R. Pennaand Y. Zhu, “Energy, momentum and mass outflows and feedback from thick accretion discs around rotating black holes”, Monthly Notices of the Royal Astronomical Society, vol. 436, no. 4. Oxford University Press (OUP), pp. 3856–3874, Nov. 16, 2013. doi: 10.1093/mnras/stt1881.*  
  
*A. Tchekhovskoy, B. D. Metzger, D. Gianniosand L. Z. Kelley, “Swift J1644+57 gone MAD: the case for dynamically important magnetic flux threading the black hole in a jetted tidal disruption event”, Monthly Notices of the Royal Astronomical Society, vol. 437, no. 3. Oxford University Press (OUP), pp. 2744–2760, Nov. 30, 2013. doi: 10.1093/mnras/stt2085.*  
  
*S. R. Harmon and J. D. Mckinney, “Precision Broadband RF Signal Recovery in Subsampled Analog Optical Links”, IEEE Photonics Technology Letters, vol. 27, no. 6. Institute of Electrical and Electronics Engineers (IEEE), pp. 620–623, Mar. 15, 2015. doi: 10.1109/lpt.2014.2386657.*  
  
*S. R. Harmon and J. D. McKinney, “Broadband RF disambiguation in subsampled analog optical links via intentionally-introduced sampling jitter”, Optics Express, vol. 22, no. 20. The Optical Society, p. 23928, Sep. 23, 2014. doi: 10.1364/oe.22.023928.*  
  
*M. N. Hutchinson, J. M. Singley, V. J. Urick, S. R. Harmon, J. D. McKinneyand N. J. Frigo, “Mitigation of Photodiode Induced Even-Order Distortion in Photonic Links With Predistortion Modulation”, Journal of Lightwave Technology, vol. 32, no. 20. Institute of Electrical and Electronics Engineers (IEEE), pp. 3885–3892, Oct. 15, 2014. doi: 10.1109/jlt.2014.2321481.*  
  
*J. D. McKinney, “Photonics illuminates the future of radar”, Nature, vol. 507, no. 7492. Springer Science and Business Media LLC, pp. 310–312, Mar. 19, 2014. doi: 10.1038/507310a.*  
  
*J. Meeßen, “Effects of UVC254 nm on the photosynthetic activity of photobionts from the astrobiologically relevant lichens Buellia frigida and Circinaria gyrosa”, International Journal of Astrobiology, vol. 13, no. 4. Cambridge University Press (CUP), pp. 340–352, Oct. 2014. doi: 10.1017/s1473550414000275.*  
  
*J. Meeßen, F. J. Sánchez, A. Sadowsky, R. de la Torre, S. Ottand J.-P. de Vera, “Extremotolerance and Resistance of Lichens: Comparative Studies on Five Species Used in Astrobiological Research II. Secondary Lichen Compounds”, Origins of Life and Evolution of Biospheres, vol. 43, no. 6. Springer Science and Business Media LLC, pp. 501–526, Dec. 2013. doi: 10.1007/s11084-013-9348-z.*  
  
*V. J. Urick, J. F. Diehl, M. N. Draa, J. D. McKinneyand K. J. Williams, “Wideband analog photonic links: some performance limits and considerations for multi-octave implementations”, SPIE Proceedings. SPIE, Feb. 23, 2012. doi: 10.1117/12.912528.*  
  
*V. J. Urick, J. D. McKinney, J. F. Diehland K. J. Williams, “Equations for Two-Tone Analog Optical Phase Modulation With an Asymmetric Interferometer”, IEEE Photonics Technology Letters, vol. 25, no. 15. Institute of Electrical and Electronics Engineers (IEEE), pp. 1527–1530, Aug. 2013. doi: 10.1109/lpt.2013.2270432.*  
  
*K. Vierdayanti, A. Sadowski, S. Mineshigeand M. Bursa, “Inner disc obscuration in GRS 1915+105 based on relativistic slim disc model”, Monthly Notices of the Royal Astronomical Society, vol. 436, no. 1. Oxford University Press (OUP), pp. 71–81, Sep. 26, 2013. doi: 10.1093/mnras/stt1467.*  
  
*C. H. Fu, Y. B. Guo, J. McKinneyand X. T. Wei, “Process Mechanics of Low Plasticity Burnishing of Nitinol Alloy”, Journal of Materials Engineering and Performance, vol. 21, no. 12. Springer Science and Business Media LLC, pp. 2607–2617, Aug. 07, 2012. doi: 10.1007/s11665-012-0313-1.*  
  
*A. V. Bilous, “A LOFAR census of non-recycled pulsars: average profiles, dispersion measures, flux densities, and spectra”, Astronomy & Astrophysics, vol. 591. EDP Sciences, p. A134, Jun. 30, 2016. doi: 10.1051/0004-6361/201527702.*  
  
*J. W. Broderick, “Low-radio-frequency eclipses of the redback pulsar J2215+5135 observed in the image plane with LOFAR”, Monthly Notices of the Royal Astronomical Society, vol. 459, no. 3. Oxford University Press (OUP), pp. 2681–2689, Apr. 08, 2016. doi: 10.1093/mnras/stw794.*  
  
*D. Carbone, “New methods to constrain the radio transient rate: results from a survey of four fields with LOFAR”, Monthly Notices of the Royal Astronomical Society, vol. 459, no. 3. Oxford University Press (OUP), pp. 3161–3174, Mar. 07, 2016. doi: 10.1093/mnras/stw539.*  
  
*A. Chael, R. Narayanand M. D. Johnson, “Two-temperature, Magnetically Arrested Disc simulations of the jet from the supermassive black hole in M87”, Monthly Notices of the Royal Astronomical Society, vol. 486, no. 2. Oxford University Press (OUP), pp. 2873–2895, Apr. 08, 2019. doi: 10.1093/mnras/stz988.*  
  
*V. J. Urick, M. N. Hutchinson, J. M. Singley, J. D. McKinneyand K. J. Williams, “Suppression of even-order photodiode distortions via predistortion linearization with a bias-shifted Mach-Zehnder modulator”, Optics Express, vol. 21, no. 12. The Optical Society, p. 14368, Jun. 10, 2013. doi: 10.1364/oe.21.014368.*  
  
*A. A. Chael, R. Narayanand A. Sa̧dowski, “Evolving non-thermal electrons in simulations of black hole accretion”, Monthly Notices of the Royal Astronomical Society, vol. 470, no. 2. Oxford University Press (OUP), pp. 2367–2386, Jul. 06, 2017. doi: 10.1093/mnras/stx1345.*  
  
*A. Chael, M. Rowan, R. Narayan, M. Johnsonand L. Sironi, “The role of electron heating physics in images and variability of the Galactic Centre black hole Sagittarius A*”, *Monthly Notices of the Royal Astronomical Society*, vol. 478, no. 4. Oxford University Press (OUP), pp. 5209–5229, Jun. 28, 2018. doi: 10.1093/mnras/sty1261.  
  
I. Contopoulos, A. Nathanail, A. Sądowski, D. Kazanasand R. Narayan, “Numerical simulations of the Cosmic Battery in accretion flows around astrophysical black holes”, *Monthly Notices of the Royal Astronomical Society*, vol. 473, no. 1. Oxford University Press (OUP), pp. 721–727, Sep. 04, 2017. doi: 10.1093/mnras/stx2249.  
  
B. Curd and R. Narayan, “GRRMHD Simulations of Tidal Disruption Event Accretion Disks around Supermassive Black Holes: Jet Formation, Spectra, and Detectability”, *Monthly Notices of the Royal Astronomical Society*. Oxford University Press (OUP), Nov. 18, 2018. doi: 10.1093/mnras/sty3134.  
  
X. Guo, L. Sironiand R. Narayan, “Electron Heating in Low Mach Number Perpendicular Shocks. II. Dependence on the Pre-shock Conditions”, *The Astrophysical Journal*, vol. 858, no. 2. American Astronomical Society, p. 95, May 10, 2018. doi: 10.3847/1538-4357/aab6ad.  
  
R. Narayan, Y. Zhu, D. Psaltisand A. Sa̧dowski, “heroic: 3D general relativistic radiative post-processor with comptonization for black hole accretion discs”, *Monthly Notices of the Royal Astronomical Society*, vol. 457, no. 1. Oxford University Press (OUP), pp. 608–628, Jan. 22, 2016. doi: 10.1093/mnras/stv2979.  
  
M. E. Rowan, L. Sironiand R. Narayan, “Electron and Proton Heating in Transrelativistic Magnetic Reconnection”, *The Astrophysical Journal*, vol. 850, no. 1. American Astronomical Society, p. 29, Nov. 14, 2017. doi: 10.3847/1538-4357/aa9380.  
  
A. Sądowski, “Thin accretion discs are stabilized by a strong magnetic field”, *Monthly Notices of the Royal Astronomical Society*, vol. 459, no. 4. Oxford University Press (OUP), pp. 4397–4407, Apr. 20, 2016. doi: 10.1093/mnras/stw913.  
  
A. Sądowski, J.-P. Lasota, M. A. Abramowiczand R. Narayan, “Energy flows in thick accretion discs and their consequences for black hole feedback”, *Monthly Notices of the Royal Astronomical Society*, vol. 456, no. 4. Oxford University Press (OUP), pp. 3915–3928, Jan. 14, 2016. doi: 10.1093/mnras/stv2854.  
  
A. Sądowski and R. Narayan, “Powerful radiative jets in supercritical accretion discs around non-spinning black holes”, *Monthly Notices of the Royal Astronomical Society*, vol. 453, no. 3. Oxford University Press (OUP), pp. 3214–3222, Sep. 04, 2015. doi: 10.1093/mnras/stv1802.  
  
A. Sądowski and R. Narayan, “Photon-conserving Comptonization in simulations of accretion discs around black holes”, *Monthly Notices of the Royal Astronomical Society*, vol. 454, no. 3. Oxford University Press (OUP), pp. 2372–2380, Oct. 13, 2015. doi: 10.1093/mnras/stv2022.  
  
A. Sądowski and R. Narayan, “Three-dimensional simulations of supercritical black hole accretion discs – luminosities, photon trapping and variability”, *Monthly Notices of the Royal Astronomical Society*, vol. 456, no. 4. Oxford University Press (OUP), pp. 3929–3947, Jan. 14, 2016. doi: 10.1093/mnras/stv2941.  
  
A. Sądowski, E. Tejeda, E. Gafton, S. Rosswogand D. Abarca, “Magnetohydrodynamical simulations of a deep tidal disruption in general relativity”, *Monthly Notices of the Royal Astronomical Society*, vol. 458, no. 4. Oxford University Press (OUP), pp. 4250–4268, Mar. 11, 2016. doi: 10.1093/mnras/stw589.  
  
A. Sądowski, M. Wielgus, R. Narayan, D. Abarca, J. C. McKinneyand A. Chael, “Radiative, two-temperature simulations of low-luminosity black hole accretion flows in general relativity”, *Monthly Notices of the Royal Astronomical Society*, vol. 466, no. 1. Oxford University Press (OUP), pp. 705–725, Dec. 01, 2016. doi: 10.1093/mnras/stw3116.  
  
M. Siwek, A. Sądowski, R. Narayan, T. P. Robertsand R. Soria, “Optical and X-ray luminosities of expanding nebulae around ultraluminous X-ray sources”, *Monthly Notices of the Royal Astronomical Society*, vol. 470, no. 1. Oxford University Press (OUP), pp. 361–371, May 17, 2017. doi: 10.1093/mnras/stx1185.  
  
F. Yuan, Z. Gan, R. Narayan, A. Sadowski, D. Buand X.-N. Bai, “NUMERICAL SIMULATION OF HOT ACCRETION FLOWS. III. REVISITING WIND PROPERTIES USING THE TRAJECTORY APPROACH”, *The Astrophysical Journal*, vol. 804, no. 2. American Astronomical Society, p. 101, May 06, 2015. doi: 10.1088/0004-637x/804/2/101.  
  
Y. Zhu, R. Narayan, A. Sadowskiand D. Psaltis, “hero – A 3D general relativistic radiative post-processor for accretion discs around black holes”, *Monthly Notices of the Royal Astronomical Society*, vol. 451, no. 2. Oxford University Press (OUP), pp. 1661–1681, Jun. 08, 2015. doi: 10.1093/mnras/stv1046.  
  
T. G. Bisbas, “starbench: the D-type expansion of an H ii region”, *Monthly Notices of the Royal Astronomical Society*, vol. 453, no. 2. Oxford University Press (OUP), pp. 1324–1343, Aug. 25, 2015. doi: 10.1093/mnras/stv1659.  
  
J. W. Lynn, E. Quataert, B. D. G. Chandranand I. J. Parrish, “ACCELERATION OF RELATIVISTIC ELECTRONS BY MAGNETOHYDRODYNAMIC TURBULENCE: IMPLICATIONS FOR NON-THERMAL EMISSION FROM BLACK HOLE ACCRETION DISKS”, *The Astrophysical Journal*, vol. 791, no. 1. American Astronomical Society, p. 71, Jul. 28, 2014. doi: 10.1088/0004-637x/791/1/71.  
  
M. A. Riquelme, E. Quataert, P. Sharmaand A. Spitkovsky, “LOCAL TWO-DIMENSIONAL PARTICLE-IN-CELL SIMULATIONS OF THE COLLISIONLESS MAGNETOROTATIONAL INSTABILITY”, *The Astrophysical Journal*, vol. 755, no. 1. American Astronomical Society, p. 50, Jul. 25, 2012. doi: 10.1088/0004-637x/755/1/50.  
  
M. A. Riquelme, E. Quataertand D. Verscharen, “PARTICLE-IN-CELL SIMULATIONS OF CONTINUOUSLY DRIVEN MIRROR AND ION CYCLOTRON INSTABILITIES IN HIGH BETA ASTROPHYSICAL AND HELIOSPHERIC PLASMAS”, *The Astrophysical Journal*, vol. 800, no. 1. American Astronomical Society, p. 27, Feb. 05, 2015. doi: 10.1088/0004-637x/800/1/27.  
  
K. Ahn, I. T. Iliev, P. R. Shapiroand C. Srisawat, “Non-linear bias of cosmological halo formation in the early universe”, *Monthly Notices of the Royal Astronomical Society*, vol. 450, no. 2. Oxford University Press (OUP), pp. 1486–1502, Apr. 25, 2015. doi: 10.1093/mnras/stv704.  
  
K. Ahn, “Cosmological Reionization by the First Stars in the H[sub 2]-Dissociating Background”, *AIP Conference Proceedings*. AIP, 2010. doi: 10.1063/1.3518862.  
  
D. Aubert, “The Inhomogeneous Reionization Times of Present-day Galaxies”, *The Astrophysical Journal*, vol. 856, no. 2. American Astronomical Society, p. L22, Mar. 26, 2018. doi: 10.3847/2041-8213/aab14d.  
  
K. K. Datta, M. M. Friedrich, G. Mellema, I. T. Ilievand P. R. Shapiro, “Prospects of observing a quasar H ii region during the epoch of reionization with the redshifted 21-cm signal”, *Monthly Notices of the Royal Astronomical Society*, vol. 424, no. 1. Oxford University Press (OUP), pp. 762–778, Jun. 19, 2012. doi: 10.1111/j.1365-2966.2012.21268.x.  
  
K. K. Datta, “Light cone effect on the reionization 21-cm signal – II. Evolution, anisotropies and observational implications”, *Monthly Notices of the Royal Astronomical Society*, vol. 442, no. 2. Oxford University Press (OUP), pp. 1491–1506, Jun. 16, 2014. doi: 10.1093/mnras/stu927.  
  
K. K. Datta, G. Mellema, Y. Mao, I. T. Iliev, P. R. Shapiroand K. Ahn, “Light-cone effect on the reionization 21-cm power spectrum”, *Monthly Notices of the Royal Astronomical Society*, vol. 424, no. 3. Oxford University Press (OUP), pp. 1877–1891, Jul. 03, 2012. doi: 10.1111/j.1365-2966.2012.21293.x.  
  
T. Dawoodbhoy, “Suppression of star formation in low-mass galaxies caused by the reionization of their local neighbourhood”, *Monthly Notices of the Royal Astronomical Society*, vol. 480, no. 2. Oxford University Press (OUP), pp. 1740–1753, Jul. 20, 2018. doi: 10.1093/mnras/sty1945.  
  
V. Desjacques, U. Seljak, I. T. Iliev, J.-M. Alimiand A. Fuözfa, “Effect of primordial non-Gaussianity on halo bias and mass function”, *AIP Conference Proceedings*. AIP, 2010. doi: 10.1063/1.3462723.  
  
K. L. Dixon, “Reionization of the Milky Way, M31, and their satellites – I. Reionization history and star formation”, *Monthly Notices of the Royal Astronomical Society*, vol. 477, no. 1. Oxford University Press (OUP), pp. 867–881, Feb. 27, 2018. doi: 10.1093/mnras/sty494.  
  
K. L. Dixon, I. T. Iliev, G. Mellema, K. Ahnand P. R. Shapiro, “The large-scale observational signatures of low-mass galaxies during reionization”, *Monthly Notices of the Royal Astronomical Society*, vol. 456, no. 3. Oxford University Press (OUP), pp. 3011–3029, Dec. 31, 2015. doi: 10.1093/mnras/stv2887.  
  
E. Fernandez, I. T. Iliev, E. Komatsu, H. Doleand P. Shapiro, “Using the cosmic infrared background to deduce properties of high redshift stars”, *AIP Conference Proceedings*. AIP, 2012. doi: 10.1063/1.4754368.  
  
E. R. Fernandez, S. Zaroubi, I. T. Iliev, G. Mellemaand V. Jelić, “Stars and reionization: the cross-correlation of the 21 cm line and the near-infrared background”, *Monthly Notices of the Royal Astronomical Society*, vol. 440, no. 1. Oxford University Press (OUP), pp. 298–306, Mar. 08, 2014. doi: 10.1093/mnras/stu261.  
  
M. M. Friedrich, G. Mellema, M. A. Alvarez, P. R. Shapiroand I. T. Iliev, “Topology and sizes of H ii regions during cosmic reionization”, *Monthly Notices of the Royal Astronomical Society*, vol. 413, no. 2. Oxford University Press (OUP), pp. 1353–1372, Mar. 15, 2011. doi: 10.1111/j.1365-2966.2011.18219.x.  
  
M. M. Friedrich, G. Mellema, I. T. Ilievand P. R. Shapiro, “Radiative transfer of energetic photons: X-rays and helium ionization in C2-Ray”, *Monthly Notices of the Royal Astronomical Society*, vol. 421, no. 3. Oxford University Press (OUP), pp. 2232–2250, Feb. 09, 2012. doi: 10.1111/j.1365-2966.2012.20449.x.  
  
R. Ghara, G. Mellema, S. K. Giri, T. R. Choudhury, K. K. Dattaand S. Majumdar, “Prediction of the 21-cm signal from reionization: comparison between 3D and 1D radiative transfer schemes”, *Monthly Notices of the Royal Astronomical Society*, vol. 476, no. 2. Oxford University Press (OUP), pp. 1741–1755, Feb. 07, 2018. doi: 10.1093/mnras/sty314.  
  
S. K. Giri, G. Mellema, K. L. Dixonand I. T. Iliev, “Bubble size statistics during reionization from 21-cm tomography”, *Monthly Notices of the Royal Astronomical Society*, vol. 473, no. 3. Oxford University Press (OUP), pp. 2949–2964, Oct. 02, 2017. doi: 10.1093/mnras/stx2539.  
  
B. F. Griffen, M. J. Drinkwater, I. T. Iliev, P. A. Thomasand G. Mellema, “The inhomogeneous reionization of the local intergalactic medium by metal-poor globular clusters”, *Monthly Notices of the Royal Astronomical Society*, vol. 431, no. 4. Oxford University Press (OUP), pp. 3087–3102, Apr. 03, 2013. doi: 10.1093/mnras/stt382.  
  
J. Harnois-Deraps, U.-L. Pen, I. T. Iliev, H. Merz, J. D. Embersonand V. Desjacques, “High-performance P3M N-body code: CUBEP3M”, *Monthly Notices of the Royal Astronomical Society*, vol. 436, no. 1. Oxford University Press (OUP), pp. 540–559, Sep. 17, 2013. doi: 10.1093/mnras/stt1591.  
  
S. Hotchkiss, “The Jubilee ISW Project - II. Observed and simulated imprints of voids and superclusters on the cosmic microwave background”, *Monthly Notices of the Royal Astronomical Society*, vol. 446, no. 2. Oxford University Press (OUP), pp. 1321–1334, Nov. 19, 2014. doi: 10.1093/mnras/stu2072.  
  
K. Ichikawa, R. Barkana, I. T. Iliev, G. Mellemaand P. R. Shapiro, “Measuring the history of cosmic reionization using the 21-cm probability distribution function from simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 406, no. 4. Oxford University Press (OUP), pp. 2521–2532, May 26, 2010. doi: 10.1111/j.1365-2966.2010.16828.x.  
  
C. Ilie, K. Freese, M. Valluri, I. T. Ilievand P. R. Shapiro, “Observing supermassive dark stars with James Webb Space Telescope”, *Monthly Notices of the Royal Astronomical Society*, vol. 422, no. 3. Oxford University Press (OUP), pp. 2164–2186, Apr. 10, 2012. doi: 10.1111/j.1365-2966.2012.20760.x.  
  
I. T. Iliev, G. Mellema, K. Ahn, P. R. Shapiro, Y. Maoand U.-L. Pen, “Simulating cosmic reionization: how large a volume is large enough?”, *Monthly Notices of the Royal Astronomical Society*, vol. 439, no. 1. Oxford University Press (OUP), pp. 725–743, Jan. 23, 2014. doi: 10.1093/mnras/stt2497.  
  
I. T. Iliev, “Can 21-cm observations discriminate between high-mass and low-mass galaxies as reionization sources?”, *Monthly Notices of the Royal Astronomical Society*, vol. 423, no. 3. Oxford University Press (OUP), pp. 2222–2253, May 07, 2012. doi: 10.1111/j.1365-2966.2012.21032.x.  
  
I. T. Iliev, B. Moore, S. Gottlöber, G. Yepes, Y. Hoffmanand G. Mellema, “Reionization of the Local Group of galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 413, no. 3. Oxford University Press (OUP), pp. 2093–2102, Mar. 08, 2011. doi: 10.1111/j.1365-2966.2011.18292.x.  
  
V. Jelić, “A cross-correlation study between the cosmological 21 cm signal and the kinetic Sunyaev-Zel’dovich effect”, *Monthly Notices of the Royal Astronomical Society*, vol. 402, no. 4. Oxford University Press (OUP), pp. 2279–2290, Mar. 2010. doi: 10.1111/j.1365-2966.2009.16086.x.  
  
H. Jensen, “Probing reionization with LOFAR using 21-cm redshift space distortions”, *Monthly Notices of the Royal Astronomical Society*, vol. 435, no. 1. Oxford University Press (OUP), pp. 460–474, Aug. 19, 2013. doi: 10.1093/mnras/stt1341.  
  
H. Jensen, M. Hayes, I. T. Iliev, P. Laursen, G. Mellemaand E. Zackrisson, “Studying reionization with the next generation of Lyα emitter surveys”, *Monthly Notices of the Royal Astronomical Society*, vol. 444, no. 3. Oxford University Press (OUP), pp. 2114–2127, Sep. 09, 2014. doi: 10.1093/mnras/stu1600.  
  
H. Jensen, P. Laursen, G. Mellema, I. T. Iliev, J. Sommer-Larsenand P. R. Shapiro, “On the use of Lyα emitters as probes of reionization”, *Monthly Notices of the Royal Astronomical Society*, vol. 428, no. 2. Oxford University Press (OUP), pp. 1366–1381, Nov. 01, 2012. doi: 10.1093/mnras/sts116.  
  
H. Jensen, S. Majumdar, G. Mellema, A. Lidz, I. T. Ilievand K. L. Dixon, “The wedge bias in reionization 21-cm power spectrum measurements”, *Monthly Notices of the Royal Astronomical Society*, vol. 456, no. 1. Oxford University Press (OUP), pp. 66–70, Dec. 11, 2015. doi: 10.1093/mnras/stv2679.  
  
K. Kakiichi, “Recovering the H ii region size statistics from 21-cm tomography”, *Monthly Notices of the Royal Astronomical Society*, vol. 471, no. 2. Oxford University Press (OUP), pp. 1936–1954, Jun. 22, 2017. doi: 10.1093/mnras/stx1568.  
  
J. Koda and P. R. Shapiro, “Gravothermal collapse of isolated self-interacting dark matter haloes: N-body simulation versus the fluid model”, *Monthly Notices of the Royal Astronomical Society*, vol. 415, no. 2. Oxford University Press (OUP), pp. 1125–1137, Jun. 27, 2011. doi: 10.1111/j.1365-2966.2011.18684.x.  
  
B. Li, P. R. Shapiroand T. Rindler-Daller, “Bose-Einstein-condensed scalar field dark matter and the gravitational wave background from inflation: New cosmological constraints and its detectability by LIGO”, *Physical Review D*, vol. 96, no. 6. American Physical Society (APS), Sep. 08, 2017. doi: 10.1103/physrevd.96.063505.  
  
S. Majumdar, “Effects of the sources of reionization on 21-cm redshift-space distortions”, *Monthly Notices of the Royal Astronomical Society*, vol. 456, no. 2. Oxford University Press (OUP), pp. 2080–2094, Dec. 30, 2015. doi: 10.1093/mnras/stv2812.  
  
S. Majumdar, “On the use of seminumerical simulations in predicting the 21-cm signal from the epoch of reionization”, *Monthly Notices of the Royal Astronomical Society*, vol. 443, no. 4. Oxford University Press (OUP), pp. 2843–2861, Aug. 05, 2014. doi: 10.1093/mnras/stu1342.  
  
S. Majumdar, J. R. Pritchard, R. Mondal, C. A. Watkinson, S. Bharadwajand G. Mellema, “Quantifying the non-Gaussianity in the EoR 21-cm signal through bispectrum”, *Monthly Notices of the Royal Astronomical Society*, vol. 476, no. 3. Oxford University Press (OUP), pp. 4007–4024, Feb. 27, 2018. doi: 10.1093/mnras/sty535.  
  
Y. Mao, “The impact of inhomogeneous subgrid clumping on cosmic reionization”, *Monthly Notices of the Royal Astronomical Society*, vol. 491, no. 2. Oxford University Press (OUP), pp. 1600–1621, Oct. 24, 2019. doi: 10.1093/mnras/stz2986.  
  
Y. Mao, P. R. Shapiro, G. Mellema, I. T. Iliev, J. Kodaand K. Ahn, “Redshift-space distortion of the 21-cm background from the epoch of reionization - I. Methodology re-examined”, *Monthly Notices of the Royal Astronomical Society*, vol. 422, no. 2. Oxford University Press (OUP), pp. 926–954, Apr. 04, 2012. doi: 10.1111/j.1365-2966.2012.20471.x.  
  
G. Mellema, “Reionization and the Cosmic Dawn with the Square Kilometre Array”, *Experimental Astronomy*, vol. 36, no. 1–2. Springer Science and Business Media LLC, pp. 235–318, Apr. 27, 2013. doi: 10.1007/s10686-013-9334-5.  
  
S. Nadathur, “Self-similarity and universality of void density profiles in simulation and SDSS data”, *Monthly Notices of the Royal Astronomical Society*, vol. 449, no. 4. Oxford University Press (OUP), pp. 3997–4009, Apr. 10, 2015. doi: 10.1093/mnras/stv513.  
  
G. Paciga, “The GMRT Epoch of Reionization experiment: a new upper limit on the neutral hydrogen power spectrum at z≈ 8.6”, *Monthly Notices of the Royal Astronomical Society*, vol. 413, no. 2. Oxford University Press (OUP), pp. 1174–1183, Mar. 01, 2011. doi: 10.1111/j.1365-2966.2011.18208.x.  
  
H. E. Ross, K. Dixon, I. Ilievand G. Mellema, “New simulation of QSO X-ray heating during the Cosmic Dawn”, *Proceedings of the International Astronomical Union*, vol. 12, no. S333. Cambridge University Press (CUP), pp. 34–38, Oct. 2017. doi: 10.1017/s1743921317011115.  
  
H. E. Ross, K. L. Dixon, I. T. Ilievand G. Mellema, “Simulating the impact of X-ray heating during the cosmic dawn”, *Monthly Notices of the Royal Astronomical Society*, vol. 468, no. 4. Oxford University Press (OUP), pp. 3785–3797, Mar. 22, 2017. doi: 10.1093/mnras/stx649.  
  
P. R. Shapiro, “Simulating cosmic reionization and the radiation backgrounds from the epoch of reionization”, *AIP Conference Proceedings*. AIP, 2012. doi: 10.1063/1.4754363.  
  
H. Shukla, G. Mellema, I. T. Ilievand P. R. Shapiro, “The effects of Lyman-limit systems on the evolution and observability of the epoch of reionization”, *Monthly Notices of the Royal Astronomical Society*, vol. 458, no. 1. Oxford University Press (OUP), pp. 135–150, Feb. 02, 2016. doi: 10.1093/mnras/stw249.  
  
D. Sullivan, I. T. Ilievand K. L. Dixon, “Using artificial neural networks to constrain the halo baryon fraction during reionization”, *Monthly Notices of the Royal Astronomical Society*, vol. 473, no. 1. Oxford University Press (OUP), pp. 38–58, Sep. 07, 2017. doi: 10.1093/mnras/stx2324.  
  
D. Vrbanec, “Predictions for the 21 cm-galaxy cross-power spectrum observable with LOFAR and Subaru”, *Monthly Notices of the Royal Astronomical Society*, vol. 457, no. 1. Oxford University Press (OUP), pp. 666–675, Jan. 22, 2016. doi: 10.1093/mnras/stv2993.  
  
W. A. Watson, “The Jubilee ISW project – I. Simulated ISW and weak lensing maps and initial power spectra results”, *Monthly Notices of the Royal Astronomical Society*, vol. 438, no. 1. Oxford University Press (OUP), pp. 412–425, Dec. 12, 2013. doi: 10.1093/mnras/stt2208.  
  
W. A. Watson, I. T. Iliev, A. D’Aloisio, A. Knebe, P. R. Shapiroand G. Yepes, “The halo mass function through the cosmic ages”, *Monthly Notices of the Royal Astronomical Society*, vol. 433, no. 2. Oxford University Press (OUP), pp. 1230–1245, Jun. 04, 2013. doi: 10.1093/mnras/stt791.  
  
W. A. Watson, “Statistics of extreme objects in the Juropa Hubble Volume simulation★”, *Monthly Notices of the Royal Astronomical Society*, vol. 437, no. 4. Oxford University Press (OUP), pp. 3776–3786, Dec. 07, 2013. doi: 10.1093/mnras/stt2173.  
  
R. Wojtak, “Cosmic variance of the local Hubble flow in large-scale cosmological simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 438, no. 2. Oxford University Press (OUP), pp. 1805–1812, Dec. 31, 2013. doi: 10.1093/mnras/stt2321.  
  
E. Zackrisson, “Observational constraints on supermassive dark stars”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 407, no. 1. Oxford University Press (OUP), pp. L74–L78, Jul. 21, 2010. doi: 10.1111/j.1745-3933.2010.00908.x.  
  
P. Ocvirk, “Cosmic Dawn (CoDa): the first radiation-hydrodynamics simulation of reionization and galaxy formation in the Local Universe”, *Monthly Notices of the Royal Astronomical Society*, vol. 463, no. 2. Oxford University Press (OUP), pp. 1462–1485, Aug. 30, 2016. doi: 10.1093/mnras/stw2036.  
  
P. F. Hopkins, “A new class of accurate, mesh-free hydrodynamic simulation methods”, *Monthly Notices of the Royal Astronomical Society*, vol. 450, no. 1. Oxford University Press (OUP), pp. 53–110, Apr. 15, 2015. doi: 10.1093/mnras/stv195.  
  
F. van de Voort, T. A. Davis, D. Kereš, E. Quataert, C.-A. Faucher-Giguèreand P. F. Hopkins, “The creation and persistence of a misaligned gas disc in a simulated early-type galaxy”, *Monthly Notices of the Royal Astronomical Society*, vol. 451, no. 3. Oxford University Press (OUP), pp. 3269–3277, Jun. 19, 2015. doi: 10.1093/mnras/stv1217.  
  
D. Lecoanet, “A validated non-linear Kelvin–Helmholtz benchmark for numerical hydrodynamics”, *Monthly Notices of the Royal Astronomical Society*, vol. 455, no. 4. Oxford University Press (OUP), pp. 4274–4288, Dec. 22, 2015. doi: 10.1093/mnras/stv2564.  
  
A.-M. Madigan and M. McCourt, “A new inclination instability reshapes Keplerian discs into cones: application to the outer Solar system”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 457, no. 1. Oxford University Press (OUP), pp. L89–L93, Jan. 20, 2016. doi: 10.1093/mnrasl/slv203.  
  
K. Beckwith, P. Greteand B. W. O’Shea, “Correlations and Cascades in Magnetized Turbulence”, *IEEE Transactions on Plasma Science*, vol. 47, no. 5. Institute of Electrical and Electronics Engineers (IEEE), pp. 2020–2031, May 2019. doi: 10.1109/tps.2019.2891934.  
  
P. Grete, B. W. O’Sheaand K. Beckwith, “As a Matter of Force—Systematic Biases in Idealized Turbulence Simulations”, *The Astrophysical Journal*, vol. 858, no. 2. American Astronomical Society, p. L19, May 10, 2018. doi: 10.3847/2041-8213/aac0f5.  
  
P. Grete, B. W. O’Sheaand K. Beckwith, “As a Matter of State: The Role of Thermodynamics in Magnetohydrodynamic Turbulence”, *The Astrophysical Journal*, vol. 889, no. 1. American Astronomical Society, p. 19, Jan. 21, 2020. doi: 10.3847/1538-4357/ab5aec.  
  
B. F. Griffen, G. A. Dooley, A. P. Ji, B. W. O’Shea, F. A. Gómezand A. Frebel, “Tracing the first stars and galaxies of the Milky Way”, *Monthly Notices of the Royal Astronomical Society*, vol. 474, no. 1. Oxford University Press (OUP), pp. 443–459, Oct. 25, 2017. doi: 10.1093/mnras/stx2749.  
  
M. S. Peeples, “Figuring Out Gas & Galaxies in Enzo (FOGGIE). I. Resolving Simulated Circumgalactic Absorption at 2 ≤ *z* ≤ 2.5”, *The Astrophysical Journal*, vol. 873, no. 2. American Astronomical Society, p. 129, Mar. 13, 2019. doi: 10.3847/1538-4357/ab0654.  
  
G. R. Meece, G. M. Voitand B. W. O’Shea, “Triggering and Delivery Algorithms for AGN Feedback”, *The Astrophysical Journal*, vol. 841, no. 2. American Astronomical Society, p. 133, Jun. 05, 2017. doi: 10.3847/1538-4357/aa6fb1.  
  
J. M. Blondin and R. A. Chevalier, “Pulsar Wind Bubble Blowout from a Supernova”, *The Astrophysical Journal*, vol. 845, no. 2. American Astronomical Society, p. 139, Aug. 21, 2017. doi: 10.3847/1538-4357/aa8267.  
  
J. M. Blondin, E. Gipson, S. Harrisand A. Mezzacappa, “The Standing Accretion Shock Instability: Enhanced Growth in Rotating Progenitors”, *The Astrophysical Journal*, vol. 835, no. 2. American Astronomical Society, p. 170, Jan. 27, 2017. doi: 10.3847/1538-4357/835/2/170.  
  
C. Kolb, J. Blondin, P. Slaneand T. Temim, “Evolution of a Pulsar Wind Nebula within a Composite Supernova Remnant”, *The Astrophysical Journal*, vol. 844, no. 1. American Astronomical Society, p. 1, Jul. 17, 2017. doi: 10.3847/1538-4357/aa75ce.  
  
B. J. Williams, “The Three-dimensional Expansion of the Ejecta from Tycho’s Supernova Remnant”, *The Astrophysical Journal*, vol. 842, no. 1. American Astronomical Society, p. 28, Jun. 08, 2017. doi: 10.3847/1538-4357/aa7384.  
  
M. W. Kunz and G. Lesur, “Magnetic self-organization in Hall-dominated magnetorotational turbulence”, *Monthly Notices of the Royal Astronomical Society*, vol. 434, no. 3. Oxford University Press (OUP), pp. 2295–2312, Jul. 27, 2013. doi: 10.1093/mnras/stt1171.  
  
G. Lesur, M. W. Kunzand S. Fromang, “Thanatology in protoplanetary discs”, *Astronomy & Astrophysics*, vol. 566. EDP Sciences, p. A56, Jun. 2014. doi: 10.1051/0004-6361/201423660.  
  
J. B. Simon, P. J. Armitageand K. Beckwith, “TURBULENT LINEWIDTHS IN PROTOPLANETARY DISKS: PREDICTIONS FROM NUMERICAL SIMULATIONS”, *The Astrophysical Journal*, vol. 743, no. 1. American Astronomical Society, p. 17, Nov. 18, 2011. doi: 10.1088/0004-637x/743/1/17.  
  
J. B. Simon, X.-N. Bai, J. M. Stone, P. J. Armitageand K. Beckwith, “TURBULENCE IN THE OUTER REGIONS OF PROTOPLANETARY DISKS. I. WEAK ACCRETION WITH NO VERTICAL MAGNETIC FLUX”, *The Astrophysical Journal*, vol. 764, no. 1. American Astronomical Society, p. 66, Jan. 28, 2013. doi: 10.1088/0004-637x/764/1/66.  
  
J. B. Simon, K. Beckwithand P. J. Armitage, “Emergent mesoscale phenomena in magnetized accretion disc turbulence”, *Monthly Notices of the Royal Astronomical Society*, vol. 422, no. 3. Oxford University Press (OUP), pp. 2685–2700, Apr. 11, 2012. doi: 10.1111/j.1365-2966.2012.20835.x.  
  
T. Barclay, “A sub-Mercury-sized exoplanet”, *Nature*, vol. 494, no. 7438. Springer Science and Business Media LLC, pp. 452–454, Feb. 20, 2013. doi: 10.1038/nature11914.  
  
M. Bazot, “The radius and mass of the close solar twin 18 Scorpii derived from asteroseismology and interferometry”, *Astronomy & Astrophysics*, vol. 526. EDP Sciences, p. L4, Dec. 13, 2010. doi: 10.1051/0004-6361/201015679.  
  
I. M. Brandão, “Asteroseismic modelling of the solar-type subgiant star*β* Hydri”, *Astronomy & Astrophysics*, vol. 527. EDP Sciences, p. A37, Jan. 21, 2011. doi: 10.1051/0004-6361/201015370.  
  
A. Brandenburg, S. Mathurand T. S. Metcalfe, “Evolution of Co-existing Long and Short Period Stellar Activity Cycles”, *The Astrophysical Journal*, vol. 845, no. 1. American Astronomical Society, p. 79, Aug. 14, 2017. doi: 10.3847/1538-4357/aa7cfa.  
  
T. L. Campante, “*TESS* Asteroseismology of the Known Red-giant Host Stars HD 212771 and HD 203949”, *The Astrophysical Journal*, vol. 885, no. 1. American Astronomical Society, p. 31, Oct. 29, 2019. doi: 10.3847/1538-4357/ab44a8.  
  
J. A. Carter, “Kepler-36: A Pair of Planets with Neighboring Orbits and Dissimilar Densities”, *Science*, vol. 337, no. 6094. American Association for the Advancement of Science (AAAS), pp. 556–559, Aug. 03, 2012. doi: 10.1126/science.1223269.  
  
T. Ceillier, “Rotation periods and seismic ages of KOIs – comparison with stars without detected planets from*Kepler*observations”, *Monthly Notices of the Royal Astronomical Society*, vol. 456, no. 1. Oxford University Press (OUP), pp. 119–125, Dec. 11, 2015. doi: 10.1093/mnras/stv2622.  
  
W. J. Chaplin, “ASTEROSEISMIC FUNDAMENTAL PROPERTIES OF SOLAR-TYPE STARS OBSERVED BY THE NASA *KEPLER* MISSION”, *The Astrophysical Journal Supplement Series*, vol. 210, no. 1. American Astronomical Society, p. 1, Dec. 11, 2013. doi: 10.1088/0067-0049/210/1/1.  
  
W. J. Chaplin, “Age dating of an early Milky Way merger via asteroseismology of the naked-eye star ν Indi”, *Nature Astronomy*, vol. 4, no. 4. Springer Science and Business Media LLC, pp. 382–389, Jan. 13, 2020. doi: 10.1038/s41550-019-0975-9.  
  
O. L. Creevey, “Characterizing solar-type stars from full-length *Kepler* data sets using the Asteroseismic Modeling Portal”, *Astronomy & Astrophysics*, vol. 601. EDP Sciences, p. A67, May 2017. doi: 10.1051/0004-6361/201629496.  
  
G. R. Davies, “Asteroseismic inference on rotation, gyrochronology and planetary system dynamics of 16 Cygni”, *Monthly Notices of the Royal Astronomical Society*, vol. 446, no. 3. Oxford University Press (OUP), pp. 2959–2966, Nov. 29, 2014. doi: 10.1093/mnras/stu2331.  
  
R. A. García, “Rotation and magnetism of*Kepler*pulsating solar-like stars”, *Astronomy & Astrophysics*, vol. 572. EDP Sciences, p. A34, Nov. 25, 2014. doi: 10.1051/0004-6361/201423888.  
  
J. A. Guzik, “DETECTION OF SOLAR-LIKE OSCILLATIONS, OBSERVATIONAL CONSTRAINTS, AND STELLAR MODELS FOR*θ*CYG, THE BRIGHTEST STAR OBSERVED BY THE*KEPLER*MISSION”, *The Astrophysical Journal*, vol. 831, no. 1. American Astronomical Society, p. 17, Oct. 21, 2016. doi: 10.3847/0004-637x/831/1/17.  
  
P. G. Judge, R. Egeland, T. S. Metcalfe, E. Guinanand S. Engle, “The Magnetic Future of the Sun”, *The Astrophysical Journal*, vol. 848, no. 1. American Astronomical Society, p. 43, Oct. 10, 2017. doi: 10.3847/1538-4357/aa8d6a.  
  
C. Karoff, “Sounding stellar cycles with Kepler – II. Ground-based observations★”, *Monthly Notices of the Royal Astronomical Society*, vol. 433, no. 4. Oxford University Press (OUP), pp. 3227–3238, Jun. 22, 2013. doi: 10.1093/mnras/stt964.  
  
C. Karoff, “Sounding stellar cycles with Kepler – III. Comparative analysis of chromospheric, photometric, and asteroseismic variability”, *Monthly Notices of the Royal Astronomical Society*, vol. 485, no. 4. Oxford University Press (OUP), pp. 5096–5104, Mar. 16, 2019. doi: 10.1093/mnras/stz782.  
  
C. Karoff, “The Influence of Metallicity on Stellar Differential Rotation and Magnetic Activity”, *The Astrophysical Journal*, vol. 852, no. 1. American Astronomical Society, p. 46, Jan. 05, 2018. doi: 10.3847/1538-4357/aaa026.  
  
G. W. Marcy, “MASSES, RADII, AND ORBITS OF SMALL *KEPLER* PLANETS: THE TRANSITION FROM GASEOUS TO ROCKY PLANETS”, *The Astrophysical Journal Supplement Series*, vol. 210, no. 2. American Astronomical Society, p. 20, Jan. 13, 2014. doi: 10.1088/0067-0049/210/2/20.  
  
S. Mathur, “Magnetic activity of F stars observed by*Kepler*”, *Astronomy & Astrophysics*, vol. 562. EDP Sciences, p. A124, Feb. 2014. doi: 10.1051/0004-6361/201322707.  
  
A. Mazumdar, “Acoustic glitches in solar-type stars from*Kepler*”, *Astronomische Nachrichten*, vol. 333, no. 10. Wiley, pp. 1040–1043, Dec. 2012. doi: 10.1002/asna.201211825.  
  
T. S. Metcalfe, O. L. Creeveyand G. R. Davies, “ASTEROSEISMIC MODELING OF 16 Cyg A & B USING THE COMPLETE *KEPLER* DATA SET”, *The Astrophysical Journal*, vol. 811, no. 2. American Astronomical Society, p. L37, Sep. 29, 2015. doi: 10.1088/2041-8205/811/2/l37.  
  
T. S. Metcalfe, “PROPERTIES OF 42 SOLAR-TYPE *KEPLER* TARGETS FROM THE ASTEROSEISMIC MODELING PORTAL”, *The Astrophysical Journal Supplement Series*, vol. 214, no. 2. American Astronomical Society, p. 27, Oct. 01, 2014. doi: 10.1088/0067-0049/214/2/27.  
  
T. S. Metcalfe and R. Egeland, “Understanding the Limitations of Gyrochronology for Old Field Stars”, *The Astrophysical Journal*, vol. 871, no. 1. American Astronomical Society, p. 39, Jan. 21, 2019. doi: 10.3847/1538-4357/aaf575.  
  
T. S. Metcalfe, R. Egelandand J. van Saders, “STELLAR EVIDENCE THAT THE SOLAR DYNAMO MAY BE IN TRANSITION”, *The Astrophysical Journal*, vol. 826, no. 1. American Astronomical Society, p. L2, Jul. 13, 2016. doi: 10.3847/2041-8205/826/1/l2.  
  
T. S. Metcalfe and J. van Saders, “Magnetic Evolution and the Disappearance of Sun-Like Activity Cycles”, *Solar Physics*, vol. 292, no. 9. Springer Science and Business Media LLC, Aug. 29, 2017. doi: 10.1007/s11207-017-1157-5.  
  
D. R. Reese, “SpaceInn hare-and-hounds exercise: Estimation of stellar properties using space-based asteroseismic data”, *Astronomy & Astrophysics*, vol. 592. EDP Sciences, p. A14, Jul. 05, 2016. doi: 10.1051/0004-6361/201527987.  
  
D. Salabert, “Photospheric and chromospheric magnetic activity of seismic solar analogs”, *Astronomy & Astrophysics*, vol. 596. EDP Sciences, p. A31, Nov. 25, 2016. doi: 10.1051/0004-6361/201628583.  
  
D. Salabert, “Magnetic variability in the young solar analog KIC 10644253”, *Astronomy & Astrophysics*, vol. 589. EDP Sciences, p. A118, Apr. 22, 2016. doi: 10.1051/0004-6361/201527978.  
  
A. R. G. Santos, “Signatures of Magnetic Activity: On the Relation between Stellar Properties and p-mode Frequency Variations”, *The Astrophysical Journal*, vol. 883, no. 1. American Astronomical Society, p. 65, Sep. 20, 2019. doi: 10.3847/1538-4357/ab397a.  
  
V. Silva Aguirre, “Ages and fundamental properties of*Kepler*exoplanet host stars from asteroseismology”, *Monthly Notices of the Royal Astronomical Society*, vol. 452, no. 2. Oxford University Press (OUP), pp. 2127–2148, Jul. 24, 2015. doi: 10.1093/mnras/stv1388.  
  
J. L. van Saders, “Weakened magnetic braking as the origin of anomalously rapid rotation in old field stars”, *Nature*, vol. 529, no. 7585. Springer Science and Business Media LLC, pp. 181–184, Jan. 04, 2016. doi: 10.1038/nature16168.  
  
T. R. White, “*Kepler*observations of the asteroseismic binary HD 176465”, *Astronomy & Astrophysics*, vol. 601. EDP Sciences, p. A82, May 2017. doi: 10.1051/0004-6361/201628706.  
  
O. L. Creevey, “Fundamental properties of five*Kepler*stars using global asteroseismic quantities and ground-based observations”, *Astronomy & Astrophysics*, vol. 537. EDP Sciences, p. A111, Jan. 2012. doi: 10.1051/0004-6361/201117037.  
  
M. E. Escobar, “Precise modeling of the exoplanet host star and CoRoT main target HD 52265”, *Astronomy & Astrophysics*, vol. 543. EDP Sciences, p. A96, Jul. 2012. doi: 10.1051/0004-6361/201218969.  
  
S. Mathur, “Study of HD 169392A observed by CoRoT and HARPS”, *Astronomy & Astrophysics*, vol. 549. EDP Sciences, p. A12, Dec. 06, 2012. doi: 10.1051/0004-6361/201219678.  
  
S. Mathur, “Constraining magnetic-activity modulations in three solar-like stars observed by CoRoT and NARVAL”, *Astronomy & Astrophysics*, vol. 550. EDP Sciences, p. A32, Jan. 21, 2013. doi: 10.1051/0004-6361/201117913.  
  
M. E. Caplan, A. S. Schneider, C. J. Horowitzand D. K. Berry, “Pasta nucleosynthesis: Molecular dynamics simulations of nuclear statistical equilibrium”, *Physical Review C*, vol. 91, no. 6. American Physical Society (APS), Jun. 22, 2015. doi: 10.1103/physrevc.91.065802.  
  
C. J. Horowitz, D. K. Berry, C. M. Briggs, M. E. Caplan, A. Cummingand A. S. Schneider, “Disordered Nuclear Pasta, Magnetic Field Decay, and Crust Cooling in Neutron Stars”, *Physical Review Letters*, vol. 114, no. 3. American Physical Society (APS), Jan. 22, 2015. doi: 10.1103/physrevlett.114.031102.  
  
A. S. Schneider, D. K. Berry, C. M. Briggs, M. E. Caplanand C. J. Horowitz, “Nuclear “waffles””, *Physical Review C*, vol. 90, no. 5. American Physical Society (APS), Nov. 24, 2014. doi: 10.1103/physrevc.90.055805.  
  
A. S. Schneider, C. J. Horowitz, J. Hughtoand D. K. Berry, “Nuclear “pasta” formation”, *Physical Review C*, vol. 88, no. 6. American Physical Society (APS), Dec. 20, 2013. doi: 10.1103/physrevc.88.065807.  
  
X.-N. Bai, D. Caprioli, L. Sironiand A. Spitkovsky, “MAGNETOHYDRODYNAMIC-PARTICLE-IN-CELL METHOD FOR COUPLING COSMIC RAYS WITH A THERMAL PLASMA: APPLICATION TO NON-RELATIVISTIC SHOCKS”, *The Astrophysical Journal*, vol. 809, no. 1. American Astronomical Society, p. 55, Aug. 10, 2015. doi: 10.1088/0004-637x/809/1/55.  
  
D. Caprioli, D. T. Yiand A. Spitkovsky, “Chemical Enhancements in Shock-Accelerated Particles: *Ab initio* Simulations”, *Physical Review Letters*, vol. 119, no. 17. American Physical Society (APS), Oct. 23, 2017. doi: 10.1103/physrevlett.119.171101.  
  
D. Caprioli, H. Zhangand A. Spitkovsky, “Diffusive shock re-acceleration”, *Journal of Plasma Physics*, vol. 84, no. 3. Cambridge University Press (CUP), May 22, 2018. doi: 10.1017/s0022377818000478.  
  
R. M. T. Connors, “Mass-scaling as a method to constrain outflows and particle acceleration from low-luminosity accreting black holes”, *Monthly Notices of the Royal Astronomical Society*. Oxford University Press (OUP), p. stw3150, Dec. 05, 2016. doi: 10.1093/mnras/stw3150.  
  
R. M. T. Connors, “Combining timing characteristics with physical broad-band spectral modelling of black hole X-ray binary GX 339–4”, *Monthly Notices of the Royal Astronomical Society*, vol. 485, no. 3. Oxford University Press (OUP), pp. 3696–3714, Mar. 02, 2019. doi: 10.1093/mnras/stz604.  
  
P. Crumley, D. Caprioli, S. Markoffand A. Spitkovsky, “Kinetic simulations of mildly relativistic shocks – I. Particle acceleration in high Mach number shocks”, *Monthly Notices of the Royal Astronomical Society*, vol. 485, no. 4. Oxford University Press (OUP), pp. 5105–5119, Jan. 30, 2019. doi: 10.1093/mnras/stz232.  
  
P. Crumley, C. Ceccobello, R. M. T. Connorsand Y. Cavecchi, “The jet-disk symbiosis without*maximal jets*: 1D hydrodynamical jets revisited”, *Astronomy & Astrophysics*, vol. 601. EDP Sciences, p. A87, May 2017. doi: 10.1051/0004-6361/201630229.  
  
N. L. Kugland, “Self-organized electromagnetic field structures in laser-produced counter-streaming plasmas”, *Nature Physics*, vol. 8, no. 11. Springer Science and Business Media LLC, pp. 809–812, Sep. 30, 2012. doi: 10.1038/nphys2434.  
  
R. Kumar, E. J. Zirnsteinand A. Spitkovsky, “Energy Distribution of Pickup Ions at the Solar Wind Termination Shock”, *The Astrophysical Journal*, vol. 860, no. 2. American Astronomical Society, p. 156, Jun. 22, 2018. doi: 10.3847/1538-4357/aabf96.  
  
M. Lucchini, S. Markoff, P. Crumley, F. Kraußand R. M. T. Connors, “Breaking degeneracy in jet dynamics: multi-epoch joint modelling of the BL Lac PKS 2155–304”, *Monthly Notices of the Royal Astronomical Society*, vol. 482, no. 4. Oxford University Press (OUP), pp. 4798–4812, Oct. 30, 2018. doi: 10.1093/mnras/sty2929.  
  
W. Lu, J. Krolik, P. Crumleyand P. Kumar, “Radiative interaction between the relativistic jet and optically thick envelope in tidal disruption events”, *Monthly Notices of the Royal Astronomical Society*, vol. 471, no. 1. Oxford University Press (OUP), pp. 1141–1152, Jul. 04, 2017. doi: 10.1093/mnras/stx1668.  
  
J. Park, D. Caprioliand A. Spitkovsky, “Simultaneous Acceleration of Protons and Electrons at Nonrelativistic Quasiparallel Collisionless Shocks”, *Physical Review Letters*, vol. 114, no. 8. American Physical Society (APS), Feb. 27, 2015. doi: 10.1103/physrevlett.114.085003.  
  
A. A. Philippov and R. R. Rafikov, “Radial Transport and Meridional Circulation in Accretion Disks”, *The Astrophysical Journal*, vol. 837, no. 2. American Astronomical Society, p. 101, Mar. 08, 2017. doi: 10.3847/1538-4357/aa60ca.  
  
A. A. Philippov, R. R. Rafikovand J. M. Stone, “SPREADING LAYERS IN ACCRETING OBJECTS: ROLE OF ACOUSTIC WAVES FOR ANGULAR MOMENTUM TRANSPORT, MIXING, AND THERMODYNAMICS”, *The Astrophysical Journal*, vol. 817, no. 1. American Astronomical Society, p. 62, Jan. 20, 2016. doi: 10.3847/0004-637x/817/1/62.  
  
R. Kumar, D. Eichler, M. Gaspariand A. Spitkovsky, “Preferential Heating and Acceleration of Heavy Ions in Impulsive Solar Flares”, *The Astrophysical Journal*, vol. 835, no. 2. American Astronomical Society, p. 295, Feb. 02, 2017. doi: 10.3847/1538-4357/835/2/295.  
  
B. D. Metzger, D. Caprioli, I. Vurm, A. M. Beloborodov, I. Bartosand A. Vlasov, “Novae as Tevatrons: prospects for CTA and IceCube”, *Monthly Notices of the Royal Astronomical Society*, vol. 457, no. 2. Oxford University Press (OUP), pp. 1786–1795, Feb. 04, 2016. doi: 10.1093/mnras/stw123.  
  
S. K. Sarbadhicary, C. Badenes, L. Chomiuk, D. Caprioliand D. Huizenga, “Supernova remnants in the Local Group – I. A model for the radio luminosity function and visibility times of supernova remnants”, *Monthly Notices of the Royal Astronomical Society*, vol. 464, no. 2. Oxford University Press (OUP), pp. 2326–2340, Oct. 08, 2016. doi: 10.1093/mnras/stw2566.  
  
L. B. Wilson, D. G. Sibeck, D. L. Turner, A. Osmane, D. Caprioliand V. Angelopoulos, “Relativistic Electrons Produced by Foreshock Disturbances Observed Upstream of Earth’s Bow Shock”, *Physical Review Letters*, vol. 117, no. 21. American Physical Society (APS), Nov. 14, 2016. doi: 10.1103/physrevlett.117.215101.  
  
C. Byrohl, R. Fisherand D. Townsley, “The Intrinsic Stochasticity of the 56Ni Distribution of Single-degenerate Near-Chandrasekhar-mass SN Ia”, *The Astrophysical Journal*, vol. 878, no. 1. American Astronomical Society, p. 67, Jun. 14, 2019. doi: 10.3847/1538-4357/ab1f73.  
  
P. Dave, R. Kashyap, R. Fisher, F. Timmes, D. Townsleyand C. Byrohl, “Constraining the Single-degenerate Channel of Type Ia Supernovae with Stable Iron-group Elements in SNR 3C 397”, *The Astrophysical Journal*, vol. 841, no. 1. American Astronomical Society, p. 58, May 24, 2017. doi: 10.3847/1538-4357/aa7134.  
  
R. Fisher, P. Mozumdarand G. Casabona, “Carbon Detonation Initiation in Turbulent Electron-degenerate Matter”, *The Astrophysical Journal*, vol. 876, no. 1. American Astronomical Society, p. 64, May 06, 2019. doi: 10.3847/1538-4357/ab15d8.  
  
O. Graur, “A year-long plateau in the late-time near-infrared light curves of type Ia supernovae”, *Nature Astronomy*, vol. 4, no. 2. Springer Science and Business Media LLC, pp. 188–195, Oct. 07, 2019. doi: 10.1038/s41550-019-0901-1.  
  
O. Graur, “Observations of SN 2015F Suggest a Correlation between the Intrinsic Luminosity of Type Ia Supernovae and the Shape of Their Light Curves >900 Days after Explosion”, *The Astrophysical Journal*, vol. 859, no. 2. American Astronomical Society, p. 79, May 25, 2018. doi: 10.3847/1538-4357/aabe25.  
  
R. Kashyap, R. Fisher, E. García-Berro, G. Aznar-Siguán, S. Jiand P. Lorén-Aguilar, “One-armed Spiral Instability in Double-degenerate Post-merger Accretion Disks”, *The Astrophysical Journal*, vol. 840, no. 1. American Astronomical Society, p. 16, Apr. 28, 2017. doi: 10.3847/1538-4357/aa6afb.  
  
R. Kashyap, T. Haque, P. Lorén-Aguilar, E. García-Berroand R. Fisher, “Double-degenerate Carbon–Oxygen and Oxygen–Neon White Dwarf Mergers: A New Mechanism for Faint and Rapid Type Ia Supernovae”, *The Astrophysical Journal*, vol. 869, no. 2. American Astronomical Society, p. 140, Dec. 19, 2018. doi: 10.3847/1538-4357/aaedb7.  
  
D. Abarca, A. Sądowskiand L. Sironi, “Simulating the effect of the Sgr A\* accretion flow on the appearance of G2 after pericentre”, *Monthly Notices of the Royal Astronomical Society*, vol. 440, no. 2. Oxford University Press (OUP), pp. 1125–1137, Mar. 19, 2014. doi: 10.1093/mnras/stu244.  
  
O. Bromberg and A. Tchekhovskoy, “Relativistic MHD simulations of core-collapse GRB jets: 3D instabilities and magnetic dissipation”, *Monthly Notices of the Royal Astronomical Society*, vol. 456, no. 2. Oxford University Press (OUP), pp. 1739–1760, Dec. 24, 2015. doi: 10.1093/mnras/stv2591.  
  
A. Ciesielski, “Stability of radiation-pressure dominated disks”, *Astronomy & Astrophysics*, vol. 538. EDP Sciences, p. A148, Feb. 2012. doi: 10.1051/0004-6361/201117478.  
  
L. Z. Kelley, A. Tchekhovskoyand R. Narayan, “Tidal disruption and magnetic flux capture: powering a jet from a quiescent black hole”, *Monthly Notices of the Royal Astronomical Society*, vol. 445, no. 4. Oxford University Press (OUP), pp. 3919–3938, Oct. 31, 2014. doi: 10.1093/mnras/stu2041.  
  
J. Li, A. Spitkovskyand A. Tchekhovskoy, “ON THE SPIN-DOWN OF INTERMITTENT PULSARS”, *The Astrophysical Journal*, vol. 746, no. 2. American Astronomical Society, p. L24, Feb. 02, 2012. doi: 10.1088/2041-8205/746/2/l24.  
  
J. Li, A. Spitkovskyand A. Tchekhovskoy, “Resistivity and dissipation in pulsar magnetospheres”, *Proceedings of the International Astronomical Union*, vol. 8, no. S291. Cambridge University Press (CUP), pp. 287–290, Aug. 2012. doi: 10.1017/s1743921312023885.  
  
R. Narayan, A. Sądowski, R. F. Pennaand A. K. Kulkarni, “GRMHD simulations of magnetized advection-dominated accretion on a non-spinning black hole: role of outflows”, *Monthly Notices of the Royal Astronomical Society*, vol. 426, no. 4. Oxford University Press (OUP), pp. 3241–3259, Oct. 17, 2012. doi: 10.1111/j.1365-2966.2012.22002.x.  
  
R. S. Nemmen and A. Tchekhovskoy, “On the efficiency of jet production in radio galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 449, no. 1. Oxford University Press (OUP), pp. 316–327, Mar. 17, 2015. doi: 10.1093/mnras/stv260.  
  
J.-U. Ness, “FROM X-RAY DIPS TO ECLIPSE: WITNESSING DISK REFORMATION IN THE RECURRENT NOVA U Sco”, *The Astrophysical Journal*, vol. 745, no. 1. American Astronomical Society, p. 43, Dec. 28, 2011. doi: 10.1088/0004-637x/745/1/43.  
  
A. Philippov, A. Tchekhovskoyand J. G. Li, “Time evolution of pulsar obliquity angle from 3D simulations of magnetospheres”, *Monthly Notices of the Royal Astronomical Society*, vol. 441, no. 3. Oxford University Press (OUP), pp. 1879–1887, May 12, 2014. doi: 10.1093/mnras/stu591.  
  
S. M. Ressler, A. Tchekhovskoy, E. Quataert, M. Chandraand C. F. Gammie, “Electron thermodynamics in GRMHD simulations of low-luminosity black hole accretion”, *Monthly Notices of the Royal Astronomical Society*, vol. 454, no. 2. Oxford University Press (OUP), pp. 1848–1870, Oct. 08, 2015. doi: 10.1093/mnras/stv2084.  
  
S. M. Ressler, A. Tchekhovskoy, E. Quataertand C. F. Gammie, “The disc-jet symbiosis emerges: modelling the emission of Sagittarius A\* with electron thermodynamics”, *Monthly Notices of the Royal Astronomical Society*, vol. 467, no. 3. Oxford University Press (OUP), pp. 3604–3619, Feb. 11, 2017. doi: 10.1093/mnras/stx364.  
  
A. Sądowski, R. Narayan, L. Sironiand F. Özel, “Location of the bow shock ahead of cloud G2 at the Galactic Centre”, *Monthly Notices of the Royal Astronomical Society*, vol. 433, no. 3. Oxford University Press (OUP), pp. 2165–2171, Jun. 17, 2013. doi: 10.1093/mnras/stt879.  
  
F. J. Sánchez, “UV-C tolerance of symbiotic*Trebouxia*sp. in the space-tested lichen species*Rhizocarpon geographicum*and*Circinaria gyrosa*: role of the hydration state and cortex/screening substances”, *International Journal of Astrobiology*, vol. 13, no. 1. Cambridge University Press (CUP), pp. 1–18, Sep. 06, 2013. doi: 10.1017/s147355041300027x.  
  
A. Tchekhovskoy and J. C. McKinney, “Prograde and retrograde black holes: whose jet is more powerful?”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 423, no. 1. Oxford University Press (OUP), pp. L55–L59, Apr. 19, 2012. doi: 10.1111/j.1745-3933.2012.01256.x.  
  
A. Tchekhovskoy, A. Spitkovskyand J. G. Li, “Time-dependent 3D magnetohydrodynamic pulsar magnetospheres: oblique rotators”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 435, no. 1. Oxford University Press (OUP), pp. L1–L5, Aug. 19, 2013. doi: 10.1093/mnrasl/slt076.  
  
K. Parfrey and A. Tchekhovskoy, “General-relativistic Simulations of Four States of Accretion onto Millisecond Pulsars”, *The Astrophysical Journal*, vol. 851, no. 2. American Astronomical Society, p. L34, Dec. 15, 2017. doi: 10.3847/2041-8213/aa9c85.  
  
J. Oñorbe, “Forged in fire: cusps, cores and baryons in low-mass dwarf galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 454, no. 2. Oxford University Press (OUP), pp. 2092–2106, Oct. 13, 2015. doi: 10.1093/mnras/stv2072.  
  
A. Bauer, “Hydrogen reionization in the Illustris universe”, *Monthly Notices of the Royal Astronomical Society*, vol. 453, no. 4. Oxford University Press (OUP), pp. 3594–3611, Sep. 09, 2015. doi: 10.1093/mnras/stv1893.  
  
A. D. Bray, “Modelling galactic conformity with the colour–halo age relation in the Illustris simulation”, *Monthly Notices of the Royal Astronomical Society*, vol. 455, no. 1. Oxford University Press (OUP), pp. 185–198, Nov. 02, 2015. doi: 10.1093/mnras/stv2316.  
  
S. Genel, “Introducing the Illustris project: the evolution of galaxy populations across cosmic time”, *Monthly Notices of the Royal Astronomical Society*, vol. 445, no. 1. Oxford University Press (OUP), pp. 175–200, Sep. 24, 2014. doi: 10.1093/mnras/stu1654.  
  
M. Haider, “Large-scale mass distribution in the Illustris simulation”, *Monthly Notices of the Royal Astronomical Society*, vol. 457, no. 3. Oxford University Press (OUP), pp. 3024–3035, Feb. 24, 2016. doi: 10.1093/mnras/stw077.  
  
D. Nelson, “The illustris simulation: Public data release”, *Astronomy and Computing*, vol. 13. Elsevier BV, pp. 12–37, Nov. 2015. doi: 10.1016/j.ascom.2015.09.003.  
  
A. Pillepich, “Halo mass and assembly history exposed in the faint outskirts: the stellar and dark matter haloes of Illustris galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 444, no. 1. Oxford University Press (OUP), pp. 237–249, Aug. 14, 2014. doi: 10.1093/mnras/stu1408.  
  
V. Rodriguez-Gomez, “The merger rate of galaxies in the Illustris simulation: a comparison with observations and semi-empirical models”, *Monthly Notices of the Royal Astronomical Society*, vol. 449, no. 1. Oxford University Press (OUP), pp. 49–64, Mar. 14, 2015. doi: 10.1093/mnras/stv264.  
  
V. Rodriguez-Gomez, “The stellar mass assembly of galaxies in the Illustris simulation: growth by mergers and the spatial distribution of accreted stars”, *Monthly Notices of the Royal Astronomical Society*, vol. 458, no. 3. Oxford University Press (OUP), pp. 2371–2390, Feb. 26, 2016. doi: 10.1093/mnras/stw456.  
  
L. V. Sales, “The colours of satellite galaxies in the Illustris simulation”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 447, no. 1. Oxford University Press (OUP), pp. L6–L10, Nov. 24, 2014. doi: 10.1093/mnrasl/slu173.  
  
D. Sijacki, “The Illustris simulation: the evolving population of black holes across cosmic time”, *Monthly Notices of the Royal Astronomical Society*, vol. 452, no. 1. Oxford University Press (OUP), pp. 575–596, Jul. 06, 2015. doi: 10.1093/mnras/stv1340.  
  
G. F. Snyder, “Galaxy morphology and star formation in the Illustris Simulation at*z* = 0”, *Monthly Notices of the Royal Astronomical Society*, vol. 454, no. 2. Oxford University Press (OUP), pp. 1886–1908, Oct. 08, 2015. doi: 10.1093/mnras/stv2078.  
  
M. Sparre, “The star formation main sequence and stellar mass assembly of galaxies in the Illustris simulation”, *Monthly Notices of the Royal Astronomical Society*, vol. 447, no. 4. Oxford University Press (OUP), pp. 3548–3563, Jan. 24, 2015. doi: 10.1093/mnras/stu2713.  
  
P. Torrey, “Synthetic galaxy images and spectra from the Illustris simulation”, *Monthly Notices of the Royal Astronomical Society*, vol. 447, no. 3. Oxford University Press (OUP), pp. 2753–2771, Jan. 10, 2015. doi: 10.1093/mnras/stu2592.  
  
M. Vogelsberger, “Introducing the Illustris Project: simulating the coevolution of dark and visible matter in the Universe”, *Monthly Notices of the Royal Astronomical Society*, vol. 444, no. 2. Oxford University Press (OUP), pp. 1518–1547, Aug. 29, 2014. doi: 10.1093/mnras/stu1536.  
  
M. Vogelsberger, “Properties of galaxies reproduced by a hydrodynamic simulation”, *Nature*, vol. 509, no. 7499. Springer Science and Business Media LLC, pp. 177–182, May 07, 2014. doi: 10.1038/nature13316.  
  
S. Wellons, “The diverse evolutionary paths of simulated high-*z*massive, compact galaxies to*z*= 0”, *Monthly Notices of the Royal Astronomical Society*, vol. 456, no. 1. Oxford University Press (OUP), pp. 1030–1048, Dec. 18, 2015. doi: 10.1093/mnras/stv2738.  
  
S. Wellons, “The formation of massive, compact galaxies at z = 2 in the Illustris simulation”, *Monthly Notices of the Royal Astronomical Society*, vol. 449, no. 1. Oxford University Press (OUP), pp. 361–372, Mar. 17, 2015. doi: 10.1093/mnras/stv303.  
  
M. V. Medvedev, “On the dynamics of non-relativistic flavor-mixed particles”, *Journal of Cosmology and Astroparticle Physics*, vol. 2014, no. 6. IOP Publishing, pp. 063–063, Jun. 27, 2014. doi: 10.1088/1475-7516/2014/06/063.  
  
A. S. Graus, J. S. Bullock, M. Boylan-Kolchinand D. R. Weisz, “Push it to the limit: Local Group constraints on high-redshift stellar mass functions for*M*⋆≥ 105 M⊙”, *Monthly Notices of the Royal Astronomical Society*, vol. 456, no. 1. Oxford University Press (OUP), pp. 477–484, Dec. 16, 2015. doi: 10.1093/mnras/stv2728.  
  
K. D. Gordon, “THE PANCHROMATIC HUBBLE ANDROMEDA TREASURY. XV. THE BEAST: BAYESIAN EXTINCTION AND STELLAR TOOL”, *The Astrophysical Journal*, vol. 826, no. 2. American Astronomical Society, p. 104, Jul. 26, 2016. doi: 10.3847/0004-637x/826/2/104.  
  
C. A. Cole, Z.-C. Wang, T. P. Snowand V. M. Bierbaum, “GAS-PHASE CHEMISTRY OF THE CYANATE ION, OCN−”, *The Astrophysical Journal*, vol. 812, no. 1. American Astronomical Society, p. 77, Oct. 09, 2015. doi: 10.1088/0004-637x/812/1/77.  
  
Z.-C. Wang, C. A. Cole, N. J. Demarais, T. P. Snowand V. M. Bierbaum, “Reactions of Azine Anions with Nitrogen and Oxygen Atoms: Implications for Titan’s Upper Atmosphere and Interstellar Chemistry”, *Journal of the American Chemical Society*, vol. 137, no. 33. American Chemical Society (ACS), pp. 10700–10709, Aug. 17, 2015. doi: 10.1021/jacs.5b06089.  
  
J.-H. Choi, I. Shlosmanand M. C. Begelman, “Supermassive black hole formation at high redshifts via direct collapse in a cosmological context”, *Monthly Notices of the Royal Astronomical Society*, vol. 450, no. 4. Oxford University Press (OUP), pp. 4411–4423, May 22, 2015. doi: 10.1093/mnras/stv694.  
  
H. Yajima, I. Shlosman, E. Romano-Díazand K. Nagamine, “Observational properties of simulated galaxies in overdense and average regions at redshifts z ≃ 6–12”, *Monthly Notices of the Royal Astronomical Society*, vol. 451, no. 1. Oxford University Press (OUP), pp. 418–432, May 27, 2015. doi: 10.1093/mnras/stv974.  
  
D. Ball, L. Sironiand F. Özel, “Electron and Proton Acceleration in Trans-relativistic Magnetic Reconnection: Dependence on Plasma Beta and Magnetization”, *The Astrophysical Journal*, vol. 862, no. 1. American Astronomical Society, p. 80, Jul. 25, 2018. doi: 10.3847/1538-4357/aac820.  
  
D. Kagan, L. Sironi, B. Ceruttiand D. Giannios, “Relativistic Magnetic Reconnection in Pair Plasmas and Its Astrophysical Applications”, *Space Science Reviews*, vol. 191, no. 1–4. Springer Science and Business Media LLC, pp. 545–573, Jan. 13, 2015. doi: 10.1007/s11214-014-0132-9.  
  
A. Marcowith, “The microphysics of collisionless shock waves”, *Reports on Progress in Physics*, vol. 79, no. 4. IOP Publishing, p. 046901, Mar. 23, 2016. doi: 10.1088/0034-4885/79/4/046901.  
  
L. Sironi, U. Keshetand M. Lemoine, “Relativistic Shocks: Particle Acceleration and Magnetization”, *Space Science Reviews*, vol. 191, no. 1–4. Springer Science and Business Media LLC, pp. 519–544, Sep. 02, 2015. doi: 10.1007/s11214-015-0181-8.  
  
L. Sironi, M. Petropoulouand D. Giannios, “Relativistic jets shine through shocks or magnetic reconnection?”, *Monthly Notices of the Royal Astronomical Society*, vol. 450, no. 1. Oxford University Press (OUP), pp. 183–191, Apr. 15, 2015. doi: 10.1093/mnras/stv641.  
  
N. Ivanova, S. Justham, J. L. A. Nandezand J. C. Lombardi Jr., “Identification of the Long-Sought Common-Envelope Events”, *Science*, vol. 339, no. 6118. American Association for the Advancement of Science (AAAS), pp. 433–435, Jan. 25, 2013. doi: 10.1126/science.1225540.  
  
J. C. Lombardi Jr, W. G. McInallyand J. A. Faber, “An efficient radiative cooling approximation for use in hydrodynamic simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 447, no. 1. Oxford University Press (OUP), pp. 25–35, Dec. 12, 2014. doi: 10.1093/mnras/stu2432.  
  
K. J. Walsh and H. F. Levison, “FORMATION AND EVOLUTION OF PLUTO’S SMALL SATELLITES”, *The Astronomical Journal*, vol. 150, no. 1. American Astronomical Society, p. 11, Jun. 18, 2015. doi: 10.1088/0004-6256/150/1/11.  
  
J. S. Ritter, A. Sluder, C. Safranek-Shrader, M. Milosavljevi and V. Bromm, “Metal transport and chemical heterogeneity in early star forming systems”, *Monthly Notices of the Royal Astronomical Society*, vol. 451, no. 2. Oxford University Press (OUP), pp. 1190–1198, Jun. 10, 2015. doi: 10.1093/mnras/stv982.  
  
C. Safranek-Shrader, M. Milosavljevićand V. Bromm, “Star formation in the first galaxies – II. Clustered star formation and the influence of metal line cooling”, *Monthly Notices of the Royal Astronomical Society*, vol. 438, no. 2. Oxford University Press (OUP), pp. 1669–1685, Jan. 03, 2014. doi: 10.1093/mnras/stt2307.  
  
T. K. Chan, “Cosmic ray feedback in the FIRE simulations: constraining cosmic ray propagation with GeV γ-ray emission”, *Monthly Notices of the Royal Astronomical Society*, vol. 488, no. 3. Oxford University Press (OUP), pp. 3716–3744, Jul. 10, 2019. doi: 10.1093/mnras/stz1895.  
  
T. K. Chan, “The origin of ultra diffuse galaxies: stellar feedback and quenching”, *Monthly Notices of the Royal Astronomical Society*, vol. 478, no. 1. Oxford University Press (OUP), pp. 906–925, May 04, 2018. doi: 10.1093/mnras/sty1153.  
  
R. K. Cochrane, “Predictions for the spatial distribution of the dust continuum emission in **1** **<** **z** **<** **5** star-forming galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 488, no. 2. Oxford University Press (OUP), pp. 1779–1789, Jun. 25, 2019. doi: 10.1093/mnras/stz1736.  
  
R. Feldmann, C.-A. Faucher-Giguèreand D. Kereš, “The Galaxy–Halo Connection in Low-mass Halos”, *The Astrophysical Journal*, vol. 871, no. 2. American Astronomical Society, p. L21, Jan. 25, 2019. doi: 10.3847/2041-8213/aafe80.  
  
Z. Hafen, “The origins of the circumgalactic medium in the FIRE simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 488, no. 1. Oxford University Press (OUP), pp. 1248–1272, Jun. 28, 2019. doi: 10.1093/mnras/stz1773.  
  
L. Liang, “On the dust temperatures of high-redshift galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 489, no. 1. Oxford University Press (OUP), pp. 1397–1422, Aug. 02, 2019. doi: 10.1093/mnras/stz2134.  
  
D. Narayanan, “The formation of submillimetre-bright galaxies from gas infall over a billion years”, *Nature*, vol. 525, no. 7570. Springer Science and Business Media LLC, pp. 496–499, Sep. 23, 2015. doi: 10.1038/nature15383.  
  
M. E. Orr, “What FIREs up star formation: the emergence of the Kennicutt–Schmidt law from feedback”, *Monthly Notices of the Royal Astronomical Society*, vol. 478, no. 3. Oxford University Press (OUP), pp. 3653–3673, May 14, 2018. doi: 10.1093/mnras/sty1241.  
  
C. Wheeler, “The no-spin zone: rotation versus dispersion support in observed and simulated dwarf galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 465, no. 2. Oxford University Press (OUP), pp. 2420–2431, Oct. 08, 2016. doi: 10.1093/mnras/stw2583.  
  
T. K. Chan, “The impact of baryonic physics on the structure of dark matter haloes: the view from the FIRE cosmological simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 454, no. 3. Oxford University Press (OUP), pp. 2981–3001, Oct. 17, 2015. doi: 10.1093/mnras/stv2165.  
  
R. Davé, M. H. Rafieferantsoa, R. J. Thompsonand P. F. Hopkins, “Mufasa: Galaxy star formation, gas, and metal properties across cosmic time”, *Monthly Notices of the Royal Astronomical Society*. Oxford University Press (OUP), p. stx108, Jan. 14, 2017. doi: 10.1093/mnras/stx108.  
  
R. Davé, R. Thompsonand P. F. Hopkins, “mufasa: galaxy formation simulations with meshless hydrodynamics”, *Monthly Notices of the Royal Astronomical Society*, vol. 462, no. 3. Oxford University Press (OUP), pp. 3265–3284, Jul. 30, 2016. doi: 10.1093/mnras/stw1862.  
  
C. Federrath, M. Krumholzand P. F. Hopkins, “Converging on the Initial Mass Function of Stars”, *Journal of Physics: Conference Series*, vol. 837. IOP Publishing, p. 012007, May 30, 2017. doi: 10.1088/1742-6596/837/1/012007.  
  
D. Guszejnov, P. F. Hopkinsand X. Ma, “Comparing models for IMF variation across cosmological time in Milky Way-like galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 472, no. 2. Oxford University Press (OUP), pp. 2107–2116, Aug. 14, 2017. doi: 10.1093/mnras/stx2067.  
  
D. Guszejnov, M. R. Krumholzand P. F. Hopkins, “The necessity of feedback physics in setting the peak of the initial mass function”, *Monthly Notices of the Royal Astronomical Society*, vol. 458, no. 1. Oxford University Press (OUP), pp. 673–680, Feb. 10, 2016. doi: 10.1093/mnras/stw315.  
  
P. F. Hopkins, “A constrained-gradient method to control divergence errors in numerical MHD”, *Monthly Notices of the Royal Astronomical Society*, vol. 462, no. 1. Oxford University Press (OUP), pp. 576–587, Jul. 04, 2016. doi: 10.1093/mnras/stw1578.  
  
P. F. Hopkins, “Anisotropic diffusion in mesh-free numerical magnetohydrodynamics”, *Monthly Notices of the Royal Astronomical Society*, vol. 466, no. 3. Oxford University Press (OUP), pp. 3387–3405, Dec. 20, 2016. doi: 10.1093/mnras/stw3306.  
  
P. F. Hopkins and M. J. Raives, “Accurate, meshless methods for magnetohydrodynamics”, *Monthly Notices of the Royal Astronomical Society*, vol. 455, no. 1. Oxford University Press (OUP), pp. 51–88, Nov. 02, 2015. doi: 10.1093/mnras/stv2180.  
  
P. F. Hopkins, P. Torrey, C.-A. Faucher-Giguère, E. Quataertand N. Murray, “Stellar and quasar feedback in concert: effects on AGN accretion, obscuration, and outflows”, *Monthly Notices of the Royal Astronomical Society*, vol. 458, no. 1. Oxford University Press (OUP), pp. 816–831, Feb. 09, 2016. doi: 10.1093/mnras/stw289.  
  
X. Ma, “The origin and evolution of the galaxy mass–metallicity relation”, *Monthly Notices of the Royal Astronomical Society*, vol. 456, no. 2. Oxford University Press (OUP), pp. 2140–2156, Dec. 30, 2015. doi: 10.1093/mnras/stv2659.  
  
X. Ma, “The difficulty of getting high escape fractions of ionizing photons from high-redshift galaxies: a view from the FIRE cosmological simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 453, no. 1. Oxford University Press (OUP), pp. 960–975, Aug. 22, 2015. doi: 10.1093/mnras/stv1679.  
  
X. Ma, “Dust attenuation, dust emission, and dust temperature in galaxies at z ≥ 5: a view from the FIRE-2 simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 487, no. 2. Oxford University Press (OUP), pp. 1844–1864, May 14, 2019. doi: 10.1093/mnras/stz1324.  
  
L. Blecha, A. Loeband R. Narayan, “Double-peaked narrow-line signatures of dual supermassive black holes in galaxy merger simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 429, no. 3. Oxford University Press (OUP), pp. 2594–2616, Jan. 09, 2013. doi: 10.1093/mnras/sts533.  
  
K. S. S. Barrow, A. Aykutalpand J. H. Wise, “Observational signatures of massive black hole formation in the early Universe”, *Nature Astronomy*, vol. 2, no. 12. Springer Science and Business Media LLC, pp. 987–994, Sep. 10, 2018. doi: 10.1038/s41550-018-0569-y.  
  
K. S. S. Barrow, J. H. Wise, A. Aykutalp, B. W. O’Shea, M. L. Normanand H. Xu, “First light – II. Emission line extinction, population III stars, and X-ray binaries”, *Monthly Notices of the Royal Astronomical Society*, vol. 474, no. 2. Oxford University Press (OUP), pp. 2617–2634, Nov. 17, 2017. doi: 10.1093/mnras/stx2973.  
  
K. S. S. Barrow, J. H. Wise, M. L. Norman, B. W. O’Sheaand H. Xu, “First light: exploring the spectra of high-redshift galaxies in the Renaissance Simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 469, no. 4. Oxford University Press (OUP), pp. 4863–4878, May 15, 2017. doi: 10.1093/mnras/stx1181.  
  
G. Chiaki and J. H. Wise, “Seeding the second star: enrichment from population III, dust evolution, and cloud collapse”, *Monthly Notices of the Royal Astronomical Society*, vol. 482, no. 3. Oxford University Press (OUP), pp. 3933–3949, Nov. 03, 2018. doi: 10.1093/mnras/sty2984.  
  
L. Corlies, K. V. Johnstonand J. H. Wise, “Exploring simulated early star formation in the context of the ultrafaint dwarf galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 475, no. 4. Oxford University Press (OUP), pp. 4868–4880, Jan. 10, 2018. doi: 10.1093/mnras/sty064.  
  
B. Côté, D. W. Silvia, B. W. O’Shea, B. Smithand J. H. Wise, “Validating Semi-analytic Models of High-redshift Galaxy Formation Using Radiation Hydrodynamical Simulations”, *The Astrophysical Journal*, vol. 859, no. 1. American Astronomical Society, p. 67, May 24, 2018. doi: 10.3847/1538-4357/aabe8f.  
  
C. B. Hummels, “The Impact of Enhanced Halo Resolution on the Simulated Circumgalactic Medium”, *The Astrophysical Journal*, vol. 882, no. 2. American Astronomical Society, p. 156, Sep. 13, 2019. doi: 10.3847/1538-4357/ab378f.  
  
J.-. hoon . Kim, J. H. Wise, T. Abel, Y. Jo, J. R. Primackand P. F. Hopkins, “High-redshift Galaxy Formation with Self-consistently Modeled Stars and Massive Black Holes: Stellar Feedback and Quasar Growth”, *The Astrophysical Journal*, vol. 887, no. 2. American Astronomical Society, p. 120, Dec. 16, 2019. doi: 10.3847/1538-4357/ab510b.  
  
D. Koh and J. H. Wise, “Amplification of magnetic fields in a primordial H ii region and supernova”, *Monthly Notices of the Royal Astronomical Society*, vol. 462, no. 1. Oxford University Press (OUP), pp. 81–91, Jul. 13, 2016. doi: 10.1093/mnras/stw1673.  
  
D. Koh and J. H. Wise, “Extending semi-numeric reionization models to the first stars and galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 474, no. 3. Oxford University Press (OUP), pp. 3817–3824, Nov. 23, 2017. doi: 10.1093/mnras/stx3018.  
  
M. L. Norman, P. Chen, J. H. Wiseand H. Xu, “Fully Coupled Simulation of Cosmic Reionization. III. Stochastic Early Reionization by the Smallest Galaxies”, *The Astrophysical Journal*, vol. 867, no. 1. American Astronomical Society, p. 27, Oct. 26, 2018. doi: 10.3847/1538-4357/aae30b.  
  
B. W. O’Shea, J. H. Wise, H. Xuand M. L. Norman, “PROBING THE ULTRAVIOLET LUMINOSITY FUNCTION OF THE EARLIEST GALAXIES WITH THE RENAISSANCE SIMULATIONS”, *The Astrophysical Journal*, vol. 807, no. 1. American Astronomical Society, p. L12, Jun. 30, 2015. doi: 10.1088/2041-8205/807/1/l12.  
  
Y. Qiu, T. Bogdanović, Y. Li, K. Parkand J. H. Wise, “The Interplay of Kinetic and Radiative Feedback in Galaxy Clusters”, *The Astrophysical Journal*, vol. 877, no. 1. American Astronomical Society, p. 47, May 23, 2019. doi: 10.3847/1538-4357/ab18fd.  
  
J. A. Regan, P. H. Johanssonand J. H. Wise, “The effect of dark matter resolution on the collapse of baryons in high-redshift numerical simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 449, no. 4. Oxford University Press (OUP), pp. 3766–3779, Apr. 10, 2015. doi: 10.1093/mnras/stv610.  
  
J. A. Regan, P. H. Johanssonand J. H. Wise, “Positive or negative? The impact of X-ray feedback on the formation of direct collapse black hole seeds”, *Monthly Notices of the Royal Astronomical Society*, vol. 461, no. 1. Oxford University Press (OUP), pp. 111–125, Jun. 15, 2016. doi: 10.1093/mnras/stw1307.  
  
J. A. Regan, E. Visbal, J. H. Wise, Z. Haiman, P. H. Johanssonand G. L. Bryan, “Rapid formation of massive black holes in close proximity to embryonic protogalaxies”, *Nature Astronomy*, vol. 1, no. 4. Springer Science and Business Media LLC, Mar. 13, 2017. doi: 10.1038/s41550-017-0075.  
  
J. A. Regan, J. H. Wise, B. W. O’Sheaand M. L. Norman, “The emergence of the first star-free atomic cooling haloes in the Universe”, *Monthly Notices of the Royal Astronomical Society*, vol. 492, no. 2. Oxford University Press (OUP), pp. 3021–3031, Jan. 09, 2020. doi: 10.1093/mnras/staa035.  
  
B. D. Smith, J. A. Regan, T. P. Downes, M. L. Norman, B. W. O’Sheaand J. H. Wise, “The growth of black holes from Population III remnants in the Renaissance simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 480, no. 3. Oxford University Press (OUP), pp. 3762–3773, Aug. 02, 2018. doi: 10.1093/mnras/sty2103.  
  
B. D. Smith, J. H. Wise, B. W. O’Shea, M. L. Normanand S. Khochfar, “The first Population II stars formed in externally enriched mini-haloes”, *Monthly Notices of the Royal Astronomical Society*, vol. 452, no. 3. Oxford University Press (OUP), pp. 2822–2836, Jul. 29, 2015. doi: 10.1093/mnras/stv1509.  
  
J. H. Wise, “The birth of a galaxy – III. Propelling reionization with the faintest galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 442, no. 3. Oxford University Press (OUP), pp. 2560–2579, Jun. 26, 2014. doi: 10.1093/mnras/stu979.  
  
J. H. Wise, J. A. Regan, B. W. O’Shea, M. L. Norman, T. P. Downesand H. Xu, “Formation of massive black holes in rapidly growing pre-galactic gas clouds”, *Nature*, vol. 566, no. 7742. Springer Science and Business Media LLC, pp. 85–88, Jan. 23, 2019. doi: 10.1038/s41586-019-0873-4.  
  
H. Xu, J. H. Wise, M. L. Norman, K. Ahnand B. W. O’Shea, “GALAXY PROPERTIES AND UV ESCAPE FRACTIONS DURING THE EPOCH OF REIONIZATION: RESULTS FROM THE RENAISSANCE SIMULATIONS”, *The Astrophysical Journal*, vol. 833, no. 1. American Astronomical Society, p. 84, Dec. 08, 2016. doi: 10.3847/1538-4357/833/1/84.  
  
M. L. Norman, D. R. Reynolds, G. C. So, R. P. Harknessand J. H. Wise, “FULLY COUPLED SIMULATION OF COSMIC REIONIZATION. I. NUMERICAL METHODS AND TESTS”, *The Astrophysical Journal Supplement Series*, vol. 216, no. 1. American Astronomical Society, p. 16, Jan. 09, 2015. doi: 10.1088/0067-0049/216/1/16.  
  
K. Finlator, J. A. Muñoz, B. D. Oppenheimer, S. P. Oh, F. Özeland R. Davé, “The host haloes of O i absorbers in the reionization epoch”, *Monthly Notices of the Royal Astronomical Society*, vol. 436, no. 2. Oxford University Press (OUP), pp. 1818–1835, Oct. 01, 2013. doi: 10.1093/mnras/stt1697.  
  
K. Finlator, B. D. Oppenheimer, R. Davé, E. Zackrisson, R. Thompsonand S. Huang, “The Soft, Fluctuating UVB at*z*∼ 6 as Traced by C IV, Si IV, and C II”, *Monthly Notices of the Royal Astronomical Society*. Oxford University Press (OUP), p. stw805, Apr. 07, 2016. doi: 10.1093/mnras/stw805.  
  
L. Chamandy, “Accretion in common envelope evolution”, *Monthly Notices of the Royal Astronomical Society*, vol. 480, no. 2. Oxford University Press (OUP), pp. 1898–1911, Jul. 20, 2018. doi: 10.1093/mnras/sty1950.  
  
L. Chamandy, “Energy budget and core-envelope motion in common envelope evolution”, *Monthly Notices of the Royal Astronomical Society*, vol. 486, no. 1. Oxford University Press (OUP), pp. 1070–1085, Mar. 27, 2019. doi: 10.1093/mnras/stz887.  
  
Z. Chen, E. G. Blackman, J. Nordhaus, A. Frankand J. Carroll-Nellenback, “Wind-accelerated orbital evolution in binary systems with giant stars”, *Monthly Notices of the Royal Astronomical Society*, vol. 473, no. 1. Oxford University Press (OUP), pp. 747–756, Sep. 09, 2017. doi: 10.1093/mnras/stx2335.  
  
Z. Chen, A. Frank, E. G. Blackman, J. Nordhausand J. Carroll-Nellenback, “Mass transfer and disc formation in AGB binary systems”, *Monthly Notices of the Royal Astronomical Society*, vol. 468, no. 4. Oxford University Press (OUP), pp. 4465–4477, Mar. 17, 2017. doi: 10.1093/mnras/stx680.  
  
Z. Chen, A. Frank, E. G. Blackman, J. Nordhausand J. Carroll-Nellenback, “Mass transfer and disc formation in AGB binary systems”, *Monthly Notices of the Royal Astronomical Society*, vol. 468, no. 4. Oxford University Press (OUP), pp. 4465–4477, Mar. 17, 2017. doi: 10.1093/mnras/stx680.  
  
A. Debrecht, J. Carroll-Nellenback, A. Frank, L. Fossati, E. G. Blackmanand I. Dobbs-Dixon, “Generation of a circumstellar gas disc by hot Jupiter WASP-12b”, *Monthly Notices of the Royal Astronomical Society*, vol. 478, no. 2. Oxford University Press (OUP), pp. 2592–2598, May 04, 2018. doi: 10.1093/mnras/sty1164.  
  
A. Debrecht, J. Carroll-Nellenback, A. Frank, J. McCann, R. Murray-Clayand E. G. Blackman, “Photoevaporative flows from exoplanet atmospheres: a 3D radiative hydrodynamic parameter study”, *Monthly Notices of the Royal Astronomical Society*, vol. 483, no. 2. Oxford University Press (OUP), pp. 1481–1495, Nov. 27, 2018. doi: 10.1093/mnras/sty3212.  
  
A. Frank, Z. Chen, T. Reichardt, O. De Marco, E. Blackmanand J. Nordhaus, “Planetary Nebulae Shaped by Common Envelope Evolution”, *Galaxies*, vol. 6, no. 4. MDPI AG, p. 113, Oct. 26, 2018. doi: 10.3390/galaxies6040113.  
  
M. Huarte-Espinosa, J. Carroll-Nellenback, J. Nordhaus, A. Frankand E. G. Blackman, “The formation and evolution of wind-capture discs in binary systems”, *Monthly Notices of the Royal Astronomical Society*, vol. 433, no. 1. Oxford University Press (OUP), pp. 295–306, May 29, 2013. doi: 10.1093/mnras/stt725.  
  
Z. Chen, A. Frank, E. G. Blackmanand J. Nordhaus, “The creation of AGB fallback shells”, *Monthly Notices of the Royal Astronomical Society*, vol. 457, no. 3. Oxford University Press (OUP), pp. 3219–3224, Feb. 22, 2016. doi: 10.1093/mnras/stw012.  
  
Z. Chen, J. Nordhaus, A. Frank, E. G. Blackmanand B. Balick, “Three-dimensional hydrodynamic simulations of*L*2Puppis”, *Monthly Notices of the Royal Astronomical Society*, vol. 460, no. 4. Oxford University Press (OUP), pp. 4182–4187, Jun. 07, 2016. doi: 10.1093/mnras/stw1305.  
  
A. Frank, “Planetary Evaporation and the Dynamics of Planet Wind/Stellar Wind Bow Shocks”, *Proceedings of the International Astronomical Union*, vol. 10, no. S314. Cambridge University Press (CUP), pp. 237–240, Nov. 2015. doi: 10.1017/s1743921315006675.  
  
E. C. Hansen, A. Frank, P. Hartiganand K. Yirak, “Numerical simulations of Mach stem formation via intersecting bow shocks”, *High Energy Density Physics*, vol. 17. Elsevier BV, pp. 135–139, Dec. 2015. doi: 10.1016/j.hedp.2014.12.005.  
  
E. C. Hansen, A. Frankand P. Hartigan, “MAGNETOHYDRODYNAMIC EFFECTS ON PULSED YOUNG STELLAR OBJECT JETS. I. 2.5D SIMULATIONS”, *The Astrophysical Journal*, vol. 800, no. 1. American Astronomical Society, p. 41, Feb. 06, 2015. doi: 10.1088/0004-637x/800/1/41.  
  
D. A. Gole and J. B. Simon, “The Nature of Turbulence in the Outer Regions of Protoplanetary Disks”, *The Astrophysical Journal*, vol. 869, no. 1. American Astronomical Society, p. 84, Dec. 13, 2018. doi: 10.3847/1538-4357/aae823.  
  
J. B. Simon and P. J. Armitage, “EFFICIENCY OF PARTICLE TRAPPING IN THE OUTER REGIONS OF PROTOPLANETARY DISKS”, *The Astrophysical Journal*, vol. 784, no. 1. American Astronomical Society, p. 15, Feb. 26, 2014. doi: 10.1088/0004-637x/784/1/15.  
  
J. B. Simon, P. J. Armitage, A. N. Youdinand R. Li, “Evidence for Universality in the Initial Planetesimal Mass Function”, *The Astrophysical Journal*, vol. 847, no. 2. American Astronomical Society, p. L12, Sep. 22, 2017. doi: 10.3847/2041-8213/aa8c79.  
  
J. B. Simon, X.-N. Bai, P. J. Armitage, J. M. Stoneand K. Beckwith, “TURBULENCE IN THE OUTER REGIONS OF PROTOPLANETARY DISKS. II. STRONG ACCRETION DRIVEN BY A VERTICAL MAGNETIC FIELD”, *The Astrophysical Journal*, vol. 775, no. 1. American Astronomical Society, p. 73, Sep. 05, 2013. doi: 10.1088/0004-637x/775/1/73.  
  
J. B. Simon, X.-N. Bai, K. M. Flahertyand A. M. Hughes, “Origin of Weak Turbulence in the Outer Regions of Protoplanetary Disks”, *The Astrophysical Journal*, vol. 865, no. 1. American Astronomical Society, p. 10, Sep. 17, 2018. doi: 10.3847/1538-4357/aad86d.  
  
A. D’Aloisio, P. R. Upton Sanderbeck, M. McQuinn, H. Tracand P. R. Shapiro, “On the contribution of active galactic nuclei to the high-redshift metagalactic ionizing background”, *Monthly Notices of the Royal Astronomical Society*, vol. 468, no. 4. Oxford University Press (OUP), pp. 4691–4701, Mar. 24, 2017. doi: 10.1093/mnras/stx711.  
  
F. B. Davies, S. R. Furlanettoand M. McQuinn, “Quasar ionization front Lyα emission in an inhomogeneous intergalactic medium”, *Monthly Notices of the Royal Astronomical Society*, vol. 457, no. 3. Oxford University Press (OUP), pp. 3006–3023, Feb. 18, 2016. doi: 10.1093/mnras/stw055.  
  
I. S. Khrykin, J. F. Hennawiand M. McQuinn, “The Thermal Proximity Effect: A New Probe of the He ii Reionization History and Quasar Lifetime”, *The Astrophysical Journal*, vol. 838, no. 2. American Astronomical Society, p. 96, Mar. 30, 2017. doi: 10.3847/1538-4357/aa6621.  
  
M. McQuinn and P. R. Upton Sanderbeck, “On the intergalactic temperature–density relation”, *Monthly Notices of the Royal Astronomical Society*, vol. 456, no. 1. Oxford University Press (OUP), pp. 47–54, Dec. 11, 2015. doi: 10.1093/mnras/stv2675.  
  
M. McQuinn and M. White, “Cosmological perturbation theory in 1+1 dimensions”, *Journal of Cosmology and Astroparticle Physics*, vol. 2016, no. 1. IOP Publishing, pp. 043–043, Jan. 22, 2016. doi: 10.1088/1475-7516/2016/01/043.  
  
M. McQuinn and G. Worseck, “The case against large intensity fluctuations in the z ∼ 2.5 He舁ii Lyα forest”, *Monthly Notices of the Royal Astronomical Society*, vol. 440, no. 3. Oxford University Press (OUP), pp. 2406–2418, Mar. 31, 2014. doi: 10.1093/mnras/stu242.  
  
Y. Noh and M. McQuinn, “A physical understanding of how reionization suppresses accretion on to dwarf haloes”, *Monthly Notices of the Royal Astronomical Society*, vol. 444, no. 1. Oxford University Press (OUP), pp. 503–514, Aug. 18, 2014. doi: 10.1093/mnras/stu1412.  
  
J. L. Hoffman, “Reconstructing the Scene: New Views of Supernovae and Progenitors from the SNSPOL Project”, *Proceedings of the International Astronomical Union*, vol. 12, no. S329. Cambridge University Press (CUP), pp. 54–58, Nov. 2016. doi: 10.1017/s1743921317003052.  
  
L. Huk, “Time Lapse Spectropolarimetry: Constraining the Nature and Progenitors of Interacting CCSNe”, *Proceedings of the International Astronomical Union*, vol. 12, no. S329. Cambridge University Press (CUP), pp. 408–408, Nov. 2016. doi: 10.1017/s1743921317002939.  
  
M. Shrestha and J. L. Hoffman, “Polarization Signatures of Bow Shocks in Stellar Winds”, *EAS Publications Series*, vol. 71–72. EDP Sciences, pp. 293–295, 2015. doi: 10.1051/eas/1571066.  
  
M. Shrestha, H. R. Neilson, J. L. Hoffmanand R. Ignace, “Polarization simulations of stellar wind bow-shock nebulae – I. The case of electron scattering”, *Monthly Notices of the Royal Astronomical Society*, vol. 477, no. 1. Oxford University Press (OUP), pp. 1365–1382, Mar. 20, 2018. doi: 10.1093/mnras/sty724.  
  
L. Arzamasskiy, Z. Zhuand J. M. Stone, “Three-dimensional disc–satellite interaction: torques, migration, and observational signatures”, *Monthly Notices of the Royal Astronomical Society*, vol. 475, no. 3. Oxford University Press (OUP), pp. 3201–3212, Jan. 05, 2018. doi: 10.1093/mnras/sty001.  
  
T. Birnstiel, “The Disk Substructures at High Angular Resolution Project (DSHARP). V. Interpreting ALMA Maps of Protoplanetary Disks in Terms of a Dust Model”, *The Astrophysical Journal*, vol. 869, no. 2. American Astronomical Society, p. L45, Dec. 26, 2018. doi: 10.3847/2041-8213/aaf743.  
  
I. Crnkovic-Rubsamen, Z. Zhuand J. M. Stone, “Survival and structure of dusty vortices in protoplanetary discs”, *Monthly Notices of the Royal Astronomical Society*, vol. 450, no. 4. Oxford University Press (OUP), pp. 4285–4291, May 21, 2015. doi: 10.1093/mnras/stv828.  
  
R. Dong (董若冰), Z. Zhu (朱照寰), R. R. Rafikovand J. M. Stone, “OBSERVATIONAL SIGNATURES OF PLANETS IN PROTOPLANETARY DISKS: SPIRAL ARMS OBSERVED IN SCATTERED LIGHT IMAGING CAN BE INDUCED BY PLANETS”, *The Astrophysical Journal*, vol. 809, no. 1. American Astronomical Society, p. L5, Aug. 05, 2015. doi: 10.1088/2041-8205/809/1/l5.  
  
C. P. Dullemond, “The Disk Substructures at High Angular Resolution Project (DSHARP). VI. Dust Trapping in Thin-ringed Protoplanetary Disks”, *The Astrophysical Journal*, vol. 869, no. 2. American Astronomical Society, p. L46, Dec. 26, 2018. doi: 10.3847/2041-8213/aaf742.  
  
V. V. Guzmán, “The Disk Substructures at High Angular Resolution Program (DSHARP). VIII. The Rich Ringed Substructures in the AS 209 Disk”, *The Astrophysical Journal*, vol. 869, no. 2. American Astronomical Society, p. L48, Dec. 26, 2018. doi: 10.3847/2041-8213/aaedae.  
  
X. Hu, “Nonideal MHD Simulation of HL Tau Disk: Formation of Rings”, *The Astrophysical Journal*, vol. 885, no. 1. American Astronomical Society, p. 36, Oct. 29, 2019. doi: 10.3847/1538-4357/ab44cb.  
  
W. Ju, J. M. Stoneand Z. Zhu, “Global MHD Simulations of Accretion Disks in Cataclysmic Variables (CVs). II. The Relative Importance of MRI and Spiral Shocks”, *The Astrophysical Journal*, vol. 841, no. 1. American Astronomical Society, p. 29, May 19, 2017. doi: 10.3847/1538-4357/aa705d.  
  
N. T. Kurtovic, “The Disk Substructures at High Angular Resolution Project (DSHARP). IV. Characterizing Substructures and Interactions in Disks around Multiple Star Systems”, *The Astrophysical Journal*, vol. 869, no. 2. American Astronomical Society, p. L44, Dec. 26, 2018. doi: 10.3847/2041-8213/aaf746.  
  
L. M. Pérez, “The Disk Substructures at High Angular Resolution Project (DSHARP). X. Multiple Rings, a Misaligned Inner Disk, and a Bright Arc in the Disk around the T Tauri star HD 143006”, *The Astrophysical Journal*, vol. 869, no. 2. American Astronomical Society, p. L50, Dec. 26, 2018. doi: 10.3847/2041-8213/aaf745.  
  
J.-M. Shi, Z. Zhu, J. M. Stoneand E. Chiang, “Dust dynamics in 2D gravito-turbulent discs”, *Monthly Notices of the Royal Astronomical Society*, vol. 459, no. 1. Oxford University Press (OUP), pp. 982–998, Mar. 28, 2016. doi: 10.1093/mnras/stw692.  
  
C.-C. Yang (楊朝欽) and Z. Zhu (朱照寰), “Morphological signatures induced by dust back reaction in discs with an embedded planet”, *Monthly Notices of the Royal Astronomical Society*, vol. 491, no. 4. Oxford University Press (OUP), pp. 4702–4718, Nov. 19, 2019. doi: 10.1093/mnras/stz3232.  
  
S. Zhang, “The Disk Substructures at High Angular Resolution Project (DSHARP). VII. The Planet–Disk Interactions Interpretation”, *The Astrophysical Journal*, vol. 869, no. 2. American Astronomical Society, p. L47, Dec. 26, 2018. doi: 10.3847/2041-8213/aaf744.  
  
Z. Zhu, “Inclined massive planets in a protoplanetary disc: gap opening, disc breaking, and observational signatures”, *Monthly Notices of the Royal Astronomical Society*, vol. 483, no. 3. Oxford University Press (OUP), pp. 4221–4241, Dec. 12, 2018. doi: 10.1093/mnras/sty3358.  
  
Z. Zhu and C. Baruteau, “Gas and dust hydrodynamical simulations of massive lopsided transition discs – I. Gas distribution”, *Monthly Notices of the Royal Astronomical Society*, vol. 458, no. 4. Oxford University Press (OUP), pp. 3918–3926, Apr. 07, 2016. doi: 10.1093/mnras/stw202.  
  
Z. Zhu, W. Juand J. M. Stone, “SHOCK-DRIVEN ACCRETION IN CIRCUMPLANETARY DISKS: OBSERVABLES AND SATELLITE FORMATION”, *The Astrophysical Journal*, vol. 832, no. 2. American Astronomical Society, p. 193, Dec. 01, 2016. doi: 10.3847/0004-637x/832/2/193.  
  
Z. Zhu and J. M. Stone, “DUST TRAPPING BY VORTICES IN TRANSITIONAL DISKS: EVIDENCE FOR NON-IDEAL MAGNETOHYDRODYNAMIC EFFECTS IN PROTOPLANETARY DISKS”, *The Astrophysical Journal*, vol. 795, no. 1. American Astronomical Society, p. 53, Oct. 13, 2014. doi: 10.1088/0004-637x/795/1/53.  
  
Z. Zhu and J. M. Stone, “Global Evolution of an Accretion Disk with a Net Vertical Field: Coronal Accretion, Flux Transport, and Disk Winds”, *The Astrophysical Journal*, vol. 857, no. 1. American Astronomical Society, p. 34, Apr. 10, 2018. doi: 10.3847/1538-4357/aaafc9.  
  
Z. Zhu, J. M. Stoneand X.-N. Bai, “DUST TRANSPORT IN MRI TURBULENT DISKS: IDEAL AND NON-IDEAL MHD WITH AMBIPOLAR DIFFUSION”, *The Astrophysical Journal*, vol. 801, no. 2. American Astronomical Society, p. 81, Mar. 05, 2015. doi: 10.1088/0004-637x/801/2/81.  
  
B. Burkhart, A. Lazarian, D. Balsara, C. Meyerand J. Cho, “ALFVÉNIC TURBULENCE BEYOND THE AMBIPOLAR DIFFUSION SCALE”, *The Astrophysical Journal*, vol. 805, no. 2. American Astronomical Society, p. 118, May 27, 2015. doi: 10.1088/0004-637x/805/2/118.  
  
J. Kim, D. S. Balsara, M. Lyutikovand S. S. Komissarov, “On the linear stability of sheared and magnetized jets without current sheets – non-relativistic case”, *Monthly Notices of the Royal Astronomical Society*, vol. 461, no. 1. Oxford University Press (OUP), pp. 728–741, May 03, 2016. doi: 10.1093/mnras/stw1051.  
  
J. Kim, D. S. Balsara, M. Lyutikov, S. S. Komissarov, D. Georgeand P. K. Siddireddy, “On the linear stability of magnetized jets without current sheets – non-relativistic case”, *Monthly Notices of the Royal Astronomical Society*, vol. 450, no. 1. Oxford University Press (OUP), pp. 982–997, Apr. 21, 2015. doi: 10.1093/mnras/stv606.  
  
S. Caldwell and P. Chang, “The accelerating pace of star formation”, *Monthly Notices of the Royal Astronomical Society*, vol. 474, no. 4. Oxford University Press (OUP), pp. 4818–4823, Nov. 24, 2017. doi: 10.1093/mnras/stx3037.  
  
P. Chang, A. E. Broderick, C. Pfrommer, E. Puchwein, A. Lambertsand M. Shalaby, “THE EFFECT OF NONLINEAR LANDAU DAMPING ON ULTRARELATIVISTIC BEAM PLASMA INSTABILITIES”, *The Astrophysical Journal*, vol. 797, no. 2. American Astronomical Society, p. 110, Dec. 05, 2014. doi: 10.1088/0004-637x/797/2/110.  
  
P. Chang and Z. B. Etienne, “General relativistic hydrodynamics on a moving-mesh I: static space–times”, *Monthly Notices of the Royal Astronomical Society*, vol. 496, no. 1. Oxford University Press (OUP), pp. 206–214, Jun. 03, 2020. doi: 10.1093/mnras/staa1532.  
  
P. Chang and N. Murray, “GW170817: a neutron star merger in a mass-transferring triple system”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 474, no. 1. Oxford University Press (OUP), pp. L12–L16, Nov. 21, 2017. doi: 10.1093/mnrasl/slx186.  
  
P. Chang, J. Wadsleyand T. R. Quinn, “A moving-mesh hydrodynamic solver for ChaNGa”, *Monthly Notices of the Royal Astronomical Society*, vol. 471, no. 3. Oxford University Press (OUP), pp. 3577–3589, Jul. 18, 2017. doi: 10.1093/mnras/stx1809.  
  
U. Garg and P. Chang, “A Semi-analytic Criterion for the Spontaneous Initiation of Carbon Detonations in White Dwarfs”, *The Astrophysical Journal*, vol. 836, no. 2. American Astronomical Society, p. 189, Feb. 21, 2017. doi: 10.3847/1538-4357/aa5d58.  
  
A. Lamberts, P. Chang, C. Pfrommer, E. Puchwein, A. E. Broderickand M. Shalaby, “PATCHY BLAZAR HEATING: DIVERSIFYING THE THERMAL HISTORY OF THE INTERGALACTIC MEDIUM”, *The Astrophysical Journal*, vol. 811, no. 1. American Astronomical Society, p. 19, Sep. 16, 2015. doi: 10.1088/0004-637x/811/1/19.  
  
E. J. Lee, P. Changand N. Murray, “TIME-VARYING DYNAMICAL STAR FORMATION RATE”, *The Astrophysical Journal*, vol. 800, no. 1. American Astronomical Society, p. 49, Feb. 09, 2015. doi: 10.1088/0004-637x/800/1/49.  
  
A. Lipnicky, S. Chakrabartiand P. Chang, “Relating the H i gas structure of spiral discs to passing satellites”, *Monthly Notices of the Royal Astronomical Society*, vol. 481, no. 2. Oxford University Press (OUP), pp. 2590–2600, Aug. 27, 2018. doi: 10.1093/mnras/sty2330.  
  
D. W. Murray, P. Chang, N. W. Murrayand J. Pittman, “Collapse in self-gravitating turbulent fluids”, *Monthly Notices of the Royal Astronomical Society*, vol. 465, no. 2. Oxford University Press (OUP), pp. 1316–1335, Nov. 02, 2016. doi: 10.1093/mnras/stw2796.  
  
D. Murray, S. Goyaland P. Chang, “The effects of protostellar jet feedback on turbulent collapse”, *Monthly Notices of the Royal Astronomical Society*, vol. 475, no. 1. Oxford University Press (OUP), pp. 1023–1035, Dec. 08, 2017. doi: 10.1093/mnras/stx3153.  
  
N. Murray and P. Chang, “STAR FORMATION IN SELF-GRAVITATING TURBULENT FLUIDS”, *The Astrophysical Journal*, vol. 804, no. 1. American Astronomical Society, p. 44, Apr. 29, 2015. doi: 10.1088/0004-637x/804/1/44.  
  
M. Shalaby, A. E. Broderick, P. Chang, C. Pfrommer, A. Lambertsand E. Puchwein, “SHARP: A Spatially Higher-order, Relativistic Particle-in-cell Code”, *The Astrophysical Journal*, vol. 841, no. 1. American Astronomical Society, p. 52, May 23, 2017. doi: 10.3847/1538-4357/aa6d13.  
  
M. Shalaby, A. E. Broderick, P. Chang, C. Pfrommer, A. Lambertsand E. Puchwein, “Growth of Beam–Plasma Instabilities in the Presence of Background Inhomogeneity”, *The Astrophysical Journal*, vol. 859, no. 1. American Astronomical Society, p. 45, May 23, 2018. doi: 10.3847/1538-4357/aabe92.  
  
P. Tiede, “Bow Ties in the Sky. II. Searching for Gamma-Ray Halos in the*Fermi*Sky Using Anisotropy”, *The Astrophysical Journal*, vol. 850, no. 2. American Astronomical Society, p. 157, Nov. 28, 2017. doi: 10.3847/1538-4357/aa9375.  
  
C. Zhu, R. Pakmor, M. H. van . Kerkwijkand P. Chang, “MAGNETIZED MOVING MESH MERGER OF A CARBON–OXYGEN WHITE DWARF BINARY”, *The Astrophysical Journal*, vol. 806, no. 1. American Astronomical Society, p. L1, Jun. 02, 2015. doi: 10.1088/2041-8205/806/1/l1.  
  
M. Delbo’, K. Walsh, B. Bolin, C. Avdellidouand A. Morbidelli, “Identification of a primordial asteroid family constrains the original planetesimal population”, *Science*, vol. 357, no. 6355. American Association for the Advancement of Science (AAAS), pp. 1026–1029, Sep. 08, 2017. doi: 10.1126/science.aam6036.  
  
B. C. Johnson, K. J. Walsh, D. A. Minton, A. N. Krotand H. F. Levison, “Timing of the formation and migration of giant planets as constrained by CB chondrites”, *Science Advances*, vol. 2, no. 12. American Association for the Advancement of Science (AAAS), Dec. 02, 2016. doi: 10.1126/sciadv.1601658.  
  
K. J. Walsh and H. F. Levison, “Planetesimals to terrestrial planets: Collisional evolution amidst a dissipating gas disk”, *Icarus*, vol. 329. Elsevier BV, pp. 88–100, Sep. 2019. doi: 10.1016/j.icarus.2019.03.031.  
  
K. E. Andrade, Q. Minor, A. Nierenbergand M. Kaplinghat, “Detecting dark matter cores in galaxy clusters with strong lensing”, *Monthly Notices of the Royal Astronomical Society*, vol. 487, no. 2. Oxford University Press (OUP), pp. 1905–1926, May 17, 2019. doi: 10.1093/mnras/stz1360.  
  
Q. E. Minor, A. B. Pace, J. L. Marshalland L. E. Strigari, “Robust velocity dispersion and binary population modelling of the ultrafaint dwarf galaxy Reticulum II”, *Monthly Notices of the Royal Astronomical Society*, vol. 487, no. 2. Oxford University Press (OUP), pp. 2961–2968, Jun. 03, 2019. doi: 10.1093/mnras/stz1468.  
  
E. A. Gómez, “Magnetohydrodynamics of Mira’s cometary tail”, *Astronomy & Astrophysics*, vol. 558. EDP Sciences, p. A107, Oct. 2013. doi: 10.1051/0004-6361/201322080.  
  
D. Yoon and S. Heinz, “GLOBAL SIMULATIONS OF THE INTERACTION OF MICROQUASAR JETS WITH A STELLAR WIND IN HIGH-MASS X-RAY BINARIES”, *The Astrophysical Journal*, vol. 801, no. 1. American Astronomical Society, p. 55, Mar. 04, 2015. doi: 10.1088/0004-637x/801/1/55.  
  
T. H. Greif, V. Springeland V. Bromm, “On the operation of the chemothermal instability in primordial star-forming clouds”, *Monthly Notices of the Royal Astronomical Society*, vol. 434, no. 4. Oxford University Press (OUP), pp. 3408–3422, Aug. 03, 2013. doi: 10.1093/mnras/stt1251.  
  
E. Buie II, M. Fumagalliand E. Scannapieco, “Interpreting Observations of Absorption Lines in the Circumgalactic Medium with a Turbulent Medium”, *The Astrophysical Journal*, vol. 890, no. 1. American Astronomical Society, p. 33, Feb. 10, 2020. doi: 10.3847/1538-4357/ab65bc.  
  
E. Buie II, W. J. Grayand E. Scannapieco, “Modeling Photoionized Turbulent Material in the Circumgalactic Medium”, *The Astrophysical Journal*, vol. 864, no. 2. American Astronomical Society, p. 114, Sep. 05, 2018. doi: 10.3847/1538-4357/aad8bd.  
  
M. Safarzadeh, R. Sarmentoand E. Scannapieco, “On Neutron Star Mergers as the Source of *r*-process-enhanced Metal-poor Stars in the Milky Way”, *The Astrophysical Journal*, vol. 876, no. 1. American Astronomical Society, p. 28, Apr. 30, 2019. doi: 10.3847/1538-4357/ab1341.  
  
R. Sarmento, E. Scannapiecoand B. Côté, “Following the Cosmic Evolution of Pristine Gas. III. The Observational Consequences of the Unknown Properties of Population III Stars”, *The Astrophysical Journal*, vol. 871, no. 2. American Astronomical Society, p. 206, Feb. 01, 2019. doi: 10.3847/1538-4357/aafa1a.  
  
J. Cottle, E. Scannapiecoand M. Brüggen, “Column Density Profiles of Cold Clouds Driven by Galactic Outflows”, *The Astrophysical Journal*, vol. 864, no. 1. American Astronomical Society, p. 96, Sep. 04, 2018. doi: 10.3847/1538-4357/aad55c.  
  
A. Dubey, “Pragmatic optimizations for better scientific utilization of large supercomputers”, *The International Journal of High Performance Computing Applications*, vol. 27, no. 3. SAGE Publications, pp. 360–373, Nov. 21, 2012. doi: 10.1177/1094342012464404.  
  
M. Huarte-Espinosa and A. Frank, “Magnetic towers and binary-formed disks: New results for planetary nebula evolution”, *Proceedings of the International Astronomical Union*, vol. 7, no. S283. Cambridge University Press (CUP), pp. 164–167, Jul. 2011. doi: 10.1017/s1743921312010885.  
  
P. F. Hopkins, “But what about…: cosmic rays, magnetic fields, conduction, and viscosity in galaxy formation”, *Monthly Notices of the Royal Astronomical Society*, vol. 492, no. 3. Oxford University Press (OUP), pp. 3465–3498, Dec. 05, 2019. doi: 10.1093/mnras/stz3321.  
  
C. Ricci, “Growing supermassive black holes in the late stages of galaxy mergers are heavily obscured”, *Monthly Notices of the Royal Astronomical Society*. Oxford University Press (OUP), p. stx173, Jan. 23, 2017. doi: 10.1093/mnras/stx173.  
  
S. Satyapal, “Buried AGNs in Advanced Mergers: Mid-infrared Color Selection as a Dual AGN Candidate Finder”, *The Astrophysical Journal*, vol. 848, no. 2. American Astronomical Society, p. 126, Oct. 23, 2017. doi: 10.3847/1538-4357/aa88ca.  
  
S. Adhikari, S. Shanderaand N. Dalal, “Higher moments of primordial non-Gaussianity and N-body simulations”, *Journal of Cosmology and Astroparticle Physics*, vol. 2014, no. 6. IOP Publishing, pp. 052–052, Jun. 23, 2014. doi: 10.1088/1475-7516/2014/06/052.  
  
C. T. Richardson, “Interpreting the ionization sequence in star-forming galaxy emission-line spectra”, *Monthly Notices of the Royal Astronomical Society*, vol. 458, no. 1. Oxford University Press (OUP), pp. 988–1012, Mar. 11, 2016. doi: 10.1093/mnras/stw100.  
  
C. T. Richardson, J. T. Allen, J. A. Baldwin, P. C. Hewettand G. J. Ferland, “Interpreting the ionization sequence in AGN emission-line spectra”, *Monthly Notices of the Royal Astronomical Society*, vol. 437, no. 3. Oxford University Press (OUP), pp. 2376–2403, Nov. 26, 2013. doi: 10.1093/mnras/stt2056.  
  
M. W. Kunz, J. M. Stoneand X.-N. Bai, “Pegasus: A new hybrid-kinetic particle-in-cell code for astrophysical plasma dynamics”, *Journal of Computational Physics*, vol. 259. Elsevier BV, pp. 154–174, Feb. 2014. doi: 10.1016/j.jcp.2013.11.035.  
  
L. Arzamasskiy, M. W. Kunz, B. D. G. Chandranand E. Quataert, “Hybrid-kinetic Simulations of Ion Heating in Alfvénic Turbulence”, *The Astrophysical Journal*, vol. 879, no. 1. American Astronomical Society, p. 53, Jul. 03, 2019. doi: 10.3847/1538-4357/ab20cc.  
  
B. Burkhart, D. C. Collinsand A. Lazarian, “OBSERVATIONAL DIAGNOSTICS OF SELF-GRAVITATING MHD TURBULENCE IN GIANT MOLECULAR CLOUDS”, *The Astrophysical Journal*, vol. 808, no. 1. American Astronomical Society, p. 48, Jul. 17, 2015. doi: 10.1088/0004-637x/808/1/48.  
  
H. H.-H. Chen, B. Burkhart, A. Goodmanand D. C. Collins, “The Anatomy of the Column Density Probability Distribution Function (N-PDF)”, *The Astrophysical Journal*, vol. 859, no. 2. American Astronomical Society, p. 162, Jun. 04, 2018. doi: 10.3847/1538-4357/aabaf6.  
  
B. Hristov, D. C. Collins, P. Hoeflich, C. A. Weatherfordand T. R. Diamond, “Magnetohydrodynamical Effects on Nuclear Deflagration Fronts in Type Ia Supernovae”, *The Astrophysical Journal*, vol. 858, no. 1. American Astronomical Society, p. 13, Apr. 27, 2018. doi: 10.3847/1538-4357/aab7f2.  
  
W. Schmidt, D. C. Collinsand A. G. Kritsuk, “Local support against gravity in magnetoturbulent fluids”, *Monthly Notices of the Royal Astronomical Society*, vol. 431, no. 4. Oxford University Press (OUP), pp. 3196–3215, Apr. 03, 2013. doi: 10.1093/mnras/stt399.  
  
A. Castrejon, W. Lyra, A. J. W. Richertand M. Kuchner, “Disentangling Planets from Photoelectric Instability in Gas-rich Optically Thin Dusty Disks”, *The Astrophysical Journal*, vol. 887, no. 1. American Astronomical Society, p. 6, Dec. 04, 2019. doi: 10.3847/1538-4357/ab3f3b.  
  
B. Hord, W. Lyra, M. Flock, N. J. Turnerand M.-M. Mac Low, “On Shocks Driven by High-mass Planets in Radiatively Inefficient Disks. III. Observational Signatures in Thermal Emission and Scattered Light”, *The Astrophysical Journal*, vol. 849, no. 2. American Astronomical Society, p. 164, Nov. 10, 2017. doi: 10.3847/1538-4357/aa8fcf.  
  
W. Lyra, C. P. McNally, T. Heinemannand F. Masset, “Orbital Advection with Magnetohydrodynamics and Vector Potential”, *The Astronomical Journal*, vol. 154, no. 4. American Astronomical Society, p. 146, Sep. 15, 2017. doi: 10.3847/1538-3881/aa8811.  
  
W. Lyra, N. Raettigand H. Klahr, “Pebble-trapping Backreaction Does Not Destroy Vortices”, *Research Notes of the AAS*, vol. 2, no. 4. American Astronomical Society, p. 195, Oct. 26, 2018. doi: 10.3847/2515-5172/aaeac9.  
  
W. Lyra, N. J. Turnerand C. P. McNally, “Rossby wave instability does not require sharp resistivity gradients”, *Astronomy & Astrophysics*, vol. 574. EDP Sciences, p. A10, Jan. 16, 2015. doi: 10.1051/0004-6361/201424919.  
  
W. Lyra and O. M. Umurhan, “The Initial Conditions for Planet Formation: Turbulence Driven by Hydrodynamical Instabilities in Disks around Young Stars”, *Publications of the Astronomical Society of the Pacific*, vol. 131, no. 1001. IOP Publishing, p. 072001, Jun. 12, 2019. doi: 10.1088/1538-3873/aaf5ff.  
  
C. J. Manser, “A planetesimal orbiting within the debris disc around a white dwarf star”, *Science*, vol. 364, no. 6435. American Association for the Advancement of Science (AAAS), pp. 66–69, Apr. 05, 2019. doi: 10.1126/science.aat5330.  
  
C. J. Manser, “A planetesimal orbiting within the debris disc around a white dwarf star”, *Science*, vol. 364, no. 6435. American Association for the Advancement of Science (AAAS), pp. 66–69, Apr. 05, 2019. doi: 10.1126/science.aat5330.  
  
B. McKernan, K. E. S. Ford, B. Kocsis, W. Lyraand L. M. Winter, “Intermediate-mass black holes in AGN discs – II. Model predictions and observational constraints”, *Monthly Notices of the Royal Astronomical Society*, vol. 441, no. 1. Oxford University Press (OUP), pp. 900–909, May 02, 2014. doi: 10.1093/mnras/stu553.  
  
C. P. McNally, R. P. Nelson, S.-J. Paardekooper, O. Gresseland W. Lyra, “Low mass planet migration in magnetically torqued dead zones – I. Static migration torque”, *Monthly Notices of the Royal Astronomical Society*, vol. 472, no. 2. Oxford University Press (OUP), pp. 1565–1575, Aug. 18, 2017. doi: 10.1093/mnras/stx2136.  
  
N. Raettig, H. Klahrand W. Lyra, “PARTICLE TRAPPING AND STREAMING INSTABILITY IN VORTICES IN PROTOPLANETARY DISKS”, *The Astrophysical Journal*, vol. 804, no. 1. American Astronomical Society, p. 35, Apr. 28, 2015. doi: 10.1088/0004-637x/804/1/35.  
  
A. J. W. Richert, W. Lyra, A. Boley, M.-M. M. Lowand N. Turner, “ON SHOCKS DRIVEN BY HIGH-MASS PLANETS IN RADIATIVELY INEFFICIENT DISKS. I. TWO-DIMENSIONAL GLOBAL DISK SIMULATIONS”, *The Astrophysical Journal*, vol. 804, no. 2. American Astronomical Society, p. 95, May 06, 2015. doi: 10.1088/0004-637x/804/2/95.  
  
A. J. W. Richert, W. Lyraand M. J. Kuchner, “The Interplay between Radiation Pressure and the Photoelectric Instability in Optically Thin Disks of Gas and Dust”, *The Astrophysical Journal*, vol. 856, no. 1. American Astronomical Society, p. 41, Mar. 22, 2018. doi: 10.3847/1538-4357/aaadaa.  
  
A. Secunda, “Orbital Migration of Interacting Stellar Mass Black Holes in Disks around Supermassive Black Holes”, *The Astrophysical Journal*, vol. 878, no. 2. American Astronomical Society, p. 85, Jun. 18, 2019. doi: 10.3847/1538-4357/ab20ca.  
  
D. Anglés-Alcázar, C.-A. Faucher-Giguère, D. Kereš, P. F. Hopkins, E. Quataertand N. Murray, “The cosmic baryon cycle and galaxy mass assembly in the FIRE simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 470, no. 4. Oxford University Press (OUP), pp. 4698–4719, Jun. 20, 2017. doi: 10.1093/mnras/stx1517.  
  
D. Anglés-Alcázar, “Black holes on FIRE: stellar feedback limits early feeding of galactic nuclei”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 472, no. 1. Oxford University Press (OUP), pp. L109–L114, Oct. 05, 2017. doi: 10.1093/mnrasl/slx161.  
  
B. Bozek, “Warm FIRE: simulating galaxy formation with resonant sterile neutrino dark matter”, *Monthly Notices of the Royal Astronomical Society*, vol. 483, no. 3. Oxford University Press (OUP), pp. 4086–4099, Dec. 12, 2018. doi: 10.1093/mnras/sty3300.  
  
V. P. Debattista, “Formation, vertex deviation, and age of the Milky Way’s bulge: input from a cosmological simulation with a late-forming bar”, *Monthly Notices of the Royal Astronomical Society*, vol. 485, no. 4. Oxford University Press (OUP), pp. 5073–5085, Mar. 15, 2019. doi: 10.1093/mnras/stz746.  
  
K. El-Badry, “Gas kinematics in FIRE simulated galaxies compared to spatially unresolved H i observations”, *Monthly Notices of the Royal Astronomical Society*, vol. 477, no. 2. Oxford University Press (OUP), pp. 1536–1548, Mar. 24, 2018. doi: 10.1093/mnras/sty730.  
  
K. El-Badry, “Gas kinematics, morphology and angular momentum in the FIRE simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 473, no. 2. Oxford University Press (OUP), pp. 1930–1955, Sep. 26, 2017. doi: 10.1093/mnras/stx2482.  
  
I. Escala, “Modelling chemical abundance distributions for dwarf galaxies in the Local Group: the impact of turbulent metal diffusion”, *Monthly Notices of the Royal Astronomical Society*, vol. 474, no. 2. Oxford University Press (OUP), pp. 2194–2211, Nov. 06, 2017. doi: 10.1093/mnras/stx2858.  
  
C.-A. Faucher-Giguère, “Recent progress in simulating galaxy formation from the largest to the smallest scales”, *Nature Astronomy*, vol. 2, no. 5. Springer Science and Business Media LLC, pp. 368–373, Apr. 09, 2018. doi: 10.1038/s41550-018-0427-y.  
  
C.-A. Faucher-Giguère, “A model for the origin of bursty star formation in galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 473, no. 3. Oxford University Press (OUP), pp. 3717–3731, Oct. 09, 2017. doi: 10.1093/mnras/stx2595.  
  
C.-A. Faucher-Giguère, “A cosmic UV/X-ray background model update”, *Monthly Notices of the Royal Astronomical Society*, vol. 493, no. 2. Oxford University Press (OUP), pp. 1614–1632, Jan. 31, 2020. doi: 10.1093/mnras/staa302.  
  
C.-A. Faucher-Giguère, R. Feldmann, E. Quataert, D. Kereš, P. F. Hopkinsand N. Murray, “A stellar feedback origin for neutral hydrogen in high-redshift quasar-mass haloes”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 461, no. 1. Oxford University Press (OUP), pp. L32–L36, May 11, 2016. doi: 10.1093/mnrasl/slw091.  
  
C.-A. Faucher-Giguère, P. F. Hopkins, D. Kereš, A. L. Muratov, E. Quataertand N. Murray, “Neutral hydrogen in galaxy haloes at the peak of the cosmic star formation history”, *Monthly Notices of the Royal Astronomical Society*, vol. 449, no. 1. Oxford University Press (OUP), pp. 987–1003, Mar. 19, 2015. doi: 10.1093/mnras/stv336.  
  
R. Feldmann, E. Quataert, P. F. Hopkins, C.-A. Faucher-Giguèreand D. Kereš, “Colours, star formation rates and environments of star-forming and quiescent galaxies at the cosmic noon”, *Monthly Notices of the Royal Astronomical Society*, vol. 470, no. 1. Oxford University Press (OUP), pp. 1050–1072, May 10, 2017. doi: 10.1093/mnras/stx1120.  
  
D. Fielding, E. Quataert, D. Martizziand C.-A. Faucher-Giguère, “How supernovae launch galactic winds?”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 470, no. 1. Oxford University Press (OUP), pp. L39–L43, May 10, 2017. doi: 10.1093/mnrasl/slx072.  
  
A. Fitts, “Dwarf galaxies in CDM, WDM, and SIDM: disentangling baryons and dark matter physics”, *Monthly Notices of the Royal Astronomical Society*, vol. 490, no. 1. Oxford University Press (OUP), pp. 962–977, Sep. 19, 2019. doi: 10.1093/mnras/stz2613.  
  
S. Garrison-Kimmel, “The Local Group on FIRE: dwarf galaxy populations across a suite of hydrodynamic simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 487, no. 1. Oxford University Press (OUP), pp. 1380–1399, May 16, 2019. doi: 10.1093/mnras/stz1317.  
  
S. Garrison-Kimmel, “Star formation histories of dwarf galaxies in the FIRE simulations: dependence on mass and Local Group environment”, *Monthly Notices of the Royal Astronomical Society*, vol. 489, no. 4. Oxford University Press (OUP), pp. 4574–4588, Sep. 10, 2019. doi: 10.1093/mnras/stz2507.  
  
A. González-Samaniego, “Dwarf galaxy mass estimators versus cosmological simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 472, no. 4. Oxford University Press (OUP), pp. 4786–4796, Sep. 07, 2017. doi: 10.1093/mnras/stx2322.  
  
A. S. Graus, “A predicted correlation between age gradient and star formation history in FIRE dwarf galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 490, no. 1. Oxford University Press (OUP), pp. 1186–1201, Sep. 21, 2019. doi: 10.1093/mnras/stz2649.  
  
M. Y. Grudić, P. F. Hopkins, C.-A. Faucher-Giguère, E. Quataert, N. Murrayand D. Kereš, “When feedback fails: the scaling and saturation of star formation efficiency”, *Monthly Notices of the Royal Astronomical Society*, vol. 475, no. 3. Oxford University Press (OUP), pp. 3511–3528, Jan. 08, 2018. doi: 10.1093/mnras/sty035.  
  
M. Y. Grudić, P. F. Hopkins, E. J. Lee, N. Murray, C.-A. Faucher-Giguèreand L. C. Johnson, “On the nature of variations in the measured star formation efficiency of molecular clouds”, *Monthly Notices of the Royal Astronomical Society*, vol. 488, no. 2. Oxford University Press (OUP), pp. 1501–1518, Jun. 26, 2019. doi: 10.1093/mnras/stz1758.  
  
D. Guszejnov, “Evolution of giant molecular clouds across cosmic time”, *Monthly Notices of the Royal Astronomical Society*, vol. 492, no. 1. Oxford University Press (OUP), pp. 488–502, Dec. 17, 2019. doi: 10.1093/mnras/stz3527.  
  
Z. Hafen, “Low-redshift Lyman limit systems as diagnostics of cosmological inflows and outflows”, *Monthly Notices of the Royal Astronomical Society*, vol. 469, no. 2. Oxford University Press (OUP), pp. 2292–2304, Apr. 21, 2017. doi: 10.1093/mnras/stx952.  
  
M. H. Hani, “Variations in the slope of the resolved star-forming main sequence: a tool for constraining the mass of star-forming regions”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 493, no. 1. Oxford University Press (OUP), pp. L87–L91, Jan. 23, 2020. doi: 10.1093/mnrasl/slaa013.  
  
P. F. Hopkins, “Radiative stellar feedback in galaxy formation: Methods and physics”, *Monthly Notices of the Royal Astronomical Society*, vol. 491, no. 3. Oxford University Press (OUP), pp. 3702–3729, Nov. 12, 2019. doi: 10.1093/mnras/stz3129.  
  
P. F. Hopkins, “Galaxies on FIRE (Feedback In Realistic Environments): stellar feedback explains cosmologically inefficient star formation”, *Monthly Notices of the Royal Astronomical Society*, vol. 445, no. 1. Oxford University Press (OUP), pp. 581–603, Sep. 29, 2014. doi: 10.1093/mnras/stu1738.  
  
P. F. Hopkins, “How to model supernovae in simulations of star and galaxy formation”, *Monthly Notices of the Royal Astronomical Society*, vol. 477, no. 2. Oxford University Press (OUP), pp. 1578–1603, Mar. 14, 2018. doi: 10.1093/mnras/sty674.  
  
J. C. Howk, “Project AMIGA: A Minimal Covering Factor for Optically Thick Circumgalactic Gas around the Andromeda Galaxy”, *The Astrophysical Journal*, vol. 846, no. 2. American Astronomical Society, p. 141, Sep. 12, 2017. doi: 10.3847/1538-4357/aa87b4.  
  
J.-. hoon . Kim, “Formation of globular cluster candidates in merging proto-galaxies at high redshift: a view from the FIRE cosmological simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 474, no. 3. Oxford University Press (OUP), pp. 4232–4244, Nov. 23, 2017. doi: 10.1093/mnras/stx2994.  
  
L. Liang, “Submillimetre flux as a probe of molecular ISM mass in high-z galaxies”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 478, no. 1. Oxford University Press (OUP), pp. L83–L88, Apr. 27, 2018. doi: 10.1093/mnrasl/sly071.  
  
X. Ma, “Self-consistent proto-globular cluster formation in cosmological simulations of high-redshift galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 493, no. 3. Oxford University Press (OUP), pp. 4315–4332, Feb. 21, 2020. doi: 10.1093/mnras/staa527.  
  
X. Ma, “Simulating galaxies in the reionization era with FIRE-2: morphologies and sizes”, *Monthly Notices of the Royal Astronomical Society*, vol. 477, no. 1. Oxford University Press (OUP), pp. 219–229, Mar. 15, 2018. doi: 10.1093/mnras/sty684.  
  
X. Ma, “Binary stars can provide the ‘missing photons’ needed for reionization”, *Monthly Notices of the Royal Astronomical Society*, vol. 459, no. 4. Oxford University Press (OUP), pp. 3614–3619, Apr. 21, 2016. doi: 10.1093/mnras/stw941.  
  
A. L. Muratov, “Metal flows of the circumgalactic medium, and the metal budget in galactic haloes”, *Monthly Notices of the Royal Astronomical Society*, vol. 468, no. 4. Oxford University Press (OUP), pp. 4170–4188, Mar. 17, 2017. doi: 10.1093/mnras/stx667.  
  
M. E. Orr, “Stacked Star Formation Rate Profiles of Bursty Galaxies Exhibit “Coherent” Star Formation”, *The Astrophysical Journal*, vol. 849, no. 1. American Astronomical Society, p. L2, Oct. 20, 2017. doi: 10.3847/2041-8213/aa8f93.  
  
S. H. Price, “Testing the Recovery of Intrinsic Galaxy Sizes and Masses of *z* ∼ 2 Massive Galaxies Using Cosmological Simulations”, *The Astrophysical Journal*, vol. 844, no. 1. American Astronomical Society, p. L6, Jul. 17, 2017. doi: 10.3847/2041-8213/aa7d4b.  
  
A. Richings and C.-A. Faucher-Giguere, “Molecular Emission Lines From Simulations Of Agn-Driven Molecular Outflows”, *Zenodo*, Mar. 2018, doi: 10.5281/ZENODO.1209445.  
  
A. J. Richings and C.-A. Faucher-Giguère, “Radiative cooling of swept-up gas in AGN-driven galactic winds and its implications for molecular outflows”, *Monthly Notices of the Royal Astronomical Society*, vol. 478, no. 3. Oxford University Press (OUP), pp. 3100–3119, May 16, 2018. doi: 10.1093/mnras/sty1285.  
  
V. H. Robles, “SIDM on fire: hydrodynamical self-interacting dark matter simulations of low-mass dwarf galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 472, no. 3. Oxford University Press (OUP), pp. 2945–2954, Sep. 05, 2017. doi: 10.1093/mnras/stx2253.  
  
J. Samuel, “A profile in FIRE: resolving the radial distributions of satellite galaxies in the Local Group with simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 491, no. 1. Oxford University Press (OUP), pp. 1471–1490, Oct. 31, 2019. doi: 10.1093/mnras/stz3054.  
  
R. E. Sanderson, “Synthetic *Gaia* Surveys from the FIRE Cosmological Simulations of Milky Way-mass Galaxies”, *The Astrophysical Journal Supplement Series*, vol. 246, no. 1. American Astronomical Society, p. 6, Jan. 06, 2020. doi: 10.3847/1538-4365/ab5b9d.  
  
A. Smith, “The physics of Lyman α escape from high-redshift galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 484, no. 1. Oxford University Press (OUP), pp. 39–59, Dec. 22, 2018. doi: 10.1093/mnras/sty3483.  
  
N. Sravan, “Strongly time-variable ultraviolet metal-line emission from the circum-galactic medium of high-redshift galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 463, no. 1. Oxford University Press (OUP), pp. 120–133, Aug. 08, 2016. doi: 10.1093/mnras/stw1962.  
  
J. Stern, C.-A. Faucher-Giguère, J. F. Hennawi, Z. Hafen, S. D. Johnsonand D. Fielding, “Does Circumgalactic O vi Trace Low-pressure Gas Beyond the Accretion Shock? Clues from H i and Low-ion Absorption, Line Kinematics, and Dust Extinction”, *The Astrophysical Journal*, vol. 865, no. 2. American Astronomical Society, p. 91, Sep. 25, 2018. doi: 10.3847/1538-4357/aac884.  
  
J. Stern, D. Fielding, C.-A. Faucher-Giguèreand E. Quataert, “Cooling flow solutions for the circumgalactic medium”, *Monthly Notices of the Royal Astronomical Society*, vol. 488, no. 2. Oxford University Press (OUP), pp. 2549–2572, Jul. 11, 2019. doi: 10.1093/mnras/stz1859.  
  
J. Stern, D. Fielding, C.-A. Faucher-Giguèreand E. Quataert, “The maximum accretion rate of hot gas in dark matter haloes”, *Monthly Notices of the Royal Astronomical Society*, vol. 492, no. 4. Oxford University Press (OUP), pp. 6042–6058, Jan. 28, 2020. doi: 10.1093/mnras/staa198.  
  
K. R. Stewart, “High Angular Momentum Halo Gas: A Feedback and Code-independent Prediction of LCDM”, *The Astrophysical Journal*, vol. 843, no. 1. American Astronomical Society, p. 47, Jun. 30, 2017. doi: 10.3847/1538-4357/aa6dff.  
  
K.-Y. Su, C. C. Hayward, P. F. Hopkins, E. Quataert, C.-A. Faucher-Giguèreand D. Kereš, “Stellar feedback strongly alters the amplification and morphology of galactic magnetic fields”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 473, no. 1. Oxford University Press (OUP), pp. L111–L115, Oct. 17, 2017. doi: 10.1093/mnrasl/slx172.  
  
K.-Y. Su, “Feedback first: the surprisingly weak effects of magnetic fields, viscosity, conduction and metal diffusion on sub-L\* galaxy formation”, *Monthly Notices of the Royal Astronomical Society*, vol. 471, no. 1. Oxford University Press (OUP), pp. 144–166, Jun. 13, 2017. doi: 10.1093/mnras/stx1463.  
  
K.-Y. Su, “Cosmic rays or turbulence can suppress cooling flows (where thermal heating or momentum injection fail)”, *Monthly Notices of the Royal Astronomical Society*, vol. 491, no. 1. Oxford University Press (OUP), pp. 1190–1212, Nov. 05, 2019. doi: 10.1093/mnras/stz3011.  
  
K.-Y. Su, “Discrete Effects in Stellar Feedback: Individual Supernovae, Hypernovae, and IMF Sampling in Dwarf Galaxies”, *Monthly Notices of the Royal Astronomical Society*. Oxford University Press (OUP), Jul. 23, 2018. doi: 10.1093/mnras/sty1928.  
  
K.-Y. Su, “The failure of stellar feedback, magnetic fields, conduction, and morphological quenching in maintaining red galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 487, no. 3. Oxford University Press (OUP), pp. 4393–4408, Jun. 03, 2019. doi: 10.1093/mnras/stz1494.  
  
F. van de Voort, “On the deuterium abundance and the importance of stellar mass loss in the interstellar and intergalactic medium”, *Monthly Notices of the Royal Astronomical Society*, vol. 477, no. 1. Oxford University Press (OUP), pp. 80–92, Mar. 06, 2018. doi: 10.1093/mnras/sty591.  
  
F. van de Voort, E. Quataert, P. F. Hopkins, D. Kerešand C.-A. Faucher-Giguère, “Galactic r-process enrichment by neutron star mergers in cosmological simulations of a Milky Way-mass galaxy”, *Monthly Notices of the Royal Astronomical Society*, vol. 447, no. 1. Oxford University Press (OUP), pp. 140–148, Dec. 12, 2014. doi: 10.1093/mnras/stu2404.  
  
A. R. Wetzel, P. F. Hopkins, J.-. hoon . Kim, C.-A. Faucher-Giguère, D. Kerešand E. Quataert, “RECONCILING DWARF GALAXIES WITH ΛCDM COSMOLOGY: SIMULATING A REALISTIC POPULATION OF SATELLITES AROUND A MILKY WAY–MASS GALAXY”, *The Astrophysical Journal*, vol. 827, no. 2. American Astronomical Society, p. L23, Aug. 11, 2016. doi: 10.3847/2041-8205/827/2/l23.  
  
C. Wheeler, “Be it therefore resolved: cosmological simulations of dwarf galaxies with 30 solar mass resolution”, *Monthly Notices of the Royal Astronomical Society*, vol. 490, no. 3. Oxford University Press (OUP), pp. 4447–4463, Oct. 16, 2019. doi: 10.1093/mnras/stz2887.  
  
S. Yu, “Stars made in outflows may populate the stellar halo of the Milky Way”, *Monthly Notices of the Royal Astronomical Society*, vol. 494, no. 2. Oxford University Press (OUP), pp. 1539–1559, Mar. 03, 2020. doi: 10.1093/mnras/staa522.  
  
Y.-F. Jiang, J. M. Stoneand S. W. Davis, “A GLOBAL THREE-DIMENSIONAL RADIATION MAGNETO-HYDRODYNAMIC SIMULATION OF SUPER-EDDINGTON ACCRETION DISKS”, *The Astrophysical Journal*, vol. 796, no. 2. American Astronomical Society, p. 106, Nov. 12, 2014. doi: 10.1088/0004-637x/796/2/106.  
  
Y.-F. Jiang, J. M. Stoneand S. W. Davis, “AN ALGORITHM FOR RADIATION MAGNETOHYDRODYNAMICS BASED ON SOLVING THE TIME-DEPENDENT TRANSFER EQUATION”, *The Astrophysical Journal Supplement Series*, vol. 213, no. 1. American Astronomical Society, p. 7, Jun. 18, 2014. doi: 10.1088/0067-0049/213/1/7.  
  
K. J. Walsh and H. F. Levison, “TERRESTRIAL PLANET FORMATION FROM AN ANNULUS”, *The Astronomical Journal*, vol. 152, no. 3. American Astronomical Society, p. 68, Aug. 31, 2016. doi: 10.3847/0004-6256/152/3/68.  
  
S. Dong, B. Katz, D. Kushnirand J. L. Prieto, “Type Ia supernovae with bimodal explosions are common – possible smoking gun for direct collisions of white dwarfs”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 454, no. 1. Oxford University Press (OUP), pp. L61–L65, Oct. 01, 2015. doi: 10.1093/mnrasl/slv129.  
  
M. Blank, M. R. Morris, A. Frank, J. J. Carroll-Nellenbackand W. J. Duschl, “The inner cavity of the circumnuclear disc”, *Monthly Notices of the Royal Astronomical Society*, vol. 459, no. 2. Oxford University Press (OUP), pp. 1721–1736, Apr. 05, 2016. doi: 10.1093/mnras/stw771.  
  
A. Crider, C. Richardsonand B. Kaiser, “Detecting H II Regions in “Pure” Starburst Galaxies with SDSS Data”, *Proceedings of the International Astronomical Union*, vol. 11, no. S315. Cambridge University Press (CUP), Aug. 2015. doi: 10.1017/s1743921316007766.  
  
M. W. Abruzzo and Z. Haiman, “The impact of photometric redshift errors on lensing statistics in ray-tracing simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 486, no. 2. Oxford University Press (OUP), pp. 2730–2753, Apr. 18, 2019. doi: 10.1093/mnras/stz1016.  
  
W. R. Coulton, J. Liu, M. S. Madhavacheril, V. Böhmand D. N. Spergel, “Constraining neutrino mass with the tomographic weak lensing bispectrum”, *Journal of Cosmology and Astroparticle Physics*, vol. 2019, no. 5. IOP Publishing, pp. 043–043, May 24, 2019. doi: 10.1088/1475-7516/2019/05/043.  
  
A. Gupta, J. M. Z. Matilla, D. Hsuand Z. Haiman, “Non-Gaussian information from weak lensing data via deep learning”, *Physical Review D*, vol. 97, no. 10. American Physical Society (APS), May 18, 2018. doi: 10.1103/physrevd.97.103515.  
  
C. D. Kreisch, “Massive neutrinos leave fingerprints on cosmic voids”, *Monthly Notices of the Royal Astronomical Society*, vol. 488, no. 3. Oxford University Press (OUP), pp. 4413–4426, Jul. 17, 2019. doi: 10.1093/mnras/stz1944.  
  
J. Liu, “MassiveNuS: cosmological massive neutrino simulations”, *Journal of Cosmology and Astroparticle Physics*, vol. 2018, no. 3. IOP Publishing, pp. 049–049, Mar. 29, 2018. doi: 10.1088/1475-7516/2018/03/049.  
  
J. Liu and M. S. Madhavacheril, “Constraining neutrino mass with the tomographic weak lensing one-point probability distribution function and power spectrum”, *Physical Review D*, vol. 99, no. 8. American Physical Society (APS), Apr. 09, 2019. doi: 10.1103/physrevd.99.083508.  
  
T. Lu and Z. Haiman, “The matter fluctuation amplitude inferred from the weak lensing power spectrum and correlation function in CFHTLenS data”, *Monthly Notices of the Royal Astronomical Society*, vol. 490, no. 4. Oxford University Press (OUP), pp. 5033–5042, Oct. 18, 2019. doi: 10.1093/mnras/stz2931.  
  
G. A. Marques, J. Liu, J. M. Z. Matilla, Z. Haiman, A. Bernuiand C. P. Novaes, “Constraining neutrino mass with weak lensing Minkowski Functionals”, *Journal of Cosmology and Astroparticle Physics*, vol. 2019, no. 6. IOP Publishing, pp. 019–019, Jun. 07, 2019. doi: 10.1088/1475-7516/2019/06/019.  
  
A. Petri, “Mocking the weak lensing universe: The LensTools Python computing package”, *Astronomy and Computing*, vol. 17. Elsevier BV, pp. 73–79, Oct. 2016. doi: 10.1016/j.ascom.2016.06.001.  
  
A. Petri, Z. Haimanand M. May, “Sample variance in weak lensing: How many simulations are required?”, *Physical Review D*, vol. 93, no. 6. American Physical Society (APS), Mar. 24, 2016. doi: 10.1103/physrevd.93.063524.  
  
A. Petri, Z. Haimanand M. May, “Validity of the Born approximation for beyond Gaussian weak lensing observables”, *Physical Review D*, vol. 95, no. 12. American Physical Society (APS), Jun. 06, 2017. doi: 10.1103/physrevd.95.123503.  
  
A. Petri, M. Mayand Z. Haiman, “Cosmology with photometric weak lensing surveys: Constraints with redshift tomography of convergence peaks and moments”, *Physical Review D*, vol. 94, no. 6. American Physical Society (APS), Sep. 30, 2016. doi: 10.1103/physrevd.94.063534.  
  
D. Ribli, B. Á. Pataki, J. M. Zorrilla Matilla, D. Hsu, Z. Haimanand I. Csabai, “Weak lensing cosmology with convolutional neural networks on noisy data”, *Monthly Notices of the Royal Astronomical Society*, vol. 490, no. 2. Oxford University Press (OUP), pp. 1843–1860, Sep. 17, 2019. doi: 10.1093/mnras/stz2610.  
  
V. Böhm, B. D. Sherwin, J. Liu, J. C. Hill, M. Schmittfulland T. Namikawa, “Effect of non-Gaussian lensing deflections on CMB lensing measurements”, *Physical Review D*, vol. 98, no. 12. American Physical Society (APS), Dec. 13, 2018. doi: 10.1103/physrevd.98.123510.  
  
Z. Li, J. Liu, J. M. Z. Matillaand W. R. Coulton, “Constraining neutrino mass with tomographic weak lensing peak counts”, *Physical Review D*, vol. 99, no. 6. American Physical Society (APS), Mar. 25, 2019. doi: 10.1103/physrevd.99.063527.  
  
Y.-H. Chen, S. Heinzand T. A. Enßlin, “Jets, bubbles, and heat pumps in galaxy clusters”, *Monthly Notices of the Royal Astronomical Society*, vol. 489, no. 2. Oxford University Press (OUP), pp. 1939–1949, Aug. 14, 2019. doi: 10.1093/mnras/stz2256.  
  
M. Lang, K. Holley-Bockelmannand M. Sinha, “BAR FORMATION FROM GALAXY FLYBYS”, *The Astrophysical Journal*, vol. 790, no. 2. American Astronomical Society, p. L33, Jul. 21, 2014. doi: 10.1088/2041-8205/790/2/l33.  
  
M. B. Eide, M. Gronke, M. Dijkstraand M. Hayes, “Unlocking the Full Potential of Extragalactic Ly*α* through Its Polarization Properties”, *The Astrophysical Journal*, vol. 856, no. 2. American Astronomical Society, p. 156, Apr. 04, 2018. doi: 10.3847/1538-4357/aab5b7.  
  
M. Gronke, M. Dijkstra, M. McCourtand S. P. Oh, “FROM MIRRORS TO WINDOWS: LYMAN-ALPHA RADIATIVE TRANSFER IN A VERY CLUMPY MEDIUM”, *The Astrophysical Journal*, vol. 833, no. 2. American Astronomical Society, p. L26, Dec. 19, 2016. doi: 10.3847/2041-8213/833/2/l26.  
  
M. Gronke, M. Dijkstra, M. McCourtand S. Peng Oh, “Resonant line transfer in a fog: using Lyman-alpha to probe tiny structures in atomic gas”, *Astronomy & Astrophysics*, vol. 607. EDP Sciences, p. A71, Nov. 2017. doi: 10.1051/0004-6361/201731013.  
  
M. McCourt, R. M. O’Leary, A.-M. Madiganand E. Quataert, “Magnetized gas clouds can survive acceleration by a hot wind”, *Monthly Notices of the Royal Astronomical Society*, vol. 449, no. 1. Oxford University Press (OUP), pp. 2–7, Mar. 14, 2015. doi: 10.1093/mnras/stv355.  
  
S. Ji (季索清), S. P. Oh, M. Ruszkowskiand M. Markevitch, “The efficiency of magnetic field amplification at shocks by turbulence”, *Monthly Notices of the Royal Astronomical Society*, vol. 463, no. 4. Oxford University Press (OUP), pp. 3989–4003, Sep. 14, 2016. doi: 10.1093/mnras/stw2320.  
  
A. Bonaca, C. Conroy, A. Wetzel, P. F. Hopkinsand D. Kereš, “*Gaia*Reveals a Metal-rich, in situ Component of the Local Stellar Halo”, *The Astrophysical Journal*, vol. 845, no. 2. American Astronomical Society, p. 101, Aug. 16, 2017. doi: 10.3847/1538-4357/aa7d0c.  
  
K. El-Badry, “Where are the most ancient stars in the Milky Way?”, *Monthly Notices of the Royal Astronomical Society*, vol. 480, no. 1. Oxford University Press (OUP), pp. 652–668, Jul. 14, 2018. doi: 10.1093/mnras/sty1864.  
  
K. El-Badry, “When the Jeans do not Fit: How Stellar Feedback Drives Stellar Kinematics and Complicates Dynamical Modeling in Low-mass Galaxies”, *The Astrophysical Journal*, vol. 835, no. 2. American Astronomical Society, p. 193, Jan. 31, 2017. doi: 10.3847/1538-4357/835/2/193.  
  
Y. Feng, T. Di-Matteo, R. A. Croft, S. Bird, N. Battagliaand S. Wilkins, “The BlueTides simulation: first galaxies and reionization”, *Monthly Notices of the Royal Astronomical Society*, vol. 455, no. 3. Oxford University Press (OUP), pp. 2778–2791, Nov. 25, 2015. doi: 10.1093/mnras/stv2484.  
  
Y. Feng, “THE FORMATION OF MILKY WAY–MASS DISK GALAXIES IN THE FIRST 500 MILLION YEARS OF A COLD DARK MATTER UNIVERSE”, *The Astrophysical Journal*, vol. 808, no. 1. American Astronomical Society, p. L17, Jul. 20, 2015. doi: 10.1088/2041-8205/808/1/l17.  
  
A. Fitts, “fire in the field: simulating the threshold of galaxy formation”, *Monthly Notices of the Royal Astronomical Society*, vol. 471, no. 3. Oxford University Press (OUP), pp. 3547–3562, Jul. 14, 2017. doi: 10.1093/mnras/stx1757.  
  
S. Garrison-Kimmel, “Not so lumpy after all: modelling the depletion of dark matter subhaloes by Milky Way-like galaxies ”, *Monthly Notices of the Royal Astronomical Society*, vol. 471, no. 2. Oxford University Press (OUP), pp. 1709–1727, Jul. 08, 2017. doi: 10.1093/mnras/stx1710.  
  
P. F. Hopkins, “FIRE-2 simulations: physics versus numerics in galaxy formation”, *Monthly Notices of the Royal Astronomical Society*, vol. 480, no. 1. Oxford University Press (OUP), pp. 800–863, Jun. 28, 2018. doi: 10.1093/mnras/sty1690.  
  
C.-L. Hung, “What drives the evolution of gas kinematics in star-forming galaxies?”, *Monthly Notices of the Royal Astronomical Society*, vol. 482, no. 4. Oxford University Press (OUP), pp. 5125–5137, Nov. 03, 2018. doi: 10.1093/mnras/sty2970.  
  
A. Lamberts, “Predicting the binary black hole population of the Milky Way with cosmological simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 480, no. 2. Oxford University Press (OUP), pp. 2704–2718, Jul. 27, 2018. doi: 10.1093/mnras/sty2035.  
  
X. Ma, “The structure and dynamical evolution of the stellar disc of a simulated Milky Way-mass galaxy”, *Monthly Notices of the Royal Astronomical Society*, vol. 467, no. 2. Oxford University Press (OUP), pp. 2430–2444, Feb. 01, 2017. doi: 10.1093/mnras/stx273.  
  
E. O. Nadler, Y.-Y. Mao, R. H. Wechsler, S. Garrison-Kimmeland A. Wetzel, “Modeling the Impact of Baryons on Subhalo Populations with Machine Learning”, *The Astrophysical Journal*, vol. 859, no. 2. American Astronomical Society, p. 129, Jun. 01, 2018. doi: 10.3847/1538-4357/aac266.  
  
R. E. Sanderson, “Reconciling Observed and Simulated Stellar Halo Masses”, *The Astrophysical Journal*, vol. 869, no. 1. American Astronomical Society, p. 12, Dec. 06, 2018. doi: 10.3847/1538-4357/aaeb33.  
  
R. Sanderson, A. Wetzel, S. Sharmaand P. Hopkins, “Better Galactic Mass Models through Chemistry”, *Galaxies*, vol. 5, no. 3. MDPI AG, p. 43, Aug. 21, 2017. doi: 10.3390/galaxies5030043.  
  
J. Li, A. Spitkovskyand A. Tchekhovskoy, “RESISTIVE SOLUTIONS FOR PULSAR MAGNETOSPHERES”, *The Astrophysical Journal*, vol. 746, no. 1. American Astronomical Society, p. 60, Jan. 25, 2012. doi: 10.1088/0004-637x/746/1/60.  
  
R. Narayan, J. E. McClintockand A. Tchekhovskoy, “Energy Extraction from Spinning Black Holes Via Relativistic Jets”, *General Relativity, Cosmology and Astrophysics*. Springer International Publishing, pp. 523–535, 2014. doi: 10.1007/978-3-319-06349-2\_25.  
  
A. Sądowski, L. Sironi, D. Abarca, X. Guo, F. Özeland R. Narayan, “Radio light curves during the passage of cloud G2 near Sgr A*”, Monthly Notices of the Royal Astronomical Society, vol. 432, no. 1. Oxford University Press (OUP), pp. 478–491, Apr. 12, 2013. doi: 10.1093/mnras/stt495.*  
  
*M. Boylan-Kolchin, J. S. Bullockand S. Garrison-Kimmel, “Near-field limits on the role of faint galaxies in cosmic reionization”, Monthly Notices of the Royal Astronomical Society: Letters, vol. 443, no. 1. Oxford University Press (OUP), pp. L44–L48, Jun. 26, 2014. doi: 10.1093/mnrasl/slu079.*  
  
*M. Boylan-Kolchin, D. R. Weisz, B. D. Johnson, J. S. Bullock, C. Conroyand A. Fitts, “The Local Group as a time machine: studying the high-redshift Universe with nearby galaxies”, Monthly Notices of the Royal Astronomical Society, vol. 453, no. 2. Oxford University Press (OUP), pp. 1503–1512, Aug. 25, 2015. doi: 10.1093/mnras/stv1736.*  
  
*A. Deason, A. Wetzeland S. Garrison-Kimmel, “SATELLITE DWARF GALAXIES IN A HIERARCHICAL UNIVERSE: THE PREVALENCE OF DWARF-DWARF MAJOR MERGERS”, The Astrophysical Journal, vol. 794, no. 2. American Astronomical Society, p. 115, Sep. 30, 2014. doi: 10.1088/0004-637x/794/2/115.*  
  
*A. J. Deason, A. R. Wetzel, S. Garrison-Kimmeland V. Belokurov, “Satellites of LMC-mass dwarfs: close friendships ruined by Milky Way mass haloes”, Monthly Notices of the Royal Astronomical Society, vol. 453, no. 4. Oxford University Press (OUP), pp. 3569–3575, Sep. 09, 2015. doi: 10.1093/mnras/stv1939.*  
  
*S. P. Fillingham, M. C. Cooper, C. Wheeler, S. Garrison-Kimmel, M. Boylan-Kolchinand J. S. Bullock, “Taking care of business in a flash : constraining the time-scale for low-mass satellite quenching with ELVIS”, Monthly Notices of the Royal Astronomical Society, vol. 454, no. 2. Oxford University Press (OUP), pp. 2039–2049, Oct. 13, 2015. doi: 10.1093/mnras/stv2058.*  
  
*A. Fitts, “No assembly required: mergers are mostly irrelevant for the growth of low-mass dwarf galaxies”, Monthly Notices of the Royal Astronomical Society, vol. 479, no. 1. Oxford University Press (OUP), pp. 319–331, Jun. 06, 2018. doi: 10.1093/mnras/sty1488.*  
  
*S. Garrison-Kimmel, “The origin of the diverse morphologies and kinematics of Milky Way-mass galaxies in the FIRE-2 simulations”, Monthly Notices of the Royal Astronomical Society, vol. 481, no. 3. Oxford University Press (OUP), pp. 4133–4157, Sep. 14, 2018. doi: 10.1093/mnras/sty2513.*  
  
*S. Horiuchi, P. J. Humphrey, J. Oñorbe, K. N. Abazajian, M. Kaplinghatand S. Garrison-Kimmel, “Sterile neutrino dark matter bounds from galaxies of the Local Group”, Physical Review D, vol. 89, no. 2. American Physical Society (APS), Jan. 28, 2014. doi: 10.1103/physrevd.89.025017.*  
  
*P. Mocz, “Galaxy formation with BECDM – I. Turbulence and relaxation of idealized haloes”, Monthly Notices of the Royal Astronomical Society, vol. 471, no. 4. Oxford University Press (OUP), pp. 4559–4570, Jul. 25, 2017. doi: 10.1093/mnras/stx1887.*  
  
*A. R. Wetzel, A. J. Deasonand S. Garrison-Kimmel, “SATELLITE DWARF GALAXIES IN A HIERARCHICAL UNIVERSE: INFALL HISTORIES, GROUP PREPROCESSING, AND REIONIZATION”, The Astrophysical Journal, vol. 807, no. 1. American Astronomical Society, p. 49, Jun. 30, 2015. doi: 10.1088/0004-637x/807/1/49.*  
  
*B. Yniguez, S. Garrison-Kimmel, M. Boylan-Kolchinand J. S. Bullock, “On the stark difference in satellite distributions around the Milky Way and Andromeda”, Monthly Notices of the Royal Astronomical Society, vol. 439, no. 1. Oxford University Press (OUP), pp. 73–82, Feb. 04, 2014. doi: 10.1093/mnras/stt2058.*  
  
*S. Ji (季索清), S. P. Ohand P. Masterson, “Simulations of radiative turbulent mixing layers”, Monthly Notices of the Royal Astronomical Society, vol. 487, no. 1. Oxford University Press (OUP), pp. 737–754, May 09, 2019. doi: 10.1093/mnras/stz1248.*  
  
*S. A. Mortazavi, J. M. Lotz, J. E. Barnesand G. F. Snyder, “Modeling the initial conditions of interacting galaxy pairs using Identikit”, Monthly Notices of the Royal Astronomical Society, vol. 455, no. 3. Oxford University Press (OUP), pp. 3058–3074, Nov. 26, 2015. doi: 10.1093/mnras/stv2364.*  
  
*A. Kashi, K. Davidsonand R. M. Humphreys, “Recovery From Giant Eruptions in Massive Stars”, EAS Publications Series, vol. 71–72. EDP Sciences, pp. 275–277, 2015. doi: 10.1051/eas/1571061.*  
  
*A. Kashi, K. Davidsonand R. M. Humphreys, “RECOVERY FROM GIANT ERUPTIONS IN VERY MASSIVE STARS”, The Astrophysical Journal, vol. 817, no. 1. American Astronomical Society, p. 66, Jan. 22, 2016. doi: 10.3847/0004-637x/817/1/66.*  
  
*M. Bergemann, “Two chemically similar stellar overdensities on opposite sides of the plane of the Galactic disk”, Nature, vol. 555, no. 7696. Springer Science and Business Media LLC, pp. 334–337, Feb. 26, 2018. doi: 10.1038/nature25490.*  
  
*C. F. P. Laporte, K. V. Johnston, F. A. Gómez, N. Garavito-Camargoand G. Besla, “The influence of Sagittarius and the Large Magellanic Cloud on the stellar disc of the Milky Way Galaxy”, Monthly Notices of the Royal Astronomical Society, vol. 481, no. 1. Oxford University Press (OUP), pp. 286–306, Jun. 14, 2018. doi: 10.1093/mnras/sty1574.*  
  
*C. F. P. Laporte, K. V. Johnstonand A. Tzanidakis, “Stellar disc streams as probes of the Galactic potential and satellite impacts”, Monthly Notices of the Royal Astronomical Society, vol. 483, no. 2. Oxford University Press (OUP), pp. 1427–1436, Aug. 30, 2018. doi: 10.1093/mnras/sty2362.*  
  
*C. F. P. Laporte, I. Minchev, K. V. Johnstonand F. A. Gómez, “Footprints of the Sagittarius dwarf galaxy in the Gaia data set”, Monthly Notices of the Royal Astronomical Society, vol. 485, no. 3. Oxford University Press (OUP), pp. 3134–3152, Feb. 28, 2019. doi: 10.1093/mnras/stz583.*  
  
*A. A. Sheffield, A. M. Price-Whelan, A. Tzanidakis, K. V. Johnston, C. F. P. Laporteand B. Sesar, “A Disk Origin for the Monoceros Ring and A13 Stellar Overdensities”, The Astrophysical Journal, vol. 854, no. 1. American Astronomical Society, p. 47, Feb. 09, 2018. doi: 10.3847/1538-4357/aaa4b6.*  
  
*G. F. Thomas, “A-type stars in the Canada–France Imaging Survey – II. Tracing the height of the disc at large distances with Blue Stragglers”, Monthly Notices of the Royal Astronomical Society, vol. 483, no. 3. Oxford University Press (OUP), pp. 3119–3126, Dec. 07, 2018. doi: 10.1093/mnras/sty3334.*  
  
*A. M. Price-Whelan, K. V. Johnston, A. A. Sheffield, C. F. P. Laporteand B. Sesar, “A reinterpretation of the Triangulum–Andromeda stellar clouds: a population of halo stars kicked out of the Galactic disc”, Monthly Notices of the Royal Astronomical Society, vol. 452, no. 1. Oxford University Press (OUP), pp. 676–685, Jul. 07, 2015. doi: 10.1093/mnras/stv1324.*  
  
*J. C. Becker and F. C. Adams, “Oscillations of relative inclination angles in compact extrasolar planetary systems”, Monthly Notices of the Royal Astronomical Society, vol. 455, no. 3. Oxford University Press (OUP), pp. 2980–2993, Nov. 26, 2015. doi: 10.1093/mnras/stv2444.*  
  
*J. C. Becker and F. C. Adams, “Effects of unseen additional planetary perturbers on compact extrasolar planetary systems”, Monthly Notices of the Royal Astronomical Society, vol. 468, no. 1. Oxford University Press (OUP), pp. 549–563, Feb. 22, 2017. doi: 10.1093/mnras/stx461.*  
  
*J. C. Becker, A. Vanderburg, F. C. Adams, T. Khainand M. Bryan, “Exterior Companions to Hot Jupiters Orbiting Cool Stars Are Coplanar”, The Astronomical Journal, vol. 154, no. 6. American Astronomical Society, p. 230, Nov. 16, 2017. doi: 10.3847/1538-3881/aa9176.*  
  
*J. C. Becker, A. Vanderburg, F. C. Adams, S. A. Rappaportand H. M. Schwengeler, “WASP-47: A HOT JUPITER SYSTEM WITH TWO ADDITIONAL PLANETS DISCOVERED BY K2”, The Astrophysical Journal, vol. 812, no. 2. American Astronomical Society, p. L18, Oct. 12, 2015. doi: 10.1088/2041-8205/812/2/l18.*  
  
*J. C. Becker, “A Discrete Set of Possible Transit Ephemerides for Two Long-period Gas Giants Orbiting HIP 41378”, The Astronomical Journal, vol. 157, no. 1. American Astronomical Society, p. 19, Dec. 21, 2018. doi: 10.3847/1538-3881/aaf0a2.*  
  
*J. E. Rodriguez, “A Compact Multi-planet System with a Significantly Misaligned Ultra Short Period Planet”, The Astronomical Journal, vol. 156, no. 5. American Astronomical Society, p. 245, Nov. 02, 2018. doi: 10.3847/1538-3881/aae530.*  
  
*A. Vanderburg, “Precise Masses in the WASP-47 System”, The Astronomical Journal, vol. 154, no. 6. American Astronomical Society, p. 237, Nov. 16, 2017. doi: 10.3847/1538-3881/aa918b.*  
  
*A. Vanderburg, “FIVE PLANETS TRANSITING A NINTH MAGNITUDE STAR”, The Astrophysical Journal, vol. 827, no. 1. American Astronomical Society, p. L10, Aug. 04, 2016. doi: 10.3847/2041-8205/827/1/l10.*  
  
*J. C. Becker, F. C. Adams, T. Khain, S. J. Hamiltonand D. Gerdes, “Evaluating the Dynamical Stability of Outer Solar System Objects in the Presence of Planet Nine”, The Astronomical Journal, vol. 154, no. 2. American Astronomical Society, p. 61, Jul. 19, 2017. doi: 10.3847/1538-3881/aa7aa2.*  
  
*J. Zrake and W. E. East, “FREELY DECAYING TURBULENCE IN FORCE-FREE ELECTRODYNAMICS”, The Astrophysical Journal, vol. 817, no. 2. American Astronomical Society, p. 89, Jan. 22, 2016. doi: 10.3847/0004-637x/817/2/89.*  
  
*D. Zhang and S. W. Davis, “Radiation Hydrodynamic Simulations of Dust-driven Winds”, The Astrophysical Journal, vol. 839, no. 1. American Astronomical Society, p. 54, Apr. 13, 2017. doi: 10.3847/1538-4357/aa6935.*  
  
*D. Zhang, S. W. Davis, Y.-F. Jiangand J. M. Stone, “Dusty Cloud Acceleration by Radiation Pressure in Rapidly Star-forming Galaxies”, The Astrophysical Journal, vol. 854, no. 2. American Astronomical Society, p. 110, Feb. 16, 2018. doi: 10.3847/1538-4357/aaa8e4.*  
  
*S. A. Mortazavi, J. M. Lotz, J. E. Barnes, G. C. Privonand G. F. Snyder, “H I versus H α – comparing the kinematic tracers in modelling the initial conditions of the Mice”, Monthly Notices of the Royal Astronomical Society, vol. 474, no. 3. Oxford University Press (OUP), pp. 3423–3434, Nov. 20, 2017. doi: 10.1093/mnras/stx2964.*  
  
*A. Tenerani, M. Velli, A. F. Rappazzoand F. Pucci, “MAGNETIC RECONNECTION: RECURSIVE CURRENT SHEET COLLAPSE TRIGGERED BY “IDEAL” TEARING”, The Astrophysical Journal, vol. 813, no. 2. American Astronomical Society, p. L32, Nov. 04, 2015. doi: 10.1088/2041-8205/813/2/l32.*  
  
*J. Bae, R. P. Nelsonand L. Hartmann, “THE SPIRAL WAVE INSTABILITY INDUCED BY A GIANT PLANET. I. PARTICLE STIRRING IN THE INNER REGIONS OF PROTOPLANETARY DISKS”, The Astrophysical Journal, vol. 833, no. 2. American Astronomical Society, p. 126, Dec. 13, 2016. doi: 10.3847/1538-4357/833/2/126.*  
  
*J. Bae, R. P. Nelson, L. Hartmannand S. Richard, “SELF-DESTRUCTING SPIRAL WAVES: GLOBAL SIMULATIONS OF A SPIRAL-WAVE INSTABILITY IN ACCRETION DISKS”, The Astrophysical Journal, vol. 829, no. 1. American Astronomical Society, p. 13, Sep. 14, 2016. doi: 10.3847/0004-637x/829/1/13.*  
  
*J. Bae, Z. Zhuand L. Hartmann, “On the Formation of Multiple Concentric Rings and Gaps in Protoplanetary Disks”, The Astrophysical Journal, vol. 850, no. 2. American Astronomical Society, p. 201, Dec. 04, 2017. doi: 10.3847/1538-4357/aa9705.*  
  
*R. K. Yadav, U. R. Christensen, S. J. Wolkand K. Poppenhaeger, “MAGNETIC CYCLES IN A DYNAMO SIMULATION OF FULLY CONVECTIVE M-STAR PROXIMA CENTAURI”, The Astrophysical Journal, vol. 833, no. 2. American Astronomical Society, p. L28, Dec. 19, 2016. doi: 10.3847/2041-8213/833/2/l28.*  
  
*A. M. Nierenberg, T. Treu, N. Menci, Y. Lu, P. Torreyand M. Vogelsberger, “The missing satellite problem in 3D”, Monthly Notices of the Royal Astronomical Society, vol. 462, no. 4. Oxford University Press (OUP), pp. 4473–4481, Jul. 30, 2016. doi: 10.1093/mnras/stw1860.*  
  
*P. Torrey, “An instability of feedback-regulated star formation in galactic nuclei”, Monthly Notices of the Royal Astronomical Society, vol. 467, no. 2. Oxford University Press (OUP), pp. 2301–2314, Feb. 01, 2017. doi: 10.1093/mnras/stx254.*  
  
*P. Torrey, S. Wellons, C.-P. Ma, P. F. Hopkinsand M. Vogelsberger, “Forward and backward galaxy evolution in comoving cumulative number density space”, Monthly Notices of the Royal Astronomical Society, vol. 467, no. 4. Oxford University Press (OUP), pp. 4872–4885, Feb. 16, 2017. doi: 10.1093/mnras/stx370.*  
  
*F. Soubiran and B. Militzer, “THE PROPERTIES OF HEAVY ELEMENTS IN GIANT PLANET ENVELOPES”, The Astrophysical Journal, vol. 829, no. 1. American Astronomical Society, p. 14, Sep. 14, 2016. doi: 10.3847/0004-637x/829/1/14.*  
  
*G. Dunn, K. Holley-Bockelmannand J. Bellovary, “The Role of Gravitational Recoil in the Assembly of Massive Black Hole Seeds”, The Astrophysical Journal, vol. 896, no. 1. American Astronomical Society, p. 72, Jun. 15, 2020. doi: 10.3847/1538-4357/ab7cd2.*  
  
*B. Paxton, “Modules for Experiments in Stellar Astrophysics (MESA): Convective Boundaries, Element Diffusion, and Massive Star Explosions”, The Astrophysical Journal Supplement Series, vol. 234, no. 2. American Astronomical Society, p. 34, Feb. 06, 2018. doi: 10.3847/1538-4365/aaa5a8.*  
  
*C. Shi, A. Tenerani, M. Velliand S. Lu, “Fast Recursive Reconnection and the Hall Effect: Hall-MHD Simulations”, The Astrophysical Journal, vol. 883, no. 2. American Astronomical Society, p. 172, Oct. 01, 2019. doi: 10.3847/1538-4357/ab33ff.*  
  
*C. Shi, M. Velliand A. Tenerani, “Marginal Stability of Sweet–Parker Type Current Sheets at Low Lundquist Numbers”, The Astrophysical Journal, vol. 859, no. 2. American Astronomical Society, p. 83, May 25, 2018. doi: 10.3847/1538-4357/aabd83.*  
  
*C. Shi, M. Velli, A. Tenerani, F. Rappazzoand V. Réville, “Propagation of Alfvén Waves in the Expanding Solar Wind with the Fast–Slow Stream Interaction”, The Astrophysical Journal, vol. 888, no. 2. American Astronomical Society, p. 68, Jan. 09, 2020. doi: 10.3847/1538-4357/ab5fce.*  
  
*A. Tenerani and M. Velli, “Nonlinear Firehose Relaxation and Constant- B Field Fluctuations”, The Astrophysical Journal, vol. 867, no. 2. American Astronomical Society, p. L26, Nov. 08, 2018. doi: 10.3847/2041-8213/aaec01.*  
  
*K. Finlator, C. Doughty, Z. Caiand G. Díaz, “The faint host galaxies of C IV absorbers at z &gt; 5”, Monthly Notices of the Royal Astronomical Society, vol. 493, no. 3. Oxford University Press (OUP), pp. 3223–3237, Feb. 18, 2020. doi: 10.1093/mnras/staa377.*  
  
*C. Doughty and K. Finlator, “Evolution of neutral oxygen during the epoch of reionization and its use in estimating the neutral hydrogen fraction”, Monthly Notices of the Royal Astronomical Society, vol. 489, no. 2. Oxford University Press (OUP), pp. 2755–2768, Aug. 22, 2019. doi: 10.1093/mnras/stz2331.*  
  
*M. Molaro, R. Davé, S. Hassan, M. G. Santosand K. Finlator, “Artist: fast radiative transfer for large-scale simulations of the epoch of reionization”, Monthly Notices of the Royal Astronomical Society, vol. 489, no. 4. Oxford University Press (OUP), pp. 5594–5611, Aug. 14, 2019. doi: 10.1093/mnras/stz2171.*  
  
*K. Finlator, L. Keating, B. D. Oppenheimer, R. Davéand E. Zackrisson, “Reionization in Technicolor”, Monthly Notices of the Royal Astronomical Society, vol. 480, no. 2. Oxford University Press (OUP), pp. 2628–2649, Jul. 25, 2018. doi: 10.1093/mnras/sty1949.*  
  
*D. Fielding, E. Quataertand D. Martizzi, “Clustered supernovae drive powerful galactic winds after superbubble breakout”, Monthly Notices of the Royal Astronomical Society, vol. 481, no. 3. Oxford University Press (OUP), pp. 3325–3347, Sep. 07, 2018. doi: 10.1093/mnras/sty2466.*  
  
*D. Martizzi, E. Quataert, C.-A. Faucher-Giguèreand D. Fielding, “Simulations of jet heating in galaxy clusters: successes and challenges”, Monthly Notices of the Royal Astronomical Society, vol. 483, no. 2. Oxford University Press (OUP), pp. 2465–2486, Nov. 30, 2018. doi: 10.1093/mnras/sty3273.*  
  
*A. Danehkar, “Bi-Abundance Ionisation Structure of the Wolf–Rayet Planetary Nebula PB 8”, Publications of the Astronomical Society of Australia, vol. 35. Cambridge University Press (CUP), 2018. doi: 10.1017/pasa.2018.1.*  
  
*A. Danehkar, “The Ultra-fast Outflow of the Quasar PG 1211+143 as Viewed by Time-averagedChandraGrating Spectroscopy”, The Astrophysical Journal, vol. 853, no. 2. American Astronomical Society, p. 165, Feb. 02, 2018. doi: 10.3847/1538-4357/aaa427.*  
  
*A. Danehkar, M. A. Nowak, J. C. Leeand R. K. Smith, “MPI\_XSTAR: MPI-based Parallelization of the XSTAR Photoionization Program”, Publications of the Astronomical Society of the Pacific, vol. 130, no. 984. IOP Publishing, p. 024501, Dec. 29, 2017. doi: 10.1088/1538-3873/aa9dff.*  
  
*G. A. Kriss, “Discovery of an Ultraviolet Counterpart to an Ultrafast X-Ray Outflow in the Quasar PG 1211+143”, The Astrophysical Journal, vol. 853, no. 2. American Astronomical Society, p. 166, Feb. 02, 2018. doi: 10.3847/1538-4357/aaa42b.*  
  
*A. K. Dupree, “NGC 1866: First Spectroscopic Detection of Fast-rotating Stars in a Young LMC Cluster”, The Astrophysical Journal, vol. 846, no. 1. American Astronomical Society, p. L1, Aug. 23, 2017. doi: 10.3847/2041-8213/aa85dd.*  
  
*A. J. Richings and C.-A. Faucher-Giguère, “The origin of fast molecular outflows in quasars: molecule formation in AGN-driven galactic winds”, Monthly Notices of the Royal Astronomical Society, vol. 474, no. 3. Oxford University Press (OUP), pp. 3673–3699, Nov. 23, 2017. doi: 10.1093/mnras/stx3014.*  
  
*B. Robertson and P. Goldreich, “Dense Regions in Supersonic Isothermal Turbulence”, The Astrophysical Journal, vol. 854, no. 2. American Astronomical Society, p. 88, Feb. 15, 2018. doi: 10.3847/1538-4357/aaa89e.*  
  
*R. H. Hewins, C. Condie, M. Morris, M. L. A. Richardson, N. Ouelletteand M. Metcalf, “Thermal History of CB b Chondrules and Cooling Rate Distributions of Ejecta Plumes”, The Astrophysical Journal, vol. 855, no. 2. American Astronomical Society, p. L17, Mar. 07, 2018. doi: 10.3847/2041-8213/aab15b.*  
  
*V. Rodriguez-Gomez, “Vrodgom/Statmorph: First Release”. Zenodo, Oct. 19, 2017. doi: 10.5281/ZENODO.1026011.*  
  
*V. Rodriguez-Gomez, “The optical morphologies of galaxies in the IllustrisTNG simulation: a comparison to Pan-STARRS observations”, Monthly Notices of the Royal Astronomical Society, vol. 483, no. 3. Oxford University Press (OUP), pp. 4140–4159, Dec. 10, 2018. doi: 10.1093/mnras/sty3345.*  
  
*Snyder, Gregory F., “Illustris Simulated Deep Fields (”ILLUSTRIS”)”. STScI/MAST, 2017. doi: 10.17909/T98385.*  
  
*E. Buie II, W. J. Gray, E. Scannapiecoand M. Safarzadeh, “Modeling Photoionized Turbulent Material in the Circumgalactic Medium. II. Effect of Turbulence within a Stratified Medium”, The Astrophysical Journal, vol. 896, no. 2. American Astronomical Society, p. 136, Jun. 22, 2020. doi: 10.3847/1538-4357/ab9535.*  
  
*J. Cottle, E. Scannapieco, M. Brüggen, W. Banda-Barragánand C. Federrath, “The Launching of Cold Clouds by Galaxy Outflows. III. The Influence of Magnetic Fields”, The Astrophysical Journal, vol. 892, no. 1. American Astronomical Society, p. 59, Mar. 27, 2020. doi: 10.3847/1538-4357/ab76d1.*  
  
*M. Safarzadeh and B. Côté, “On the impact of neutron star binaries’ natal-kick distribution on the Galactic r-process enrichment”, Monthly Notices of the Royal Astronomical Society, vol. 471, no. 4. Oxford University Press (OUP), pp. 4488–4493, Jul. 26, 2017. doi: 10.1093/mnras/stx1897.*  
  
*M. Safarzadeh and E. Scannapieco, “Simulating neutron star mergers as r-process sources in ultrafaint dwarf galaxies”, Monthly Notices of the Royal Astronomical Society, vol. 471, no. 2. Oxford University Press (OUP), pp. 2088–2096, Jul. 08, 2017. doi: 10.1093/mnras/stx1706.*  
  
*R. Sarmento, E. Scannapiecoand L. Pan, “FOLLOWING THE COSMIC EVOLUTION OF PRISTINE GAS. I. IMPLICATIONS FOR MILKY WAY HALO STARS”, The Astrophysical Journal, vol. 834, no. 1. American Astronomical Society, p. 23, Dec. 27, 2016. doi: 10.3847/1538-4357/834/1/23.*  
  
*C. M. Mauney and D. Lazzati, “The formation of astrophysical Mg-rich silicate dust”, Molecular Astrophysics, vol. 12. Elsevier BV, pp. 1–9, Sep. 2018. doi: 10.1016/j.molap.2018.03.002.*  
  
*J. Squire, M. W. Kunz, E. Quataertand A. A. Schekochihin, “Kinetic Simulations of the Interruption of Large-Amplitude Shear-Alfvén Waves in a High- Plasma”, Physical Review Letters, vol. 119, no. 15. American Physical Society (APS), Oct. 12, 2017. doi: 10.1103/physrevlett.119.155101.*  
  
*J. Squire, E. Quataertand M. W. Kunz, “Pressure-anisotropy-induced nonlinearities in the kinetic magnetorotational instability”, Journal of Plasma Physics, vol. 83, no. 6. Cambridge University Press (CUP), Dec. 2017. doi: 10.1017/s0022377817000940.*  
  
*J. Squire, A. A. Schekochihin, E. Quataertand M. W. Kunz, “Magneto-immutable turbulence in weakly collisional plasmas”, Journal of Plasma Physics, vol. 85, no. 1. Cambridge University Press (CUP), Feb. 2019. doi: 10.1017/s0022377819000114.*  
  
*N. S. Kern, A. Liu, A. R. Parsons, A. Mesingerand B. Greig, “Emulating Simulations of Cosmic Dawn for 21 cm Power Spectrum Constraints on Cosmology, Reionization, and X-Ray Heating”, The Astrophysical Journal, vol. 848, no. 1. American Astronomical Society, p. 23, Oct. 09, 2017. doi: 10.3847/1538-4357/aa8bb4.*  
  
*J. Bae and Z. Zhu, “Planet-driven Spiral Arms in Protoplanetary Disks. I. Formation Mechanism”, The Astrophysical Journal, vol. 859, no. 2. American Astronomical Society, p. 118, May 30, 2018. doi: 10.3847/1538-4357/aabf8c.*  
  
*J. Bae and Z. Zhu, “Planet-driven Spiral Arms in Protoplanetary Disks. II. Implications”, The Astrophysical Journal, vol. 859, no. 2. American Astronomical Society, p. 119, May 30, 2018. doi: 10.3847/1538-4357/aabf93.*  
  
*G. Witzel, “Variability Timescale and Spectral Index of Sgr A* in the Near Infrared: Approximate Bayesian Computation Analysis of the Variability of the Closest Supermassive Black Hole”, *The Astrophysical Journal*, vol. 863, no. 1. American Astronomical Society, p. 15, Aug. 07, 2018. doi: 10.3847/1538-4357/aace62.  
  
J. M. Stone, K. Tomida, C. J. Whiteand K. G. Felker, “The Athena++ Adaptive Mesh Refinement Framework: Design and Magnetohydrodynamic Solvers”, *The Astrophysical Journal Supplement Series*, vol. 249, no. 1. American Astronomical Society, p. 4, Jun. 26, 2020. doi: 10.3847/1538-4365/ab929b.  
  
C. J. White, J. Dexter, O. Blaesand E. Quataert, “The Effects of Tilt on the Images of Black Hole Accretion Flows”, *The Astrophysical Journal*, vol. 894, no. 1. American Astronomical Society, p. 14, Apr. 30, 2020. doi: 10.3847/1538-4357/ab8463.  
  
C. J. White, E. Quataertand O. Blaes, “Tilted Disks around Black Holes: A Numerical Parameter Survey for Spin and Inclination Angle”, *The Astrophysical Journal*, vol. 878, no. 1. American Astronomical Society, p. 51, Jun. 12, 2019. doi: 10.3847/1538-4357/ab089e.  
  
C. J. White, E. Quataertand C. F. Gammie, “The Structure of Radiatively Inefficient Black Hole Accretion Flows”, *The Astrophysical Journal*, vol. 891, no. 1. American Astronomical Society, p. 63, Mar. 04, 2020. doi: 10.3847/1538-4357/ab718e.  
  
P. Mocz, L. Lancaster, A. Fialkov, F. Becerraand P.-H. Chavanis, “Schrödinger-Poisson–Vlasov-Poisson correspondence”, *Physical Review D*, vol. 97, no. 8. American Physical Society (APS), Apr. 25, 2018. doi: 10.1103/physrevd.97.083519.  
  
S. Adhikari, A.-S. Deutschand S. Shandera, “Statistical anisotropies in temperature and polarization fluctuations from a scale-dependent trispectrum”, *Physical Review D*, vol. 98, no. 2. American Physical Society (APS), Jul. 16, 2018. doi: 10.1103/physrevd.98.023520.  
  
S. Adhikari and D. Huterer, “A new measure of tension between experiments”, *Journal of Cosmology and Astroparticle Physics*, vol. 2019, no. 1. IOP Publishing, pp. 036–036, Jan. 18, 2019. doi: 10.1088/1475-7516/2019/01/036.  
  
P. Mocz, “First Star-Forming Structures in Fuzzy Cosmic Filaments”, *Physical Review Letters*, vol. 123, no. 14. American Physical Society (APS), Oct. 02, 2019. doi: 10.1103/physrevlett.123.141301.  
  
P. D. Mullen and C. F. Gammie, “A Magnetized, Moon-forming Giant Impact”, *The Astrophysical Journal*, vol. 903, no. 1. American Astronomical Society, p. L15, Oct. 29, 2020. doi: 10.3847/2041-8213/abbffd.  
  
A. Ricarte, B. S. Prather, G. N. Wong, R. Narayan, C. Gammieand M. D. Johnson, “Decomposing the internal faraday rotation of black hole accretion flows”, *Monthly Notices of the Royal Astronomical Society*, vol. 498, no. 4. Oxford University Press (OUP), pp. 5468–5488, Sep. 07, 2020. doi: 10.1093/mnras/staa2692.  
  
F. Roelofs, “SYMBA: An end-to-end VLBI synthetic data generation pipeline”, *Astronomy & Astrophysics*, vol. 636. EDP Sciences, p. A5, Apr. 2020. doi: 10.1051/0004-6361/201936622.  
  
B. R. Ryan, S. M. Ressler, J. C. Dolence, C. Gammieand E. Quataert, “Two-temperature GRRMHD Simulations of M87”, *The Astrophysical Journal*, vol. 864, no. 2. American Astronomical Society, p. 126, Sep. 07, 2018. doi: 10.3847/1538-4357/aad73a.  
  
R. Yarza, G. N. Wong, B. R. Ryanand C. F. Gammie, “Bremsstrahlung in GRMHD Models of Accreting Black Holes”, *The Astrophysical Journal*, vol. 898, no. 1. American Astronomical Society, p. 50, Jul. 22, 2020. doi: 10.3847/1538-4357/ab9808.  
  
R. J. Beachley, M. Mistysyn, J. A. Faber, S. J. Weinsteinand N. S. Barlow, “Accurate closed-form trajectories of light around a Kerr black hole using asymptotic approximants”, *Classical and Quantum Gravity*, vol. 35, no. 20. IOP Publishing, p. 205009, Oct. 01, 2018. doi: 10.1088/1361-6382/aae0cd.  
  
C. Bustard, S. A. Pardy, E. D’Onghia, E. G. Zweibeland J. S. Gallagher III, “The Fate of Supernova-heated Gas in Star-forming Regions of the LMC: Lessons for Galaxy Formation?”, *The Astrophysical Journal*, vol. 863, no. 1. American Astronomical Society, p. 49, Aug. 09, 2018. doi: 10.3847/1538-4357/aad08f.  
  
J. D. Alvarado-Gómez, “Coronal Response to Magnetically Suppressed CME Events in M-dwarf Stars”, *The Astrophysical Journal Letters*, vol. 884, no. 1. American Astronomical Society, p. L13, Oct. 07, 2019. doi: 10.3847/2041-8213/ab44d0.  
  
P. La Plante, A. Lidz, J. Aguirreand S. Kohn, “The 21 cm kSZ–kSZ Bispectrum during the Epoch of Reionization”, *The Astrophysical Journal*, vol. 899, no. 1. American Astronomical Society, p. 40, Aug. 11, 2020. doi: 10.3847/1538-4357/aba2ed.  
  
S. Hassan, A. Liu, S. Kohnand P. L. Plante, “Identifying Reionization Sources from 21cm Maps using Convolutional Neural Networks”, *Monthly Notices of the Royal Astronomical Society*. Oxford University Press (OUP), Dec. 03, 2018. doi: 10.1093/mnras/sty3282.  
  
J. Kerrigan, “Optimizing sparse RFI prediction using deep learning”, *Monthly Notices of the Royal Astronomical Society*, vol. 488, no. 2. Oxford University Press (OUP), pp. 2605–2615, Jul. 08, 2019. doi: 10.1093/mnras/stz1865.  
  
S. Bird, Y. Ali-Haïmoud, Y. Fengand J. Liu, “An efficient and accurate hybrid method for simulating non-linear neutrino structure”, *Monthly Notices of the Royal Astronomical Society*, vol. 481, no. 2. Oxford University Press (OUP), pp. 1486–1500, Aug. 31, 2018. doi: 10.1093/mnras/sty2376.  
  
S. Bird, K. K. Rogers, H. V. Peiris, L. Verde, A. Font-Riberaand A. Pontzen, “An emulator for the Lyman-α forest”, *Journal of Cosmology and Astroparticle Physics*, vol. 2019, no. 2. IOP Publishing, pp. 050–050, Feb. 26, 2019. doi: 10.1088/1475-7516/2019/02/050.  
  
K. K. Rogers, H. V. Peiris, A. Pontzen, S. Bird, L. Verdeand A. Font-Ribera, “Bayesian emulator optimisation for cosmology: application to the Lyman-alpha forest”, *Journal of Cosmology and Astroparticle Physics*, vol. 2019, no. 2. IOP Publishing, pp. 031–031, Feb. 14, 2019. doi: 10.1088/1475-7516/2019/02/031.  
  
V. Réville, A. Teneraniand M. Velli, “Parametric Decay and the Origin of the Low-frequency Alfvénic Spectrum of the Solar Wind”, *The Astrophysical Journal*, vol. 866, no. 1. American Astronomical Society, p. 38, Oct. 08, 2018. doi: 10.3847/1538-4357/aadb8f.  
  
V. Réville, “The Role of Alfvén Wave Dynamics on the Large-scale Properties of the Solar Wind: Comparing an MHD Simulation with Parker Solar Probe E1 Data”, *The Astrophysical Journal Supplement Series*, vol. 246, no. 2. American Astronomical Society, p. 24, Feb. 01, 2020. doi: 10.3847/1538-4365/ab4fef.  
  
C. Wang, Y. Liand M. Ruszkowski, “AGN feedback and multiphase gas in giant elliptical galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 482, no. 3. Oxford University Press (OUP), pp. 3576–3590, Oct. 27, 2018. doi: 10.1093/mnras/sty2906.  
  
M. Gronke and S. P. Oh, “The growth and entrainment of cold gas in a hot wind”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 480, no. 1. Oxford University Press (OUP), pp. L111–L115, Jul. 20, 2018. doi: 10.1093/mnrasl/sly131.  
  
C. M. Liepold, “The MASSIVE Survey. XV. A Stellar Dynamical Mass Measurement of the Supermassive Black Hole in Massive Elliptical Galaxy NGC 1453”, *The Astrophysical Journal*, vol. 891, no. 1. American Astronomical Society, p. 4, Feb. 27, 2020. doi: 10.3847/1538-4357/ab6f71.  
  
M. E. Quenneville, C. M. Liepoldand C.-P. Ma, “Dynamical Modeling of Galaxies and Supermassive Black Holes: Axisymmetry in Triaxial Schwarzschild Orbit Superposition Models”, *The Astrophysical Journal Supplement Series*, vol. 254, no. 2. American Astronomical Society, p. 25, May 17, 2021. doi: 10.3847/1538-4365/abe6a0.  
  
K. S. S. Barrow, “Blue galaxies: modelling nebular He ii emission in high redshift galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 491, no. 3. Oxford University Press (OUP), pp. 4509–4522, Nov. 26, 2019. doi: 10.1093/mnras/stz3290.  
  
R. Teague, J. Baeand E. A. Bergin, “Meridional flows in the disk around a young star”, *Nature*, vol. 574, no. 7778. Springer Science and Business Media LLC, pp. 378–381, Oct. 16, 2019. doi: 10.1038/s41586-019-1642-0.  
  
X. Zhang and C. Liang, “An Open Boundary Condition for High-order Solutions of Magnetohydrodynamics on Unstructured Grids”, *International Journal of Computational Fluid Dynamics*, vol. 34, no. 6. Informa UK Limited, pp. 438–456, Jul. 02, 2020. doi: 10.1080/10618562.2020.1791835.  
  
D. Agarwal, K. Aggarwal, S. Burke-Spolaor, D. R. Lorimerand N. Garver-Daniels, “FETCH: A deep-learning based classifier for fast transient classification”, *Monthly Notices of the Royal Astronomical Society*, vol. 497, no. 2. Oxford University Press (OUP), pp. 1661–1674, Jun. 27, 2020. doi: 10.1093/mnras/staa1856.  
  
S. Hassan, S. Andrianomenaand C. Doughty, “Constraining the astrophysics and cosmology from 21 cm tomography using deep learning with the SKA”, *Monthly Notices of the Royal Astronomical Society*, vol. 494, no. 4. Oxford University Press (OUP), pp. 5761–5774, May 04, 2020. doi: 10.1093/mnras/staa1151.  
  
S. Hassan, K. Finlator, R. Davé, C. W. Churchilland J. X. Prochaska, “Testing galaxy formation simulations with damped Lyman-α abundance and metallicity evolution”, *Monthly Notices of the Royal Astronomical Society*, vol. 492, no. 2. Oxford University Press (OUP), pp. 2835–2846, Jan. 09, 2020. doi: 10.1093/mnras/staa056.  
  
T. Mangena, S. Hassanand M. G. Santos, “Constraining the reionization history using deep learning from 21-cm tomography with the Square Kilometre Array”, *Monthly Notices of the Royal Astronomical Society*, vol. 494, no. 1. Oxford University Press (OUP), pp. 600–606, Mar. 19, 2020. doi: 10.1093/mnras/staa750.  
  
E. Heintz, C. Bustardand E. G. Zweibel, “The Role of the Parker Instability in Structuring the Interstellar Medium”, *The Astrophysical Journal*, vol. 891, no. 2. American Astronomical Society, p. 157, Mar. 16, 2020. doi: 10.3847/1538-4357/ab7453.  
  
C. Binggeli, “Balmer breaks in simulated galaxies at z>6”, *Monthly Notices of the Royal Astronomical Society*. Oxford University Press (OUP), Sep. 05, 2019. doi: 10.1093/mnras/stz2387.  
  
X. Ma, “Simulating galaxies in the reionization era with FIRE-2: galaxy scaling relations, stellar mass functions, and luminosity functions”, *Monthly Notices of the Royal Astronomical Society*, vol. 478, no. 2. Oxford University Press (OUP), pp. 1694–1715, Apr. 21, 2018. doi: 10.1093/mnras/sty1024.  
  
P. Prem, D. M. Hurley, D. B. Goldsteinand P. L. Varghese, “The Evolution of a Spacecraft‐Generated Lunar Exosphere”, *Journal of Geophysical Research: Planets*, vol. 125, no. 8. American Geophysical Union (AGU), Aug. 2020. doi: 10.1029/2020je006464.  
  
A. J. Shajib, “STRIDES: a 3.9 per cent measurement of the Hubble constant from the strong lens system DES J0408−5354”, *Monthly Notices of the Royal Astronomical Society*, vol. 494, no. 4. Oxford University Press (OUP), pp. 6072–6102, Mar. 28, 2020. doi: 10.1093/mnras/staa828.  
  
P. Pjanka and J. M. Stone, “Stratified Global MHD Models of Accretion Disks in Semidetached Binaries”, *The Astrophysical Journal*, vol. 904, no. 2. American Astronomical Society, p. 90, Nov. 24, 2020. doi: 10.3847/1538-4357/abbe07.  
  
M. S. Clement, S. N. Raymond, N. A. Kaib, R. Deienno, J. E. Chambersand A. Izidoro, “Born eccentric: Constraints on Jupiter and Saturn’s pre-instability orbits”, *Icarus*, vol. 355. Elsevier BV, p. 114122, Feb. 2021. doi: 10.1016/j.icarus.2020.114122.  
  
F. Feng, “Search for Nearby Earth Analogs .III. Detection of 10 New Planets, 3 Planet Candidates, and Confirmation of 3 Planets around 11 Nearby M Dwarfs”, *The Astrophysical Journal Supplement Series*, vol. 250, no. 2. American Astronomical Society, p. 29, Oct. 01, 2020. doi: 10.3847/1538-4365/abb139.  
  
G. Lapenta, M. El Alaoui, J. Berchemand R. Walker, “Multiscale MHD‐Kinetic PIC Study of Energy Fluxes Caused by Reconnection”, *Journal of Geophysical Research: Space Physics*, vol. 125, no. 3. American Geophysical Union (AGU), Feb. 28, 2020. doi: 10.1029/2019ja027276.  
  
M. Zhou, “Suprathermal Electron Acceleration in a Reconnecting Magnetotail: Large‐Scale Kinetic Simulation”, *Journal of Geophysical Research: Space Physics*, vol. 123, no. 10. American Geophysical Union (AGU), pp. 8087–8108, Oct. 2018. doi: 10.1029/2018ja025502.  
  
J. M. Keeler, “Dynamics of Cloud-Top Generating Cells in Winter Cyclones. Part I: Idealized Simulations in the Context of Field Observations”, *Journal of the Atmospheric Sciences*, vol. 73, no. 4. American Meteorological Society, pp. 1507–1527, Feb. 24, 2016. doi: 10.1175/jas-d-15-0126.1.  
  
J. M. Keeler, “Dynamics of Cloud-Top Generating Cells in Winter Cyclones. Part II: Radiative and Instability Forcing”, *Journal of the Atmospheric Sciences*, vol. 73, no. 4. American Meteorological Society, pp. 1529–1553, Feb. 24, 2016. doi: 10.1175/jas-d-15-0127.1.  
  
A. Goldner, M. Huber, N. Diffenbaughand R. Caballero, “Implications of the permanent El Niño teleconnection &quot;blueprint&quot; for past global and North American hydroclimatology”, *Climate of the Past*, vol. 7, no. 3. Copernicus GmbH, pp. 723–743, Jul. 13, 2011. doi: 10.5194/cp-7-723-2011.  
  
P. Zhu, A. Bhattacharjee, A. Sangari, Z. Wangand P. Bonofiglo, “Three-dimensional geometry of magnetic reconnection induced by ballooning instability in a generalized Harris sheet”, *Physics of Plasmas*, vol. 24, no. 2. AIP Publishing, p. 024503, Feb. 2017. doi: 10.1063/1.4976994.  
  
G. J. Kooperman, M. S. Pritchardand R. C. J. Somerville, “Robustness and sensitivities of central U.S. summer convection in the super-parameterized CAM: Multi-model intercomparison with a new regional EOF index”, *Geophysical Research Letters*, vol. 40, no. 12. American Geophysical Union (AGU), pp. 3287–3291, Jun. 18, 2013. doi: 10.1002/grl.50597.  
  
L. Orf, E. Kantorand E. Savory, “Simulation of a downburst-producing thunderstorm using a very high-resolution three-dimensional cloud model”, *Journal of Wind Engineering and Industrial Aerodynamics*, vol. 104–106. Elsevier BV, pp. 547–557, May 2012. doi: 10.1016/j.jweia.2012.02.020.  
  
H. Li, “Projected climate change scenario over California by a regional ocean–atmosphere coupled model system”, *Climatic Change*, vol. 122, no. 4. Springer Science and Business Media LLC, pp. 609–619, Dec. 12, 2013. doi: 10.1007/s10584-013-1025-8.  
  
H. Li, M. Kanamitsu, S.-Y. Hong, K. Yoshimura, D. R. Cayanand V. Misra, “A high-resolution ocean-atmosphere coupled downscaling of the present climate over California”, *Climate Dynamics*, vol. 42, no. 3–4. Springer Science and Business Media LLC, pp. 701–714, Jan. 26, 2013. doi: 10.1007/s00382-013-1670-7.  
  
H. W. Chen, R. B. Alleyand F. Zhang, “Interannual Arctic sea ice variability and associated winter weather patterns: A regional perspective for 1979-2014”, *Journal of Geophysical Research: Atmospheres*, vol. 121, no. 24. American Geophysical Union (AGU), pp. 14, 433–14, 455, Dec. 27, 2016. doi: 10.1002/2016jd024769.  
  
X. Chen, O. M. Pauluis, L. R. Leungand F. Zhang, “Multiscale Atmospheric Overturning of the Indian Summer Monsoon as Seen through Isentropic Analysis”, *Journal of the Atmospheric Sciences*, vol. 75, no. 9. American Meteorological Society, pp. 3011–3030, Aug. 15, 2018. doi: 10.1175/jas-d-18-0068.1.  
  
X. Chen, O. M. Pauluis, L. R. Leungand F. Zhang, “Significant Contribution of Mesoscale Overturning to Tropical Mass and Energy Transport Revealed by the ERA5 Reanalysis”, *Geophysical Research Letters*, vol. 47, no. 1. American Geophysical Union (AGU), Jan. 16, 2020. doi: 10.1029/2019gl085333.  
  
X. Chen, O. M. Pauluisand F. Zhang, “Regional simulation of Indian summer monsoon intraseasonal oscillations at gray-zone resolution”, *Atmospheric Chemistry and Physics*, vol. 18, no. 2. Copernicus GmbH, pp. 1003–1022, Jan. 26, 2018. doi: 10.5194/acp-18-1003-2018.  
  
X. Chen, O. M. Pauluisand F. Zhang, “Atmospheric Overturning across Multiple Scales of an MJO Event during the CINDY/DYNAMO Campaign”, *Journal of the Atmospheric Sciences*, vol. 75, no. 2. American Meteorological Society, pp. 381–399, Jan. 19, 2018. doi: 10.1175/jas-d-17-0060.1.  
  
X. Chen, F. Zhangand K. Zhao, “Influence of Monsoonal Wind Speed and Moisture Content on Intensity and Diurnal Variations of the Mei-Yu Season Coastal Rainfall over South China”, *Journal of the Atmospheric Sciences*, vol. 74, no. 9. American Meteorological Society, pp. 2835–2856, Aug. 24, 2017. doi: 10.1175/jas-d-17-0081.1.  
  
Y. Chen, F. Zhang, B. W. Greenand X. Yu, “Impacts of Ocean Cooling and Reduced Wind Drag on Hurricane Katrina (2005) Based on Numerical Simulations”, *Monthly Weather Review*, vol. 146, no. 1. American Meteorological Society, pp. 287–306, Jan. 01, 2018. doi: 10.1175/mwr-d-17-0170.1.  
  
L. Dong and F. Zhang, “OBEST: An Observation-Based Ensemble Subsetting Technique for Tropical Cyclone Track Prediction”, *Weather and Forecasting*, vol. 31, no. 1. American Meteorological Society, pp. 57–70, Jan. 28, 2016. doi: 10.1175/waf-d-15-0056.1.  
  
K. Emanuel and F. Zhang, “On the Predictability and Error Sources of Tropical Cyclone Intensity Forecasts”, *Journal of the Atmospheric Sciences*, vol. 73, no. 9. American Meteorological Society, pp. 3739–3747, Sep. 01, 2016. doi: 10.1175/jas-d-16-0100.1.  
  
K. Emanuel and F. Zhang, “The Role of Inner-Core Moisture in Tropical Cyclone Predictability and Practical Forecast Skill”, *Journal of the Atmospheric Sciences*, vol. 74, no. 7. American Meteorological Society, pp. 2315–2324, Jul. 01, 2017. doi: 10.1175/jas-d-17-0008.1.  
  
J. Fang, O. Pauluisand F. Zhang, “Isentropic Analysis on the Intensification of Hurricane Edouard (2014)”, *Journal of the Atmospheric Sciences*, vol. 74, no. 12. American Meteorological Society, pp. 4177–4197, Dec. 01, 2017. doi: 10.1175/jas-d-17-0092.1.  
  
J. Fang and F. Zhang, “Contribution of Tropical Waves to the Formation of Supertyphoon Megi (2010)”, *Journal of the Atmospheric Sciences*, vol. 73, no. 11. American Meteorological Society, pp. 4387–4405, Oct. 20, 2016. doi: 10.1175/jas-d-15-0179.1.  
  
B. W. Green and F. Zhang, “Impacts of Air–Sea Flux Parameterizations on the Intensity and Structure of Tropical Cyclones”, *Monthly Weather Review*, vol. 141, no. 7. American Meteorological Society, pp. 2308–2324, Jul. 01, 2013. doi: 10.1175/mwr-d-12-00274.1.  
  
B. W. Green and F. Zhang, “Sensitivity of Tropical Cyclone Simulations to Parametric Uncertainties in Air–Sea Fluxes and Implications for Parameter Estimation”, *Monthly Weather Review*, vol. 142, no. 6. American Meteorological Society, pp. 2290–2308, May 28, 2014. doi: 10.1175/mwr-d-13-00208.1.  
  
B. W. Green and F. Zhang, “Idealized Large-Eddy Simulations of a Tropical Cyclone–like Boundary Layer”, *Journal of the Atmospheric Sciences*, vol. 72, no. 5. American Meteorological Society, pp. 1743–1764, May 01, 2015. doi: 10.1175/jas-d-14-0244.1.  
  
B. W. Green and F. Zhang, “Numerical simulations of Hurricane Katrina (2005) in the turbulent gray zone”, *Journal of Advances in Modeling Earth Systems*, vol. 7, no. 1. American Geophysical Union (AGU), pp. 142–161, Feb. 11, 2015. doi: 10.1002/2014ms000399.  
  
N. Hayatbini, K.-. lin . Hsu, S. Sorooshian, Y. Zhangand F. Zhang, “Effective Cloud Detection and Segmentation Using a Gradient-Based Algorithm for Satellite Imagery: Application to Improve PERSIANN-CCS”, *Journal of Hydrometeorology*, vol. 20, no. 5. American Meteorological Society, pp. 901–913, May 01, 2019. doi: 10.1175/jhm-d-18-0197.1.  
  
X.-M. Hu, D. C. Doughty, K. J. Sanchez, E. Josephand J. D. Fuentes, “Ozone variability in the atmospheric boundary layer in Maryland and its implications for vertical transport model”, *Atmospheric Environment*, vol. 46. Elsevier BV, pp. 354–364, Jan. 2012. doi: 10.1016/j.atmosenv.2011.09.054.  
  
X.-M. Hu, J. D. Fuentesand F. Zhang, “Downward transport and modification of tropospheric ozone through moist convection”, *Journal of Atmospheric Chemistry*, vol. 65, no. 1. Springer Science and Business Media LLC, pp. 13–35, Jan. 2010. doi: 10.1007/s10874-010-9179-5.  
  
X.-M. Hu, J. W. Nielsen-Gammonand F. Zhang, “Evaluation of Three Planetary Boundary Layer Schemes in the WRF Model”, *Journal of Applied Meteorology and Climatology*, vol. 49, no. 9. American Meteorological Society, pp. 1831–1844, Sep. 01, 2010. doi: 10.1175/2010jamc2432.1.  
  
X.-M. Hu, J. M. Siglerand J. D. Fuentes, “Variability of ozone in the marine boundary layer of the equatorial Pacific Ocean”, *Journal of Atmospheric Chemistry*, vol. 66, no. 3. Springer Science and Business Media LLC, pp. 117–136, Jul. 2010. doi: 10.1007/s10874-011-9196-z.  
  
X.-M. Hu, F. Zhangand J. W. Nielsen-Gammon, “Ensemble-based simultaneous state and parameter estimation for treatment of mesoscale model error: A real-data study”, *Geophysical Research Letters*, vol. 37, no. 8. American Geophysical Union (AGU), Apr. 2010. doi: 10.1029/2010gl043017.  
  
X.-M. Hu, F. Zhang, G. Yu, J. D. Fuentesand L. Wu, “Contribution of mixed-phase boundary layer clouds to the termination of ozone depletion events in the Arctic”, *Geophysical Research Letters*, vol. 38, no. 21. American Geophysical Union (AGU), p. n/a–n/a, Nov. 2011. doi: 10.1029/2011gl049229.  
  
J. Li and F. Zhang, “Geometry-Sensitive Ensemble Mean Based on Wasserstein Barycenters: Proof-of-Concept on Cloud Simulations”, *Journal of Computational and Graphical Statistics*, vol. 27, no. 4. Informa UK Limited, pp. 785–797, Oct. 02, 2018. doi: 10.1080/10618600.2018.1448831.  
  
M. Li, F. Zhang, Q. Zhang, J. Y. Harringtonand M. R. Kumjian, “Nonlinear response of hail precipitation rate to environmental moisture content: A real case modeling study of an episodic midlatitude severe convective event”, *Journal of Geophysical Research: Atmospheres*, vol. 122, no. 13. American Geophysical Union (AGU), pp. 6729–6747, Jul. 04, 2017. doi: 10.1002/2016jd026373.  
  
M. Li, Q. Zhangand F. Zhang, “Hail Day Frequency Trends and Associated Atmospheric Circulation Patterns over China during 1960–2012”, *Journal of Climate*, vol. 29, no. 19. American Meteorological Society, pp. 7027–7044, Sep. 15, 2016. doi: 10.1175/jcli-d-15-0500.1.  
  
S. Liu, D. Tao, K. Zhao, M. Minamideand F. Zhang, “Dynamics and Predictability of the Rapid Intensification of Super Typhoon Usagi (2013)”, *Journal of Geophysical Research: Atmospheres*, vol. 123, no. 14. American Geophysical Union (AGU), pp. 7462–7481, Jul. 20, 2018. doi: 10.1029/2018jd028561.  
  
Y. Lu and F. Zhang, “A Novel Channel‐Synthesizing Method for Reducing Uncertainties in Satellite Radiative Transfer Modeling”, *Geophysical Research Letters*, vol. 45, no. 10. American Geophysical Union (AGU), pp. 5115–5125, May 17, 2018. doi: 10.1029/2018gl077342.  
  
C. Melhauser and F. Zhang, “Diurnal Radiation Cycle Impact on the Pregenesis Environment of Hurricane Karl (2010)”, *Journal of the Atmospheric Sciences*, vol. 71, no. 4. American Meteorological Society, pp. 1241–1259, Mar. 27, 2014. doi: 10.1175/jas-d-13-0116.1.  
  
C. Melhauser and F. Zhang, “Development and Application of a Simplified Coplane Wind Retrieval Algorithm Using Dual-Beam Airborne Doppler Radar Observations for Tropical Cyclone Prediction”, *Monthly Weather Review*, vol. 144, no. 7. American Meteorological Society, pp. 2645–2666, Jun. 23, 2016. doi: 10.1175/mwr-d-15-0323.1.  
  
C. Melhauser, F. Zhang, Y. Weng, Y. Jin, H. Jinand Q. Zhao, “A Multiple-Model Convection-Permitting Ensemble Examination of the Probabilistic Prediction of Tropical Cyclones: Hurricanes Sandy (2012) and Edouard (2014)”, *Weather and Forecasting*, vol. 32, no. 2. American Meteorological Society, pp. 665–688, Mar. 21, 2017. doi: 10.1175/waf-d-16-0082.1.  
  
Z. Meng, F. Zhang, P. Markowski, D. Wuand K. Zhao, “A Modeling Study on the Development of a Bowing Structure and Associated Rear Inflow within a Squall Line over South China”, *Journal of the Atmospheric Sciences*, vol. 69, no. 4. American Meteorological Society, pp. 1182–1207, Mar. 30, 2012. doi: 10.1175/jas-d-11-0121.1.  
  
M. Minamide and F. Zhang, “Adaptive Observation Error Inflation for Assimilating All-Sky Satellite Radiance”, *Monthly Weather Review*, vol. 145, no. 3. American Meteorological Society, pp. 1063–1081, Mar. 2017. doi: 10.1175/mwr-d-16-0257.1.  
  
E. B. Munsell and F. Zhang, “Prediction and uncertainty of Hurricane Sandy (2012) explored through a real-time cloud-permitting ensemble analysis and forecast system assimilating airborne Doppler radar observations”, *Journal of Advances in Modeling Earth Systems*, vol. 6, no. 1. American Geophysical Union (AGU), pp. 38–58, Jan. 28, 2014. doi: 10.1002/2013ms000297.  
  
E. B. Munsell, F. Zhang, S. A. Braun, J. A. Sippeland A. C. Didlake, “The Inner-Core Temperature Structure of Hurricane Edouard (2014): Observations and Ensemble Variability”, *Monthly Weather Review*, vol. 146, no. 1. American Meteorological Society, pp. 135–155, Jan. 01, 2018. doi: 10.1175/mwr-d-17-0095.1.  
  
E. B. Munsell, F. Zhang, J. A. Sippel, S. A. Braunand Y. Weng, “Dynamics and Predictability of the Intensification of Hurricane Edouard (2014)”, *Journal of the Atmospheric Sciences*, vol. 74, no. 2. American Meteorological Society, pp. 573–595, Feb. 01, 2017. doi: 10.1175/jas-d-16-0018.1.  
  
J. W. Nielsen-Gammon, X.-M. Hu, F. Zhangand J. E. Pleim, “Evaluation of Planetary Boundary Layer Scheme Sensitivities for the Purpose of Parameter Estimation”, *Monthly Weather Review*, vol. 138, no. 9. American Meteorological Society, pp. 3400–3417, Sep. 01, 2010. doi: 10.1175/2010mwr3292.1.  
  
R. G. Nystrom, “Predictability and Dynamics of Hurricane Joaquin (2015) Explored through Convection-Permitting Ensemble Sensitivity Experiments”, *Journal of the Atmospheric Sciences*, vol. 75, no. 2. American Meteorological Society, pp. 401–424, Jan. 19, 2018. doi: 10.1175/jas-d-17-0137.1.  
  
J. Pan, “Dynamics of local extreme rainfall of super Typhoon Soudelor (2015) in East China”, *Science China Earth Sciences*, vol. 61, no. 5. Springer Science and Business Media LLC, pp. 572–594, Feb. 03, 2018. doi: 10.1007/s11430-017-9135-6.  
  
O. M. Pauluis and F. Zhang, “Reconstruction of Thermodynamic Cycles in a High-Resolution Simulation of a Hurricane”, *Journal of the Atmospheric Sciences*, vol. 74, no. 10. American Meteorological Society, pp. 3367–3381, Sep. 28, 2017. doi: 10.1175/jas-d-16-0353.1.  
  
J. Poterjoy and F. Zhang, “Dynamics and Structure of Forecast Error Covariance in the Core of a Developing Hurricane”, *Journal of the Atmospheric Sciences*, vol. 68, no. 8. American Meteorological Society, pp. 1586–1606, Aug. 01, 2011. doi: 10.1175/2011jas3681.1.  
  
J. Poterjoy and F. Zhang, “Intercomparison and Coupling of Ensemble and Four-Dimensional Variational Data Assimilation Methods for the Analysis and Forecasting of Hurricane Karl (2010)”, *Monthly Weather Review*, vol. 142, no. 9. American Meteorological Society, pp. 3347–3364, Sep. 2014. doi: 10.1175/mwr-d-13-00394.1.  
  
J. Poterjoy and F. Zhang, “Predictability and Genesis of Hurricane Karl (2010) Examined through the EnKF Assimilation of Field Observations Collected during PREDICT”, *Journal of the Atmospheric Sciences*, vol. 71, no. 4. American Meteorological Society, pp. 1260–1275, Mar. 27, 2014. doi: 10.1175/jas-d-13-0291.1.  
  
J. Poterjoy and F. Zhang, “Systematic Comparison of Four-Dimensional Data Assimilation Methods With and Without the Tangent Linear Model Using Hybrid Background Error Covariance: E4DVar versus 4DEnVar”, *Monthly Weather Review*, vol. 143, no. 5. American Meteorological Society, pp. 1601–1621, May 01, 2015. doi: 10.1175/mwr-d-14-00224.1.  
  
J. Poterjoy and F. Zhang, “Comparison of Hybrid Four-Dimensional Data Assimilation Methods with and without the Tangent Linear and Adjoint Models for Predicting the Life Cycle of Hurricane Karl (2010)”, *Monthly Weather Review*, vol. 144, no. 4. American Meteorological Society, pp. 1449–1468, Mar. 29, 2016. doi: 10.1175/mwr-d-15-0116.1.  
  
J. Poterjoy, F. Zhangand Y. Weng, “The Effects of Sampling Errors on the EnKF Assimilation of Inner-Core Hurricane Observations”, *Monthly Weather Review*, vol. 142, no. 4. American Meteorological Society, pp. 1609–1630, Mar. 27, 2014. doi: 10.1175/mwr-d-13-00305.1.  
  
S. B. Sieron, E. E. Clothiaux, F. Zhang, Y. Luand J. A. Otkin, “Comparison of using distribution‐specific versus effective radius methods for hydrometeor single‐scattering properties for all‐sky microwave satellite radiance simulations with different microphysics parameterization schemes”, *Journal of Geophysical Research: Atmospheres*, vol. 122, no. 13. American Geophysical Union (AGU), pp. 7027–7046, Jul. 06, 2017. doi: 10.1002/2017jd026494.  
  
S. B. Sieron, F. Zhang, E. E. Clothiaux, L. N. Zhangand Y. Lu, “Representing Precipitation Ice Species With Both Spherical and Nonspherical Particles for Radiative Transfer Modeling of Microphysics‐Consistent Cloud Microwave Scattering Properties”, *Journal of Advances in Modeling Earth Systems*, vol. 10, no. 4. American Geophysical Union (AGU), pp. 1011–1028, Apr. 2018. doi: 10.1002/2017ms001226.  
  
Y. Q. Sun, R. Rotunnoand F. Zhang, “Contributions of Moist Convection and Internal Gravity Waves to Building the Atmospheric −5/3 Kinetic Energy Spectra”, *Journal of the Atmospheric Sciences*, vol. 74, no. 1. American Meteorological Society, pp. 185–201, Jan. 01, 2017. doi: 10.1175/jas-d-16-0097.1.  
  
Y. Q. Sun and F. Zhang, “Intrinsic versus Practical Limits of Atmospheric Predictability and the Significance of the Butterfly Effect”, *Journal of the Atmospheric Sciences*, vol. 73, no. 3. American Meteorological Society, pp. 1419–1438, Feb. 19, 2016. doi: 10.1175/jas-d-15-0142.1.  
  
X. Tang, Z.-M. Tan, J. Fang, Y. Q. Sunand F. Zhang, “Impact of the Diurnal Radiation Cycle on Secondary Eyewall Formation”, *Journal of the Atmospheric Sciences*, vol. 74, no. 9. American Meteorological Society, pp. 3079–3098, Aug. 31, 2017. doi: 10.1175/jas-d-17-0020.1.  
  
X. Tang and F. Zhang, “Impacts of the Diurnal Radiation Cycle on the Formation, Intensity, and Structure of Hurricane Edouard (2014)”, *Journal of the Atmospheric Sciences*, vol. 73, no. 7. American Meteorological Society, pp. 2871–2892, Jul. 01, 2016. doi: 10.1175/jas-d-15-0283.1.  
  
D. Tao and F. Zhang, “Effect of environmental shear, sea‐surface temperature, and ambient moisture on the formation and predictability of tropical cyclones: An ensemble‐mean perspective”, *Journal of Advances in Modeling Earth Systems*, vol. 6, no. 2. American Geophysical Union (AGU), pp. 384–404, May 27, 2014. doi: 10.1002/2014ms000314.  
  
S. Wang, A. H. Sobel, F. Zhang, Y. Q. Sun, Y. Yueand L. Zhou, “Regional Simulation of the October and November MJO Events Observed during the CINDY/DYNAMO Field Campaign at Gray Zone Resolution”, *Journal of Climate*, vol. 28, no. 6. American Meteorological Society, pp. 2097–2119, Mar. 13, 2015. doi: 10.1175/jcli-d-14-00294.1.  
  
J. Wei and F. Zhang, “Tracking gravity waves in moist baroclinic jet-front systems”, *Journal of Advances in Modeling Earth Systems*, vol. 7, no. 1. American Geophysical Union (AGU), pp. 67–91, Jan. 20, 2015. doi: 10.1002/2014ms000395.  
  
J. Wei, F. Zhangand J. H. Richter, “An Analysis of Gravity Wave Spectral Characteristics in Moist Baroclinic Jet–Front Systems”, *Journal of the Atmospheric Sciences*, vol. 73, no. 8. American Meteorological Society, pp. 3133–3155, Jul. 25, 2016. doi: 10.1175/jas-d-15-0316.1.  
  
Y. Weng and F. Zhang, “Assimilating Airborne Doppler Radar Observations with an Ensemble Kalman Filter for Convection-Permitting Hurricane Initialization and Prediction: Katrina (2005)”, *Monthly Weather Review*, vol. 140, no. 3. American Meteorological Society, pp. 841–859, Feb. 01, 2012. doi: 10.1175/2011mwr3602.1.  
  
Y. WENG and F. ZHANG, “Advances in Convection-Permitting Tropical Cyclone Analysis and Prediction through EnKF Assimilation of Reconnaissance Aircraft Observations”, *Journal of the Meteorological Society of Japan. Ser. II*, vol. 94, no. 4. Meteorological Society of Japan, pp. 345–358, 2016. doi: 10.2151/jmsj.2016-018.  
  
B. Xie and F. Zhang, “Impacts of Typhoon Track and Island Topography on the Heavy Rainfalls in Taiwan Associated with Morakot (2009)”, *Monthly Weather Review*, vol. 140, no. 10. American Meteorological Society, pp. 3379–3394, Oct. 01, 2012. doi: 10.1175/mwr-d-11-00240.1.  
  
B. Xie, F. Zhang, Q. Zhang, J. Poterjoyand Y. Weng, “Observing Strategy and Observation Targeting for Tropical Cyclones Using Ensemble-Based Sensitivity Analysis and Data Assimilation”, *Monthly Weather Review*, vol. 141, no. 5. American Meteorological Society, pp. 1437–1453, May 01, 2013. doi: 10.1175/mwr-d-12-00188.1.  
  
Y. Ying and F. Zhang, “An adaptive covariance relaxation method for ensemble data assimilation”, *Quarterly Journal of the Royal Meteorological Society*, vol. 141, no. 692. Wiley, pp. 2898–2906, Aug. 07, 2015. doi: 10.1002/qj.2576.  
  
Y. Ying and F. Zhang, “Practical and Intrinsic Predictability of Multiscale Weather and Convectively Coupled Equatorial Waves during the Active Phase of an MJO”, *Journal of the Atmospheric Sciences*, vol. 74, no. 11. American Meteorological Society, pp. 3771–3785, Nov. 01, 2017. doi: 10.1175/jas-d-17-0157.1.  
  
Y. Ying and F. Zhang, “Potentials in Improving Predictability of Multiscale Tropical Weather Systems Evaluated through Ensemble Assimilation of Simulated Satellite-Based Observations”, *Journal of the Atmospheric Sciences*, vol. 75, no. 5. American Meteorological Society, pp. 1675–1698, May 2018. doi: 10.1175/jas-d-17-0245.1.  
  
Y. Ying, F. Zhangand J. L. Anderson, “On the Selection of Localization Radius in Ensemble Filtering for Multiscale Quasigeostrophic Dynamics”, *Monthly Weather Review*, vol. 146, no. 2. American Meteorological Society, pp. 543–560, Feb. 2018. doi: 10.1175/mwr-d-17-0336.1.  
  
Y. Yun, Q. Zeng, B. W. Greenand F. Zhang, “Mitigating atmospheric effects in InSAR measurements through high-resolution data assimilation and numerical simulations with a weather prediction model”, *International Journal of Remote Sensing*, vol. 36, no. 8. Informa UK Limited, pp. 2129–2147, Apr. 18, 2015. doi: 10.1080/01431161.2015.1034894.  
  
F. Zhang and K. Emanuel, “On the Role of Surface Fluxes and WISHE in Tropical Cyclone Intensification”, *Journal of the Atmospheric Sciences*, vol. 73, no. 5. American Meteorological Society, pp. 2011–2019, Apr. 22, 2016. doi: 10.1175/jas-d-16-0011.1.  
  
F. Zhang, M. Minamideand E. E. Clothiaux, “Potential impacts of assimilating all‐sky infrared satellite radiances from GOES‐R on convection‐permitting analysis and prediction of tropical cyclones”, *Geophysical Research Letters*, vol. 43, no. 6. American Geophysical Union (AGU), pp. 2954–2963, Mar. 24, 2016. doi: 10.1002/2016gl068468.  
  
F. Zhang and D. Tao, “Effects of Vertical Wind Shear on the Predictability of Tropical Cyclones”, *Journal of the Atmospheric Sciences*, vol. 70, no. 3. American Meteorological Society, pp. 975–983, Mar. 01, 2013. doi: 10.1175/jas-d-12-0133.1.  
  
F. Zhang, D. Tao, Y. Q. Sunand J. D. Kepert, “Dynamics and predictability of secondary eyewall formation in sheared tropical cyclones”, *Journal of Advances in Modeling Earth Systems*, vol. 9, no. 1. American Geophysical Union (AGU), pp. 89–112, Jan. 22, 2017. doi: 10.1002/2016ms000729.  
  
F. Zhang, S. Taraphdarand S. Wang, “The role of global circumnavigating mode in the MJO initiation and propagation”, *Journal of Geophysical Research: Atmospheres*, vol. 122, no. 11. American Geophysical Union (AGU), pp. 5837–5856, Jun. 10, 2017. doi: 10.1002/2016jd025665.  
  
F. Zhang, “Aircraft measurements of gravity waves in the upper troposphere and lower stratosphere during the START08 Field Experiment”, *[]*. Copernicus GmbH, Feb. 20, 2015. doi: 10.5194/acpd-15-4725-2015.  
  
F. Zhang and Y. Weng, “Predicting Hurricane Intensity and Associated Hazards: A Five-Year Real-Time Forecast Experiment with Assimilation of Airborne Doppler Radar Observations”, *Bulletin of the American Meteorological Society*, vol. 96, no. 1. American Meteorological Society, pp. 25–33, Jan. 01, 2015. doi: 10.1175/bams-d-13-00231.1.  
  
F. Zhang and Y. Weng, “Predicting Hurricane Intensity and Associated Hazards: A Five-Year Real-Time Forecast Experiment with Assimilation of Airborne Doppler Radar Observations”, *Bulletin of the American Meteorological Society*, vol. 96, no. 1. American Meteorological Society, pp. 25–33, Jan. 01, 2015. doi: 10.1175/bams-d-13-00231.1.  
  
F. Zhang, Y. Weng, J. F. Gamacheand F. D. Marks, “Performance of convection-permitting hurricane initialization and prediction during 2008-2010 with ensemble data assimilation of inner-core airborne Doppler radar observations”, *Geophysical Research Letters*, vol. 38, no. 15. American Geophysical Union (AGU), Aug. 2011. doi: 10.1029/2011gl048469.  
  
F. Zhang, Y. Weng, Y.-H. Kuo, J. S. Whitakerand B. Xie, “Predicting Typhoon Morakot’s Catastrophic Rainfall with a Convection-Permitting Mesoscale Ensemble System”, *Weather and Forecasting*, vol. 25, no. 6. American Meteorological Society, pp. 1816–1825, Dec. 01, 2010. doi: 10.1175/2010waf2222414.1.  
  
Y. Zhang, Z. Meng, F. Zhangand Y. Weng, “Predictability of Tropical Cyclone Intensity Evaluated through 5-yr Forecasts with a Convection-Permitting Regional-Scale Model in the Atlantic Basin”, *Weather and Forecasting*, vol. 29, no. 4. American Meteorological Society, pp. 1003–1023, Jul. 22, 2014. doi: 10.1175/waf-d-13-00085.1.  
  
Y. Zhang, F. Zhang, C. A. Davisand J. Sun, “Diurnal Evolution and Structure of Long-Lived Mesoscale Convective Vortices along the Mei-Yu Front over the East China Plains”, *Journal of the Atmospheric Sciences*, vol. 75, no. 3. American Meteorological Society, pp. 1005–1025, Mar. 01, 2018. doi: 10.1175/jas-d-17-0197.1.  
  
Y. Zhang, F. Zhang, D. J. Stensrudand Z. Meng, “Practical Predictability of the 20 May 2013 Tornadic Thunderstorm Event in Oklahoma: Sensitivity to Synoptic Timing and Topographical Influence”, *Monthly Weather Review*, vol. 143, no. 8. American Meteorological Society, pp. 2973–2997, Aug. 01, 2015. doi: 10.1175/mwr-d-14-00394.1.  
  
Y. Zhang, F. Zhang, D. J. Stensrudand Z. Meng, “Intrinsic Predictability of the 20 May 2013 Tornadic Thunderstorm Event in Oklahoma at Storm Scales”, *Monthly Weather Review*, vol. 144, no. 4. American Meteorological Society, pp. 1273–1298, Mar. 23, 2016. doi: 10.1175/mwr-d-15-0105.1.  
  
L. Zhu, X. Chenand L. Bai, “Relative Roles of Low‐Level Wind Speed and Moisture in the Diurnal Cycle of Rainfall Over a Tropical Island Under Monsoonal Flows”, *Geophysical Research Letters*, vol. 47, no. 8. American Geophysical Union (AGU), Apr. 15, 2020. doi: 10.1029/2020gl087467.  
  
L. Zhu, Z. Meng, F. Zhangand P. M. Markowski, “The influence of sea- and land-breeze circulations on the diurnal variability of precipitation over a tropical island”, *[]*. Copernicus GmbH, Apr. 24, 2017. doi: 10.5194/acp-2017-332.  
  
L. Zhu, “Prediction and Predictability of High-Impact Western Pacific Landfalling Tropical Cyclone Vicente (2012) through Convection-Permitting Ensemble Assimilation of Doppler Radar Velocity”, *Monthly Weather Review*, vol. 144, no. 1. American Meteorological Society, pp. 21–43, Dec. 22, 2015. doi: 10.1175/mwr-d-14-00403.1.  
  
H. Li and V. Misra, “Global seasonal climate predictability in a two tiered forecast system. Part II: boreal winter and spring seasons”, *Climate Dynamics*, vol. 42, no. 5–6. Springer Science and Business Media LLC, pp. 1449–1468, Jun. 13, 2013. doi: 10.1007/s00382-013-1813-x.  
  
V. Misra and H. Li, “The seasonal predictability of the Asian summer monsoon in a two-tiered forecast system”, *Climate Dynamics*, vol. 42, no. 9–10. Springer Science and Business Media LLC, pp. 2491–2507, Jun. 20, 2013. doi: 10.1007/s00382-013-1838-1.  
  
A. McGovern, “Using Artificial Intelligence to Improve Real-Time Decision-Making for High-Impact Weather”, *Bulletin of the American Meteorological Society*, vol. 98, no. 10. American Meteorological Society, pp. 2073–2090, Oct. 01, 2017. doi: 10.1175/bams-d-16-0123.1.  
  
N. Goldenson, S. J. Doherty, C. M. Bitz, M. M. Holland, B. Lightand A. J. Conley, “Arctic climate response to forcing from light-absorbing particles in snow and sea ice in CESM”, *Atmospheric Chemistry and Physics*, vol. 12, no. 17. Copernicus GmbH, pp. 7903–7920, Sep. 05, 2012. doi: 10.5194/acp-12-7903-2012.  
  
K. E. McCusker, K. C. Armour, C. M. Bitzand D. S. Battisti, “Rapid and extensive warming following cessation of solar radiation management”, *Environmental Research Letters*, vol. 9, no. 2. IOP Publishing, p. 024005, Jan. 01, 2014. doi: 10.1088/1748-9326/9/2/024005.  
  
K. E. McCusker, D. S. Battistiand C. M. Bitz, “Inability of stratospheric sulfate aerosol injections to preserve the West Antarctic Ice Sheet”, *Geophysical Research Letters*, vol. 42, no. 12. American Geophysical Union (AGU), pp. 4989–4997, Jun. 24, 2015. doi: 10.1002/2015gl064314.  
  
L. Zhao, “Developing an integrated end-to-end TeraGrid climate modeling environment”, *Proceedings of the 2011 TeraGrid Conference: Extreme Digital Discovery*. ACM, Jul. 18, 2011. doi: 10.1145/2016741.2016790.  
  
S. Bastola and V. Misra, “Evaluation of dynamically downscaled reanalysis precipitation data for hydrological application”, *Hydrological Processes*, vol. 28, no. 4. Wiley, pp. 1989–2002, Mar. 05, 2013. doi: 10.1002/hyp.9734.  
  
C. Selman, V. Misra, L. Stefanova, S. Dinapoliand T. J. Smith III, “On the twenty-first-century wet season projections over the Southeastern United States”, *Regional Environmental Change*, vol. 13, no. S1. Springer Science and Business Media LLC, pp. 153–164, May 22, 2013. doi: 10.1007/s10113-013-0477-8.  
  
J. Um and G. M. McFarquhar, “Optimal numerical methods for determining the orientation averages of single-scattering properties of atmospheric ice crystals”, *Journal of Quantitative Spectroscopy and Radiative Transfer*, vol. 127. Elsevier BV, pp. 207–223, Sep. 2013. doi: 10.1016/j.jqsrt.2013.05.020.  
  
C. Zhang, “How Well Does an FV3‐Based Model Predict Precipitation at a Convection‐Allowing Resolution? Results From CAPS Forecasts for the 2018 NOAA Hazardous Weather Test Bed With Different Physics Combinations”, *Geophysical Research Letters*, vol. 46, no. 6. American Geophysical Union (AGU), pp. 3523–3531, Mar. 25, 2019. doi: 10.1029/2018gl081702.  
  
G. Thompson, “Explicitly-coupled cloud physics and radiation parameterizations and subsequent evaluation in WRF high-resolution convective forecasts”, *Atmospheric Research*, vol. 168. Elsevier BV, pp. 92–104, Feb. 2016. doi: 10.1016/j.atmosres.2015.09.005.  
  
B. Roberts and M. Xue, “The Role of Surface Drag in Mesocyclone Intensification Leading to Tornadogenesis within an Idealized Supercell Simulation”, *Journal of the Atmospheric Sciences*, vol. 74, no. 9. American Meteorological Society, pp. 3055–3077, Aug. 31, 2017. doi: 10.1175/jas-d-16-0364.1.  
  
B. Roberts, M. Xue, A. D. Schenkmanand D. T. Dawson II, “The Role of Surface Drag in Tornadogenesis within an Idealized Supercell Simulation”, *Journal of the Atmospheric Sciences*, vol. 73, no. 9. American Meteorological Society, pp. 3371–3395, Aug. 04, 2016. doi: 10.1175/jas-d-15-0332.1.  
  
A. C. Fletcher, Y. S. Dimant, M. M. Oppenheimand J. M. Fontenla, “Effects of Ion Magnetization on the Farley–Buneman Instability in the Solar Chromosphere”, *The Astrophysical Journal*, vol. 857, no. 2. American Astronomical Society, p. 129, Apr. 24, 2018. doi: 10.3847/1538-4357/aab71a.  
  
G. Guttormsen, A. C. Fletcherand M. M. Oppenheim, “Atomic‐Scale Simulations of Meteor Ablation”, *Journal of Geophysical Research: Space Physics*, vol. 125, no. 9. American Geophysical Union (AGU), Sep. 2020. doi: 10.1029/2020ja028229.  
  
J. Liu, W. Wang, A. Burns, M. Oppenheimand Y. Dimant, “Faster Traveling Atmosphere Disturbances Caused by Polar Ionosphere Turbulence Heating”, *Journal of Geophysical Research: Space Physics*. American Geophysical Union (AGU), Mar. 09, 2018. doi: 10.1002/2017ja024746.  
  
J. Liu, W. Wang, M. Oppenheim, Y. Dimant, M. Wiltbergerand S. Merkin, “Anomalous electron heating effects on the *E* region ionosphere in TIEGCM”, *Geophysical Research Letters*, vol. 43, no. 6. American Geophysical Union (AGU), pp. 2351–2358, Mar. 19, 2016. doi: 10.1002/2016gl068010.  
  
W. J. Longley, P. J. Erickson, J. Vierinen, M. M. Oppenheim, F. D. Lindand Y. S. Dimant, “Millstone Hill ISR Measurements of Small Aspect Angle Spectra”, *Journal of Geophysical Research: Space Physics*, vol. 125, no. 6. American Geophysical Union (AGU), Jun. 2020. doi: 10.1029/2019ja027708.  
  
W. J. Longley, M. M. Oppenheimand Y. S. Dimant, “Nonlinear Effects of Electron‐Electron Collisions on ISR Temperature Measurements”, *Journal of Geophysical Research: Space Physics*, vol. 124, no. 7. American Geophysical Union (AGU), pp. 6313–6329, Jul. 2019. doi: 10.1029/2019ja026753.  
  
W. J. Longley, M. M. Oppenheim, A. C. Fletcherand Y. S. Dimant, “ISR Spectra Simulations With Electron‐Ion Coulomb Collisions”, *Journal of Geophysical Research: Space Physics*, vol. 123, no. 4. Wiley, pp. 2990–3004, Apr. 2018. doi: 10.1002/2017ja025015.  
  
W. J. Longley, M. M. Oppenheim, N. M. Pedatellaand Y. S. Dimant, “The Photoelectron‐Driven Upper Hybrid Instability as the Cause of 150‐km Echoes”, *Geophysical Research Letters*, vol. 47, no. 8. American Geophysical Union (AGU), Apr. 16, 2020. doi: 10.1029/2020gl087391.  
  
M. M. Oppenheim and Y. S. Dimant, “Kinetic simulations of 3-D Farley-Buneman turbulence and anomalous electron heating”, *Journal of Geophysical Research: Space Physics*, vol. 118, no. 3. American Geophysical Union (AGU), pp. 1306–1318, Mar. 2013. doi: 10.1002/jgra.50196.  
  
M. M. Oppenheim and Y. S. Dimant, “First 3-D simulations of meteor plasma dynamics and turbulence”, *Geophysical Research Letters*, vol. 42, no. 3. American Geophysical Union (AGU), pp. 681–687, Feb. 09, 2015. doi: 10.1002/2014gl062411.  
  
M. M. Oppenheim and Y. S. Dimant, “Photoelectron‐induced waves: A likely source of 150 km radar echoes and enhanced electron modes”, *Geophysical Research Letters*, vol. 43, no. 8. American Geophysical Union (AGU), pp. 3637–3644, Apr. 27, 2016. doi: 10.1002/2016gl068179.  
  
M. Oppenheim, Y. Dimant, W. Longleyand A. C. Fletcher, “Newly Discovered Source of Turbulence and Heating in the Solar Chromosphere”, *The Astrophysical Journal*, vol. 891, no. 1. American Astronomical Society, p. L9, Feb. 27, 2020. doi: 10.3847/2041-8213/ab75bc.  
  
S. Perkins, “Mysterious radar echoes in the sky explained?”, *Science*. American Association for the Advancement of Science (AAAS), May 05, 2016. doi: 10.1126/science.aaf9863.  
  
G. Sugar, M. M. Oppenheim, Y. S. Dimantand S. Close, “Formation of Plasma Around a Small Meteoroid: Simulation and Theory”, *Journal of Geophysical Research: Space Physics*, vol. 123, no. 5. American Geophysical Union (AGU), pp. 4080–4093, May 2018. doi: 10.1002/2018ja025265.  
  
G. Sugar, M. M. Oppenheim, Y. S. Dimantand S. Close, “Formation of Plasma Around a Small Meteoroid: Electrostatic Simulations”, *Journal of Geophysical Research: Space Physics*, vol. 124, no. 5. American Geophysical Union (AGU), pp. 3810–3826, May 2019. doi: 10.1029/2018ja026434.  
  
M. Wiltberger, “Effects of electrojet turbulence on a magnetosphere‐ionosphere simulation of a geomagnetic storm”, *Journal of Geophysical Research: Space Physics*, vol. 122, no. 5. American Geophysical Union (AGU), pp. 5008–5027, May 2017. doi: 10.1002/2016ja023700.  
  
M. A. Young, M. M. Oppenheimand Y. S. Dimant, “Hybrid simulations of coupled Farley‐Buneman/gradient drift instabilities in the equatorial *E* region ionosphere”, *Journal of Geophysical Research: Space Physics*, vol. 122, no. 5. American Geophysical Union (AGU), pp. 5768–5781, May 2017. doi: 10.1002/2017ja024161.  
  
M. A. Young, M. M. Oppenheimand Y. S. Dimant, “The Farley‐Buneman Spectrum in 2‐D and 3‐D Particle‐in‐Cell Simulations”, *Journal of Geophysical Research: Space Physics*, vol. 125, no. 1. American Geophysical Union (AGU), Jan. 2020. doi: 10.1029/2019ja027326.  
  
D. A. Jacobsen and I. Senocak, “Multi-level parallelism for incompressible flow computations on GPU clusters”, *Parallel Computing*, vol. 39, no. 1. Elsevier BV, pp. 1–20, Jan. 2013. doi: 10.1016/j.parco.2012.10.002.  
  
B. R. Bzdek, J. W. DePalmaand M. V. Johnston, “Mechanisms of Atmospherically Relevant Cluster Growth”, *Accounts of Chemical Research*, vol. 50, no. 8. American Chemical Society (ACS), pp. 1965–1975, Jul. 12, 2017. doi: 10.1021/acs.accounts.7b00213.  
  
B. R. Bzdek, J. W. DePalma, D. P. Ridge, J. Laskinand M. V. Johnston, “Fragmentation Energetics of Clusters Relevant to Atmospheric New Particle Formation”, *Journal of the American Chemical Society*, vol. 135, no. 8. American Chemical Society (ACS), pp. 3276–3285, Feb. 12, 2013. doi: 10.1021/ja3124509.  
  
J. W. DePalma, B. R. Bzdek, D. J. Dorenand M. V. Johnston, “Structure and Energetics of Nanometer Size Clusters of Sulfuric Acid with Ammonia and Dimethylamine”, *The Journal of Physical Chemistry A*, vol. 116, no. 3. American Chemical Society (ACS), pp. 1030–1040, Jan. 11, 2012. doi: 10.1021/jp210127w.  
  
J. W. DePalma, B. R. Bzdek, D. J. Dorenand M. V. Johnston, “Structure and Energetics of Nanometer Size Clusters of Sulfuric Acid with Ammonia and Dimethylamine”, *The Journal of Physical Chemistry A*, vol. 116, no. 3. American Chemical Society (ACS), pp. 1030–1040, Jan. 11, 2012. doi: 10.1021/jp210127w.  
  
J. W. DePalma, B. R. Bzdek, D. P. Ridgeand M. V. Johnston, “Activation Barriers in the Growth of Molecular Clusters Derived from Sulfuric Acid and Ammonia”, *The Journal of Physical Chemistry A*, vol. 118, no. 49. American Chemical Society (ACS), pp. 11547–11554, Nov. 26, 2014. doi: 10.1021/jp507769b.  
  
J. W. DePalma, D. J. Dorenand M. V. Johnston, “Formation and Growth of Molecular Clusters Containing Sulfuric Acid, Water, Ammonia, and Dimethylamine”, *The Journal of Physical Chemistry A*, vol. 118, no. 29. American Chemical Society (ACS), pp. 5464–5473, Jul. 09, 2014. doi: 10.1021/jp503348b.  
  
J. W. DePalma, A. J. Horan, W. A. Hall IVand M. V. Johnston, “Thermodynamics of oligomer formation: implications for secondary organic aerosol formation and reactivity”, *Physical Chemistry Chemical Physics*, vol. 15, no. 18. Royal Society of Chemistry (RSC), p. 6935, 2013. doi: 10.1039/c3cp44586k.  
  
J. W. DePalma, J. Wang, A. S. Wexlerand M. V. Johnston, “Growth of Ammonium Bisulfate Clusters by Adsorption of Oxygenated Organic Molecules”, *The Journal of Physical Chemistry A*, vol. 119, no. 45. American Chemical Society (ACS), pp. 11191–11198, Oct. 30, 2015. doi: 10.1021/acs.jpca.5b07744.  
  
J. M. Thomas, S. He, C. Larriba-Andaluz, J. W. DePalma, M. V. Johnstonand C. J. Hogan Jr., “Ion mobility spectrometry-mass spectrometry examination of the structures, stabilities, and extents of hydration of dimethylamine–sulfuric acid clusters”, *Physical Chemistry Chemical Physics*, vol. 18, no. 33. Royal Society of Chemistry (RSC), pp. 22962–22972, 2016. doi: 10.1039/c6cp03432b.  
  
N. Jeevanjee and D. M. Romps, “Convective self-aggregation, cold pools, and domain size”, *Geophysical Research Letters*, vol. 40, no. 5. American Geophysical Union (AGU), pp. 994–998, Mar. 13, 2013. doi: 10.1002/grl.50204.  
  
D. Higdon, “Computer Model Calibration Using the Ensemble Kalman Filter”, *Technometrics*, vol. 55, no. 4. Informa UK Limited, pp. 488–500, Nov. 2013. doi: 10.1080/00401706.2013.842936.  
  
C. S. Jackson and G. Huerta, “Empirical Bayes approach to climate model calibration”, *[]*. Copernicus GmbH, Mar. 04, 2016. doi: 10.5194/gmd-2016-20.  
  
A. Nosedal-Sanchez, C. S. Jacksonand G. Huerta, “A new metric for climate models that includes field and spatial dependencies using Gaussian Markov Random Fields”, *[]*. Copernicus GmbH, Jan. 15, 2016. doi: 10.5194/gmd-2015-250.  
  
Y. Qian, “Uncertainty Quantification in Climate Modeling and Projection”, *Bulletin of the American Meteorological Society*, vol. 97, no. 5. American Meteorological Society, pp. 821–824, May 01, 2016. doi: 10.1175/bams-d-15-00297.1.  
  
T. Yokohata, “Reliability and importance of structural diversity of climate model ensembles”, *Climate Dynamics*, vol. 41, no. 9–10. Springer Science and Business Media LLC, pp. 2745–2763, Apr. 04, 2013. doi: 10.1007/s00382-013-1733-9.  
  
T. Yokohata, “Reliability of multi-model and structurally different single-model ensembles”, *Climate Dynamics*, vol. 39, no. 3–4. Springer Science and Business Media LLC, pp. 599–616, Oct. 12, 2011. doi: 10.1007/s00382-011-1203-1.  
  
B. P. Kirtman, “Impact of ocean model resolution on CCSM climate simulations”, *Climate Dynamics*, vol. 39, no. 6. Springer Science and Business Media LLC, pp. 1303–1328, Sep. 2012. doi: 10.1007/s00382-012-1500-3.  
  
B. P. Kirtman, “Impact of ocean model resolution on CCSM climate simulations”, *Climate Dynamics*, vol. 39, no. 6. Springer Science and Business Media LLC, pp. 1303–1328, Sep. 2012. doi: 10.1007/s00382-012-1500-3.  
  
E. M. Maddox and G. L. Mullendore, “Determination of Best Tropopause Definition for Convective Transport Studies”, *Journal of the Atmospheric Sciences*, vol. 75, no. 10. American Meteorological Society, pp. 3433–3446, Oct. 2018. doi: 10.1175/jas-d-18-0032.1.  
  
A. D. Crouch, “Resolving the Azimuthal Ambiguity in Vector Magnetogram Data with the Divergence-Free Condition: The Effects of Noise and Limited Spatial Resolution”, *Solar Physics*, vol. 282, no. 1. Springer Science and Business Media LLC, pp. 107–131, Oct. 23, 2012. doi: 10.1007/s11207-012-0149-8.  
  
T. Felipe, D. Braun, A. Crouchand A. Birch, “SCATTERING OF THE*f*-MODE BY SMALL MAGNETIC FLUX ELEMENTS FROM OBSERVATIONS AND NUMERICAL SIMULATIONS”, *The Astrophysical Journal*, vol. 757, no. 2. American Astronomical Society, p. 148, Sep. 12, 2012. doi: 10.1088/0004-637x/757/2/148.  
  
M. O. G. Hills, D. R. Durranand P. N. Blossey, “The Dissipation of Trapped Lee Waves. Part II: The Relative Importance of the Boundary Layer and the Stratosphere”, *Journal of the Atmospheric Sciences*, vol. 73, no. 3. American Meteorological Society, pp. 943–955, Feb. 05, 2016. doi: 10.1175/jas-d-15-0175.1.  
  
X. Shi and D. R. Durran, “Estimating the Response of Extreme Precipitation over Midlatitude Mountains to Global Warming”, *Journal of Climate*, vol. 28, no. 10. American Meteorological Society, pp. 4246–4262, May 12, 2015. doi: 10.1175/jcli-d-14-00750.1.  
  
X. Shi and D. Durran, “Sensitivities of Extreme Precipitation to Global Warming Are Lower over Mountains than over Oceans and Plains”, *Journal of Climate*, vol. 29, no. 13. American Meteorological Society, pp. 4779–4791, Jun. 14, 2016. doi: 10.1175/jcli-d-15-0576.1.  
  
A. Bhardwaj, “Downscaling future climate change projections over Puerto Rico using a non-hydrostatic atmospheric model”, *Climatic Change*, vol. 147, no. 1–2. Springer Science and Business Media LLC, pp. 133–147, Jan. 22, 2018. doi: 10.1007/s10584-017-2130-x.  
  
H. Li and V. Misra, “Thirty-two-year ocean–atmosphere coupled downscaling of global reanalysis over the Intra-American Seas”, *Climate Dynamics*, vol. 43, no. 9–10. Springer Science and Business Media LLC, pp. 2471–2489, Feb. 02, 2014. doi: 10.1007/s00382-014-2069-9.  
  
V. Misra, A. Mishraand H. Li, “The sensitivity of the regional coupled ocean-atmosphere simulations over the Intra-Americas seas to the prescribed bathymetry”, *Dynamics of Atmospheres and Oceans*, vol. 76. Elsevier BV, pp. 29–51, Dec. 2016. doi: 10.1016/j.dynatmoce.2016.08.007.  
  
C. Selman and V. Misra, “The impact of an extreme case of irrigation on the southeastern United States climate”, *Climate Dynamics*, vol. 48, no. 3–4. Springer Science and Business Media LLC, pp. 1309–1327, May 02, 2016. doi: 10.1007/s00382-016-3144-1.  
  
C. Selman and V. Misra, “The sensitivity of southeastern United States climate to varying irrigation vigor”, *Journal of Geophysical Research: Atmospheres*, vol. 121, no. 13. American Geophysical Union (AGU), pp. 7606–7621, Jul. 05, 2016. doi: 10.1002/2016jd025002.  
  
V. Misra, H. Li, Z. Wuand S. DiNapoli, “Global seasonal climate predictability in a two tiered forecast system: part I: boreal summer and fall seasons”, *Climate Dynamics*, vol. 42, no. 5–6. Springer Science and Business Media LLC, pp. 1425–1448, May 29, 2013. doi: 10.1007/s00382-013-1812-y.  
  
A. Subramanian, “The MJO and global warming: a study in CCSM4”, *Climate Dynamics*, vol. 42, no. 7–8. Springer Science and Business Media LLC, pp. 2019–2031, Jun. 27, 2013. doi: 10.1007/s00382-013-1846-1.  
  
J. J. Benedict, M. S. Pritchardand W. D. Collins, “Sensitivity of MJO propagation to a robust positive I ndian O cean dipole event in the superparameterized CAM”, *Journal of Advances in Modeling Earth Systems*, vol. 7, no. 4. American Geophysical Union (AGU), pp. 1901–1917, Nov. 23, 2015. doi: 10.1002/2015ms000530.  
  
E. J. Elliott, S. Yu, G. J. Kooperman, H. Morrison, M. Wangand M. S. Pritchard, “Sensitivity of summer ensembles of fledgling superparameterized U.S. mesoscale convective systems to cloud resolving model microphysics and grid configuration”, *Journal of Advances in Modeling Earth Systems*, vol. 8, no. 2. American Geophysical Union (AGU), pp. 634–649, May 01, 2016. doi: 10.1002/2015ms000567.  
  
C. R. Jones, C. S. Brethertonand M. S. Pritchard, “Mean-state acceleration of cloud-resolving models and large eddy simulations”, *Journal of Advances in Modeling Earth Systems*, vol. 7, no. 4. American Geophysical Union (AGU), pp. 1643–1660, Oct. 29, 2015. doi: 10.1002/2015ms000488.  
  
N. P. Klingaman, “Vertical structure and physical processes of the Madden‐Julian oscillation: Linking hindcast fidelity to simulated diabatic heating and moistening”, *Journal of Geophysical Research: Atmospheres*, vol. 120, no. 10. American Geophysical Union (AGU), pp. 4690–4717, May 26, 2015. doi: 10.1002/2014jd022374.  
  
G. J. Kooperman, M. S. Pritchardand R. C. J. Somerville, “The response of US summer rainfall to quadrupled CO2 climate change in conventional and superparameterized versions of the NCAR community atmosphere model”, *Journal of Advances in Modeling Earth Systems*, vol. 6, no. 3. American Geophysical Union (AGU), pp. 859–882, Aug. 20, 2014. doi: 10.1002/2014ms000306.  
  
M. S. Pritchard and C. S. Bretherton, “Causal Evidence that Rotational Moisture Advection is Critical to the Superparameterized Madden–Julian Oscillation”, *Journal of the Atmospheric Sciences*, vol. 71, no. 2. American Meteorological Society, pp. 800–815, Jan. 31, 2014. doi: 10.1175/jas-d-13-0119.1.  
  
M. S. Pritchard, C. S. Brethertonand C. A. DeMott, “Restricting 32-128 km horizontal scales hardly affects the MJO in the Superparameterized Community Atmosphere Model v.3.0 but the number of cloud-resolving grid columns constrains vertical mixing”, *Journal of Advances in Modeling Earth Systems*, vol. 6, no. 3. American Geophysical Union (AGU), pp. 723–739, Aug. 05, 2014. doi: 10.1002/2014ms000340.  
  
M. S. Pritchard and D. Yang, “Response of the Superparameterized Madden–Julian Oscillation to Extreme Climate and Basic-State Variation Challenges a Moisture Mode View”, *Journal of Climate*, vol. 29, no. 13. American Meteorological Society, pp. 4995–5008, Jun. 27, 2016. doi: 10.1175/jcli-d-15-0790.1.  
  
J. Sun and M. S. Pritchard, “Effects of Explicit Convection on Land Surface Air Temperature and Land‐Atmosphere Coupling in the Thermal Feedback Pathway”, *Journal of Advances in Modeling Earth Systems*, vol. 10, no. 10. American Geophysical Union (AGU), pp. 2376–2392, Oct. 2018. doi: 10.1029/2018ms001301.  
  
P. K. Xavier, “Vertical structure and physical processes of the Madden‐Julian Oscillation: Biases and uncertainties at short range”, *Journal of Geophysical Research: Atmospheres*, vol. 120, no. 10. American Geophysical Union (AGU), pp. 4749–4763, May 26, 2015. doi: 10.1002/2014jd022718.  
  
S. Yu and M. S. Pritchard, “The effect of large-scale model time step and multiscale coupling frequency on cloud climatology, vertical structure, and rainfall extremes in a superparameterized GCM”, *Journal of Advances in Modeling Earth Systems*, vol. 7, no. 4. American Geophysical Union (AGU), pp. 1977–1996, Dec. 2015. doi: 10.1002/2015ms000493.  
  
M. D. Fowler, M. S. Pritchardand G. J. Kooperman, “Assessing the Impact of Indian Irrigation on Precipitation in the Irrigation-Enabled Community Earth System Model”, *Journal of Hydrometeorology*, vol. 19, no. 2. American Meteorological Society, pp. 427–443, Feb. 01, 2018. doi: 10.1175/jhm-d-17-0038.1.  
  
P. Gentine, M. Pritchard, S. Rasp, G. Reinaudiand G. Yacalis, “Could Machine Learning Break the Convection Parameterization Deadlock?”, *Geophysical Research Letters*, vol. 45, no. 11. American Geophysical Union (AGU), pp. 5742–5751, Jun. 12, 2018. doi: 10.1029/2018gl078202.  
  
H. Qin, M. S. Pritchard, G. J. Koopermanand H. Parishani, “Global Effects of Superparameterization on Hydrothermal Land‐Atmosphere Coupling on Multiple Timescales”, *Journal of Advances in Modeling Earth Systems*, vol. 10, no. 2. American Geophysical Union (AGU), pp. 530–549, Feb. 2018. doi: 10.1002/2017ms001185.  
  
S. Rasp, M. S. Pritchardand P. Gentine, “Deep learning to represent subgrid processes in climate models”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 39. Proceedings of the National Academy of Sciences, pp. 9684–9689, Sep. 06, 2018. doi: 10.1073/pnas.1810286115.  
  
D. Brunner, “Comparative analysis of meteorological performance of coupled chemistry-meteorology models in the context of AQMEII phase 2”, *Atmospheric Environment*, vol. 115. Elsevier BV, pp. 470–498, Aug. 2015. doi: 10.1016/j.atmosenv.2014.12.032.  
  
C. Cai, “Incorporation of new particle formation and early growth treatments into WRF/Chem: Model improvement, evaluation, and impacts of anthropogenic aerosols over East Asia”, *Atmospheric Environment*, vol. 124. Elsevier BV, pp. 262–284, Jan. 2016. doi: 10.1016/j.atmosenv.2015.05.046.  
  
P. Campbell, “Evaluation of a multi-scale WRF-CAM5 simulation during the 2010 East Asian Summer Monsoon”, *Atmospheric Environment*, vol. 169. Elsevier BV, pp. 204–217, Nov. 2017. doi: 10.1016/j.atmosenv.2017.09.008.  
  
P. Campbell, “A multi-model assessment for the 2006 and 2010 simulations under the Air Quality Model Evaluation International Initiative (AQMEII) phase 2 over North America: Part I. Indicators of the sensitivity of O3 and PM2.5 formation regimes”, *Atmospheric Environment*, vol. 115. Elsevier BV, pp. 569–586, Aug. 2015. doi: 10.1016/j.atmosenv.2014.12.026.  
  
P. Campbell, “A multi-model assessment for the 2006 and 2010 simulations under the Air Quality Model Evaluation International Initiative (AQMEII) phase 2 over North America: Part I. Indicators of the sensitivity of O3 and PM2.5 formation regimes”, *Atmospheric Environment*, vol. 115. Elsevier BV, pp. 569–586, Aug. 2015. doi: 10.1016/j.atmosenv.2014.12.026.  
  
Y. Chen, Y. Zhang, J. Fan, L.-Y. Leung, Q. Zhangand K. He, “Application of an Online-Coupled Regional Climate Model, WRF-CAM5, over East Asia for Examination of Ice Nucleation Schemes: Part I. Comprehensive Model Evaluation and Trend Analysis for 2006 and 2011”, *Climate*, vol. 3, no. 3. MDPI AG, pp. 627–667, Aug. 18, 2015. doi: 10.3390/cli3030627.  
  
L. Giordano, “Assessment of the MACC reanalysis and its influence as chemical boundary conditions for regional air quality modeling in AQMEII-2”, *Atmospheric Environment*, vol. 115. Elsevier BV, pp. 371–388, Aug. 2015. doi: 10.1016/j.atmosenv.2015.02.034.  
  
J. He, “Multi-year application of WRF-CAM5 over East Asia-Part I: Comprehensive evaluation and formation regimes of O3 and PM2.5”, *Atmospheric Environment*, vol. 165. Elsevier BV, pp. 122–142, Sep. 2017. doi: 10.1016/j.atmosenv.2017.06.015.  
  
U. Im, “Evaluation of operational on-line-coupled regional air quality models over Europe and North America in the context of AQMEII phase 2. Part I: Ozone”, *Atmospheric Environment*, vol. 115. Elsevier BV, pp. 404–420, Aug. 2015. doi: 10.1016/j.atmosenv.2014.09.042.  
  
U. Im, “Evaluation of operational online-coupled regional air quality models over Europe and North America in the context of AQMEII phase 2. Part II: Particulate matter”, *Atmospheric Environment*, vol. 115. Elsevier BV, pp. 421–441, Aug. 2015. doi: 10.1016/j.atmosenv.2014.08.072.  
  
C. Knote, “Influence of the choice of gas-phase mechanism on predictions of key gaseous pollutants during the AQMEII phase-2 intercomparison”, *Atmospheric Environment*, vol. 115. Elsevier BV, pp. 553–568, Aug. 2015. doi: 10.1016/j.atmosenv.2014.11.066.  
  
P. Li, “High reduction of ozone and particulate matter during the 2016 G-20 summit in Hangzhou by forced emission controls of industry and traffic”, *Environmental Chemistry Letters*, vol. 15, no. 4. Springer Science and Business Media LLC, pp. 709–715, Jun. 21, 2017. doi: 10.1007/s10311-017-0642-2.  
  
X. Li, “Source contributions of urban PM2.5 in the Beijing–Tianjin–Hebei region: Changes between 2006 and 2013 and relative impacts of emissions and meteorology”, *Atmospheric Environment*, vol. 123. Elsevier BV, pp. 229–239, Dec. 2015. doi: 10.1016/j.atmosenv.2015.10.048.  
  
P. A. Makar, “Feedbacks between air pollution and weather, part 2: Effects on chemistry”, *Atmospheric Environment*, vol. 115. Elsevier BV, pp. 499–526, Aug. 2015. doi: 10.1016/j.atmosenv.2014.10.021.  
  
P. A. Makar, “Feedbacks between air pollution and weather, Part 1: Effects on weather”, *Atmospheric Environment*, vol. 115. Elsevier BV, pp. 442–469, Aug. 2015. doi: 10.1016/j.atmosenv.2014.12.003.  
  
P. K. Saha, “Quantifying the volatility of organic aerosol in the southeastern US”, *Atmospheric Chemistry and Physics*, vol. 17, no. 1. Copernicus GmbH, pp. 501–520, Jan. 11, 2017. doi: 10.5194/acp-17-501-2017.  
  
K. Wang, “A multi-model assessment for the 2006 and 2010 simulations under the Air Quality Model Evaluation International Initiative (AQMEII) Phase 2 over North America: Part II. Evaluation of column variable predictions using satellite data”, *Atmospheric Environment*, vol. 115. Elsevier BV, pp. 587–603, Aug. 2015. doi: 10.1016/j.atmosenv.2014.07.044.  
  
K. Wang, “Fine-scale application of WRF-CAM5 during a dust storm episode over East Asia: Sensitivity to grid resolutions and aerosol activation parameterizations”, *Atmospheric Environment*, vol. 176. Elsevier BV, pp. 1–20, Mar. 2018. doi: 10.1016/j.atmosenv.2017.12.014.  
  
L. Wang, Y. Zhang, K. Wang, B. Zheng, Q. Zhangand W. Wei, “Application of Weather Research and Forecasting Model with Chemistry (WRF/Chem) over northern China: Sensitivity study, comparative evaluation, and policy implications”, *Atmospheric Environment*, vol. 124. Elsevier BV, pp. 337–350, Jan. 2016. doi: 10.1016/j.atmosenv.2014.12.052.  
  
K. Yahya, T. Glotfelty, K. Wang, Y. Zhangand A. Nenes, “Modeling regional air quality and climate: improving organic aerosol and aerosol activation processes in WRF/Chem version 3.7.1”, *Geoscientific Model Development*, vol. 10, no. 6. Copernicus GmbH, pp. 2333–2363, Jun. 27, 2017. doi: 10.5194/gmd-10-2333-2017.  
  
K. Yahya, J. Heand Y. Zhang, “Multiyear applications of WRF/Chem over continental U.S.: Model evaluation, variation trend, and impacts of boundary conditions”, *Journal of Geophysical Research: Atmospheres*, vol. 120, no. 24. American Geophysical Union (AGU), pp. 12748–12777, Dec. 22, 2015. doi: 10.1002/2015jd023819.  
  
K. Yahya, K. Wang, Y. Zhangand T. E. Kleindienst, “Application of WRF/Chem over North America under the AQMEII Phase 2 – Part 2: Evaluation of 2010 application and responses of air quality and meteorology–chemistry interactions to changes in emissions and meteorology from 2006 to 2010”, *Geoscientific Model Development*, vol. 8, no. 7. Copernicus GmbH, pp. 2095–2117, Jul. 16, 2015. doi: 10.5194/gmd-8-2095-2015.  
  
Zhang, “Multiscale Applications of Two Online-Coupled Meteorology-Chemistry Models During Recent Field Campaigns in Australia, Part II: Comparison of WRF/Chem and WRF/Chem-ROMS and Impacts of Air-Sea Interactions and Boundary Conditions”, *Atmosphere*, vol. 10, no. 4. MDPI AG, p. 210, Apr. 20, 2019. doi: 10.3390/atmos10040210.  
  
Y. Zhang, Y. Chen, J. Fanand L.-Y. Leung, “Application of an Online-Coupled Regional Climate Model, WRF-CAM5, over East Asia for Examination of Ice Nucleation Schemes: Part II. Sensitivity to Heterogeneous Ice Nucleation Parameterizations and Dust Emissions”, *Climate*, vol. 3, no. 3. MDPI AG, pp. 753–774, Sep. 14, 2015. doi: 10.3390/cli3030753.  
  
Y. Zhang, K. Wangand J. He, “Multi-year application of WRF-CAM5 over East Asia-Part II: Interannual variability, trend analysis, and aerosol indirect effects”, *Atmospheric Environment*, vol. 165. Elsevier BV, pp. 222–239, Sep. 2017. doi: 10.1016/j.atmosenv.2017.06.029.  
  
Y. Zhang, “Incorporating an advanced aerosol activation parameterization into WRF-CAM5: Model evaluation and parameterization intercomparison”, *Journal of Geophysical Research: Atmospheres*, vol. 120, no. 14. American Geophysical Union (AGU), pp. 6952–6979, Jul. 22, 2015. doi: 10.1002/2014jd023051.  
  
Y. Zhang, X. Zhang, K. Wang, Q. Zhang, F. Duanand K. He, “Application of WRF/Chem over East Asia: Part II. Model improvement and sensitivity simulations”, *Atmospheric Environment*, vol. 124. Elsevier BV, pp. 301–320, Jan. 2016. doi: 10.1016/j.atmosenv.2015.07.023.  
  
Y. Zhang, X. Zhang, L. Wang, Q. Zhang, F. Duanand K. He, “Application of WRF/Chem over East Asia: Part I. Model evaluation and intercomparison with MM5/CMAQ”, *Atmospheric Environment*, vol. 124. Elsevier BV, pp. 285–300, Jan. 2016. doi: 10.1016/j.atmosenv.2015.07.022.  
  
A. Garai, J. Kleissland S. Sarkar, “Flow and heat transfer in convectively unstable turbulent channel flow with solid-wall heat conduction”, *Journal of Fluid Mechanics*, vol. 757. Cambridge University Press (CUP), pp. 57–81, Sep. 19, 2014. doi: 10.1017/jfm.2014.479.  
  
J. Berchem, R. L. Richard, C. P. Escoubet, S. Wingand F. Pitout, “Asymmetrical response of dayside ion precipitation to a large rotation of the IMF”, *Journal of Geophysical Research: Space Physics*, vol. 121, no. 1. American Geophysical Union (AGU), pp. 263–273, Jan. 2016. doi: 10.1002/2015ja021969.  
  
D. A. Schecter, “Development and Nondevelopment of Binary Mesoscale Vortices into Tropical Cyclones in Idealized Numerical Experiments”, *Journal of the Atmospheric Sciences*, vol. 73, no. 3. American Meteorological Society, pp. 1223–1254, Feb. 15, 2016. doi: 10.1175/jas-d-15-0028.1.  
  
L. A. Martínez-Tossas, M. J. Churchfieldand C. Meneveau, “Large Eddy Simulation of wind turbine wakes: detailed comparisons of two codes focusing on effects of numerics and subgrid modeling”, *Journal of Physics: Conference Series*, vol. 625. IOP Publishing, p. 012024, Jun. 18, 2015. doi: 10.1088/1742-6596/625/1/012024.  
  
R. J. A. M. Stevens, “Dependence of optimal wind turbine spacing on wind farm length”, *Wind Energy*, vol. 19, no. 4. Wiley, pp. 651–663, May 15, 2015. doi: 10.1002/we.1857.  
  
R. J. A. M. Stevens, D. F. Gaymeand C. Meneveau, “Large eddy simulation studies of the effects of alignment and wind farm length”, *Journal of Renewable and Sustainable Energy*, vol. 6, no. 2. AIP Publishing, p. 023105, Mar. 2014. doi: 10.1063/1.4869568.  
  
R. J. A. M. Stevens, D. F. Gaymeand C. Meneveau, “Coupled wake boundary layer model of wind-farms”, *Journal of Renewable and Sustainable Energy*, vol. 7, no. 2. AIP Publishing, p. 023115, Mar. 2015. doi: 10.1063/1.4915287.  
  
R. J. A. M. Stevens, D. F. Gaymeand C. Meneveau, “Effects of turbine spacing on the power output of extended wind-farms”, *Wind Energy*, vol. 19, no. 2. Wiley, pp. 359–370, Mar. 02, 2015. doi: 10.1002/we.1835.  
  
R. J. A. M. Stevens, M. Wilczekand C. Meneveau, “Large-eddy simulation study of the logarithmic law for second- and higher-order moments in turbulent wall-bounded flow”, *Journal of Fluid Mechanics*, vol. 757. Cambridge University Press (CUP), pp. 888–907, Sep. 29, 2014. doi: 10.1017/jfm.2014.510.  
  
M. Wilczek, R. J. A. M. Stevensand C. Meneveau, “Height-dependence of spatio-temporal spectra of wall-bounded turbulence – LES results and model predictions”, *Journal of Turbulence*, vol. 16, no. 10. Informa UK Limited, pp. 937–949, Jun. 04, 2015. doi: 10.1080/14685248.2015.1047497.  
  
M. Wilczek, R. J. A. M. Stevensand C. Meneveau, “Spatio-temporal spectra in the logarithmic layer of wall turbulence: large-eddy simulations and simple models”, *Journal of Fluid Mechanics*, vol. 769. Cambridge University Press (CUP), Mar. 13, 2015. doi: 10.1017/jfm.2015.116.  
  
M. Wilczek, R. J. A. M. Stevens, Y. Naritaand C. Meneveau, “A wavenumber-frequency spectral model for atmospheric boundary layers”, *Journal of Physics: Conference Series*, vol. 524. IOP Publishing, p. 012104, Jun. 16, 2014. doi: 10.1088/1742-6596/524/1/012104.  
  
Q. Pan, M. Ashour‐Abdalla, R. J. Walkerand M. El‐Alaoui, “Ion energization and transport associated with magnetic dipolarizations”, *Geophysical Research Letters*, vol. 41, no. 16. American Geophysical Union (AGU), pp. 5717–5726, Aug. 22, 2014. doi: 10.1002/2014gl061209.  
  
J. Franklin, A. J. Potts, E. C. Fisher, R. M. Cowlingand C. W. Marean, “Paleodistribution modeling in archaeology and paleoanthropology”, *Quaternary Science Reviews*, vol. 110. Elsevier BV, pp. 1–14, Feb. 2015. doi: 10.1016/j.quascirev.2014.12.015.  
  
C. W. Marean, “A new research strategy for integrating studies of paleoclimate, paleoenvironment, and paleoanthropology”, *Evolutionary Anthropology: Issues, News, and Reviews*, vol. 24, no. 2. Wiley, pp. 62–72, Mar. 04, 2015. doi: 10.1002/evan.21443.  
  
E. Shook, “Paleoscape model of coastal South Africa during modern human origins”, *Proceedings of the 2015 XSEDE Conference on Scientific Advancements Enabled by Enhanced Cyberinfrastructure - XSEDE ’15*. ACM Press, 2015. doi: 10.1145/2792745.2792747.  
  
R. J. Bombardi, “The heated condensation framework as a convective trigger in the NCEP Climate Forecast System version 2”, *Journal of Advances in Modeling Earth Systems*, vol. 8, no. 3. American Geophysical Union (AGU), pp. 1310–1329, Aug. 23, 2016. doi: 10.1002/2016ms000668.  
  
P. A. Dirmeyer, “Verification of Land–Atmosphere Coupling in Forecast Models, Reanalyses, and Land Surface Models Using Flux Site Observations”, *Journal of Hydrometeorology*, vol. 19, no. 2. American Meteorological Society, pp. 375–392, Feb. 01, 2018. doi: 10.1175/jhm-d-17-0152.1.  
  
B. Huang, “Reforecasting the ENSO Events in the Past 57 Years (1958–2014)”, *Journal of Climate*, vol. 30, no. 19. American Meteorological Society, pp. 7669–7693, Aug. 30, 2017. doi: 10.1175/jcli-d-16-0642.1.  
  
C.-S. Shin and B. Huang, “Slow and fast annual cycles of the Asian summer monsoon in the NCEP CFSv2”, *Climate Dynamics*, vol. 47, no. 1–2. Springer Science and Business Media LLC, pp. 529–553, Oct. 05, 2015. doi: 10.1007/s00382-015-2854-0.  
  
C.-S. Shin and B. Huang, “A spurious warming trend in the NMME equatorial Pacific SST hindcasts”, *Climate Dynamics*, vol. 53, no. 12. Springer Science and Business Media LLC, pp. 7287–7303, Jun. 28, 2017. doi: 10.1007/s00382-017-3777-8.  
  
R. P. Shukla and B. Huang, “Mean state and interannual variability of the Indian summer monsoon simulation by NCEP CFSv2”, *Climate Dynamics*, vol. 46, no. 11–12. Springer Science and Business Media LLC, pp. 3845–3864, Aug. 26, 2015. doi: 10.1007/s00382-015-2808-6.  
  
R. P. Shukla and J. L. Kinter, “Subseasonal Prediction of Significant Wave Heights over the Western Pacific and Indian Ocean Region”, *Weather and Forecasting*, vol. 31, no. 6. American Meteorological Society, pp. 1733–1751, Nov. 01, 2016. doi: 10.1175/waf-d-16-0078.1.  
  
R. P. Shukla, J. L. Kinterand C.-S. Shin, “Sub-seasonal prediction of significant wave heights over the Western Pacific and Indian Oceans, part II: The impact of ENSO and MJO”, *Ocean Modelling*, vol. 123. Elsevier BV, pp. 1–15, Mar. 2018. doi: 10.1016/j.ocemod.2018.01.002.  
  
B. Huang, “Climate drift of AMOC, North Atlantic salinity and arctic sea ice in CFSv2 decadal predictions”, *Climate Dynamics*, vol. 44, no. 1–2. Springer Science and Business Media LLC, pp. 559–583, Nov. 12, 2014. doi: 10.1007/s00382-014-2395-y.  
  
F. De Sales, G. S. Okin, Y. Xueand K. Dintwe, “On the effects of wildfires on precipitation in Southern Africa”, *Climate Dynamics*, vol. 52, no. 1–2. Springer Science and Business Media LLC, pp. 951–967, Mar. 16, 2018. doi: 10.1007/s00382-018-4174-7.  
  
H. Huang, Y. Gu, Y. Xue, J. Jiangand B. Zhao, “Assessing aerosol indirect effect on clouds and regional climate of East/South Asia and West Africa using NCEP GFS”, *Climate Dynamics*, vol. 52, no. 9–10. Springer Science and Business Media LLC, pp. 5759–5774, Oct. 05, 2018. doi: 10.1007/s00382-018-4476-9.  
  
J. Lee, “Evaluation of multi-decadal UCLA-CFSv2 simulation and impact of interactive atmospheric-ocean feedback on global and regional variability”, *Climate Dynamics*, vol. 52, no. 5–6. Springer Science and Business Media LLC, pp. 3683–3707, Jul. 13, 2018. doi: 10.1007/s00382-018-4351-8.  
  
Y. Liu, Y. Xue, G. MacDonald, P. Coxand Z. Zhang, “Global vegetation variability and its response to elevated CO&lt;sub&gt;2&lt;/sub&gt;, global warming, and climate variability – a study using the offline SSiB4/TRIFFID model and satellite data”, *[]*. Copernicus GmbH, Jun. 06, 2018. doi: 10.5194/esd-2018-40.  
  
Y. Liu, Y. Xue, G. MacDonald, P. Coxand Z. Zhang, “Global vegetation variability and its response to elevated CO&lt;sub&gt;2&lt;/sub&gt;, global warming, and climate variability – a study using the offline SSiB4/TRIFFID model and satellite data”, *Earth System Dynamics*, vol. 10, no. 1. Copernicus GmbH, pp. 9–29, Jan. 07, 2019. doi: 10.5194/esd-10-9-2019.  
  
W. Li, W. Guo, P.-. chi . Hsuand Y. Xue, “Influence of the Madden–Julian oscillation on Tibetan Plateau snow cover at the intraseasonal time-scale”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Jul. 28, 2016. doi: 10.1038/srep30456.  
  
J. Pierret and S. S. P. Shen, “4D Visual Delivery of Big Climate Data: A Fast Web Database Application System”, *Advances in Data Science and Adaptive Analysis*, vol. 9, no. 3. World Scientific Pub Co Pte Lt, p. 1750006, Jul. 2017. doi: 10.1142/s2424922x17500061.  
  
B. Qiu, Y. Xue, J. B. Fisher, W. Guo, J. A. Berryand Y. Zhang, “Satellite Chlorophyll Fluorescence and Soil Moisture Observations Lead to Advances in the Predictive Understanding of Global Terrestrial Coupled Carbon‐Water Cycles”, *Global Biogeochemical Cycles*, vol. 32, no. 3. American Geophysical Union (AGU), pp. 360–375, Mar. 2018. doi: 10.1002/2017gb005744.  
  
Y. Xue, “Spring Land Surface and Subsurface Temperature Anomalies and Subsequent Downstream Late Spring-Summer Droughts/Floods in North America and East Asia”, *Journal of Geophysical Research: Atmospheres*, vol. 123, no. 10. American Geophysical Union (AGU), pp. 5001–5019, May 18, 2018. doi: 10.1029/2017jd028246.  
  
T. Yao, “Recent Third Pole’s Rapid Warming Accompanies Cryospheric Melt and Water Cycle Intensification and Interactions between Monsoon and Environment: Multidisciplinary Approach with Observations, Modeling, and Analysis”, *Bulletin of the American Meteorological Society*, vol. 100, no. 3. American Meteorological Society, pp. 423–444, Mar. 2019. doi: 10.1175/bams-d-17-0057.1.  
  
Y. Zhang, T. Zouand Y. Xue, “An Arctic‐Tibetan Connection on Subseasonal to Seasonal Time Scale”, *Geophysical Research Letters*, vol. 46, no. 5. American Geophysical Union (AGU), pp. 2790–2799, Mar. 06, 2019. doi: 10.1029/2018gl081476.  
  
F. De Sales, Y. Xueand G. S. Okin, “Impact of burned areas on the northern African seasonal climate from the perspective of regional modeling”, *Climate Dynamics*, vol. 47, no. 11. Springer Science and Business Media LLC, pp. 3393–3413, Feb. 25, 2015. doi: 10.1007/s00382-015-2522-4.  
  
A. C. V. Getirana, “Water Balance in the Amazon Basin from a Land Surface Model Ensemble”, *Journal of Hydrometeorology*, vol. 15, no. 6. American Meteorological Society, pp. 2586–2614, Dec. 01, 2014. doi: 10.1175/jhm-d-14-0068.1.  
  
S. Hagos, “Assessment of uncertainties in the response of the African monsoon precipitation to land use change simulated by a regional model”, *Climate Dynamics*, vol. 43, no. 9–10. Springer Science and Business Media LLC, pp. 2765–2775, Feb. 22, 2014. doi: 10.1007/s00382-014-2092-x.  
  
B. Rodríguez-Fonseca, “Variability and Predictability of West African Droughts: A Review on the Role of Sea Surface Temperature Anomalies”, *Journal of Climate*, vol. 28, no. 10. American Meteorological Society, pp. 4034–4060, May 12, 2015. doi: 10.1175/jcli-d-14-00130.1.  
  
M. Shrestha, L. Wang, T. Koike, H. Tsutsui, Y. Xueand Y. Hirabayashi, “Correcting basin-scale snowfall in a mountainous basin using a distributed snowmelt model and remote-sensing data”, *Hydrology and Earth System Sciences*, vol. 18, no. 2. Copernicus GmbH, pp. 747–761, Feb. 21, 2014. doi: 10.5194/hess-18-747-2014.  
  
P. He, “A high order finite difference solver for massively parallel simulations of stably stratified turbulent channel flows”, *Computers & Fluids*, vol. 127. Elsevier BV, pp. 161–173, Mar. 2016. doi: 10.1016/j.compfluid.2015.12.012.  
  
P. He, C. A. Mader, J. R. R. A. Martinsand K. J. Maki, “An aerodynamic design optimization framework using a discrete adjoint approach with OpenFOAM”, *Computers & Fluids*, vol. 168. Elsevier BV, pp. 285–303, May 2018. doi: 10.1016/j.compfluid.2018.04.012.  
  
P. He, C. A. Mader, J. R. R. A. Martinsand K. Maki, “Aerothermal Optimization of Internal Cooling Passages Using a Discrete Adjoint Method”, *2018 Joint Thermophysics and Heat Transfer Conference*. American Institute of Aeronautics and Astronautics, Jun. 24, 2018. doi: 10.2514/6.2018-4080.  
  
P. He, C. A. Mader, J. R. R. A. Martinsand K. Maki, “An Object-oriented Framework for Rapid Discrete Adjoint Development using OpenFOAM”, *AIAA Scitech 2019 Forum*. American Institute of Aeronautics and Astronautics, Jan. 06, 2019. doi: 10.2514/6.2019-1210.  
  
C. M. Patricola and P. Chang, “Structure and dynamics of the Benguela low-level coastal jet”, *Climate Dynamics*, vol. 49, no. 7–8. Springer Science and Business Media LLC, pp. 2765–2788, Dec. 22, 2016. doi: 10.1007/s00382-016-3479-7.  
  
Z. Xu, P. Chang, I. Richter, W. Kimand G. Tang, “Diagnosing southeast tropical Atlantic SST and ocean circulation biases in the CMIP5 ensemble”, *Climate Dynamics*, vol. 43, no. 11. Springer Science and Business Media LLC, pp. 3123–3145, Jul. 16, 2014. doi: 10.1007/s00382-014-2247-9.  
  
Z. Xu, M. Li, C. M. Patricolaand P. Chang, “Oceanic origin of southeast tropical Atlantic biases”, *Climate Dynamics*, vol. 43, no. 11. Springer Science and Business Media LLC, pp. 2915–2930, Aug. 20, 2013. doi: 10.1007/s00382-013-1901-y.  
  
X. Ma, “Winter Extreme Flux Events in the Kuroshio and Gulf Stream Extension Regions and Relationship with Modes of North Pacific and Atlantic Variability”, *Journal of Climate*, vol. 28, no. 12. American Meteorological Society, pp. 4950–4970, Jun. 11, 2015. doi: 10.1175/jcli-d-14-00642.1.  
  
C. M. Patricola, P. Changand R. Saravanan, “Degree of simulated suppression of Atlantic tropical cyclones modulated by flavour of El Niño”, *Nature Geoscience*, vol. 9, no. 2. Springer Science and Business Media LLC, pp. 155–160, Dec. 21, 2015. doi: 10.1038/ngeo2624.  
  
C. M. Patricola, R. Saravananand P. Chang, “A teleconnection between Atlantic sea surface temperature and eastern and central North Pacific tropical cyclones”, *Geophysical Research Letters*, vol. 44, no. 2. American Geophysical Union (AGU), pp. 1167–1174, Jan. 28, 2017. doi: 10.1002/2016gl071965.  
  
J. I. Levy, “Carbon reductions and health co-benefits from US residential energy efficiency measures”, *Environmental Research Letters*, vol. 11, no. 3. IOP Publishing, p. 034017, Mar. 01, 2016. doi: 10.1088/1748-9326/11/3/034017.  
  
S. L. Penn, S. Arunachalam, M. Woody, W. Heiger-Bernays, Y. Tripodisand J. I. Levy, “Estimating State-Specific Contributions to PM 2.5 - and O 3 -Related Health Burden from Residential Combustion and Electricity Generating Unit Emissions in the United States”, *Environmental Health Perspectives*, vol. 125, no. 3. Environmental Health Perspectives, pp. 324–332, Mar. 2017. doi: 10.1289/ehp550.  
  
S. L. Penn, “Modeling variability in air pollution-related health damages from individual airport emissions”, *Environmental Research*, vol. 156. Elsevier BV, pp. 791–800, Jul. 2017. doi: 10.1016/j.envres.2017.04.031.  
  
M. A. Jisan, S. Baoand L. J. Pietrafesa, “Ensemble projection of the sea level rise impact on storm surge and inundation at the coast of Bangladesh”, *Natural Hazards and Earth System Sciences*, vol. 18, no. 1. Copernicus GmbH, pp. 351–364, Jan. 24, 2018. doi: 10.5194/nhess-18-351-2018.  
  
A. Martin, “Evaluation of Atmospheric River Predictions by the WRF Model Using Aircraft and Regional Mesonet Observations of Orographic Precipitation and Its Forcing”, *Journal of Hydrometeorology*, vol. 19, no. 7. American Meteorological Society, pp. 1097–1113, Jul. 01, 2018. doi: 10.1175/jhm-d-17-0098.1.  
  
H. Mao, Z. Yeand C. Driscoll, “Meteorological effects on Hg wet deposition in a forested site in the Adirondack region of New York during 2000–2015”, *Atmospheric Environment*, vol. 168. Elsevier BV, pp. 90–100, Nov. 2017. doi: 10.1016/j.atmosenv.2017.08.058.  
  
Z. Ye, H. Mao, C. T. Driscoll, Y. Wang, Y. Zhangand L. Jaeglé, “Evaluation of CMAQ Coupled With a State‐of‐the‐Art Mercury Chemical Mechanism (CMAQ‐newHg‐Br)”, *Journal of Advances in Modeling Earth Systems*, vol. 10, no. 3. American Geophysical Union (AGU), pp. 668–690, Mar. 2018. doi: 10.1002/2017ms001161.  
  
G. Robinson, I. Groomsand W. Kleiber, “Improving Particle Filter Performance by Smoothing Observations”, *Monthly Weather Review*, vol. 146, no. 8. American Meteorological Society, pp. 2433–2446, Jul. 17, 2018. doi: 10.1175/mwr-d-17-0349.1.  
  
R. Dang, Y. Yang, X.-M. Hu, Z. Wangand S. Zhang, “A Review of Techniques for Diagnosing the Atmospheric Boundary Layer Height (ABLH) Using Aerosol Lidar Data”, *Remote Sensing*, vol. 11, no. 13. MDPI AG, p. 1590, Jul. 04, 2019. doi: 10.3390/rs11131590.  
  
R. Dang, “Atmosphere Boundary Layer Height (ABLH) Determination under Multiple-Layer Conditions Using Micro-Pulse Lidar”, *Remote Sensing*, vol. 11, no. 3. MDPI AG, p. 263, Jan. 29, 2019. doi: 10.3390/rs11030263.  
  
J. Guo, “The Climatology of Lower Tropospheric Temperature Inversions in China from Radiosonde Measurements: Roles of Black Carbon, Local Meteorology, and Large-Scale Subsidence”, *Journal of Climate*, vol. 33, no. 21. American Meteorological Society, pp. 9327–9350, Nov. 01, 2020. doi: 10.1175/jcli-d-19-0278.1.  
  
J. Hu, “An important mechanism of regional O&lt;sub&gt;3&lt;/sub&gt; transport for summer smog over the Yangtze River Delta in East China”, *[]*. Copernicus GmbH, Jul. 26, 2018. doi: 10.5194/acp-2018-479.  
  
X. Hu, “Dynamical Downscaling of CO 2 in 2016 Over the Contiguous United States Using WRF‐VPRM, a Weather‐Biosphere‐Online‐Coupled Model”, *Journal of Advances in Modeling Earth Systems*, vol. 12, no. 4. American Geophysical Union (AGU), Apr. 2020. doi: 10.1029/2019ms001875.  
  
X.-M. Hu, J. Huang, J. D. Fuentes, R. Forkeland N. Zhang, “Advances in Boundary-Layer/Air Pollution Meteorology”, *Advances in Meteorology*, vol. 2016. Hindawi Limited, pp. 1–2, 2016. doi: 10.1155/2016/2825019.  
  
X.-M. Hu, M. Xueand X. Li, “The Use of High-Resolution Sounding Data to Evaluate and Optimize Nonlocal PBL Schemes for Simulating the Slightly Stable Upper Convective Boundary Layer”, *Monthly Weather Review*, vol. 147, no. 10. American Meteorological Society, pp. 3825–3841, Oct. 01, 2019. doi: 10.1175/mwr-d-19-0085.1.  
  
X. Hu, M. Xue, R. A. McPherson, E. Martin, D. H. Rosendahland L. Qiao, “Precipitation Dynamical Downscaling Over the Great Plains”, *Journal of Advances in Modeling Earth Systems*, vol. 10, no. 2. American Geophysical Union (AGU), pp. 421–447, Feb. 2018. doi: 10.1002/2017ms001154.  
  
P. M. Klein, X.-M. Hu, A. Shapiroand M. Xue, “Linkages Between Boundary-Layer Structure and the Development of Nocturnal Low-Level Jets in Central Oklahoma”, *Boundary-Layer Meteorology*, vol. 158, no. 3. Springer Science and Business Media LLC, pp. 383–408, Oct. 23, 2015. doi: 10.1007/s10546-015-0097-6.  
  
H. Li, “Evaluation of retrieval methods of daytime convective boundary layer height based on lidar data”, *Journal of Geophysical Research: Atmospheres*, vol. 122, no. 8. American Geophysical Union (AGU), pp. 4578–4593, Apr. 27, 2017. doi: 10.1002/2016jd025620.  
  
H. Li, Y. Yang, X.-M. Hu, Z. Huang, G. Wangand B. Zhang, “Application of Convective Condensation Level Limiter in Convective Boundary Layer Height Retrieval Based on Lidar Data”, *Atmosphere*, vol. 8, no. 4. MDPI AG, p. 79, Apr. 23, 2017. doi: 10.3390/atmos8040079.  
  
J. Li, “Reduced carbon use efficiency and increased microbial turnover with soil warming”, *Global Change Biology*, vol. 25, no. 3. Wiley, pp. 900–910, Dec. 12, 2018. doi: 10.1111/gcb.14517.  
  
C. Liu, J. Huang, E. Fedorovich, X.-M. Hu, Y. Wangand X. Lee, “The Effect of Aerosol Radiative Heating on Turbulence Statistics and Spectra in the Atmospheric Convective Boundary Layer: A Large-Eddy Simulation Study”, *Atmosphere*, vol. 9, no. 9. MDPI AG, p. 347, Sep. 05, 2018. doi: 10.3390/atmos9090347.  
  
X. Li, “Terrestrial CO 2 Fluxes, Concentrations, Sources and Budget in Northeast China: Observational and Modeling Studies”, *Journal of Geophysical Research: Atmospheres*, vol. 125, no. 6. American Geophysical Union (AGU), Mar. 17, 2020. doi: 10.1029/2019jd031686.  
  
X. Li, X.-M. Hu, Y. Ma, Y. Wang, L. Liand Z. Zhao, “Impact of planetary boundary layer structure on the formation and evolution of air-pollution episodes in Shenyang, Northeast China”, *Atmospheric Environment*, vol. 214. Elsevier BV, p. 116850, Oct. 2019. doi: 10.1016/j.atmosenv.2019.116850.  
  
X. Li, X. Hu, S. Shi, L. Shen, L. Luanand Y. Ma, “Spatiotemporal Variations and Regional Transport of Air Pollutants in Two Urban Agglomerations in Northeast China Plain”, *Chinese Geographical Science*, vol. 29, no. 6. Springer Science and Business Media LLC, pp. 917–933, Dec. 2019. doi: 10.1007/s11769-019-1081-8.  
  
X.-B. Li, “Evaluation of unmanned aerial system in measuring lower tropospheric ozone and fine aerosol particles using portable monitors”, *Atmospheric Environment*, vol. 222. Elsevier BV, p. 117134, Feb. 2020. doi: 10.1016/j.atmosenv.2019.117134.  
  
X.-B. Li, “Three-dimensional analysis of ozone and PM2.5 distributions obtained by observations of tethered balloon and unmanned aerial vehicle in Shanghai, China”, *Stochastic Environmental Research and Risk Assessment*, vol. 32, no. 5. Springer Science and Business Media LLC, pp. 1189–1203, Mar. 05, 2018. doi: 10.1007/s00477-018-1524-2.  
  
X. Sun, M. Xue, J. Brotzge, R. A. McPherson, X.-M. Huand X.-Q. Yang, “An evaluation of dynamical downscaling of Central Plains summer precipitation using a WRF-based regional climate model at a convection-permitting 4 km resolution”, *Journal of Geophysical Research: Atmospheres*, vol. 121, no. 23. American Geophysical Union (AGU), pp. 13, 801–13, 825, Dec. 02, 2016. doi: 10.1002/2016jd024796.  
  
A. Thomas, A. K. Huff, X. Huand F. Zhang, “Quantifying Uncertainties of Ground‐Level Ozone Within WRF‐Chem Simulations in the Mid‐Atlantic Region of the United States as a Response to Variability”, *Journal of Advances in Modeling Earth Systems*, vol. 11, no. 4. American Geophysical Union (AGU), pp. 1100–1116, Apr. 2019. doi: 10.1029/2018ms001457.  
  
J. Wang and X.-M. Hu, “Evaluating the performance of WRF urban schemes and PBL schemes over Dallas Fort Worth during a dry summer and a wet summer”, *Journal of Applied Meteorology and Climatology*. American Meteorological Society, Sep. 22, 2020. doi: 10.1175/jamc-d-19-0195.1.  
  
Y. Yang, X.-M. Hu, S. Gaoand Y. Wang, “Sensitivity of WRF simulations with the YSU PBL scheme to the lowest model level height for a sea fog event over the Yellow Sea”, *Atmospheric Research*, vol. 215. Elsevier BV, pp. 253–267, Jan. 2019. doi: 10.1016/j.atmosres.2018.09.004.  
  
J. Zhu, F. Kong, X.-M. Hu, Y. Guo, L. Ranand H. Lei, “Impact of Soil Moisture Uncertainty on Summertime Short-range Ensemble Forecasts”, *Advances in Atmospheric Sciences*, vol. 35, no. 7. Springer Science and Business Media LLC, pp. 839–852, May 28, 2018. doi: 10.1007/s00376-017-7107-1.  
  
P. J. Kelleher, “Trapping and Structural Characterization of the XNO2·NO3– (X = Cl, Br, I) Exit Channel Complexes in the Water-Mediated X– + N2O5 Reactions with Cryogenic Vibrational Spectroscopy”, *The Journal of Physical Chemistry Letters*, vol. 8, no. 19. American Chemical Society (ACS), pp. 4710–4715, Sep. 18, 2017. doi: 10.1021/acs.jpclett.7b02120.  
  
J. Chastang, “Deploying a Unidata JupyterHub on the NSF Jetstream Cloud, Lessons Learned and Challenges Going Forward”. figshare, 2019. doi: 10.6084/M9.FIGSHARE.8945078.V1.  
  
J. Chastang, “JupyterHub for Atmospheric Science Research and Education on the NSF Jetstream Cloud”. figshare, 2019. doi: 10.6084/M9.FIGSHARE.7590869.V1.  
  
J. Chastang, “Demonstration of Unidata Science Gateway”. figshare, 2020. doi: 10.6084/M9.FIGSHARE.12124065.V1.  
  
J. Chastang and R. Signell, “Met/Ocean Modeling Workflows on XSEDE via HPC & Cloud”. ESIP, 2017. doi: 10.6084/M9.FIGSHARE.5249845.V1.  
  
N. Wilkins-Diehr, M. Ramamurthy, E. Lingerfeltand J. Chastang, “Science Gateways in the Cloud, a Platform for Providing Modern Scientific Workflows for Reproducible Research and Collaboration”. ESIP, 2018. doi: 10.6084/M9.FIGSHARE.6856733.V1.  
  
M. Ramamurthy, J. Chastang, R. Mayand M. James, “Unidata and data-proximate analysis and visualization in the cloud”. ESIP, 2017. doi: 10.6084/M9.FIGSHARE.5249839.V1.  
  
J. K. Lundquist, K. K. DuVivier, D. Kaffineand J. M. Tomaszewski, “Costs and consequences of wind turbine wake effects arising from uncoordinated wind energy development”, *Nature Energy*, vol. 4, no. 1. Springer Science and Business Media LLC, pp. 26–34, Nov. 26, 2018. doi: 10.1038/s41560-018-0281-2.  
  
J. S. Rodrigo, “Results of the GABLS3 diurnal-cycle benchmark for wind energy applications”, *Journal of Physics: Conference Series*, vol. 854. IOP Publishing, p. 012037, May 2017. doi: 10.1088/1742-6596/854/1/012037.  
  
J. M. Tomaszewski and J. K. Lundquist, “Simulated wind farm wake sensitivity to configuration choices in the Weather Research and Forecasting model version 3.8.1”, *[]*. Copernicus GmbH, Dec. 09, 2019. doi: 10.5194/gmd-2019-302.  
  
J. M. Tomaszewski and J. K. Lundquist, “Observations and Simulations of a Wind Farm Modifying a Thunderstorm Outflow Boundary”, *[]*. Copernicus GmbH, May 04, 2020. doi: 10.5194/wes-2020-69.  
  
J. M. Tomaszewski, J. K. Lundquist, M. J. Churchfieldand P. J. Moriarty, “Do wind turbines pose roll hazards to light aircraft?”, *Wind Energy Science*, vol. 3, no. 2. Copernicus GmbH, pp. 833–843, Nov. 02, 2018. doi: 10.5194/wes-3-833-2018.  
  
M. F. Howland, A. S. Ghateand S. K. Lele, “Influence of the geostrophic wind direction on the atmospheric boundary layer flow”, *Journal of Fluid Mechanics*, vol. 883. Cambridge University Press (CUP), Nov. 26, 2019. doi: 10.1017/jfm.2019.889.  
  
B. Poduval, G. Petrieand L. Bertello, “Uncertainty Estimates of Solar Wind Prediction Using HMI Photospheric Vector and Spatial Standard Deviation Synoptic Maps”, *Solar Physics*, vol. 295, no. 10. Springer Science and Business Media LLC, Oct. 2020. doi: 10.1007/s11207-020-01704-1.  
  
F. Margairaz, M. G. Giometto, M. B. Parlangeand M. Calaf, “Comparison of dealiasing schemes in large-eddy simulation of neutrally-stratified atmospheric boundary-layer type flows”, *[]*. Copernicus GmbH, Nov. 17, 2017. doi: 10.5194/gmd-2017-272.  
  
A. Chattopadhyay, P. Hassanzadehand S. Pasha, “Predicting clustered weather patterns: A test case for applications of convolutional neural networks to spatio-temporal climate data”, *Scientific Reports*, vol. 10, no. 1. Springer Science and Business Media LLC, Jan. 28, 2020. doi: 10.1038/s41598-020-57897-9.  
  
A. Chattopadhyay, P. Hassanzadehand D. Subramanian, “Data-driven prediction of a multi-scale Lorenz 96 chaotic system using deep learning methods: Reservoir computing, ANN, and RNN-LSTM”, *[]*. California Digital Library (CDL), Jun. 19, 2019. doi: 10.31223/osf.io/fbxns.  
  
P. Hassanzadeh and Z. Kuang, “Quantifying the Annular Mode Dynamics in an Idealized Atmosphere”, *Journal of the Atmospheric Sciences*, vol. 76, no. 4. American Meteorological Society, pp. 1107–1124, Apr. 01, 2019. doi: 10.1175/jas-d-18-0268.1.  
  
M. A. Khodkar and P. Hassanzadeh, “Data-driven reduced modelling of turbulent Rayleigh–Bénard convection using DMD-enhanced fluctuation–dissipation theorem”, *Journal of Fluid Mechanics*, vol. 852. Cambridge University Press (CUP), Aug. 06, 2018. doi: 10.1017/jfm.2018.586.  
  
J. A. Aird, R. J. Barthelmie, T. J. Shepherdand S. C. Pryor, “WRF-Simulated Low-Level Jets over Iowa: Characterization and Sensitivity Studies”, *[]*. Copernicus GmbH, Nov. 14, 2020. doi: 10.5194/wes-2020-113.  
  
R. J. Barthelmie, T. J. Shepherd, J. A. Airdand S. C. Pryor, “Power and Wind Shear Implications of Large Wind Turbine Scenarios in the US Central Plains”, *Energies*, vol. 13, no. 16. MDPI AG, p. 4269, Aug. 18, 2020. doi: 10.3390/en13164269.  
  
F. W. Letson, R. J. Barthelmie, K. I. Hodgesand S. C. Pryor, “Windstorms in the Northeastern United States”, *[]*. Copernicus GmbH, Dec. 11, 2020. doi: 10.5194/nhess-2020-345.  
  
F. Letson, R. J. Barthelmieand S. C. Pryor, “RADAR-Derived Precipitation Climatology for Wind Turbine Blade Leading Edge Erosion”, *[]*. Copernicus GmbH, Aug. 13, 2019. doi: 10.5194/wes-2019-43.  
  
F. Letson, T. J. Shepherd, R. J. Barthelmieand S. C. Pryor, “WRF Modeling of Deep Convection and Hail for Wind Power Applications”, *Journal of Applied Meteorology and Climatology*, vol. 59, no. 10. American Meteorological Society, pp. 1717–1733, Oct. 01, 2020. doi: 10.1175/jamc-d-20-0033.1.  
  
S. C. Pryor, R. J. Barthelmie, M. S. Bukovsky, L. R. Leungand K. Sakaguchi, “Climate change impacts on wind power generation”, *Nature Reviews Earth & Environment*, vol. 1, no. 12. Springer Science and Business Media LLC, pp. 627–643, Oct. 20, 2020. doi: 10.1038/s43017-020-0101-7.  
  
S. C. Pryor, R. J. Barthelmieand T. J. Shepherd, “The Influence of Real‐World Wind Turbine Deployments on Local to Mesoscale Climate”, *Journal of Geophysical Research: Atmospheres*, vol. 123, no. 11. American Geophysical Union (AGU), pp. 5804–5826, Jun. 04, 2018. doi: 10.1029/2017jd028114.  
  
S. C. Pryor, R. J. Barthelmieand T. J. Shepherd, “20% of US electricity from wind will have limited impacts on system efficiency and regional climate”, *Scientific Reports*, vol. 10, no. 1. Springer Science and Business Media LLC, Jan. 17, 2020. doi: 10.1038/s41598-019-57371-1.  
  
S. C. Pryor and A. N. Hahmann, “Downscaling Wind”, *Oxford Research Encyclopedia of Climate Science*. Oxford University Press, Feb. 25, 2019. doi: 10.1093/acrefore/9780190228620.013.730.  
  
S. C. Pryor, F. W. Letsonand R. J. Barthelmie, “Variability in Wind Energy Generation across the Contiguous United States”, *Journal of Applied Meteorology and Climatology*, vol. 59, no. 12. American Meteorological Society, pp. 2021–2039, Dec. 2020. doi: 10.1175/jamc-d-20-0162.1.  
  
S. C. Pryor and J. T. Schoof, “A hierarchical analysis of the impact of methodological decisions on statistical downscaling of daily precipitation and air temperatures”, *International Journal of Climatology*, vol. 39, no. 6. Wiley, pp. 2880–2900, Jan. 25, 2019. doi: 10.1002/joc.5990.  
  
S. C. Pryor and J. T. Schoof, “Differential Credibility Assessment for Statistical Downscaling”, *Journal of Applied Meteorology and Climatology*, vol. 59, no. 8. American Meteorological Society, pp. 1333–1349, Aug. 01, 2020. doi: 10.1175/jamc-d-19-0296.1.  
  
S. C. Pryor, T. J. Shepherd, R. J. Barthelmie, A. N. Hahmannand P. Volker, “Wind Farm Wakes Simulated Using WRF”, *Journal of Physics: Conference Series*, vol. 1256, no. 1. IOP Publishing, p. 012025, Jul. 01, 2019. doi: 10.1088/1742-6596/1256/1/012025.  
  
S. C. Pryor, T. J. Shepherd, P. J. H. Volker, A. N. Hahmannand R. J. Barthelmie, ““Wind Theft” from Onshore Wind Turbine Arrays: Sensitivity to Wind Farm Parameterization and Resolution”, *Journal of Applied Meteorology and Climatology*, vol. 59, no. 1. American Meteorological Society, pp. 153–174, Jan. 2020. doi: 10.1175/jamc-d-19-0235.1.  
  
T. J. Shepherd, R. J. Barthelmieand S. C. Pryor, “Sensitivity of Wind Turbine Array Downstream Effects to the Parameterization Used in WRF”, *Journal of Applied Meteorology and Climatology*, vol. 59, no. 3. American Meteorological Society, pp. 333–361, Mar. 2020. doi: 10.1175/jamc-d-19-0135.1.  
  
N. S. Ghaisas, A. S. Ghateand S. K. Lele, “Large-eddy simulation study of multi-rotor wind turbines”, *Journal of Physics: Conference Series*, vol. 1037. IOP Publishing, p. 072021, Jun. 2018. doi: 10.1088/1742-6596/1037/7/072021.  
  
A. S. Ghate, N. Ghaisas, S. K. Leleand A. Towne, “Interaction of small scale Homogenenous Isotropic Turbulence with an Actuator Disk”, *2018 Wind Energy Symposium*. American Institute of Aeronautics and Astronautics, Jan. 07, 2018. doi: 10.2514/6.2018-0753.  
  
M. F. Howland, A. S. Ghateand S. K. Lele, “Influence of the horizontal component of Earth’s rotation on wind turbine wakes”, *Journal of Physics: Conference Series*, vol. 1037. IOP Publishing, p. 072003, Jun. 2018. doi: 10.1088/1742-6596/1037/7/072003.  
  
M. F. Howland, A. S. Ghateand S. K. Lele, “Coriolis effects within and trailing a large finite wind farm”, *AIAA Scitech 2020 Forum*. American Institute of Aeronautics and Astronautics, Jan. 05, 2020. doi: 10.2514/6.2020-0994.  
  
M. F. Howland, A. S. Ghate, S. K. Leleand J. O. Dabiri, “Optimal closed-loop wake steering, Part 1: Conventionally neutral atmospheric boundary layer conditions”, *[]*. Copernicus GmbH, Mar. 09, 2020. doi: 10.5194/wes-2020-52.  
  
Y. Cui, “Physics-based seismic hazard analysis on petascale heterogeneous supercomputers”, *Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis*. ACM, Nov. 17, 2013. doi: 10.1145/2503210.2503300.  
  
M.-G. Ascenzi, “Hyperlipidemia affects multiscale structure and strength of murine femur”, *Journal of Biomechanics*, vol. 47, no. 10. Elsevier BV, pp. 2436–2443, Jul. 2014. doi: 10.1016/j.jbiomech.2014.04.006.  
  
B. Guldur and J. F. Hajjar, “Damage Detection on Structures Using Texture Mapped Laser Point Clouds”, *Structures Congress 2014*. American Society of Civil Engineers, Apr. 02, 2014. doi: 10.1061/9780784413357.030.  
  
B. Guldur Erkal and J. F. Hajjar, “Laser-based surface damage detection and quantification using predicted surface properties”, *Automation in Construction*, vol. 83. Elsevier BV, pp. 285–302, Nov. 2017. doi: 10.1016/j.autcon.2017.08.004.  
  
V. V. Saykin, T. H. Nguyen, J. F. Hajjar, D. Denizand J. Song, “Validation of a Finite Element Approach to Modeling of Structural Collapse of Steel Structures”, *Structures Congress 2014*. American Society of Civil Engineers, Apr. 02, 2014. doi: 10.1061/9780784413357.190.  
  
V. V. Saykin, T. H. Nguyen, J. F. Hajjar, D. Denizand J. Song, “Material characterization using finite element deletion strategies for collapse modeling of steel structures”, *Engineering Structures*, vol. 147. Elsevier BV, pp. 125–133, Sep. 2017. doi: 10.1016/j.engstruct.2017.05.059.  
  
S. B. Walsh, D. J. Borello, B. Guldurand J. F. Hajjar, “Data Processing of Point Clouds for Object Detection for Structural Engineering Applications”, *Computer-Aided Civil and Infrastructure Engineering*, vol. 28, no. 7. Wiley, pp. 495–508, May 30, 2013. doi: 10.1111/mice.12016.  
  
L. Wang, M. D. Websterand J. F. Hajjar, “Behavior of Deconstructable Steel-Concrete Shear Connection in Composite Beams”, *Structures Congress 2015*. American Society of Civil Engineers, Apr. 17, 2015. doi: 10.1061/9780784479117.075.  
  
L. Wang, M. D. Websterand J. F. Hajjar, “Experimental Investigation of Deconstructable Steel-Concrete Shear Connections in Sustainable Composite Beams”, *Structures Congress 2017*. American Society of Civil Engineers, Apr. 04, 2017. doi: 10.1061/9780784480410.004.  
  
Y. Yan, B. Guldurand J. F. Hajjar, “Automated Structural Modelling of Bridges from Laser Scanning”, *Structures Congress 2017*. American Society of Civil Engineers, Apr. 04, 2017. doi: 10.1061/9780784480403.039.  
  
B. Guldur, Y. Yanand J. F. Hajjar, “Condition Assessment of Bridges Using Terrestrial Laser Scanners”, *Structures Congress 2015*. American Society of Civil Engineers, Apr. 17, 2015. doi: 10.1061/9780784479117.031.  
  
P. C. Kerr, “U.S. IOOS coastal and ocean modeling testbed: Evaluation of tide, wave, and hurricane surge response sensitivities to mesh resolution and friction in the Gulf of Mexico”, *Journal of Geophysical Research: Oceans*, vol. 118, no. 9. American Geophysical Union (AGU), pp. 4633–4661, Sep. 2013. doi: 10.1002/jgrc.20305.  
  
A. J. Fields and T. M. Keaveny, “Trabecular Architecture and Vertebral Fragility in Osteoporosis”, *Current Osteoporosis Reports*, vol. 10, no. 2. Springer Science and Business Media LLC, pp. 132–140, Apr. 11, 2012. doi: 10.1007/s11914-012-0097-0.  
  
J. D. Bayer, M. Epsteinand J. Beaumont, “FittingContinuous Parametric Surfaces to Frontiers Delimiting Physiologic Structures”, *Computational and Mathematical Methods in Medicine*, vol. 2014. Hindawi Limited, pp. 1–16, 2014. doi: 10.1155/2014/278479.  
  
A. E. Raba, J. M. Cordeiro, C. Antzelevitchand J. Beaumont, “Extending the Conditions of Application of an Inversion of the Hodgkin–Huxley Gating Model”, *Bulletin of Mathematical Biology*, vol. 75, no. 5. Springer Science and Business Media LLC, pp. 752–773, Apr. 18, 2013. doi: 10.1007/s11538-013-9832-7.  
  
C. Acevedo, “Contributions of Material Properties and Structure to Increased Bone Fragility for a Given Bone Mass in the UCD‐T2DM Rat Model of Type 2 Diabetes”, *Journal of Bone and Mineral Research*, vol. 33, no. 6. Wiley, pp. 1066–1075, Feb. 22, 2018. doi: 10.1002/jbmr.3393.  
  
T. W. Fowler, “Glucocorticoid suppression of osteocyte perilacunar remodeling is associated with subchondral bone degeneration in osteonecrosis”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Mar. 22, 2017. doi: 10.1038/srep44618.  
  
S. Nawathe, H. Yang, A. J. Fields, M. L. Bouxseinand T. M. Keaveny, “Theoretical effects of fully ductile versus fully brittle behaviors of bone tissue on the strength of the human proximal femur and vertebral body”, *Journal of Biomechanics*, vol. 48, no. 7. Elsevier BV, pp. 1264–1269, May 2015. doi: 10.1016/j.jbiomech.2015.02.066.  
  
P. G. Albal, T. A. Montidoro, O. Durand P. G. Menon, “Patient-Specific Hemodynamic Evaluation of an Aortic Coarctation under Rest and Stress Conditions”, *Statistical Atlases and Computational Models of the Heart. Imaging and Modelling Challenges*. Springer Berlin Heidelberg, pp. 83–93, 2014. doi: 10.1007/978-3-642-54268-8\_10.  
  
H. Hong, “Postsurgical Comparison of Pulsatile Hemodynamics in Five Unique Total Cavopulmonary Connections: Identifying Ideal Connection Strategies”, *The Annals of Thoracic Surgery*, vol. 96, no. 4. Elsevier BV, pp. 1398–1404, Oct. 2013. doi: 10.1016/j.athoracsur.2013.05.035.  
  
P. G. Menon, J. F. Antaki, A. Undarand K. Pekkan, “Aortic Outflow Cannula Tip Design and Orientation Impacts Cerebral Perfusion During Pediatric Cardiopulmonary Bypass Procedures”, *Annals of Biomedical Engineering*, vol. 41, no. 12. Springer Science and Business Media LLC, pp. 2588–2602, Jul. 02, 2013. doi: 10.1007/s10439-013-0857-8.  
  
P. G. Menon, N. Teslovich, C.-Y. Chen, A. Undarand K. Pekkan, “Characterization of neonatal aortic cannula jet flow regimes for improved cardiopulmonary bypass”, *Journal of Biomechanics*, vol. 46, no. 2. Elsevier BV, pp. 362–372, Jan. 2013. doi: 10.1016/j.jbiomech.2012.10.029.  
  
P. G. Menon, M. Yoshidaand K. Pekkan, “Presurgical Evaluation of Fontan Connection Options for Patients With Apicocaval Juxtaposition Using Computational Fluid Dynamics”, *Artificial Organs*, vol. 37, no. 1. Wiley, pp. E1–E8, Nov. 12, 2012. doi: 10.1111/j.1525-1594.2012.01555.x.  
  
M. Yoshida, “Total cavopulmonary connection in patients with apicocaval juxtaposition: optimal conduit route using preoperative angiogram and flow simulation†”, *European Journal of Cardio-Thoracic Surgery*, vol. 44, no. 1. Oxford University Press (OUP), pp. e46–e52, Mar. 25, 2013. doi: 10.1093/ejcts/ezt118.  
  
E. T. Filipov, “Seismic performance of highway bridges with fusing bearing components for quasi-isolation”, *Earthquake Engineering & Structural Dynamics*, vol. 42, no. 9. Wiley, pp. 1375–1394, Jan. 25, 2013. doi: 10.1002/eqe.2277.  
  
C. M. Ferreira, F. Oliveraand J. L. Irish, “Arc StormSurge: Integrating Hurricane Storm Surge Modeling and GIS”, *JAWRA Journal of the American Water Resources Association*, vol. 50, no. 1. Wiley, pp. 219–233, Oct. 08, 2013. doi: 10.1111/jawr.12127.  
  
E. Schnebele, C. Oxendine, G. Cervone, C. M. Ferreiraand N. Waters, “Using Non-authoritative Sources During Emergencies in Urban Areas”, *Computational Approaches for Urban Environments*. Springer International Publishing, pp. 337–361, Nov. 11, 2014. doi: 10.1007/978-3-319-11469-9\_14.  
  
C. Baron-Hyppolite, C. Lashley, J. Garzon, T. Miesse, C. Ferreiraand J. Bricker, “Comparison of Implicit and Explicit Vegetation Representations in SWAN Hindcasting Wave Dissipation by Coastal Wetlands in Chesapeake Bay”, *Geosciences*, vol. 9, no. 1. MDPI AG, p. 8, Dec. 24, 2018. doi: 10.3390/geosciences9010008.  
  
A. Bigalbal, A. Rezaie, J. Garzonand C. Ferreira, “Potential Impacts of Sea Level Rise and Coarse Scale Marsh Migration on Storm Surge Hydrodynamics and Waves on Coastal Protected Areas in the Chesapeake Bay”, *Journal of Marine Science and Engineering*, vol. 6, no. 3. MDPI AG, p. 86, Jul. 16, 2018. doi: 10.3390/jmse6030086.  
  
M. Borga, B. F. Tanyu, C. M. Ferreira, J. L. Garzonand M. Onufrychuk, “A geospatial framework to estimate depth of scour under buildings due to storm surge in coastal areas”, *Natural Hazards*, vol. 87, no. 3. Springer Science and Business Media LLC, pp. 1285–1311, Apr. 18, 2017. doi: 10.1007/s11069-017-2817-3.  
  
C. M. Ferreira, J. L. Irishand F. Olivera, “Quantifying the potential impact of land cover changes due to sea-level rise on storm surge on lower Texas coast bays”, *Coastal Engineering*, vol. 94. Elsevier BV, pp. 102–111, Dec. 2014. doi: 10.1016/j.coastaleng.2014.08.011.  
  
J. L. Garzon, C. M. Ferreiraand R. Padilla-Hernandez, “Evaluation of weather forecast systems for storm surge modeling in the Chesapeake Bay”, *Ocean Dynamics*, vol. 68, no. 1. Springer Science and Business Media LLC, pp. 91–107, Nov. 28, 2017. doi: 10.1007/s10236-017-1120-x.  
  
J. L. Garzon, T. Miesseand C. M. Ferreira, “Field-based numerical model investigation of wave propagation across marshes in the Chesapeake Bay under storm conditions”, *Coastal Engineering*, vol. 146. Elsevier BV, pp. 32–46, Apr. 2019. doi: 10.1016/j.coastaleng.2018.11.001.  
  
E. M. Glass, J. L. Garzon, S. Lawler, E. Paquierand C. M. Ferreira, “Potential of marshes to attenuate storm surge water level in the Chesapeake Bay”, *Limnology and Oceanography*, vol. 63, no. 2. Wiley, pp. 951–967, Oct. 17, 2017. doi: 10.1002/lno.10682.  
  
G. L. Tonn, S. D. Guikema, C. M. Ferreiraand S. M. Quiring, “Hurricane Isaac: A Longitudinal Analysis of Storm Characteristics and Power Outage Risk”, *Risk Analysis*, vol. 36, no. 10. Wiley, pp. 1936–1947, Feb. 08, 2016. doi: 10.1111/risa.12552.  
  
P. Di Achille, G. Tellides, C. A. Figueroaand J. D. Humphrey, “A haemodynamic predictor of intraluminal thrombus formation in abdominal aortic aneurysms”, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 470, no. 2172. The Royal Society, p. 20140163, Dec. 08, 2014. doi: 10.1098/rspa.2014.0163.  
  
O. E. Kadri, C. Williams III, V. Sikavitsasand R. S. Voronov, “Numerical accuracy comparison of two boundary conditions commonly used to approximate shear stress distributions in tissue engineering scaffolds cultured under flow perfusion”, *International Journal for Numerical Methods in Biomedical Engineering*, vol. 34, no. 11. Wiley, p. e3132, Aug. 17, 2018. doi: 10.1002/cnm.3132.  
  
F. E. Garcia and J. D. Bray, “Modeling the shear response of granular materials with discrete element assemblages of sphere-clusters”, *Computers and Geotechnics*, vol. 106. Elsevier BV, pp. 99–107, Feb. 2019. doi: 10.1016/j.compgeo.2018.10.003.  
  
L. Schambach, S. T. Grilli, J. T. Kirbyand F. Shi, “Landslide Tsunami Hazard Along the Upper US East Coast: Effects of Slide Deformation, Bottom Friction, and Frequency Dispersion”, *Pure and Applied Geophysics*, vol. 176, no. 7. Springer Science and Business Media LLC, pp. 3059–3098, Sep. 03, 2018. doi: 10.1007/s00024-018-1978-7.  
  
L. Schambach, S. T. Grilli, D. R. Tappin, M. D. Gangemiand G. Barbaro, “New simulations and understanding of the 1908 Messina tsunami for a dual seismic and deep submarine mass failure source”, *Marine Geology*, vol. 421. Elsevier BV, p. 106093, Mar. 2020. doi: 10.1016/j.margeo.2019.106093.  
  
Q. Shi, X. Mengand V. Prigiobbe, “Mechanistic Study of Radium Adsorption onto Goethite”, *The Journal of Physical Chemistry C*, vol. 124, no. 1. American Chemical Society (ACS), pp. 805–814, Dec. 09, 2019. doi: 10.1021/acs.jpcc.9b10451.  
  
Q. Shi, S. Zhang, G. P. Korfiatis, C. Christodoulatosand X. Meng, “Identifying the existence and molecular structure of the dissolved HCO3-Ca-As(V) complex in water”, *Science of The Total Environment*, vol. 724. Elsevier BV, p. 138216, Jul. 2020. doi: 10.1016/j.scitotenv.2020.138216.  
  
Q. Shi, G. E. Sterbinsky, V. Prigiobbeand X. Meng, “Mechanistic Study of Lead Adsorption on Activated Carbon”, *Langmuir*, vol. 34, no. 45. American Chemical Society (ACS), pp. 13565–13573, Oct. 16, 2018. doi: 10.1021/acs.langmuir.8b03096.  
  
R. Behkam, “Racioethnic differences in the biomechanical response of the lamina cribrosa”, *Acta Biomaterialia*, vol. 88. Elsevier BV, pp. 131–140, Apr. 2019. doi: 10.1016/j.actbio.2019.02.028.  
  
H. G. Kollech, “A Subdomain Method for Mapping the Heterogeneous Mechanical Properties of the Human Posterior Sclera”, *Frontiers in Bioengineering and Biotechnology*, vol. 7. Frontiers Media SA, May 31, 2019. doi: 10.3389/fbioe.2019.00129.  
  
M. D. Lee, “GToTree: a user-friendly workflow for phylogenomics”, *Bioinformatics*, vol. 35, no. 20. Oxford University Press (OUP), pp. 4162–4164, Mar. 13, 2019. doi: 10.1093/bioinformatics/btz188.  
  
M. D. Lee, “Marine *Synechococcus* isolates representing globally abundant genomic lineages demonstrate a unique evolutionary path of genome reduction without a decrease in GC content”, *Environmental Microbiology*, vol. 21, no. 5. Wiley, pp. 1677–1686, Mar. 12, 2019. doi: 10.1111/1462-2920.14552.  
  
A. O’Rourke, M. D. Lee, W. C. Nierman, R. C. Everroadand C. L. Dupont, “Genomic and phenotypic characterization of Burkholderia isolates from the potable water system of the International Space Station”, *PLOS ONE*, vol. 15, no. 2. Public Library of Science (PLoS), p. e0227152, Feb. 19, 2020. doi: 10.1371/journal.pone.0227152.  
  
J. Burridge, C. N. Jochua, A. Buckschand J. P. Lynch, “Legume shovelomics: High—Throughput phenotyping of common bean (Phaseolus vulgaris L.) and cowpea (Vigna unguiculata subsp, unguiculata) root architecture in the field”, *Field Crops Research*, vol. 192. Elsevier BV, pp. 21–32, Jun. 2016. doi: 10.1016/j.fcr.2016.04.008.  
  
J. D. Burridge, H. M. Schneider, B.-L. Huynh, P. A. Roberts, A. Buckschand J. P. Lynch, “Genome-wide association mapping and agronomic impact of cowpea root architecture”, *Theoretical and Applied Genetics*, vol. 130, no. 2. Springer Science and Business Media LLC, pp. 419–431, Nov. 18, 2016. doi: 10.1007/s00122-016-2823-y.  
  
C. L. Andersen, “Active Estrogen Receptor-alpha Signaling in Ovarian Cancer Models and Clinical Specimens”, *Clinical Cancer Research*, vol. 23, no. 14. American Association for Cancer Research (AACR), pp. 3802–3812, Jul. 13, 2017. doi: 10.1158/1078-0432.ccr-16-1501.  
  
U. R. Chandran, “TCGA Expedition: A Data Acquisition and Management System for TCGA Data”, *PLOS ONE*, vol. 11, no. 10. Public Library of Science (PLoS), p. e0165395, Oct. 27, 2016. doi: 10.1371/journal.pone.0165395.  
  
M. L. Eshbach, “The transcriptome of the *Didelphis virginiana* opossum kidney OK proximal tubule cell line”, *American Journal of Physiology-Renal Physiology*, vol. 313, no. 3. American Physiological Society, pp. F585–F595, Sep. 01, 2017. doi: 10.1152/ajprenal.00228.2017.  
  
K. A. Frahm, “Research Resource: The Dexamethasone Transcriptome in Hypothalamic Embryonic Neural Stem Cells”, *Molecular Endocrinology*, vol. 30, no. 1. The Endocrine Society, pp. 144–154, Jan. 01, 2016. doi: 10.1210/me.2015-1258.  
  
K. A. Frahm, “A comparison of the sexually dimorphic dexamethasone transcriptome in mouse cerebral cortical and hypothalamic embryonic neural stem cells”, *Molecular and Cellular Endocrinology*, vol. 471. Elsevier BV, pp. 42–50, Aug. 2018. doi: 10.1016/j.mce.2017.05.026.  
  
A. Geskin, “Needs Assessment for Research Use of High-Throughput Sequencing at a Large Academic Medical Center”, *PLOS ONE*, vol. 10, no. 6. Public Library of Science (PLoS), p. e0131166, Jun. 26, 2015. doi: 10.1371/journal.pone.0131166.  
  
S. Luthra, U. Chandran, B. Diergaarde, M. Becich, A. V. Leeand C. A. Neumann, “Expression of reactive species related genes is associated with patient survival in luminal B breast cancer”, *Free Radical Biology and Medicine*, vol. 120. Elsevier BV, pp. 170–180, May 2018. doi: 10.1016/j.freeradbiomed.2018.03.011.  
  
K. K. Mcdade, U. Chandranand R. S. Day, “Improving Cancer Gene Expression Data Quality through a TCGA Data-Driven Evaluation of Identifier Filtering”, *Cancer Informatics*, vol. 14. SAGE Publications, p. CIN.S33076, Jan. 2015. doi: 10.4137/cin.s33076.  
  
L. E. Pascal, “Conditional deletion of ELL2 induces murine prostate intraepithelial neoplasia”, *Journal of Endocrinology*, vol. 235, no. 2. Bioscientifica, pp. 123–136, Nov. 2017. doi: 10.1530/joe-17-0112.  
  
L. E. Pascal, “EAF2 and p53 Co-Regulate STAT3 Activation in Prostate Cancer”, *Neoplasia*, vol. 20, no. 4. Elsevier BV, pp. 351–363, Apr. 2018. doi: 10.1016/j.neo.2018.01.011.  
  
S. Ramaswamy, “The testicular transcriptome associated with spermatogonia differentiation initiated by gonadotrophin stimulation in the juvenile rhesus monkey (Macaca mulatta)”, *Human Reproduction*, vol. 32, no. 10. Oxford University Press (OUP), pp. 2088–2100, Aug. 30, 2017. doi: 10.1093/humrep/dex270.  
  
J. Zhong, S. Powelland J. C. Preston, “Organ boundary NAC-domain transcription factors are implicated in the evolution of petal fusion”, *Plant Biology*, vol. 18, no. 6. Wiley, pp. 893–902, Sep. 07, 2016. doi: 10.1111/plb.12493.  
  
B. Solomon and C. Kingsford, “Fast search of thousands of short-read sequencing experiments”, *Nature Biotechnology*, vol. 34, no. 3. Springer Science and Business Media LLC, pp. 300–302, Feb. 08, 2016. doi: 10.1038/nbt.3442.  
  
C. Ma, M. Shaoand C. Kingsford, “SQUID: Transcriptomic Structural Variation Detection from RNA-seq”, *[]*. Cold Spring Harbor Laboratory, Jul. 12, 2017. doi: 10.1101/162776.  
  
M. Zhu, “Molecular and systems approaches towards drought‐tolerant canola crops”, *New Phytologist*, vol. 210, no. 4. Wiley, pp. 1169–1189, Feb. 16, 2016. doi: 10.1111/nph.13866.  
  
S. A. Caplins, “Plasticity and Artificial Selection for Developmental Mode in a Poecilogonous Sea Slug”, *[]*. Cold Spring Harbor Laboratory, Mar. 08, 2020. doi: 10.1101/2020.03.06.981324.  
  
F. Asnicar, “Precise phylogenetic analysis of microbial isolates and genomes from metagenomes using PhyloPhlAn 3.0”, *Nature Communications*, vol. 11, no. 1. Springer Science and Business Media LLC, May 19, 2020. doi: 10.1038/s41467-020-16366-7.  
  
M. Balaban, S. Sarmashghiand S. Mirarab, “APPLES: Scalable Distance-based Phylogenetic Placement with or without Alignments”, *[]*. Cold Spring Harbor Laboratory, Nov. 23, 2018. doi: 10.1101/475566.  
  
E. Bolyen, “Reproducible, interactive, scalable and extensible microbiome data science using QIIME 2”, *Nature Biotechnology*, vol. 37, no. 8. Springer Science and Business Media LLC, pp. 852–857, Jul. 24, 2019. doi: 10.1038/s41587-019-0209-9.  
  
M. Estaki, “QIIME 2 Enables Comprehensive End‐to‐End Analysis of Diverse Microbiome Data and Comparative Studies with Publicly Available Data”, *Current Protocols in Bioinformatics*, vol. 70, no. 1. Wiley, Apr. 28, 2020. doi: 10.1002/cpbi.100.  
  
X. Fang, “Metagenomics-Based, Strain-Level Analysis of Escherichia coli From a Time-Series of Microbiome Samples From a Crohn’s Disease Patient”, *Frontiers in Microbiology*, vol. 9. Frontiers Media SA, Oct. 30, 2018. doi: 10.3389/fmicb.2018.02559.  
  
A. Gonzalez, “Qiita: rapid, web-enabled microbiome meta-analysis”, *Nature Methods*, vol. 15, no. 10. Springer Science and Business Media LLC, pp. 796–798, Oct. 2018. doi: 10.1038/s41592-018-0141-9.  
  
B. Hillmann, G. A. Al-Ghalith, R. R. Shields-Cutler, Q. Zhu, R. Knightand D. Knights, “SHOGUN: a modular, accurate and scalable framework for microbiome quantification”, *Bioinformatics*, vol. 36, no. 13. Oxford University Press (OUP), pp. 4088–4090, May 04, 2020. doi: 10.1093/bioinformatics/btaa277.  
  
S. Janssen, “Phylogenetic Placement of Exact Amplicon Sequences Improves Associations with Clinical Information”, *mSystems*, vol. 3, no. 3. American Society for Microbiology, Jun. 26, 2018. doi: 10.1128/msystems.00021-18.  
  
S. M. Karst, “Enabling high-accuracy long-read amplicon sequences using unique molecular identifiers with Nanopore or PacBio sequencing”, *[]*. Cold Spring Harbor Laboratory, May 24, 2019. doi: 10.1101/645903.  
  
C. A. Marotz, J. G. Sanders, C. Zuniga, L. S. Zaramela, R. Knightand K. Zengler, “Improving saliva shotgun metagenomics by chemical host DNA depletion”, *Microbiome*, vol. 6, no. 1. Springer Science and Business Media LLC, Feb. 27, 2018. doi: 10.1186/s40168-018-0426-3.  
  
R. H. Mills, “Evaluating Metagenomic Prediction of the Metaproteome in a 4.5-Year Study of a Patient with Crohn’s Disease”, *mSystems*, vol. 4, no. 1. American Society for Microbiology, Feb. 26, 2019. doi: 10.1128/msystems.00337-18.  
  
J. T. Morton, “Establishing microbial composition measurement standards with reference frames”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Jun. 20, 2019. doi: 10.1038/s41467-019-10656-5.  
  
G. D. Poore, “Microbiome analyses of blood and tissues suggest cancer diagnostic approach”, *Nature*, vol. 579, no. 7800. Springer Science and Business Media LLC, pp. 567–574, Mar. 11, 2020. doi: 10.1038/s41586-020-2095-1.  
  
A. Salosensaari, “Taxonomic Signatures of Long-Term Mortality Risk in Human Gut Microbiota”, *[]*. Cold Spring Harbor Laboratory, Jan. 02, 2020. doi: 10.1101/2019.12.30.19015842.  
  
J. G. Sanders, “Optimizing sequencing protocols for leaderboard metagenomics by combining long and short reads”, *Genome Biology*, vol. 20, no. 1. Springer Science and Business Media LLC, Oct. 31, 2019. doi: 10.1186/s13059-019-1834-9.  
  
L. Smarr, E. Hyde, D. McDonald, W. Sandbornand R. Knight, “Tracking Human Gut Microbiome Changes Resulting from a Colonoscopy”, *Methods of Information in Medicine*, vol. 56, no. 6. Georg Thieme Verlag KG, pp. 442–447, 2017. doi: 10.3414/me17-01-0036.  
  
M. Yazdani, B. C. Taylor, J. W. Debelius, W. Li, R. Knightand L. Smarr, “Using machine learning to identify major shifts in human gut microbiome protein family abundance in disease”, *2016 IEEE International Conference on Big Data (Big Data)*. IEEE, Dec. 2016. doi: 10.1109/bigdata.2016.7840731.  
  
Q. Zhu, “Phylogenomics of 10,575 genomes reveals evolutionary proximity between domains Bacteria and Archaea”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Dec. 02, 2019. doi: 10.1038/s41467-019-13443-4.  
  
Z. Sun, M. Hashemi, G. Warren, P. R. Biancoand Y. L. Lyubchenko, “Dynamics of the Interaction of RecG Protein with Stalled Replication Forks”, *Biochemistry*, vol. 57, no. 13. American Chemical Society (ACS), pp. 1967–1976, Feb. 12, 2018. doi: 10.1021/acs.biochem.7b01235.  
  
Y. Zhang, M. Hashemi, Z. Lvand Y. L. Lyubchenko, “Self-assembly of the full-length amyloid Aβ42 protein in dimers”, *Nanoscale*, vol. 8, no. 45. Royal Society of Chemistry (RSC), pp. 18928–18937, 2016. doi: 10.1039/c6nr06850b.  
  
N. Christodoulides, “Gene expression plasticity across hosts of an invasive scale insect species”, *PLOS ONE*, vol. 12, no. 5. Public Library of Science (PLoS), p. e0176956, May 04, 2017. doi: 10.1371/journal.pone.0176956.  
  
K. E. Yoh, “Repression of p63 and induction of EMT by mutant Ras in mammary epithelial cells”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 41. Proceedings of the National Academy of Sciences, Sep. 28, 2016. doi: 10.1073/pnas.1613417113.  
  
R. A. Bay, “Genetic Coupling of Female Mate Choice with Polygenic Ecological Divergence Facilitates Stickleback Speciation”, *Current Biology*, vol. 27, no. 21. Elsevier BV, pp. 3344–3349.e4, Nov. 2017. doi: 10.1016/j.cub.2017.09.037.  
  
R. A. Bay, R. J. Harrigan, V. L. Underwood, H. L. Gibbs, T. B. Smithand K. Ruegg, “Genomic signals of selection predict climate-driven population declines in a migratory bird”, *Science*, vol. 359, no. 6371. American Association for the Advancement of Science (AAAS), pp. 83–86, Jan. 05, 2018. doi: 10.1126/science.aan4380.  
  
R. A. Bay and S. R. Palumbi, “Transcriptome predictors of coral survival and growth in a highly variable environment”, *Ecology and Evolution*, vol. 7, no. 13. Wiley, pp. 4794–4803, May 25, 2017. doi: 10.1002/ece3.2685.  
  
R. A. Bay, N. H. Rose, C. A. Loganand S. R. Palumbi, “Genomic models predict successful coral adaptation if future ocean warming rates are reduced”, *Science Advances*, vol. 3, no. 11. American Association for the Advancement of Science (AAAS), Nov. 03, 2017. doi: 10.1126/sciadv.1701413.  
  
N. H. Rose, R. A. Bay, M. K. Morikawaand S. R. Palumbi, “Polygenic evolution drives species divergence and climate adaptation in corals”, *Evolution*, vol. 72, no. 1. Wiley, pp. 82–94, Nov. 24, 2017. doi: 10.1111/evo.13385.  
  
L. Thomas, “Mechanisms of Thermal Tolerance in Reef-Building Corals across a Fine-Grained Environmental Mosaic: Lessons from Ofu, American Samoa”, *Frontiers in Marine Science*, vol. 4. Frontiers Media SA, Feb. 01, 2018. doi: 10.3389/fmars.2017.00434.  
  
M. J. Sanderson, M. Nicolaeand M. M. McMahon, “Homology-aware Phylogenomics at Gigabase Scales”, *Systematic Biology*. Oxford University Press (OUP), p. syw104, Jan. 25, 2017. doi: 10.1093/sysbio/syw104.  
  
J. C. Stein, “Genomes of 13 domesticated and wild rice relatives highlight genetic conservation, turnover and innovation across the genus Oryza”, *Nature Genetics*, vol. 50, no. 2. Springer Science and Business Media LLC, pp. 285–296, Jan. 22, 2018. doi: 10.1038/s41588-018-0040-0.  
  
S. Böhm, “The Budding Yeast Ubiquitin Protease Ubp7 Is a Novel Component Involved in S Phase Progression”, *Journal of Biological Chemistry*, vol. 291, no. 9. Elsevier BV, pp. 4442–4452, Feb. 2016. doi: 10.1074/jbc.m115.671057.  
  
L. Chen, C. Cai, V. Chenand X. Lu, “Trans-species learning of cellular signaling systems with bimodal deep belief networks”, *Bioinformatics*, vol. 31, no. 18. Oxford University Press (OUP), pp. 3008–3015, May 20, 2015. doi: 10.1093/bioinformatics/btv315.  
  
M. Chikina, E. Zaslavskyand S. C. Sealfon, “CellCODE: a robust latent variable approach to differential expression analysis for heterogeneous cell populations”, *Bioinformatics*, vol. 31, no. 10. Oxford University Press (OUP), pp. 1584–1591, Jan. 11, 2015. doi: 10.1093/bioinformatics/btv015.  
  
M. Q. Ding, L. Chen, G. F. Cooper, J. D. Youngand X. Lu, “Precision Oncology beyond Targeted Therapy: Combining Omics Data with Machine Learning Matches the Majority of Cancer Cells to Effective Therapeutics”, *Molecular Cancer Research*, vol. 16, no. 2. American Association for Cancer Research (AACR), pp. 269–278, Feb. 01, 2018. doi: 10.1158/1541-7786.mcr-17-0378.  
  
A. Gough, “Biologically Relevant Heterogeneity: Metrics and Practical Insights”, *SLAS Discovery*, vol. 22, no. 3. Elsevier BV, pp. 213–237, Mar. 2017. doi: 10.1177/2472555216682725.  
  
T. Haliloglu and I. Bahar, “Adaptability of protein structures to enable functional interactions and evolutionary implications”, *Current Opinion in Structural Biology*, vol. 35. Elsevier BV, pp. 17–23, Dec. 2015. doi: 10.1016/j.sbi.2015.07.007.  
  
B. Huang, K. Zhang, J. Zhang, R. Sanchez-Romero, C. Glymourand B. Scholkopf, “Behind Distribution Shift: Mining Driving Forces of Changes and Causal Arrows”, *2017 IEEE International Conference on Data Mining (ICDM)*. IEEE, Nov. 2017. doi: 10.1109/icdm.2017.114.  
  
T. Huang, “A regulatory circuit of miR-125b/miR-20b and Wnt signalling controls glioblastoma phenotypes through FZD6-modulated pathways”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Oct. 04, 2016. doi: 10.1038/ncomms12885.  
  
D. Hu, “Interplay between arginine methylation and ubiquitylation regulates KLF4-mediated genome stability and carcinogenesis”, *Nature Communications*, vol. 6, no. 1. Springer Science and Business Media LLC, Sep. 30, 2015. doi: 10.1038/ncomms9419.  
  
A. Hyttinen, S. Plis, M. Järvisalo, F. Eberhardtand D. Danks, “A constraint optimization approach to causal discovery from subsampled time series data”, *International Journal of Approximate Reasoning*, vol. 90. Elsevier BV, pp. 208–225, Nov. 2017. doi: 10.1016/j.ijar.2017.07.009.  
  
F. Jabbari, J. Ramsey, P. Spirtesand G. Cooper, “Discovery of Causal Models that Contain Latent Variables Through Bayesian Scoring of Independence Constraints”, *Machine Learning and Knowledge Discovery in Databases*. Springer International Publishing, pp. 142–157, 2017. doi: 10.1007/978-3-319-71246-8\_9.  
  
E. Kummerfeld and J. Ramsey, “Causal Clustering for 1-Factor Measurement Models”, *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. ACM, Aug. 13, 2016. doi: 10.1145/2939672.2939838.  
  
S. Lu, “Signal-Oriented Pathway Analyses Reveal a Signaling Complex as a Synthetic Lethal Target for p53 Mutations”, *Cancer Research*, vol. 76, no. 23. American Association for Cancer Research (AACR), pp. 6785–6794, Nov. 30, 2016. doi: 10.1158/0008-5472.can-16-1740.  
  
S. Lu, “Identifying Driver Genomic Alterations in Cancers by Searching Minimum-Weight, Mutually Exclusive Sets”, *PLOS Computational Biology*, vol. 11, no. 8. Public Library of Science (PLoS), p. e1004257, Aug. 28, 2015. doi: 10.1371/journal.pcbi.1004257.  
  
S. Lu, G. Mandava, G. Yanand X. Lu, “An exact algorithm for finding cancer driver somatic genome alterations: the weighted mutually exclusive maximum set cover problem”, *Algorithms for Molecular Biology*, vol. 11, no. 1. Springer Science and Business Media LLC, May 04, 2016. doi: 10.1186/s13015-016-0073-9.  
  
D. Malinsky and P. Spirtes, “Estimating bounds on causal effects in high-dimensional and possibly confounded systems”, *International Journal of Approximate Reasoning*, vol. 88. Elsevier BV, pp. 371–384, Sep. 2017. doi: 10.1016/j.ijar.2017.06.005.  
  
A. Murray-Watters and C. Glymour, “What Is Going on Inside the Arrows? Discovering the Hidden Springs in Causal Models”, *Philosophy of Science*, vol. 82, no. 4. Cambridge University Press (CUP), pp. 556–586, Oct. 2015. doi: 10.1086/682962.  
  
M. P. Naeini and G. F. Cooper, “Binary Classifier Calibration Using an Ensemble of Near Isotonic Regression Models”, *2016 IEEE 16th International Conference on Data Mining (ICDM)*. IEEE, Dec. 2016. doi: 10.1109/icdm.2016.0047.  
  
M. P. Naeini, G. F. Cooperand M. Hauskrecht, “Binary Classifier Calibration Using a Bayesian Non-Parametric Approach”, *Proceedings of the 2015 SIAM International Conference on Data Mining*. Society for Industrial and Applied Mathematics, Jun. 30, 2015. doi: 10.1137/1.9781611974010.24.  
  
L. Nguyen, A. B. Tosun, J. L. Fine, A. V. Lee, D. L. Taylorand S. C. Chennubhotla, “Spatial Statistics for Segmenting Histological Structures in H&E Stained Tissue Images”, *IEEE Transactions on Medical Imaging*, vol. 36, no. 7. Institute of Electrical and Electronics Engineers (IEEE), pp. 1522–1532, Jul. 2017. doi: 10.1109/tmi.2017.2681519.  
  
R. Partha, “Subterranean mammals show convergent regression in ocular genes and enhancers, along with adaptation to tunneling”, *eLife*, vol. 6. eLife Sciences Publications, Ltd, Oct. 16, 2017. doi: 10.7554/elife.25884.  
  
N. Priedigkeit, N. Wolfeand N. L. Clark, “Evolutionary Signatures amongst Disease Genes Permit Novel Methods for Gene Prioritization and Construction of Informative Gene-Based Networks”, *PLOS Genetics*, vol. 11, no. 2. Public Library of Science (PLoS), p. e1004967, Feb. 13, 2015. doi: 10.1371/journal.pgen.1004967.  
  
N. Sauerwald, S. Zhang, C. Kingsfordand I. Bahar, “Chromosomal dynamics predicted by an elastic network model explains genome-wide accessibility and long-range couplings”, *Nucleic Acids Research*, vol. 45, no. 7. Oxford University Press (OUP), pp. 3663–3673, Mar. 16, 2017. doi: 10.1093/nar/gkx172.  
  
A. J. Sedgewick, I. Shi, R. M. Donovanand P. V. Benos, “Learning mixed graphical models with separate sparsity parameters and stability-based model selection”, *BMC Bioinformatics*, vol. 17, no. S5. Springer Science and Business Media LLC, Jun. 06, 2016. doi: 10.1186/s12859-016-1039-0.  
  
D. M. Spagnolo, “Platform for Quantitative Evaluation of Spatial Intratumoral Heterogeneity in Multiplexed Fluorescence Images”, *Cancer Research*, vol. 77, no. 21. American Association for Cancer Research (AACR), pp. e71–e74, Oct. 31, 2017. doi: 10.1158/0008-5472.can-17-0676.  
  
P. Spirtes and K. Zhang, “Causal discovery and inference: concepts and recent methodological advances”, *Applied Informatics*, vol. 3, no. 1. Springer Science and Business Media LLC, Feb. 18, 2016. doi: 10.1186/s40535-016-0018-x.  
  
E. V. Strobl and S. Visweswaran, “Markov Boundary Discovery with Ridge Regularized Linear Models”, *Journal of Causal Inference*, vol. 4, no. 1. Walter de Gruyter GmbH, pp. 31–48, Mar. 01, 2016. doi: 10.1515/jci-2015-0011.  
  
S. Visweswaran, A. Ferreira, G. A. Ribeiro, A. C. Oliveiraand G. F. Cooper, “Personalized Modeling for Prediction with Decision-Path Models”, *PLOS ONE*, vol. 10, no. 6. Public Library of Science (PLoS), p. e0131022, Jun. 22, 2015. doi: 10.1371/journal.pone.0131022.  
  
N. W. Wolfe and N. L. Clark, “ERC analysis: web-based inference of gene function via evolutionary rate covariation: Fig. 1.”, *Bioinformatics*. Oxford University Press (OUP), p. btv454, Aug. 04, 2015. doi: 10.1093/bioinformatics/btv454.  
  
R. Yang, P. Spirtes, R. Scheines, S. P. Reiseand M. Mansoff, “Finding Pure Submodels for Improved Differentiation of Bifactor and Second-Order Models”, *Structural Equation Modeling: A Multidisciplinary Journal*, vol. 24, no. 3. Informa UK Limited, pp. 402–413, Jan. 25, 2017. doi: 10.1080/10705511.2016.1261351.  
  
K. Zhang, B. Huang, J. Zhang, C. Glymourand B. Schölkopf, “Causal Discovery from Nonstationary/Heterogeneous Data: Skeleton Estimation and Orientation Determination”, *Proceedings of the Twenty-Sixth International Joint Conference on Artificial Intelligence*. International Joint Conferences on Artificial Intelligence Organization, Aug. 2017. doi: 10.24963/ijcai.2017/187.  
  
T. K. Chafin, B. T. Martin, S. M. Mussmann, M. R. Douglasand M. E. Douglas, “FRAGMATIC: in silico locus prediction and its utility in optimizing ddRADseq projects”, *Conservation Genetics Resources*, vol. 10, no. 3. Springer Science and Business Media LLC, pp. 325–328, Jul. 14, 2017. doi: 10.1007/s12686-017-0814-1.  
  
F. E. Anderson, “Phylogenomic analyses of Crassiclitellata support major Northern and Southern Hemisphere clades and a Pangaean origin for earthworms”, *BMC Evolutionary Biology*, vol. 17, no. 1. Springer Science and Business Media LLC, May 30, 2017. doi: 10.1186/s12862-017-0973-4.  
  
A. R. Lindgren and F. E. Anderson, “Assessing the utility of transcriptome data for inferring phylogenetic relationships among coleoid cephalopods”, *Molecular Phylogenetics and Evolution*, vol. 118. Elsevier BV, pp. 330–342, Jan. 2018. doi: 10.1016/j.ympev.2017.10.004.  
  
Y. Cao, E. K. Cartwright, G. Silvestriand A. S. Perelson, “CD8+ lymphocyte control of SIV infection during antiretroviral therapy”, *PLOS Pathogens*, vol. 14, no. 10. Public Library of Science (PLoS), p. e1007350, Oct. 11, 2018. doi: 10.1371/journal.ppat.1007350.  
  
Y. Cao, X. Lei, R. M. Ribeiro, A. S. Perelsonand J. Liang, “Probabilistic control of HIV latency and transactivation by the Tat gene circuit”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 49. Proceedings of the National Academy of Sciences, pp. 12453–12458, Nov. 19, 2018. doi: 10.1073/pnas.1811195115.  
  
B. S. Razooky, Y. Cao, M. M. K. Hansen, A. S. Perelson, M. L. Simpsonand L. S. Weinberger, “Nonlatching positive feedback enables robust bimodality by decoupling expression noise from the mean”, *PLOS Biology*, vol. 15, no. 10. Public Library of Science (PLoS), p. e2000841, Oct. 18, 2017. doi: 10.1371/journal.pbio.2000841.  
  
L. K. Johnson, H. Alexanderand C. T. Brown, “Re-assembly, quality evaluation, and annotation of 678 microbial eukaryotic reference transcriptomes”, *GigaScience*, vol. 8, no. 4. Oxford University Press (OUP), Dec. 13, 2018. doi: 10.1093/gigascience/giy158.  
  
T. Chu, “Chromatin run-on reveals the transcriptional etiology of glioblastoma multiforme”, *[]*. Cold Spring Harbor Laboratory, Sep. 07, 2017. doi: 10.1101/185991.  
  
T. Chu, “Chromatin run-on and sequencing maps the transcriptional regulatory landscape of glioblastoma multiforme”, *Nature Genetics*, vol. 50, no. 11. Springer Science and Business Media LLC, pp. 1553–1564, Oct. 22, 2018. doi: 10.1038/s41588-018-0244-3.  
  
T. Chu, Z. Wang, S. Chouand C. G. Danko, “Discovering Transcriptional Regulatory Elements From Run‐On and Sequencing Data Using the Web‐Based dREG Gateway”, *Current Protocols in Bioinformatics*, vol. 66, no. 1. Wiley, Dec. 27, 2018. doi: 10.1002/cpbi.70.  
  
Z. Wang, T. Chu, L. A. Choateand C. G. Danko, “Identification of regulatory elements from nascent transcription using dREG”, *Genome Research*, vol. 29, no. 2. Cold Spring Harbor Laboratory, pp. 293–303, Dec. 20, 2018. doi: 10.1101/gr.238279.118.  
  
Z. Wang, T. Chu, L. A. Choateand C. G. Danko, “Identification of regulatory elements from nascent transcription using dREG”, *[]*. Cold Spring Harbor Laboratory, May 14, 2018. doi: 10.1101/321539.  
  
T. K. Chafin, “Taxonomic hypotheses and the biogeography of speciation in the Tiger Whiptail complex (*Aspidoscelis tigris*: Squamata, Teiidae)”, *[]*. Cold Spring Harbor Laboratory, Oct. 07, 2020. doi: 10.1101/2020.10.05.327270.  
  
T. K. Chafin, “Spatial population genetics in heavily managed species: Separating patterns of historical translocation from contemporary gene flow in white-tailed deer”, *[]*. Cold Spring Harbor Laboratory, Sep. 22, 2020. doi: 10.1101/2020.09.22.308825.  
  
M. R. Douglas, T. K. Chafin, J. E. Claussen, D. P. Philippand M. E. Douglas, “Are populations of economically important bonefish and queen conch ‘open’ or ‘closed’ in the northern Caribbean Basin?”, *[]*. Cold Spring Harbor Laboratory, Jul. 10, 2020. doi: 10.1101/2020.07.08.194415.  
  
A. P. Sawchuk, “Noninvasive and Patient-Specific Assessment of True Severity of Renal Artery Stenosis for New Guidelines for Planning Stent Therapy”, *Journal of Vascular Surgery*, vol. 68, no. 3. Elsevier BV, pp. e64–e65, Sep. 2018. doi: 10.1016/j.jvs.2018.06.062.  
  
S. Zhou, “Study on coalescence dynamics of unequal-sized microbubbles captive on solid substrate”, *Experimental Thermal and Fluid Science*, vol. 98. Elsevier BV, pp. 362–368, Nov. 2018. doi: 10.1016/j.expthermflusci.2018.06.016.  
  
M. Balduzzi, “Reshaping Plant Biology: Qualitative and Quantitative Descriptors for Plant Morphology”, *Frontiers in Plant Science*, vol. 8. Frontiers Media SA, Feb. 03, 2017. doi: 10.3389/fpls.2017.00117.  
  
N. Busener, J. Kengkanna, P. J. Saengwilaiand A. Bucksch, “Image‐based root phenotyping links root architecture to micronutrient concentration in cassava”, *PLANTS, PEOPLE, PLANET*, vol. 2, no. 6. Wiley, pp. 678–687, Jul. 19, 2020. doi: 10.1002/ppp3.10130.  
  
J. Friesner, “The Next Generation of Training for Arabidopsis Researchers: Bioinformatics and Quantitative Biology”, *Plant Physiology*, vol. 175, no. 4. Oxford University Press (OUP), pp. 1499–1509, Dec. 2017. doi: 10.1104/pp.17.01490.  
  
J. Kengkanna, P. Jakaew, S. Amawan, N. Busener, A. Buckschand P. Saengwilai, “Phenotypic variation of cassava root traits and their responses to drought”, *Applications in Plant Sciences*, vol. 7, no. 4. Wiley, Apr. 2019. doi: 10.1002/aps3.1238.  
  
S. Liu, C. S. Barrow, M. Hanlon, J. P. Lynchand A. Bucksch, “DIRT/3D: 3D root phenotyping for field grown maize (*Zea mays*)”, *[]*. Cold Spring Harbor Laboratory, Jul. 02, 2020. doi: 10.1101/2020.06.30.180059.  
  
S. Liu, C. S. Barrow, M. Hanlon, J. P. Lynchand A. Bucksch, “DIRT/3D: 3D root phenotyping for field grown maize (*Zea mays*)”, *[]*. Cold Spring Harbor Laboratory, Jul. 02, 2020. doi: 10.1101/2020.06.30.180059.  
  
J. Salungyu, S. Thaitad, A. Bucksch, J. Kengkannaand P. J. Saengwilai, “From lab to field: Open tools facilitating the translation of maize root traits”, *Field Crops Research*, vol. 255. Elsevier BV, p. 107872, Sep. 2020. doi: 10.1016/j.fcr.2020.107872.  
  
C. Dickerson, M. Ensorand R. A. Lodder, “Establishing EDI for a Clinical Trial of a Treatment for Chikungunya”, *Lecture Notes in Computer Science*. Springer International Publishing, pp. 773–782, 2018. doi: 10.1007/978-3-319-93701-4\_61.  
  
C. Dickerson and R. A. Lodder, “The QNOAEL vs. BMD for Point of Departure”, *[]*. Cold Spring Harbor Laboratory, May 24, 2018. doi: 10.1101/329763.  
  
M. V. Tiitto and R. A. Lodder, “Working Memory and Impulsivity and Artificial Neural Networks”, *[]*. Cold Spring Harbor Laboratory, Oct. 27, 2020. doi: 10.1101/2020.10.26.355990.  
  
A. P. Aalto, “Opposing roles of microRNA Argonautes during Caenorhabditis elegans aging”, *PLOS Genetics*, vol. 14, no. 6. Public Library of Science (PLoS), p. e1007379, Jun. 21, 2018. doi: 10.1371/journal.pgen.1007379.  
  
A. L. Gladstein and M. F. Hammer, “Substructured population growth in the Ashkenazi Jews inferred with Approximate Bayesian Computation”, *[]*. Cold Spring Harbor Laboratory, Nov. 11, 2018. doi: 10.1101/467761.  
  
A. L. Gladstein and M. F. Hammer, “Substructured Population Growth in the Ashkenazi Jews Inferred with Approximate Bayesian Computation”, *Molecular Biology and Evolution*, vol. 36, no. 6. Oxford University Press (OUP), pp. 1162–1171, Mar. 06, 2019. doi: 10.1093/molbev/msz047.  
  
A. L. Gladstein, C. D. Quinto-Cortés, J. L. Pistorius, D. Christy, L. Gantnerand B. L. Joyce, “SimPrily: A Python framework to simplify high-throughput genomic simulations”, *SoftwareX*, vol. 7. Elsevier BV, pp. 335–340, Jan. 2018. doi: 10.1016/j.softx.2018.09.003.  
  
K. Levi, M. Rynge, E. Abeysingheand R. A. Edwards, “Searching the Sequence Read Archive using Jetstream and Wrangler”, *Proceedings of the Practice and Experience on Advanced Research Computing*. ACM, Jul. 22, 2018. doi: 10.1145/3219104.3229278.  
  
J. M. Doyle, “New insights into the phylogenetics and population structure of the prairie falcon (Falco mexicanus)”, *BMC Genomics*, vol. 19, no. 1. Springer Science and Business Media LLC, Apr. 04, 2018. doi: 10.1186/s12864-018-4615-z.  
  
M. Schofield, J. Duchamp, J. L. Larkin, T. J. Smyserand J. M. Doyle, “Mitochondrial genome of an Allegheny Woodrat (*Neotoma magister*)”, *Mitochondrial DNA Part B*, vol. 3, no. 1. Informa UK Limited, pp. 256–258, Jan. 02, 2018. doi: 10.1080/23802359.2018.1437806.  
  
S. A. Locke, “A new species of Clinostomum Leidy, 1856 in East Asia based on genomic and morphological data”, *Parasitology Research*, vol. 118, no. 12. Springer Science and Business Media LLC, pp. 3253–3265, Nov. 15, 2019. doi: 10.1007/s00436-019-06536-y.  
  
S. A. Locke, F. B. Drago, V. Núñez, G. T. R. e . Souzaand R. M. Takemoto, “Phylogenetic position of Diplostomum spp. from New World herons based on complete mitogenomes, rDNA operons, and DNA barcodes, including a new species with partially elucidated life cycle”, *Parasitology Research*, vol. 119, no. 7. Springer Science and Business Media LLC, pp. 2129–2137, May 30, 2020. doi: 10.1007/s00436-020-06713-4.  
  
S. A. Locke, A. V. Dam, M. Caffara, H. A. Pinto, D. López-Hernándezand C. Blanar, “Nuclear and mitochondrial phylogenomics of the Diplostomoidea and Diplostomida (Digenea, Platyhelminthes)1”, *[]*. Cold Spring Harbor Laboratory, May 30, 2018. doi: 10.1101/333518.  
  
S. A. Locke, A. Van Dam, M. Caffara, H. A. Pinto, D. López-Hernándezand C. A. Blanar, “Validity of the Diplostomoidea and Diplostomida (Digenea, Platyhelminthes) upheld in phylogenomic analysis”, *International Journal for Parasitology*, vol. 48, no. 13. Elsevier BV, pp. 1043–1059, Nov. 2018. doi: 10.1016/j.ijpara.2018.07.001.  
  
L. D. Waldrop, Y. Heand S. Khatri, “What Can Computational Modeling Tell Us about the Diversity of Odor-Capture Structures in the Pancrustacea?”, *Journal of Chemical Ecology*, vol. 44, no. 12. Springer Science and Business Media LLC, pp. 1084–1100, Sep. 21, 2018. doi: 10.1007/s10886-018-1017-2.  
  
M. C. Chambers, “An Accessible Proteogenomics Informatics Resource for Cancer Researchers”, *Cancer Research*, vol. 77, no. 21. American Association for Cancer Research (AACR), pp. e43–e46, Oct. 31, 2017. doi: 10.1158/0008-5472.can-17-0331.  
  
C. W. Easterly, “metaQuantome: An Integrated, Quantitative Metaproteomics Approach Reveals Connections Between Taxonomy and Protein Function in Complex Microbiomes”, *Molecular & Cellular Proteomics*, vol. 18, no. 8. Elsevier BV, pp. S82–S91, Aug. 2019. doi: 10.1074/mcp.ra118.001240.  
  
S. L. Hubler, “Challenges in Peptide-Spectrum Matching: A Robust and Reproducible Statistical Framework for Removing Low-Accuracy, High-Scoring Hits”, *Journal of Proteome Research*, vol. 19, no. 1. American Chemical Society (ACS), pp. 161–173, Dec. 03, 2019. doi: 10.1021/acs.jproteome.9b00478.  
  
P. Kumar, “A sectioning and database enrichment approach for improved peptide spectrum matching in large, genome-guided protein sequence databases”, *[]*. Cold Spring Harbor Laboratory, Nov. 15, 2019. doi: 10.1101/843078.  
  
T. McGowan, “Multi-omics Visualization Platform: An extensible Galaxy plug-in for multi-omics data visualization and exploration”, *GigaScience*, vol. 9, no. 4. Oxford University Press (OUP), Mar. 28, 2020. doi: 10.1093/gigascience/giaa025.  
  
S. Mehta, “Precursor intensity-based label-free quantification software tools for proteomic and multiomic analysis within the Galaxy Platform”, *[]*. Cold Spring Harbor Laboratory, Apr. 02, 2020. doi: 10.1101/2020.04.01.003988.  
  
R. Sajulga, “Survey of metaproteomics software tools for functional microbiome analysis”, *[]*. Cold Spring Harbor Laboratory, Jan. 08, 2020. doi: 10.1101/2020.01.07.897561.  
  
P. A. Stewart, “The Galaxy Platform for Reproducible Affinity Proteomic Mass Spectrometry Data Analysis”, *Methods in Molecular Biology*. Springer New York, pp. 249–261, 2019. doi: 10.1007/978-1-4939-9232-4\_16.  
  
S. Afiuni-Zadeh, “Evaluating the potential of residual Pap test fluid as a resource for the metaproteomic analysis of the cervical-vaginal microbiome”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, Jul. 18, 2018. doi: 10.1038/s41598-018-29092-4.  
  
A. Argentini, “Update on the moFF Algorithm for Label-Free Quantitative Proteomics”, *Journal of Proteome Research*, vol. 18, no. 2. American Chemical Society (ACS), pp. 728–731, Dec. 04, 2018. doi: 10.1021/acs.jproteome.8b00708.  
  
P. D. Jagtap, “BAL Fluid Metaproteome in Acute Respiratory Failure”, *American Journal of Respiratory Cell and Molecular Biology*, vol. 59, no. 5. American Thoracic Society, pp. 648–652, Nov. 2018. doi: 10.1165/rcmb.2018-0068le.  
  
J. E. Johnson, “Improve your Galaxy text life: The Query Tabular Tool”, *F1000Research*, vol. 7. F1000 Research Ltd, p. 1604, Jan. 09, 2019. doi: 10.12688/f1000research.16450.2.  
  
P. Kumar, “QuanTP: A Software Resource for Quantitative Proteo-Transcriptomic Comparative Data Analysis and Informatics”, *Journal of Proteome Research*, vol. 18, no. 2. American Chemical Society (ACS), pp. 782–790, Dec. 24, 2018. doi: 10.1021/acs.jproteome.8b00727.  
  
R. Sajulga, “Bridging the Chromosome-centric and Biology/Disease-driven Human Proteome Projects: Accessible and Automated Tools for Interpreting the Biological and Pathological Impact of Protein Sequence Variants Detected via Proteogenomics”, *Journal of Proteome Research*, vol. 17, no. 12. American Chemical Society (ACS), pp. 4329–4336, Aug. 21, 2018. doi: 10.1021/acs.jproteome.8b00404.  
  
E. Bolyen, “QIIME 2: Reproducible, interactive, scalable, and extensible microbiome data science”, *[]*. PeerJ, Dec. 03, 2018. doi: 10.7287/peerj.preprints.27295v2.  
  
E. Bolyen, “QIIME 2: Reproducible, interactive, scalable, and extensible microbiome data science”, *[]*. PeerJ, Dec. 03, 2018. doi: 10.7287/peerj.preprints.27295v2.  
  
R. Buels, “JBrowse: a dynamic web platform for genome visualization and analysis”, *Genome Biology*, vol. 17, no. 1. Springer Science and Business Media LLC, Apr. 12, 2016. doi: 10.1186/s13059-016-0924-1.  
  
R. Buels, “JBrowse: a dynamic web platform for genome visualization and analysis”, *Genome Biology*, vol. 17, no. 1. Springer Science and Business Media LLC, Apr. 12, 2016. doi: 10.1186/s13059-016-0924-1.  
  
W. Huber, “Orchestrating high-throughput genomic analysis with Bioconductor”, *Nature Methods*, vol. 12, no. 2. Springer Science and Business Media LLC, pp. 115–121, Jan. 29, 2015. doi: 10.1038/nmeth.3252.  
  
R. A. Light, “Mosquitto: server and client implementation of the MQTT protocol”, *The Journal of Open Source Software*, vol. 2, no. 13. The Open Journal, p. 265, May 26, 2017. doi: 10.21105/joss.00265.  
  
R. A. Light, “Mosquitto: server and client implementation of the MQTT protocol”, *The Journal of Open Source Software*, vol. 2, no. 13. The Open Journal, p. 265, May 26, 2017. doi: 10.21105/joss.00265.  
  
B. W. Stamps, “Metabolic Capability and Phylogenetic Diversity of Mono Lake during a Bloom of the Eukaryotic Phototroph Picocystis sp. Strain ML”, *Applied and Environmental Microbiology*, vol. 84, no. 21. American Society for Microbiology, Nov. 2018. doi: 10.1128/aem.01171-18.  
  
J. A. Goodheart, “Comparative morphology and evolution of the cnidosac in Cladobranchia (Gastropoda: Heterobranchia: Nudibranchia)”, *Frontiers in Zoology*, vol. 15, no. 1. Springer Science and Business Media LLC, Nov. 13, 2018. doi: 10.1186/s12983-018-0289-2.  
  
H. Nottebrock, M.-L. Weng, M. T. Rutterand C. B. Fenster, “Rapid evolution by spontaneous mutation increases genetic diversity facilitating plant population survival”, *[]*. Cold Spring Harbor Laboratory, Dec. 17, 2018. doi: 10.1101/497610.  
  
M.-L. Weng, “Fine-Grained Analysis of Spontaneous Mutation Spectrum and Frequency in *Arabidopsis thaliana*”, *Genetics*, vol. 211, no. 2. Oxford University Press (OUP), pp. 703–714, Dec. 04, 2018. doi: 10.1534/genetics.118.301721.  
  
S.-K. Han, “MUTE Directly Orchestrates Cell-State Switch and the Single Symmetric Division to Create Stomata”, *Developmental Cell*, vol. 45, no. 3. Elsevier BV, pp. 303–315.e5, May 2018. doi: 10.1016/j.devcel.2018.04.010.  
  
W. J. Allen, R. E. Gabr, G. B. Tefera, A. S. Pednekar, M. W. Vaughnand P. A. Narayana, “Platform for Automated Real-Time High Performance Analytics on Medical Image Data”, *IEEE Journal of Biomedical and Health Informatics*, vol. 22, no. 2. Institute of Electrical and Electronics Engineers (IEEE), pp. 318–324, Mar. 2018. doi: 10.1109/jbhi.2017.2771299.  
  
N. Shen, Y. Fanand S. Pamidighantam, “E-science infrastructures for molecular modeling and parametrization”, *Journal of Computational Science*, vol. 5, no. 4. Elsevier BV, pp. 576–589, Jul. 2014. doi: 10.1016/j.jocs.2014.01.005.  
  
P. G. Menon, K. Pekkanand S. Madan, “Quantitative Hemodynamic Evaluation in Children with Coarctation of Aorta: Phase Contrast Cardiovascular MRI versus Computational Fluid Dynamics”, *Statistical Atlases and Computational Models of the Heart. Imaging and Modelling Challenges*. Springer Berlin Heidelberg, pp. 9–16, 2013. doi: 10.1007/978-3-642-36961-2\_2.  
  
M. Burtscher and H. Rabeti, “A Scalable Heterogeneous Parallelization Framework for Iterative Local Searches”, *2013 IEEE 27th International Symposium on Parallel and Distributed Processing*. IEEE, May 2013. doi: 10.1109/ipdps.2013.27.  
  
M. Nayhouse, A. M. Amlani, V. R. Hengand G. Orkoulas, “Simulation of fluid–solid coexistence via thermodynamic integration using a modified cell model”, *Journal of Physics: Condensed Matter*, vol. 24, no. 15. IOP Publishing, p. 155101, Feb. 27, 2012. doi: 10.1088/0953-8984/24/15/155101.  
  
M. Nayhouse, A. M. Amlaniand G. Orkoulas, “A Monte Carlo study of the freezing transition of hard spheres”, *Journal of Physics: Condensed Matter*, vol. 23, no. 32. IOP Publishing, p. 325106, Jul. 28, 2011. doi: 10.1088/0953-8984/23/32/325106.  
  
M. Nayhouse, A. M. Amlaniand G. Orkoulas, “Precise simulation of the freezing transition of supercritical Lennard-Jones”, *The Journal of Chemical Physics*, vol. 135, no. 15. AIP Publishing, p. 154103, Oct. 21, 2011. doi: 10.1063/1.3651193.  
  
M. Nayhouse, V. R. Heng, A. M. Amlaniand G. Orkoulas, “Precise simulation of subcritical freezing using constrained cell models”, *Journal of Physics A: Mathematical and Theoretical*, vol. 45, no. 15. IOP Publishing, p. 155002, Mar. 30, 2012. doi: 10.1088/1751-8113/45/15/155002.  
  
G. Orkoulas and M. Nayhouse, “Communication: A simple method for simulation of freezing transitions”, *The Journal of Chemical Physics*, vol. 134, no. 17. AIP Publishing, p. 171104, May 05, 2011. doi: 10.1063/1.3587103.  
  
D. Colbry, “Reducing the barrier to entry using portable apps”, *Proceedings of the 2011 TeraGrid Conference: Extreme Digital Discovery*. ACM, Jul. 18, 2011. doi: 10.1145/2016741.2016792.  
  
Z. Gu, M. Small, X. Yuan, A. Maratheand D. K. Lowenthal, “Protocol Customization for Improving MPI Performance on RDMA-Enabled Clusters”, *International Journal of Parallel Programming*, vol. 41, no. 5. Springer Science and Business Media LLC, pp. 682–703, Feb. 28, 2013. doi: 10.1007/s10766-013-0242-0.  
  
A. L. Ferguson, N. Giovambattista, P. J. Rossky, A. Z. Panagiotopoulosand P. G. Debenedetti, “A computational investigation of the phase behavior and capillary sublimation of water confined between nanoscale hydrophobic plates”, *The Journal of Chemical Physics*, vol. 137, no. 14. AIP Publishing, p. 144501, Oct. 14, 2012. doi: 10.1063/1.4755750.  
  
J. S.-I. Kwon, M. Nayhouse, P. D. Christofidesand G. Orkoulas, “Protein Crystal Shape and Size Control in Batch Crystallization: Comparing Model Predictive Control with Conventional Operating Policies”, *Industrial & Engineering Chemistry Research*, vol. 53, no. 13. American Chemical Society (ACS), pp. 5002–5014, Jun. 11, 2013. doi: 10.1021/ie400584g.  
  
J. S.-I. Kwon, M. Nayhouse, P. D. Christofidesand G. Orkoulas, “Modeling and control of protein crystal shape and size in batch crystallization”, *AIChE Journal*, vol. 59, no. 7. Wiley, pp. 2317–2327, Mar. 04, 2013. doi: 10.1002/aic.14039.  
  
J. S.-I. Kwon, M. Nayhouse, P. D. Christofidesand G. Orkoulas, “Modeling and control of crystal shape in continuous protein crystallization”, *Chemical Engineering Science*, vol. 107. Elsevier BV, pp. 47–57, Apr. 2014. doi: 10.1016/j.ces.2013.12.005.  
  
M. Nayhouse, V. R. Heng, A. M. Amlaniand G. Orkoulas, “Simulation of phase boundaries using constrained cell models”, *Journal of Physics: Condensed Matter*, vol. 24, no. 37. IOP Publishing, p. 375105, Aug. 01, 2012. doi: 10.1088/0953-8984/24/37/375105.  
  
M. Nayhouse, J. S.-I. Kwon, V. R. Heng, A. M. Amlaniand G. Orkoulas, “Freezing Transition Studies Through Constrained Cell Model Simulation”, *International Journal of Thermophysics*, vol. 35, no. 9–10. Springer Science and Business Media LLC, pp. 1661–1676, Apr. 25, 2013. doi: 10.1007/s10765-013-1430-2.  
  
M. Nayhouse, J. S.-I. Kwonand G. Orkoulas, “Communication: Phase transitions, criticality, and three-phase coexistence in constrained cell models”, *The Journal of Chemical Physics*, vol. 136, no. 20. AIP Publishing, p. 201101, May 28, 2012. doi: 10.1063/1.4725768.  
  
M. Nayhouse, J. Sang-Il Kwon, P. D. Christofidesand G. Orkoulas, “Crystal shape modeling and control in protein crystal growth”, *Chemical Engineering Science*, vol. 87. Elsevier BV, pp. 216–223, Jan. 2013. doi: 10.1016/j.ces.2012.10.020.  
  
J. Sang-Il Kwon, M. Nayhouse, P. D. Christofidesand G. Orkoulas, “Modeling and control of shape distribution of protein crystal aggregates”, *Chemical Engineering Science*, vol. 104. Elsevier BV, pp. 484–497, Dec. 2013. doi: 10.1016/j.ces.2013.09.026.  
  
J. C. Browne, “Comprehensive, open-source resource usage measurement and analysis for HPC systems”, *Concurrency and Computation: Practice and Experience*, vol. 26, no. 13. Wiley, pp. 2191–2209, Mar. 06, 2014. doi: 10.1002/cpe.3245.  
  
J. C. Browne, “Enabling comprehensive data-driven system management for large computational facilities”, *Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis*. ACM, Nov. 17, 2013. doi: 10.1145/2503210.2503230.  
  
T. R. Furlani, “Performance metrics and auditing framework using application kernels for high‐performance computer systems”, *Concurrency and Computation: Practice and Experience*, vol. 25, no. 7. Wiley, pp. 918–931, Jun. 14, 2012. doi: 10.1002/cpe.2871.  
  
C.-D. Lu, “Comprehensive job level resource usage measurement and analysis for XSEDE HPC systems”, *Proceedings of the Conference on Extreme Science and Engineering Discovery Environment: Gateway to Discovery*. ACM, Jul. 22, 2013. doi: 10.1145/2484762.2484781.  
  
J. T. Palmer, “Open XDMoD: A Tool for the Comprehensive Management of High-Performance Computing Resources”, *Computing in Science & Engineering*, vol. 17, no. 4. Institute of Electrical and Electronics Engineers (IEEE), pp. 52–62, Jul. 2015. doi: 10.1109/mcse.2015.68.  
  
N. A. Simakov, “Slurm Simulator”, *Proceedings of the Practice and Experience on Advanced Research Computing*. ACM, Jul. 22, 2018. doi: 10.1145/3219104.3219111.  
  
N. A. Simakov, “A Quantitative Analysis of Node Sharing on HPC Clusters Using XDMoD Application Kernels”, *Proceedings of the XSEDE16 Conference on Diversity, Big Data, and Science at Scale*. ACM, Jul. 17, 2016. doi: 10.1145/2949550.2949553.  
  
J. M. Sperhac, “Managing computational gateway resources with XDMoD”, *Future Generation Computer Systems*, vol. 98. Elsevier BV, pp. 154–166, Sep. 2019. doi: 10.1016/j.future.2019.03.029.  
  
J. Sperhac, “Federating XDMoD to Monitor Affiliated Computing Resources”, *2018 IEEE International Conference on Cluster Computing (CLUSTER)*. IEEE, Sep. 2018. doi: 10.1109/cluster.2018.00074.  
  
C. A. Stewart, “Assessment of non-financial returns on cyberinfrastructure”, *Proceedings of the Humans in the Loop: Enabling and Facilitating Research on Cloud Computing*. ACM, Jul. 29, 2019. doi: 10.1145/3355738.3355749.  
  
F. Wang, “Evaluating the Scientific Impact of XSEDE”, *Proceedings of the Practice and Experience on Advanced Research Computing*. ACM, Jul. 22, 2018. doi: 10.1145/3219104.3219124.  
  
F. Wang, G. von Laszewski, G. C. Fox, T. R. Furlani, R. L. DeLeonand S. M. Gallo, “Towards a Scientific Impact Measuring Framework for Large Computing Facilities - a Case Study on XSEDE”, *Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment*. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616507.  
  
J. P. White, A. D. Kofke, R. L. DeLeon, M. Innus, M. D. Jonesand T. R. Furlani, “Automatic Characterization of HPC Job Parallel Filesystem I/O Patterns”, *Proceedings of the Practice and Experience on Advanced Research Computing*. ACM, Jul. 22, 2018. doi: 10.1145/3219104.3219121.  
  
G. Bustos Lozano, Á. Hidalgo Romero, A. Melgar Bonis, N. Ureta Velasco, C. Orbea Gallardoand C. Pallás Alonso, “Hipofosforemia precoz en recién nacidos de riesgo. Frecuencia y magnitud”, *Anales de Pediatría*, vol. 88, no. 4. Elsevier BV, pp. 216–222, Apr. 2018. doi: 10.1016/j.anpedi.2017.04.010.  
  
Á. Hidalgo Romero, E. Gómez Domínguez, R. Muñoz Gómez, C. Muñoz Codoceoand I. Fernández Vázquez, “Hipertensión portal secundaria a hemangiomatosis hepática múltiple”, *Gastroenterología y Hepatología*, vol. 41, no. 5. Elsevier BV, pp. 323–324, May 2018. doi: 10.1016/j.gastrohep.2017.06.007.  
  
W. Ibarra-Hernández, S. Hajinazar, G. Avendaño-Franco, A. Bautista-Hernández, A. N. Kolmogorovand A. H. Romero, “Structural search for stable Mg–Ca alloys accelerated with a neural network interatomic model”, *Physical Chemistry Chemical Physics*, vol. 20, no. 43. Royal Society of Chemistry (RSC), pp. 27545–27557, 2018. doi: 10.1039/c8cp05314f.  
  
N. Mottaghi, “Erratum: “Insights into the magnetic dead layer in La0.7Sr0.3MnO3 thin films from temperature, magnetic field and thickness dependence of their magnetization” [AIP Advances 8, 056319 (2018)]”, *AIP Advances*, vol. 8, no. 2. AIP Publishing, p. 029902, Feb. 2018. doi: 10.1063/1.5023228.  
  
N. Mottaghi, “Insights into the magnetic dead layer in La0.7Sr0.3MnO3 thin films from temperature, magnetic field and thickness dependence of their magnetization”, *AIP Advances*, vol. 8, no. 5. AIP Publishing, p. 056319, May 2018. doi: 10.1063/1.5005913.  
  
A. Payne, G. Avendaño-Franco, E. Bousquetand A. H. Romero, “Firefly Algorithm Applied to Noncollinear Magnetic Phase Materials Prediction”, *Journal of Chemical Theory and Computation*, vol. 14, no. 8. American Chemical Society (ACS), pp. 4455–4466, Jul. 02, 2018. doi: 10.1021/acs.jctc.8b00404.  
  
P. Pramanik, “Cubic phase stability, optical and magnetic properties of Cu-stabilized zirconia nanocrystals”, *Journal of Physics D: Applied Physics*, vol. 51, no. 22. IOP Publishing, p. 225304, May 14, 2018. doi: 10.1088/1361-6463/aac004.  
  
C. Rodríguez-Fernández, “Isotopic Heft on the *B*1*l* Silent Mode in Ultra-Narrow Gallium Nitride Nanowires”, *Nano Letters*, vol. 18, no. 8. American Chemical Society (ACS), pp. 5091–5097, Jul. 25, 2018. doi: 10.1021/acs.nanolett.8b01955.  
  
A. H. Romero and M. J. Verstraete, “From one to three, exploring the rungs of Jacob’s ladder in magnetic alloys”, *The European Physical Journal B*, vol. 91, no. 8. Springer Science and Business Media LLC, Aug. 2018. doi: 10.1140/epjb/e2018-90275-5.  
  
R. Trappen, “Electrostatic potential and valence modulation in La0.7Sr0.3MnO3 thin films”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, Sep. 25, 2018. doi: 10.1038/s41598-018-32701-x.  
  
P. Treviño, “Anharmonic contribution to the stabilization of Mg(OH)2from first principles”, *Physical Chemistry Chemical Physics*, vol. 20, no. 26. Royal Society of Chemistry (RSC), pp. 17799–17808, 2018. doi: 10.1039/c8cp02490a.  
  
A. Lenharth, D. Nguyenand K. Pingali, “Priority Queues Are Not Good Concurrent Priority Schedulers”, *Lecture Notes in Computer Science*. Springer Berlin Heidelberg, pp. 209–221, 2015. doi: 10.1007/978-3-662-48096-0\_17.  
  
D. Nguyen, A. Lenharthand K. Pingali, “A lightweight infrastructure for graph analytics”, *Proceedings of the Twenty-Fourth ACM Symposium on Operating Systems Principles*. ACM, Nov. 03, 2013. doi: 10.1145/2517349.2522739.  
  
S. Maleki, D. Nguyen, A. Lenharth, M. Garzarán, D. Paduaand K. Pingali, “DSMR”, *Proceedings of the 21st ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming*. ACM, Feb. 27, 2016. doi: 10.1145/2851141.2851183.  
  
A. N. GANSHIN, V. B. EFIMOV, G. V. KOLMAKOV, L. P. MEZHOV-DEGLINand P. V. E. McCLINTOCK, “NONLINEAR SECOND SOUND WAVES IN SUPERFLUID HELIUM: INSTABILITIES, TURBULENCE AND ROGUE WAVES”, *International Journal of Bifurcation and Chaos*, vol. 22, no. 10. World Scientific Pub Co Pte Lt, p. 1250242, Oct. 2012. doi: 10.1142/s0218127412502422.  
  
A. Gothandaraman, S. Sadatian, M. Faryniarz, O. L. Bermanand G. V. Kolmakov, “Application of Graphics Processing Units (GPUs) to the Study of Non-linear Dynamics of the Exciton Bose-Einstein Condensate in a Semiconductor Quantum Well”, *2011 Symposium on Application Accelerators in High-Performance Computing*. IEEE, Jul. 2011. doi: 10.1109/saahpc.2011.32.  
  
G. V. Kolmakov, “Using Nanoparticle-Filled Microcapsules for Site-Specific Healing of Damaged Substrates: Creating a “Repair-and-Go” System”, *ACS Nano*, vol. 4, no. 2. American Chemical Society (ACS), pp. 1115–1123, Jan. 20, 2010. doi: 10.1021/nn901296y.  
  
G. V. Kolmakov, A. Schaefer, I. Aransonand A. C. Balazs, “Designing mechano-responsive microcapsules that undergo self-propelled motion”, *Soft Matter*, vol. 8, no. 1. Royal Society of Chemistry (RSC), pp. 180–190, 2012. doi: 10.1039/c1sm06415k.  
  
R. Rong, J. Haoand J. Liu, “Performance Study of a Minimalistic Simulator on XSEDE Massively Parallel Systems”, *Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment*. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616512.  
  
S. A. Ludwig, “MapReduce-based optimization of overlay networks using particle swarm optimization”, *Proceedings of the 2014 Annual Conference on Genetic and Evolutionary Computation*. ACM, Jul. 12, 2014. doi: 10.1145/2576768.2598269.  
  
K. Ravichandran and S. Pande, “Multiverse”, *ACM SIGPLAN Notices*, vol. 48, no. 10. Association for Computing Machinery (ACM), pp. 533–552, Oct. 29, 2013. doi: 10.1145/2544173.2509525.  
  
H.-V. Dang and M. Snir, “FULT”, *Proceedings of the 47th International Conference on Parallel Processing*. ACM, Aug. 13, 2018. doi: 10.1145/3225058.3225115.  
  
M. Chabbi, M. Faganand J. Mellor-Crummey, “High performance locks for multi-level NUMA systems”, *Proceedings of the 20th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming*. ACM, Jan. 24, 2015. doi: 10.1145/2688500.2688503.  
  
D. Khaldi, P. Jouvelot, F. Irigoin, C. Ancourtand B. Chapman, “LLVM parallel intermediate representation”, *Proceedings of the Second Workshop on the LLVM Compiler Infrastructure in HPC*. ACM, Nov. 15, 2015. doi: 10.1145/2833157.2833158.  
  
S. Zeng, Z. Lyu, S. R. K. Narisetti, D. Xuand T. Joshi, “Knowledge Base Commons (KBCommons) v1.0: A multi OMICS’ web-based data integration framework for biological discoveries”, *2018 IEEE International Conference on Bioinformatics and Biomedicine (BIBM)*. IEEE, Dec. 2018. doi: 10.1109/bibm.2018.8621369.  
  
L. Chen, X. Huo, B. Ren, S. Jainand G. Agrawal, “Efficient and Simplified Parallel Graph Processing over CPU and MIC”, *2015 IEEE International Parallel and Distributed Processing Symposium*. IEEE, May 2015. doi: 10.1109/ipdps.2015.88.  
  
P. Jiang, L. Chenand G. Agrawal, “Reusing Data Reorganization for Efficient SIMD Parallelization of Adaptive Irregular Applications”, *Proceedings of the 2016 International Conference on Supercomputing*. ACM, Jun. 2016. doi: 10.1145/2925426.2926285.  
  
S. V. Perez and F. Saeed, “A Parallel Algorithm for Compression of Big Next-Generation Sequencing Datasets”, *2015 IEEE Trustcom/BigDataSE/ISPA*. IEEE, Aug. 2015. doi: 10.1109/trustcom.2015.632.  
  
S. V. Perez and F. Saeed, “Scalable data structure to compress next-generation sequencing files and its application to compressive genomics”, *2017 IEEE International Conference on Bioinformatics and Biomedicine (BIBM)*. IEEE, Nov. 2017. doi: 10.1109/bibm.2017.8217953.  
  
R. Garg, J. Cao, K. Arya, G. Coopermanand J. Vienne, “Extended Batch Sessions and Three-Phase Debugging”, *Proceedings of the XSEDE16 Conference on Diversity, Big Data, and Science at Scale*. ACM, Jul. 17, 2016. doi: 10.1145/2949550.2949645.  
  
J. Behrens, S. Jha, K. Birmanand E. Tremel, “RDMC: A Reliable RDMA Multicast for Large Objects”, *2018 48th Annual IEEE/IFIP International Conference on Dependable Systems and Networks (DSN)*. IEEE, Jun. 2018. doi: 10.1109/dsn.2018.00020.  
  
S. Jha, “Derecho”, *ACM Transactions on Computer Systems*, vol. 36, no. 2. Association for Computing Machinery (ACM), pp. 1–49, May 31, 2018. doi: 10.1145/3302258.  
  
X. Li, Y. Wang, D. Wu, L. Liu, S.-H. Boand G. Ceder, “Jahn–Teller Assisted Na Diffusion for High Performance Na Ion Batteries”, *Chemistry of Materials*, vol. 28, no. 18. American Chemical Society (ACS), pp. 6575–6583, Sep. 12, 2016. doi: 10.1021/acs.chemmater.6b02440.  
  
P. Guo and C.-. wei . Lee, “A Performance Prediction and Analysis Integrated Framework for SpMV on GPUs”, *Procedia Computer Science*, vol. 80. Elsevier BV, pp. 178–189, 2016. doi: 10.1016/j.procs.2016.05.308.  
  
P. Guo and C. Zhang, “Multi-GPU implementation and performance optimization for CSR-based sparse matrix-vector multiplication”, *2017 3rd IEEE International Conference on Computer and Communications (ICCC)*. IEEE, Dec. 2017. doi: 10.1109/compcomm.2017.8322969.  
  
L. Ning, R. Pittmanand X. Shen, “LCD: A Fast Contrastive Divergence Based Algorithm for Restricted Boltzmann Machine”, *2017 IEEE International Conference on Data Mining (ICDM)*. IEEE, Nov. 2017. doi: 10.1109/icdm.2017.131.  
  
S. Puri, A. Paudeland S. K. Prasad, “MPI-Vector-IO”, *Proceedings of the 47th International Conference on Parallel Processing*. ACM, Aug. 13, 2018. doi: 10.1145/3225058.3225105.  
  
S. Taheri, I. Briggs, M. Burtscherand G. Gopalakrishnan, “DiffTrace: Efficient Whole-Program Trace Analysis and Diffing for Debugging”, *2019 IEEE International Conference on Cluster Computing (CLUSTER)*. IEEE, Sep. 2019. doi: 10.1109/cluster.2019.8891027.  
  
S. Taheri, S. Devale, G. Gopalakrishnanand M. Burtscher, “ParLoT: Efficient Whole-Program Call Tracing for HPC Applications”, *Programming and Performance Visualization Tools*. Springer International Publishing, pp. 162–184, 2019. doi: 10.1007/978-3-030-17872-7\_10.  
  
A. Ma, M. Sun, A. McDermaid, B. Liuand Q. Ma, “MetaQUBIC: a computational pipeline for gene-level functional profiling of metagenome and metatranscriptome”, *Bioinformatics*, vol. 35, no. 21. Oxford University Press (OUP), pp. 4474–4477, May 22, 2019. doi: 10.1093/bioinformatics/btz414.  
  
B. Monier, “IRIS-EDA: An integrated RNA-Seq interpretation system for gene expression data analysis”, *PLOS Computational Biology*, vol. 15, no. 2. Public Library of Science (PLoS), p. e1006792, Feb. 14, 2019. doi: 10.1371/journal.pcbi.1006792.  
  
C. Wan, “LTMG: A novel statistical modeling of transcriptional expression states in single-cell RNA-Seq data”, *[]*. Cold Spring Harbor Laboratory, Sep. 29, 2018. doi: 10.1101/430009.  
  
J. Xie, “QUBIC2: A novel biclustering algorithm for large-scale bulk RNA-sequencing and single-cell RNA-sequencing data analysis”, *[]*. Cold Spring Harbor Laboratory, Sep. 07, 2018. doi: 10.1101/409961.  
  
A. Ma, A. McDermaid, J. Xu, Y. Changand Q. Ma, “Integrative Methods and Practical Challenges for Single-Cell Multi-omics”, *Trends in Biotechnology*, vol. 38, no. 9. Elsevier BV, pp. 1007–1022, Sep. 2020. doi: 10.1016/j.tibtech.2020.02.013.  
  
A. Ma, “IRIS3: integrated cell-type-specific regulon inference server from single-cell RNA-Seq”, *Nucleic Acids Research*, vol. 48, no. W1. Oxford University Press (OUP), pp. W275–W286, May 18, 2020. doi: 10.1093/nar/gkaa394.  
  
J. Xie, “QUBIC2: a novel and robust biclustering algorithm for analyses and interpretation of large-scale RNA-Seq data”, *Bioinformatics*, vol. 36, no. 4. Oxford University Press (OUP), pp. 1143–1149, Sep. 10, 2019. doi: 10.1093/bioinformatics/btz692.  
  
J. Yang, “Prediction of regulatory motifs from human Chip-sequencing data using a deep learning framework”, *Nucleic Acids Research*, vol. 47, no. 15. Oxford University Press (OUP), pp. 7809–7824, Aug. 02, 2019. doi: 10.1093/nar/gkz672.  
  
J. Booth and G. Bolet, “Javelin: A Scalable Implementation for Sparse Incomplete LU Factorization”, *2019 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*. IEEE, May 2019. doi: 10.1109/ipdpsw.2019.00087.  
  
H. D. Mathias and S. S. Foley, “A parallel two-stage genetic algorithm for route planning”, *Proceedings of the 2020 Genetic and Evolutionary Computation Conference Companion*. ACM, Jul. 08, 2020. doi: 10.1145/3377929.3398116.  
  
T. Phillips, X. Yu, B. Haakensonand X. Zou, “Design and Implementation of Privacy-Preserving, Flexible and Scalable Role-Based Hierarchical Access Control”, *2019 First IEEE International Conference on Trust, Privacy and Security in Intelligent Systems and Applications (TPS-ISA)*. IEEE, Dec. 2019. doi: 10.1109/tps-isa48467.2019.00015.  
  
T. Phillips, X. Zou, F. Liand N. Li, “Enhancing Biometric-Capsule-based Authentication and Facial Recognition via Deep Learning”, *Proceedings of the 24th ACM Symposium on Access Control Models and Technologies*. ACM, May 28, 2019. doi: 10.1145/3322431.3325417.  
  
L. Yang, “A 3-D model for quantification of fatigue weak-link density and strength distribution in an A713 cast aluminum alloy”, *International Journal of Fatigue*, vol. 96. Elsevier BV, pp. 185–195, Mar. 2017. doi: 10.1016/j.ijfatigue.2016.11.035.  
  
Y. Lyu, X. Zhu, N. Xiangand G. Narsimhan, “Molecular Dynamics Study of Pore Formation by Melittin in a 1,2-Dioleoyl-*sn*-glycero-3-phosphocholine and 1,2-Di(9*Z*-octadecenoyl)-*sn*-glycero-3-phospho-(1′-*rac*-glycerol) Mixed Lipid Bilayer”, *Industrial & Engineering Chemistry Research*, vol. 54, no. 42. American Chemical Society (ACS), pp. 10275–10283, Jun. 19, 2015. doi: 10.1021/acs.iecr.5b01217.  
  
A. Ashraf, Y. Wu, M. C. Wang, N. R. Aluru, S. A. Dastgheiband S. Nam, “Spectroscopic Investigation of the Wettability of Multilayer Graphene Using Highly Ordered Pyrolytic Graphite as a Model Material”, *Langmuir*, vol. 30, no. 43. American Chemical Society (ACS), pp. 12827–12836, Oct. 23, 2014. doi: 10.1021/la503089k.  
  
A. Barati Farimani and N. R. Aluru, “Existence of Multiple Phases of Water at Nanotube Interfaces”, *The Journal of Physical Chemistry C*, vol. 120, no. 41. American Chemical Society (ACS), pp. 23763–23771, Oct. 12, 2016. doi: 10.1021/acs.jpcc.6b06156.  
  
A. Barati Farimani, P. Dibaeiniaand N. R. Aluru, “DNA Origami–Graphene Hybrid Nanopore for DNA Detection”, *ACS Applied Materials & Interfaces*, vol. 9, no. 1. American Chemical Society (ACS), pp. 92–100, Dec. 22, 2016. doi: 10.1021/acsami.6b11001.  
  
A. B. Farimani, M. Heiranianand N. R. Aluru, “Nano-electro-mechanical pump: Giant pumping of water in carbon nanotubes”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, May 19, 2016. doi: 10.1038/srep26211.  
  
A. B. Farimani, Y. Wuand N. R. Aluru, “Rotational motion of a single water molecule in a buckyball”, *Physical Chemistry Chemical Physics*, vol. 15, no. 41. Royal Society of Chemistry (RSC), p. 17993, 2013. doi: 10.1039/c3cp53277a.  
  
J. Feng, “Single-layer MoS2 nanopores as nanopower generators”, *Nature*, vol. 536, no. 7615. Springer Science and Business Media LLC, pp. 197–200, Jul. 13, 2016. doi: 10.1038/nature18593.  
  
Y. Wu and N. R. Aluru, “Graphitic Carbon–Water Nonbonded Interaction Parameters”, *The Journal of Physical Chemistry B*, vol. 117, no. 29. American Chemical Society (ACS), pp. 8802–8813, Jul. 16, 2013. doi: 10.1021/jp402051t.  
  
Y. Wu, L. K. Wagnerand N. R. Aluru, “The interaction between hexagonal boron nitride and water from first principles”, *The Journal of Chemical Physics*, vol. 142, no. 23. AIP Publishing, p. 234702, Jun. 21, 2015. doi: 10.1063/1.4922491.  
  
Y. Wu, L. K. Wagnerand N. R. Aluru, “Hexagonal boron nitride and water interaction parameters”, *The Journal of Chemical Physics*, vol. 144, no. 16. AIP Publishing, p. 164118, Apr. 28, 2016. doi: 10.1063/1.4947094.  
  
S. Boone and S. Arunachalam, “Calculation of Sensitivity Coefficients for Individual Airport Emissions in the Continental U.S. using CMAQ-DDM/PM”, *Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment*. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616504.  
  
L. G. Olson, “An inverse problem approach to stiffness mapping for early detection of breast cancer: tissue phantom experiments”, *Inverse Problems in Science and Engineering*, vol. 27, no. 7. Informa UK Limited, pp. 1006–1037, Oct. 30, 2018. doi: 10.1080/17415977.2018.1538367.  
  
D. Lobo, T. J. Maloneand M. Levin, “Towards a bioinformatics of patterning: a computational approach to understanding regulative morphogenesis”, *Biology Open*, vol. 2, no. 2. The Company of Biologists, pp. 156–169, Nov. 26, 2012. doi: 10.1242/bio.20123400.  
  
D. Lobo, T. J. Maloneand M. Levin, “Planform: an application and database of graph-encoded planarian regenerative experiments”, *Bioinformatics*, vol. 29, no. 8. Oxford University Press (OUP), pp. 1098–1100, Feb. 19, 2013. doi: 10.1093/bioinformatics/btt088.  
  
M. Budnikova, J. W. Habig, D. Lobo, N. Cornia, M. Levinand T. Andersen, “Design of a flexible component gathering algorithm for converting cell-based models to graph representations for use in evolutionary search”, *BMC Bioinformatics*, vol. 15, no. 1. Springer Science and Business Media LLC, Jun. 10, 2014. doi: 10.1186/1471-2105-15-178.  
  
F. Durant, D. Lobo, J. Hammelmanand M. Levin, “Physiological controls of large‐scale patterning in planarian regeneration: a molecular and computational perspective on growth and form”, *Regeneration*, vol. 3, no. 2. Wiley, pp. 78–102, Apr. 2016. doi: 10.1002/reg2.54.  
  
M. Lobikin, D. Lobo, D. J. Blackiston, C. J. Martyniuk, E. Tkachenkoand M. Levin, “Serotonergic regulation of melanocyte conversion: A bioelectrically regulated network for stochastic all-or-none hyperpigmentation”, *Science Signaling*, vol. 8, no. 397. American Association for the Advancement of Science (AAAS), Oct. 06, 2015. doi: 10.1126/scisignal.aac6609.  
  
D. Lobo, E. B. Feldman, M. Shah, T. J. Maloneand M. Levin, “Limbform: a functional ontology-based database of limb regeneration experiments”, *Bioinformatics*, vol. 30, no. 24. Oxford University Press (OUP), pp. 3598–3600, Aug. 27, 2014. doi: 10.1093/bioinformatics/btu582.  
  
D. Lobo, E. B. Feldman, M. Shah, T. J. Maloneand M. Levin, “A bioinformatics expert system linking functional data to anatomical outcomes in limb regeneration”, *Regeneration*, vol. 1, no. 2. Wiley, pp. 37–56, Apr. 2014. doi: 10.1002/reg2.13.  
  
D. Lobo, J. Hammelmanand M. Levin, “MoCha: Molecular Characterization of Unknown Pathways”, *Journal of Computational Biology*, vol. 23, no. 4. Mary Ann Liebert Inc, pp. 291–297, Apr. 2016. doi: 10.1089/cmb.2015.0211.  
  
D. Lobo and M. Levin, “Inferring Regulatory Networks from Experimental Morphological Phenotypes: A Computational Method Reverse-Engineers Planarian Regeneration”, *PLOS Computational Biology*, vol. 11, no. 6. Public Library of Science (PLoS), p. e1004295, Jun. 04, 2015. doi: 10.1371/journal.pcbi.1004295.  
  
D. Lobo and M. Levin, “Computing a Worm: Reverse-Engineering Planarian Regeneration”, *Emergence, Complexity and Computation*. Springer International Publishing, pp. 637–654, Jul. 27, 2016. doi: 10.1007/978-3-319-33921-4\_24.  
  
D. Lobo, M. Lobikinand M. Levin, “Discovering novel phenotypes with automatically inferred dynamic models: a partial melanocyte conversion in Xenopus”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Jan. 27, 2017. doi: 10.1038/srep41339.  
  
D. Lobo, J. Morokumaand M. Levin, “Computational discovery and*in vivo*validation of*hnf4*as a regulatory gene in planarian regeneration”, *Bioinformatics*, vol. 32, no. 17. Oxford University Press (OUP), pp. 2681–2685, May 10, 2016. doi: 10.1093/bioinformatics/btw299.  
  
B. P. Rubin, “A dynamic architecture of life”, *F1000Research*, vol. 4. F1000 Research Ltd, p. 1288, Nov. 18, 2015. doi: 10.12688/f1000research.7315.1.  
  
A. B. Craig, “Getting started with high performance computing for humanities, arts, and social science”, *Proceedings of the Conference on Extreme Science and Engineering Discovery Environment: Gateway to Discovery*. ACM, Jul. 22, 2013. doi: 10.1145/2484762.2484788.  
  
R. Barnes, “Parallel Priority-Flood depression filling for trillion cell digital elevation models on desktops or clusters”, *Computers & Geosciences*, vol. 96. Elsevier BV, pp. 56–68, Nov. 2016. doi: 10.1016/j.cageo.2016.07.001.  
  
R. Barnes, “Optimal orientations of discrete global grids and the Poles of Inaccessibility”, *International Journal of Digital Earth*, vol. 13, no. 7. Informa UK Limited, pp. 803–816, Feb. 14, 2019. doi: 10.1080/17538947.2019.1576786.  
  
R. Barnes, “Accelerating a fluvial incision and landscape evolution model with parallelism”, *Geomorphology*, vol. 330. Elsevier BV, pp. 28–39, Apr. 2019. doi: 10.1016/j.geomorph.2019.01.002.  
  
R. Barnes, K. L. Callaghanand A. D. Wickert, “Computing water flow through complex landscapes, Part 2: Finding hierarchies in depressions and morphological segmentations”, *[]*. Copernicus GmbH, Jun. 17, 2019. doi: 10.5194/esurf-2019-34.  
  
J. Fischer, D. Y. Hancock, J. M. Lowe, G. Turner, W. Snapp-Childsand C. A. Stewart, “Jetstream”, *Proceedings of the 2017 ACM SIGUCCS Annual Conference*. ACM, Oct. 2017. doi: 10.1145/3123458.3123466.  
  
K. A. Agnew-Francis and C. M. Williams, “Squaramides as Bioisosteres in Contemporary Drug Design”, *Chemical Reviews*, vol. 120, no. 20. American Chemical Society (ACS), pp. 11616–11650, Sep. 15, 2020. doi: 10.1021/acs.chemrev.0c00416.  
  
A. Grushow and M. S. Reeves, “Using Computational Methods To Teach Chemical Principles: Overview”, *ACS Symposium Series*. American Chemical Society, pp. 1–10, Jan. 2019. doi: 10.1021/bk-2019-1312.ch001.  
  
C. J. Higgins and S. J. Duranceau, “Removal of Enantiomeric Ibuprofen in a Nanofiltration Membrane Process”, *Membranes*, vol. 10, no. 12. MDPI AG, p. 383, Nov. 30, 2020. doi: 10.3390/membranes10120383.  
  
J. Jung, S. Zirpoliand G. Slick, “Implementation of Computational Aids in Diels-Alder Reactions: Regioselectivity and Stereochemistry of Adduct Formation”, *The Journal of Computational Science Education*, vol. 8, no. 1. The Shodor Education Foundation, Inc., pp. 2–6, Jan. 2017. doi: 10.22369/issn.2153-4136/8/1/1.  
  
J. Lu, Z. Zhang, D. Yan, Z. Zhang, J. Guanand J. Qiao, “Synthesis of 4-Chloro-1,3-Diazobenzene Bent-Cores Liquid Crystal and Characterizations of Its Mesogenic Behaviors and Photosensitivity”, *[]*. American Chemical Society (ACS), May 11, 2020. doi: 10.26434/chemrxiv.12115878.v3.  
  
M. E. Mondejar and F. Haglind, “The potential of halogenated olefins as working fluids for organic Rankine cycle technology”, *Journal of Molecular Liquids*, vol. 310. Elsevier BV, p. 112971, Jul. 2020. doi: 10.1016/j.molliq.2020.112971.  
  
C. Morales and F. Chen, “Exploration of Substituent and Isotope Effects on Reaction Rates by a Computational Modeling Experiment”, *Journal of Chemical Education*, vol. 96, no. 4. American Chemical Society (ACS), pp. 792–796, Feb. 28, 2019. doi: 10.1021/acs.jchemed.8b00651.  
  
M. J. Perri, “Online Data Generation in Quantitative Analysis: Excel Spreadsheets and an Online HPLC Simulator Using a Jupyter Notebook on the Chem Compute Web site”, *Journal of Chemical Education*, vol. 97, no. 9. American Chemical Society (ACS), pp. 2950–2954, Aug. 13, 2020. doi: 10.1021/acs.jchemed.0c00565.  
  
A. N. Semakin, Y. V. Nelyubina, S. L. Ioffeand A. Y. Sukhorukov, “2,4,9‐Triazaadamantanes with “Clickable” Groups: Synthesis, Structure and Applications as Tripodal Platforms”, *European Journal of Organic Chemistry*, vol. 2020, no. 43. Wiley, pp. 6723–6735, Aug. 18, 2020. doi: 10.1002/ejoc.202000832.  
  
M. Fernando, D. Neilsen, E. W. Hirschmannand H. Sundar, “A scalable framework for adaptive computational general relativity on heterogeneous clusters”, *Proceedings of the ACM International Conference on Supercomputing*. ACM, Jun. 26, 2019. doi: 10.1145/3330345.3330346.  
  
N. M. Wilson, “Using a Science Gateway to Deliver SimVascular Software as a Service for Classroom Instruction”, *Proceedings of the Practice and Experience on Advanced Research Computing*. ACM, Jul. 22, 2018. doi: 10.1145/3219104.3229242.  
  
T. S. Ahmed, J. M. Grandner, B. L. H. Taylor, M. B. Herbert, K. N. Houkand R. H. Grubbs, “Metathesis and Decomposition of Fischer Carbenes of Cyclometalated *Z*-Selective Ruthenium Metathesis Catalysts”, *Organometallics*, vol. 37, no. 14. American Chemical Society (ACS), pp. 2212–2216, Jul. 10, 2018. doi: 10.1021/acs.organomet.8b00150.  
  
A. H. Asari, Y.-. hong . Lam, M. A. Tiusand K. N. Houk, “Origins of the Stereoselectivity in a Thiourea–Primary Amine-Catalyzed Nazarov Cyclization”, *Journal of the American Chemical Society*, vol. 137, no. 40. American Chemical Society (ACS), pp. 13191–13199, Oct. 01, 2015. doi: 10.1021/jacs.5b08969.  
  
S. Banerjee, “Ionic and Neutral Mechanisms for C–H Bond Silylation of Aromatic Heterocycles Catalyzed by Potassium *tert*-Butoxide”, *Journal of the American Chemical Society*, vol. 139, no. 20. American Chemical Society (ACS), pp. 6880–6887, May 12, 2017. doi: 10.1021/jacs.6b13032.  
  
J. S. Barber, E. D. Styduhar, H. V. Pham, T. C. McMahon, K. N. Houkand N. K. Garg, “Nitrone Cycloadditions of 1,2-Cyclohexadiene”, *Journal of the American Chemical Society*, vol. 138, no. 8. American Chemical Society (ACS), pp. 2512–2515, Feb. 18, 2016. doi: 10.1021/jacs.5b13304.  
  
J. S. Barber, “Diels–Alder cycloadditions of strained azacyclic allenes”, *Nature Chemistry*, vol. 10, no. 9. Springer Science and Business Media LLC, pp. 953–960, Jul. 30, 2018. doi: 10.1038/s41557-018-0080-1.  
  
G. A. Barcan, A. Patel, K. N. Houkand O. Kwon, “A Torquoselective 6π Electrocyclization Approach to Reserpine Alkaloids”, *Organic Letters*, vol. 14, no. 21. American Chemical Society (ACS), pp. 5388–5391, Oct. 05, 2012. doi: 10.1021/ol302265z.  
  
D. N. Barman, P. Liu, K. N. Houkand K. M. Nicholas, “On the Mechanism of Ligand-Assisted, Copper-Catalyzed Benzylic Amination by Chloramine-T”, *Organometallics*, vol. 29, no. 15. American Chemical Society (ACS), pp. 3404–3412, Jul. 12, 2010. doi: 10.1021/om100427s.  
  
R. D. Baxter, “Mechanistic Insights into Two-Phase Radical C–H Arylations”, *ACS Central Science*, vol. 1, no. 8. American Chemical Society (ACS), pp. 456–462, Nov. 02, 2015. doi: 10.1021/acscentsci.5b00332.  
  
C. L. Boeser, J. C. Holder, B. L. H. Taylor, K. N. Houk, B. M. Stoltzand R. N. Zare, “Mechanistic analysis of an asymmetric palladium-catalyzed conjugate addition of arylboronic acids to β-substituted cyclic enones”, *Chemical Science*, vol. 6, no. 3. Royal Society of Chemistry (RSC), pp. 1917–1922, 2015. doi: 10.1039/c4sc03337j.  
  
M. Breugst and K. N. Houk, “Computational Analysis of Cyclophane-Based Bisthiourea-Catalyzed Henry Reactions”, *The Journal of Organic Chemistry*, vol. 79, no. 13. American Chemical Society (ACS), pp. 6302–6309, Jun. 23, 2014. doi: 10.1021/jo501227m.  
  
A. M. Camelio, “Computational and Experimental Studies of Phthaloyl Peroxide-Mediated Hydroxylation of Arenes Yield a More Reactive Derivative, 4,5-Dichlorophthaloyl Peroxide”, *The Journal of Organic Chemistry*, vol. 80, no. 16. American Chemical Society (ACS), pp. 8084–8095, Aug. 06, 2015. doi: 10.1021/acs.joc.5b01079.  
  
J. S. Cannon, “Carboxylate-Assisted C(sp3)–H Activation in Olefin Metathesis-Relevant Ruthenium Complexes”, *Journal of the American Chemical Society*, vol. 136, no. 18. American Chemical Society (ACS), pp. 6733–6743, Apr. 25, 2014. doi: 10.1021/ja5021958.  
  
Y. Cao, “Why Bistetracenes Are Much Less Reactive Than Pentacenes in Diels–Alder Reactions with Fullerenes”, *Journal of the American Chemical Society*, vol. 136, no. 30. American Chemical Society (ACS), pp. 10743–10751, Jul. 17, 2014. doi: 10.1021/ja505240e.  
  
P. A. Champagne and K. N. Houk, “Origins of Selectivity and General Model for Chiral Phosphoric Acid-Catalyzed Oxetane Desymmetrizations”, *Journal of the American Chemical Society*, vol. 138, no. 38. American Chemical Society (ACS), pp. 12356–12359, Sep. 16, 2016. doi: 10.1021/jacs.6b08276.  
  
P. A. Champagne and K. N. Houk, “Influence of Endo- and Exocyclic Heteroatoms on Stabilities and 1,3-Dipolar Cycloaddition Reactivities of Mesoionic Azomethine Ylides and Imines”, *The Journal of Organic Chemistry*, vol. 82, no. 20. American Chemical Society (ACS), pp. 10980–10988, Oct. 06, 2017. doi: 10.1021/acs.joc.7b01928.  
  
F. Chen, “Mechanism of the Cycloaddition of Carbon Dioxide and Epoxides Catalyzed by Cobalt-Substituted 12-Tungstenphosphate”, *Chemistry - A European Journal*, vol. 18, no. 32. Wiley, pp. 9870–9876, Jul. 04, 2012. doi: 10.1002/chem.201201042.  
  
G.-J. Cheng, “Role of *N*-Acyl Amino Acid Ligands in Pd(II)-Catalyzed Remote C–H Activation of Tethered Arenes”, *Journal of the American Chemical Society*, vol. 136, no. 3. American Chemical Society (ACS), pp. 894–897, Jan. 10, 2014. doi: 10.1021/ja411683n.  
  
S. Chen, A. Y. Chan, M. M. Walker, J. A. Ellmanand K. N. Houk, “π-Facial Selectivities in Hydride Reductions of Hindered Endocyclic Iminium Ions”, *The Journal of Organic Chemistry*, vol. 84, no. 1. American Chemical Society (ACS), pp. 273–281, Dec. 05, 2018. doi: 10.1021/acs.joc.8b02603.  
  
S. Chen and K. N. Houk, “Origins of Stereoselectivity in Mannich Reactions Catalyzed by Chiral Vicinal Diamines”, *The Journal of Organic Chemistry*, vol. 83, no. 6. American Chemical Society (ACS), pp. 3171–3176, Feb. 13, 2018. doi: 10.1021/acs.joc.8b00037.  
  
S. Chen, X. Huang, E. Meggersand K. N. Houk, “Origins of Enantioselectivity in Asymmetric Radical Additions to Octahedral Chiral-at-Rhodium Enolates: A Computational Study”, *Journal of the American Chemical Society*, vol. 139, no. 49. American Chemical Society (ACS), pp. 17902–17907, Nov. 29, 2017. doi: 10.1021/jacs.7b08650.  
  
S. Chen, P. Yuand K. N. Houk, “Ambimodal Dipolar/Diels–Alder Cycloaddition Transition States Involving Proton Transfers”, *Journal of the American Chemical Society*, vol. 140, no. 51. American Chemical Society (ACS), pp. 18124–18131, Nov. 27, 2018. doi: 10.1021/jacs.8b11080.  
  
S. Chen, Y. Zheng, T. Cui, E. Meggersand K. N. Houk, “Arylketone π-Conjugation Controls Enantioselectivity in Asymmetric Alkynylations Catalyzed by Centrochiral Ruthenium Complexes”, *Journal of the American Chemical Society*, vol. 140, no. 15. American Chemical Society (ACS), pp. 5146–5152, Mar. 26, 2018. doi: 10.1021/jacs.8b00485.  
  
I. Chogii, “New Class of Anion-Accelerated Amino-Cope Rearrangements as Gateway to Diverse Chiral Structures”, *Journal of the American Chemical Society*, vol. 139, no. 37. American Chemical Society (ACS), pp. 13141–13146, Sep. 08, 2017. doi: 10.1021/jacs.7b07319.  
  
T. S. Chung, S. A. Lopez, K. N. Houkand M. A. Garcia-Garibay, “Stereospecific Synthesis of Substituted Aziridines by a Crystal-to-Crystal Photodenitrogenation of Δ2-1,2,3-Triazolines”, *Organic Letters*, vol. 17, no. 18. American Chemical Society (ACS), pp. 4568–4571, Sep. 04, 2015. doi: 10.1021/acs.orglett.5b02290.  
  
S. E. Denmark, W.-T. T. Chang, K. N. Houkand P. Liu, “Development of Chiral Bis-hydrazone Ligands for the Enantioselective Cross-Coupling Reactions of Aryldimethylsilanolates”, *The Journal of Organic Chemistry*, vol. 80, no. 1. American Chemical Society (ACS), pp. 313–366, Dec. 10, 2014. doi: 10.1021/jo502388r.  
  
A. Duan, “Diazo Esters as Dienophiles in Intramolecular (4 + 2) Cycloadditions: Computational Explorations of Mechanism”, *Journal of the American Chemical Society*, vol. 139, no. 7. American Chemical Society (ACS), pp. 2766–2770, Feb. 01, 2017. doi: 10.1021/jacs.6b12371.  
  
L. Fang, “Confined organization of fullerene units along high polymer chains”, *Journal of Materials Chemistry C*, vol. 1, no. 36. Royal Society of Chemistry (RSC), p. 5747, 2013. doi: 10.1039/c3tc31158a.  
  
J. S. Fell, S. A. Lopez, C. J. Higginson, M. G. Finnand K. N. Houk, “Theoretical Analysis of the Retro-Diels–Alder Reactivity of Oxanorbornadiene Thiol and Amine Adducts”, *Organic Letters*, vol. 19, no. 17. American Chemical Society (ACS), pp. 4504–4507, Aug. 17, 2017. doi: 10.1021/acs.orglett.7b02064.  
  
J. S. Fell, B. N. Martinand K. N. Houk, “Origins of the Unfavorable Activation and Reaction Energies of 1-Azadiene Heterocycles Compared to 2-Azadiene Heterocycles in Diels–Alder Reactions”, *The Journal of Organic Chemistry*, vol. 82, no. 4. American Chemical Society (ACS), pp. 1912–1919, Feb. 09, 2017. doi: 10.1021/acs.joc.6b02524.  
  
S.-S. Gao, “Phenalenone Polyketide Cyclization Catalyzed by Fungal Polyketide Synthase and Flavin-Dependent Monooxygenase”, *Journal of the American Chemical Society*, vol. 138, no. 12. American Chemical Society (ACS), pp. 4249–4259, Mar. 22, 2016. doi: 10.1021/jacs.6b01528.  
  
S.-S. Gao, “Biosynthesis of Heptacyclic Duclauxins Requires Extensive Redox Modifications of the Phenalenone Aromatic Polyketide”, *Journal of the American Chemical Society*, vol. 140, no. 22. American Chemical Society (ACS), pp. 6991–6997, May 09, 2018. doi: 10.1021/jacs.8b03705.  
  
R. Gilmour, I. Molnár, M. Holland, C. Daniliucand K. Houk, “Organocatalysis Intermediates as Platforms to Study Noncovalent Interactions: Integrating Fluorine Gauche Effects in Iminium Systems to Facilitate Acyclic Conformational Control”, *Synlett*, vol. 27, no. 7. Georg Thieme Verlag KG, pp. 1051–1055, Jan. 18, 2016. doi: 10.1055/s-0035-1561199.  
  
R. Giri, Y. Lan, P. Liu, K. N. Houkand J.-Q. Yu, “Understanding Reactivity and Stereoselectivity in Palladium-Catalyzed Diastereoselective sp3 C–H Bond Activation: Intermediate Characterization and Computational Studies”, *Journal of the American Chemical Society*, vol. 134, no. 34. American Chemical Society (ACS), pp. 14118–14126, Aug. 14, 2012. doi: 10.1021/ja304643e.  
  
J. M. Grandner, R. A. Cacho, Y. Tangand K. N. Houk, “Mechanism of the P450-Catalyzed Oxidative Cyclization in the Biosynthesis of Griseofulvin”, *ACS Catalysis*, vol. 6, no. 7. American Chemical Society (ACS), pp. 4506–4511, Jun. 14, 2016. doi: 10.1021/acscatal.6b01068.  
  
J. M. Grandner, H. Shao, R. H. Grubbs, P. Liuand K. N. Houk, “Origins of the Stereoretentive Mechanism of Olefin Metathesis with Ru-Dithiolate Catalysts”, *The Journal of Organic Chemistry*, vol. 82, no. 19. American Chemical Society (ACS), pp. 10595–10600, Sep. 26, 2017. doi: 10.1021/acs.joc.7b02129.  
  
M. N. Grayson and K. N. Houk, “Cinchona Alkaloid-Catalyzed Asymmetric Conjugate Additions: The Bifunctional Brønsted Acid–Hydrogen Bonding Model”, *Journal of the American Chemical Society*, vol. 138, no. 4. American Chemical Society (ACS), pp. 1170–1173, Jan. 21, 2016. doi: 10.1021/jacs.5b13275.  
  
M. N. Grayson, M. J. Krischeand K. N. Houk, “Ruthenium-Catalyzed Asymmetric Hydrohydroxyalkylation of Butadiene: The Role of the Formyl Hydrogen Bond in Stereochemical Control”, *Journal of the American Chemical Society*, vol. 137, no. 27. American Chemical Society (ACS), pp. 8838–8850, Jul. 06, 2015. doi: 10.1021/jacs.5b04844.  
  
M. N. Grayson, Z. Yangand K. N. Houk, “Chronology of CH···O Hydrogen Bonding from Molecular Dynamics Studies of the Phosphoric Acid-Catalyzed Allylboration of Benzaldehyde”, *Journal of the American Chemical Society*, vol. 139, no. 23. American Chemical Society (ACS), pp. 7717–7720, Jun. 06, 2017. doi: 10.1021/jacs.7b03847.  
  
A. G. Green, P. Liu, C. A. Merlicand K. N. Houk, “Distortion/Interaction Analysis Reveals the Origins of Selectivities in Iridium-Catalyzed C–H Borylation of Substituted Arenes and 5-Membered Heterocycles”, *Journal of the American Chemical Society*, vol. 136, no. 12. American Chemical Society (ACS), pp. 4575–4583, Mar. 13, 2014. doi: 10.1021/ja411699u.  
  
X. Han, S. Bian, Y. Liang, K. N. Houkand A. B. Braunschweig, “Reactions in Elastomeric Nanoreactors Reveal the Role of Force on the Kinetics of the Huisgen Reaction on Surfaces”, *Journal of the American Chemical Society*, vol. 136, no. 30. American Chemical Society (ACS), pp. 10553–10556, Jul. 18, 2014. doi: 10.1021/ja504137u.  
  
M. T. Haynes II, P. Liu, R. D. Baxter, A. J. Nett, K. N. Houkand J. Montgomery, “Dimer Involvement and Origin of Crossover in Nickel-Catalyzed Aldehyde–Alkyne Reductive Couplings”, *Journal of the American Chemical Society*, vol. 136, no. 50. American Chemical Society (ACS), pp. 17495–17504, Dec. 03, 2014. doi: 10.1021/ja508909u.  
  
C. Q. He, T. Q. Chen, A. Patel, S. Karabiyikoglu, C. A. Merlicand K. N. Houk, “Distortion, Tether, and Entropy Effects on Transannular Diels–Alder Cycloaddition Reactions of 10–18-Membered Rings”, *The Journal of Organic Chemistry*, vol. 80, no. 21. American Chemical Society (ACS), pp. 11039–11047, Oct. 28, 2015. doi: 10.1021/acs.joc.5b02288.  
  
C. Q. He, “Model for the Enantioselectivity of Asymmetric Intramolecular Alkylations by Bis-Quaternized Cinchona Alkaloid-Derived Catalysts”, *The Journal of Organic Chemistry*, vol. 82, no. 16. American Chemical Society (ACS), pp. 8645–8650, Jul. 31, 2017. doi: 10.1021/acs.joc.7b01577.  
  
M. B. Herbert, “Decomposition Pathways of *Z*-Selective Ruthenium Metathesis Catalysts”, *Journal of the American Chemical Society*, vol. 134, no. 18. American Chemical Society (ACS), pp. 7861–7866, Apr. 26, 2012. doi: 10.1021/ja301108m.  
  
M. B. Herbert, “Cyclometalated *Z*-Selective Ruthenium Metathesis Catalysts with Modified N-Chelating Groups”, *Organometallics*, vol. 34, no. 12. American Chemical Society (ACS), pp. 2858–2869, Jun. 02, 2015. doi: 10.1021/acs.organomet.5b00185.  
  
L. Hie, N. F. Fine Nathel, X. Hong, Y. Yang, K. N. Houkand N. K. Garg, “Nickel‐Catalyzed Activation of Acyl C−O Bonds of Methyl Esters”, *Angewandte Chemie*, vol. 128, no. 8. Wiley, pp. 2860–2864, Jan. 25, 2016. doi: 10.1002/ange.201511486.  
  
L. Hie, “Conversion of amides to esters by the nickel-catalysed activation of amide C–N bonds”, *Nature*, vol. 524, no. 7563. Springer Science and Business Media LLC, pp. 79–83, Jul. 22, 2015. doi: 10.1038/nature14615.  
  
D. E. Hill, “Dynamic Ligand Exchange as a Mechanistic Probe in Pd-Catalyzed Enantioselective C–H Functionalization Reactions Using Monoprotected Amino Acid Ligands”, *Journal of the American Chemical Society*, vol. 139, no. 51. American Chemical Society (ACS), pp. 18500–18503, Dec. 14, 2017. doi: 10.1021/jacs.7b11962.  
  
D. T. Hog, F. M. E. Huber, G. Jiménez-Osés, P. Mayer, K. N. Houkand D. Trauner, “Evolution of a Unified Strategy for Complex Sesterterpenoids: Progress toward Astellatol and the Total Synthesis of (−)-Nitidasin”, *Chemistry - A European Journal*, vol. 21, no. 39. Wiley, pp. 13646–13665, Aug. 20, 2015. doi: 10.1002/chem.201501423.  
  
J. C. Holder, “Mechanism and Enantioselectivity in Palladium-Catalyzed Conjugate Addition of Arylboronic Acids to β-Substituted Cyclic Enones: Insights from Computation and Experiment”, *Journal of the American Chemical Society*, vol. 135, no. 40. American Chemical Society (ACS), pp. 14996–15007, Sep. 27, 2013. doi: 10.1021/ja401713g.  
  
M. C. Holland, R. Gilmourand K. N. Houk, “Importance of Intermolecular Hydrogen Bonding for the Stereochemical Control of Allene-Enone (3+2) Annulations Catalyzed by a Bifunctional, Amino Acid Derived Phosphine Catalyst”, *Angewandte Chemie*, vol. 128, no. 6. Wiley, pp. 2062–2067, Jan. 06, 2016. doi: 10.1002/ange.201508980.  
  
K. Honda, S. A. Lopez, K. N. Houkand K. Mikami, “Mono-, Di-, and Trifluoroalkyl Substituent Effects on the Torquoselectivities of Cyclobutene and Oxetene Electrocyclic Ring Openings”, *The Journal of Organic Chemistry*, vol. 80, no. 23. American Chemical Society (ACS), pp. 11768–11772, Aug. 28, 2015. doi: 10.1021/acs.joc.5b01361.  
  
X. Hong, “Mechanism and Dynamics of Intramolecular C–H Insertion Reactions of 1-Aza-2-azoniaallene Salts”, *Journal of the American Chemical Society*, vol. 137, no. 28. American Chemical Society (ACS), pp. 9100–9107, Jul. 07, 2015. doi: 10.1021/jacs.5b04474.  
  
X. Hong, D. Holte, D. C. G. Götz, P. S. Baranand K. N. Houk, “Mechanism, Reactivity, and Selectivity of Nickel-Catalyzed [4 + 4 + 2] Cycloadditions of Dienes and Alkynes”, *The Journal of Organic Chemistry*, vol. 79, no. 24. American Chemical Society (ACS), pp. 12177–12184, Nov. 07, 2014. doi: 10.1021/jo502219d.  
  
X. Hong, H. B. Küçük, M. S. Maji, Y.-F. Yang, M. Ruepingand K. N. Houk, “Mechanism and Selectivity of *N*-Triflylphosphoramide Catalyzed (3+ + 2) Cycloaddition between Hydrazones and Alkenes”, *Journal of the American Chemical Society*, vol. 136, no. 39. American Chemical Society (ACS), pp. 13769–13780, Sep. 16, 2014. doi: 10.1021/ja506660c.  
  
X. Hong, Y. Liang, M. Brewerand K. N. Houk, “How Tethers Control the Chemo- and Regioselectivities of Intramolecular Cycloadditions between Aryl-1-aza-2-azoniaallenes and Alkenes”, *Organic Letters*, vol. 16, no. 16. American Chemical Society (ACS), pp. 4260–4263, Jul. 24, 2014. doi: 10.1021/ol501958s.  
  
X. Hong, P. Liuand K. N. Houk, “Mechanism and Origins of Ligand-Controlled Selectivities in [Ni(NHC)]-Catalyzed Intramolecular (5 + 2) Cycloadditions and Homo-Ene Reactions: A Theoretical Study”, *Journal of the American Chemical Society*, vol. 135, no. 4. American Chemical Society (ACS), pp. 1456–1462, Jan. 17, 2013. doi: 10.1021/ja309873z.  
  
X. Hong, M. C. Stevens, P. Liu, P. A. Wenderand K. N. Houk, “Reactivity and Chemoselectivity of Allenes in Rh(I)-Catalyzed Intermolecular (5 + 2) Cycloadditions with Vinylcyclopropanes: Allene-Mediated Rhodacycle Formation Can Poison Rh(I)-Catalyzed Cycloadditions”, *Journal of the American Chemical Society*, vol. 136, no. 49. American Chemical Society (ACS), pp. 17273–17283, Nov. 24, 2014. doi: 10.1021/ja5098308.  
  
X. Hong, J. Wang, Y.-F. Yang, L. He, C.-Y. Hoand K. N. Houk, “Computational Exploration of Mechanism and Selectivities of (NHC)Nickel(II)hydride-Catalyzed Hydroalkenylations of Styrene with α-Olefins”, *ACS Catalysis*, vol. 5, no. 9. American Chemical Society (ACS), pp. 5545–5555, Aug. 24, 2015. doi: 10.1021/acscatal.5b01075.  
  
J. F. Hooper, “Medium-Ring Effects on the *Endo/Exo* Selectivity of the Organocatalytic Intramolecular Diels–Alder Reaction”, *The Journal of Organic Chemistry*, vol. 80, no. 24. American Chemical Society (ACS), pp. 12058–12075, Nov. 30, 2015. doi: 10.1021/acs.joc.5b02037.  
  
K. Houk, M. White, M. Bigi, P. Liuand L. Zou, “Cafestol to Tricalysiolide B and Oxidized Analogues: Biosynthetic and Derivatization Studies Using Non-heme Iron Catalyst Fe(PDP)”, *Synlett*, vol. 23, no. 19. Georg Thieme Verlag KG, pp. 2768–2772, Nov. 14, 2012. doi: 10.1055/s-0032-1317708.  
  
X. Huang, “A Biocatalytic Platform for Synthesis of Chiral α-Trifluoromethylated Organoborons”, *[]*. American Chemical Society (ACS), Sep. 26, 2018. doi: 10.26434/chemrxiv.7130852.v1.  
  
Y. Hu, “A carbonate-forming Baeyer-Villiger monooxygenase”, *Nature Chemical Biology*, vol. 10, no. 7. Springer Science and Business Media LLC, pp. 552–554, May 18, 2014. doi: 10.1038/nchembio.1527.  
  
E. P. Jackson, “Mechanistic Basis for Regioselection and Regiodivergence in Nickel-Catalyzed Reductive Couplings”, *Accounts of Chemical Research*, vol. 48, no. 6. American Chemical Society (ACS), pp. 1736–1745, May 12, 2015. doi: 10.1021/acs.accounts.5b00096.  
  
X. Jiang, “Crystal Fluidity Reflected by Fast Rotational Motion at the Core, Branches, and Peripheral Aromatic Groups of a Dendrimeric Molecular Rotor”, *Journal of the American Chemical Society*, vol. 138, no. 13. American Chemical Society (ACS), pp. 4650–4656, Mar. 25, 2016. doi: 10.1021/jacs.6b01398.  
  
G. Jiménez-Osés, P. Liu, R. A. Matuteand K. N. Houk, “Competition Between Concerted and Stepwise Dynamics in the Triplet Di-π-Methane Rearrangement”, *Angewandte Chemie International Edition*, vol. 53, no. 33. Wiley, pp. 8664–8667, Mar. 11, 2014. doi: 10.1002/anie.201310237.  
  
G. O. Jones, P. Liu, K. N. Houkand S. L. Buchwald, “Computational Explorations of Mechanisms and Ligand-Directed Selectivities of Copper-Catalyzed Ullmann-Type Reactions”, *Journal of the American Chemical Society*, vol. 132, no. 17. American Chemical Society (ACS), pp. 6205–6213, Apr. 13, 2010. doi: 10.1021/ja100739h.  
  
R. S. Jordan, “Synthesis of *N* = 8 Armchair Graphene Nanoribbons from Four Distinct Polydiacetylenes”, *Journal of the American Chemical Society*, vol. 139, no. 44. American Chemical Society (ACS), pp. 15878–15890, Oct. 30, 2017. doi: 10.1021/jacs.7b08800.  
  
M. E. Jung, C. A. Roberts, F. Perez, H. V. Pham, L. Zouand K. N. Houk, “Thermodynamic Control of Isomerizations of Bicyclic Radicals: Interplay of Ring Strain and Radical Stabilization”, *Organic Letters*, vol. 18, no. 1. American Chemical Society (ACS), pp. 32–35, Dec. 15, 2015. doi: 10.1021/acs.orglett.5b03112.  
  
D. N. Kamber, “1,2,4-Triazines Are Versatile Bioorthogonal Reagents”, *Journal of the American Chemical Society*, vol. 137, no. 26. American Chemical Society (ACS), pp. 8388–8391, Jun. 25, 2015. doi: 10.1021/jacs.5b05100.  
  
E. H. Krenske, “Concerted Ring Opening and Cycloaddition of Chiral Epoxy Enolsilanes with Dienes”, *Angewandte Chemie International Edition*, vol. 54, no. 25. Wiley, pp. 7422–7425, May 07, 2015. doi: 10.1002/anie.201503003.  
  
E. H. Krenske, A. Pateland K. N. Houk, “Does Nature Click? Theoretical Prediction of an Enzyme-Catalyzed Transannular 1,3-Dipolar Cycloaddition in the Biosynthesis of Lycojaponicumins A and B”, *Journal of the American Chemical Society*, vol. 135, no. 46. American Chemical Society (ACS), pp. 17638–17642, Nov. 06, 2013. doi: 10.1021/ja409928z.  
  
P. Kumar, A. Thakur, X. Hong, K. N. Houkand J. Louie, “Ni(NHC)]-Catalyzed Cycloaddition of Diynes and Tropone: Apparent Enone Cycloaddition Involving an 8π Insertion”, *Journal of the American Chemical Society*, vol. 136, no. 51. American Chemical Society (ACS), pp. 17844–17851, Dec. 05, 2014. doi: 10.1021/ja5105206.  
  
Y.-. hong . Lam, M. N. Grayson, M. C. Holland, A. Simonand K. N. Houk, “Theory and Modeling of Asymmetric Catalytic Reactions”, *Accounts of Chemical Research*, vol. 49, no. 4. American Chemical Society (ACS), pp. 750–762, Mar. 11, 2016. doi: 10.1021/acs.accounts.6b00006.  
  
Y.-. hong . Lam and K. N. Houk, “How Cinchona Alkaloid-Derived Primary Amines Control Asymmetric Electrophilic Fluorination of Cyclic Ketones”, *Journal of the American Chemical Society*, vol. 136, no. 27. American Chemical Society (ACS), pp. 9556–9559, Jun. 26, 2014. doi: 10.1021/ja504714m.  
  
Y.-. hong . Lam and K. N. Houk, “Origins of Stereoselectivity in Intramolecular Aldol Reactions Catalyzed by Cinchona Amines”, *Journal of the American Chemical Society*, vol. 137, no. 5. American Chemical Society (ACS), pp. 2116–2127, Jan. 28, 2015. doi: 10.1021/ja513096x.  
  
Y. Lan, P. Liu, S. G. Newman, M. Lautensand K. N. Houk, “Theoretical study of Pd(0)-catalyzed carbohalogenation of alkenes: mechanism and origins of reactivities and selectivities in alkyl halide reductive elimination from Pd(ii) species”, *Chemical Science*, vol. 3, no. 6. Royal Society of Chemistry (RSC), p. 1987, 2012. doi: 10.1039/c2sc20103h.  
  
M. H. Larsen, K. N. Houkand A. S. K. Hashmi, “Dual Gold Catalysis: Stepwise Catalyst Transfer via Dinuclear Clusters”, *Journal of the American Chemical Society*, vol. 137, no. 33. American Chemical Society (ACS), pp. 10668–10676, Aug. 17, 2015. doi: 10.1021/jacs.5b05773.  
  
J. Lee, J. M. Grandner, K. M. Engle, K. N. Houkand R. H. Grubbs, “In Situ Catalyst Modification in Atom Transfer Radical Reactions with Ruthenium Benzylidene Complexes”, *Journal of the American Chemical Society*, vol. 138, no. 22. American Chemical Society (ACS), pp. 7171–7177, May 26, 2016. doi: 10.1021/jacs.6b03767.  
  
B. J. Levandowski, L. Zouand K. N. Houk, “Schleyer hyperconjugative aromaticity and Diels-Alder reactivity of 5-substituted cyclopentadienes”, *Journal of Computational Chemistry*, vol. 37, no. 1. Wiley, pp. 117–123, Oct. 07, 2015. doi: 10.1002/jcc.24191.  
  
R. D. Lewis, “Catalytic iron-carbene intermediate revealed in a cytochrome *c* carbene transferase”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 28. Proceedings of the National Academy of Sciences, pp. 7308–7313, Jun. 26, 2018. doi: 10.1073/pnas.1807027115.  
  
Y. Liang, X. Hong, P. Yuand K. N. Houk, “Why Alkynyl Substituents Dramatically Accelerate Hexadehydro-Diels–Alder (HDDA) Reactions: Stepwise Mechanisms of HDDA Cycloadditions”, *Organic Letters*, vol. 16, no. 21. American Chemical Society (ACS), pp. 5702–5705, Oct. 20, 2014. doi: 10.1021/ol502780w.  
  
G. Li, “Overriding Traditional Electronic Effects in Biocatalytic Baeyer–Villiger Reactions by Directed Evolution”, *Journal of the American Chemical Society*, vol. 140, no. 33. American Chemical Society (ACS), pp. 10464–10472, Jul. 25, 2018. doi: 10.1021/jacs.8b04742.  
  
H.-C. Lin, “P450-Mediated Coupling of Indole Fragments To Forge Communesin and Unnatural Isomers”, *Journal of the American Chemical Society*, vol. 138, no. 12. American Chemical Society (ACS), pp. 4002–4005, Mar. 18, 2016. doi: 10.1021/jacs.6b01413.  
  
J. B. Lin, E. R. Darzi, R. Jasti, I. Yavuzand K. N. Houk, “Solid-State Order and Charge Mobility in [5]- to [12]Cycloparaphenylenes”, *Journal of the American Chemical Society*, vol. 141, no. 2. American Chemical Society (ACS), pp. 952–960, Dec. 13, 2018. doi: 10.1021/jacs.8b10699.  
  
J. B. Lin, Y. Jin, S. A. Lopez, N. Druckerman, S. E. Wheelerand K. N. Houk, “Torsional Barriers to Rotation and Planarization in Heterocyclic Oligomers of Value in Organic Electronics”, *Journal of Chemical Theory and Computation*, vol. 13, no. 11. American Chemical Society (ACS), pp. 5624–5638, Oct. 31, 2017. doi: 10.1021/acs.jctc.7b00709.  
  
F. Liu, Y. Liangand K. N. Houk, “Theoretical Elucidation of the Origins of Substituent and Strain Effects on the Rates of Diels–Alder Reactions of 1,2,4,5-Tetrazines”, *Journal of the American Chemical Society*, vol. 136, no. 32. American Chemical Society (ACS), pp. 11483–11493, Jul. 29, 2014. doi: 10.1021/ja505569a.  
  
F. Liu, Z. Yang, Y. Yu, Y. Meiand K. N. Houk, “Bimodal Evans–Polanyi Relationships in Dioxirane Oxidations of sp3 C–H: Non-perfect Synchronization in Generation of Delocalized Radical Intermediates”, *Journal of the American Chemical Society*, vol. 139, no. 46. American Chemical Society (ACS), pp. 16650–16656, Nov. 09, 2017. doi: 10.1021/jacs.7b07988.  
  
P. Liu and K. N. Houk, “Theoretical studies of regioselectivity of Ni- and Rh-catalyzed C–C bond forming reactions with unsymmetrical alkynes”, *Inorganica Chimica Acta*, vol. 369, no. 1. Elsevier BV, pp. 2–14, Apr. 2011. doi: 10.1016/j.ica.2010.12.042.  
  
P. Liu, M. J. Krischeand K. N. Houk, “Mechanism and Origins of Regio- and Enantioselectivities in RhI-Catalyzed Hydrogenative Couplings of 1,3-Diynes and Activated Carbonyl Partners: Intervention of a Cumulene Intermediate”, *Chemistry - A European Journal*, vol. 17, no. 14. Wiley, pp. 4021–4029, Mar. 01, 2011. doi: 10.1002/chem.201002741.  
  
P. Liu, P. McCarren, P. H.-Y. Cheong, T. F. Jamisonand K. N. Houk, “Origins of Regioselectivity and Alkene-Directing Effects in Nickel-Catalyzed Reductive Couplings of Alkynes and Aldehydes”, *Journal of the American Chemical Society*, vol. 132, no. 6. American Chemical Society (ACS), pp. 2050–2057, Jan. 22, 2010. doi: 10.1021/ja909562y.  
  
P. Liu, J. Montgomeryand K. N. Houk, “Ligand Steric Contours To Understand the Effects of *N*-Heterocyclic Carbene Ligands on the Reversal of Regioselectivity in Ni-Catalyzed Reductive Couplings of Alkynes and Aldehydes”, *Journal of the American Chemical Society*, vol. 133, no. 18. American Chemical Society (ACS), pp. 6956–6959, Apr. 20, 2011. doi: 10.1021/ja202007s.  
  
P. Liu and K. M. Nicholas, “Mechanism of Sulfite-Driven, MeReO3-Catalyzed Deoxydehydration of Glycols”, *Organometallics*, vol. 32, no. 6. American Chemical Society (ACS), pp. 1821–1831, Feb. 26, 2013. doi: 10.1021/om301251z.  
  
P. Liu, “Electronic and Steric Control of Regioselectivities in Rh(I)-Catalyzed (5 + 2) Cycloadditions: Experiment and Theory”, *Journal of the American Chemical Society*, vol. 132, no. 29. American Chemical Society (ACS), pp. 10127–10135, Jun. 30, 2010. doi: 10.1021/ja103253d.  
  
P. Liu, B. L. H. Taylor, J. Garcia-Lopezand K. N. Houk, “Computational Studies of Ruthenium-Catalyzed Olefin Metathesis”, *Handbook of Metathesis*. Wiley-VCH Verlag GmbH & Co. KGaA, pp. 199–252, Mar. 27, 2015. doi: 10.1002/9783527674107.ch7.  
  
P. Liu, “*Z*-Selectivity in Olefin Metathesis with Chelated Ru Catalysts: Computational Studies of Mechanism and Selectivity”, *Journal of the American Chemical Society*, vol. 134, no. 3. American Chemical Society (ACS), pp. 1464–1467, Jan. 17, 2012. doi: 10.1021/ja2108728.  
  
P. Liu, X. Yang, V. B. Birmanand K. N. Houk, “Origin of Enantioselectivity in Benzotetramisole-Catalyzed Dynamic Kinetic Resolution of Azlactones”, *Organic Letters*, vol. 14, no. 13. American Chemical Society (ACS), pp. 3288–3291, Jun. 11, 2012. doi: 10.1021/ol301243f.  
  
W.-B. Liu, “Potassium *tert*-Butoxide-Catalyzed Dehydrogenative C–H Silylation of Heteroaromatics: A Combined Experimental and Computational Mechanistic Study”, *Journal of the American Chemical Society*, vol. 139, no. 20. American Chemical Society (ACS), pp. 6867–6879, May 12, 2017. doi: 10.1021/jacs.6b13031.  
  
S. A. Lopez and K. N. Houk, “Substituent Effects on Rates and Torquoselectivities of Electrocyclic Ring-Openings of *N*-Substituted 2-Azetines”, *The Journal of Organic Chemistry*, vol. 79, no. 13. American Chemical Society (ACS), pp. 6189–6195, Jun. 12, 2014. doi: 10.1021/jo500919s.  
  
S. A. Lopez, M. Pourati, H.-J. Gaisand K. N. Houk, “How Torsional Effects Cause Attack at Sterically Crowded Concave Faces of Bicyclic Alkenes”, *The Journal of Organic Chemistry*, vol. 79, no. 17. American Chemical Society (ACS), pp. 8304–8312, Aug. 21, 2014. doi: 10.1021/jo501557z.  
  
S.-X. Luo, “An Initiation Kinetics Prediction Model Enables Rational Design of Ruthenium Olefin Metathesis Catalysts Bearing Modified Chelating Benzylidenes”, *ACS Catalysis*, vol. 8, no. 5. American Chemical Society (ACS), pp. 4600–4611, Apr. 10, 2018. doi: 10.1021/acscatal.8b00843.  
  
J. T. Ly, “Oxidation of rubrene, and implications for device stability”, *Journal of Materials Chemistry C*, vol. 6, no. 14. Royal Society of Chemistry (RSC), pp. 3757–3761, 2018. doi: 10.1039/c7tc05775j.  
  
R. Maji, P. A. Champagne, K. N. Houkand S. E. Wheeler, “Activation Mode and Origin of Selectivity in Chiral Phosphoric Acid-Catalyzed Oxacycle Formation by Intramolecular Oxetane Desymmetrizations”, *ACS Catalysis*, vol. 7, no. 10. American Chemical Society (ACS), pp. 7332–7339, Sep. 26, 2017. doi: 10.1021/acscatal.7b02993.  
  
H. A. Malik, “Non-directed allylic C–H acetoxylation in the presence of Lewis basic heterocycles”, *Chemical Science*, vol. 5, no. 6. Royal Society of Chemistry (RSC), p. 2352, 2014. doi: 10.1039/c3sc53414f.  
  
S. J. B. Mallinson, “A promiscuous cytochrome P450 aromatic O-demethylase for lignin bioconversion”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Jun. 27, 2018. doi: 10.1038/s41467-018-04878-2.  
  
X.-M. Mao, “Efficient Biosynthesis of Fungal Polyketides Containing the Dioxabicyclo-octane Ring System”, *Journal of the American Chemical Society*, vol. 137, no. 37. American Chemical Society (ACS), pp. 11904–11907, Sep. 10, 2015. doi: 10.1021/jacs.5b07816.  
  
D. Martinez-Solorio, “Design, Synthesis, and Validation of an Effective, Reusable Silicon-Based Transfer Agent for Room-Temperature Pd-Catalyzed Cross-Coupling Reactions of Aryl and Heteroaryl Chlorides with Readily Available Aryl Lithium Reagents”, *Journal of the American Chemical Society*, vol. 138, no. 6. American Chemical Society (ACS), pp. 1836–1839, Feb. 02, 2016. doi: 10.1021/jacs.5b13260.  
  
R. A. Matute, M. A. Garcia-Garibayand K. N. Houk, “Theory of Substituent Effects on the Regioselectivity of Di-π-methane Rearrangements of Dibenzobarrelenes”, *Organic Letters*, vol. 16, no. 19. American Chemical Society (ACS), pp. 5232–5234, Sep. 19, 2014. doi: 10.1021/ol5024823.  
  
Z.-X. Ma, A. Patel, K. N. Houkand R. P. Hsung, “Highly Torquoselective Electrocyclizations and Competing 1,7-Hydrogen Shifts of 1-Azatrienes with Silyl Substitution at the Allylic Carbon”, *Organic Letters*, vol. 17, no. 9. American Chemical Society (ACS), pp. 2138–2141, Apr. 10, 2015. doi: 10.1021/acs.orglett.5b00727.  
  
J. M. Medina, J. L. Mackey, N. K. Gargand K. N. Houk, “The Role of Aryne Distortions, Steric Effects, and Charges in Regioselectivities of Aryne Reactions”, *Journal of the American Chemical Society*, vol. 136, no. 44. American Chemical Society (ACS), pp. 15798–15805, Oct. 23, 2014. doi: 10.1021/ja5099935.  
  
J. M. Medina, T. C. McMahon, G. Jiménez-Osés, K. N. Houkand N. K. Garg, “Cycloadditions of Cyclohexynes and Cyclopentyne”, *Journal of the American Chemical Society*, vol. 136, no. 42. American Chemical Society (ACS), pp. 14706–14709, Oct. 10, 2014. doi: 10.1021/ja508635v.  
  
S.-S. Meng, “Chiral Phosphoric Acid Catalyzed Highly Enantioselective Desymmetrization of 2-Substituted and 2,2-Disubstituted 1,3-Diols via Oxidative Cleavage of Benzylidene Acetals”, *Journal of the American Chemical Society*, vol. 136, no. 35. American Chemical Society (ACS), pp. 12249–12252, Aug. 25, 2014. doi: 10.1021/ja507332x.  
  
T. Mesganaw, “Nickel-catalyzed amination of aryl carbamates and sequential site-selective cross-couplings”, *Chemical Science*, vol. 2, no. 9. Royal Society of Chemistry (RSC), p. 1766, 2011. doi: 10.1039/c1sc00230a.  
  
M. S. Messina, J. H. Ko, Z. Yang, M. J. Strouse, K. N. Houkand H. D. Maynard, “Effect of trehalose polymer regioisomers on protein stabilization”, *Polymer Chemistry*, vol. 8, no. 33. Royal Society of Chemistry (RSC), pp. 4781–4788, 2017. doi: 10.1039/c7py00700k.  
  
H. Miyazaki, “*Z*-Selective Ethenolysis with a Ruthenium Metathesis Catalyst: Experiment and Theory”, *Journal of the American Chemical Society*, vol. 135, no. 15. American Chemical Society (ACS), pp. 5848–5858, Apr. 02, 2013. doi: 10.1021/ja4010267.  
  
A. R. H. Narayan, “Enzymatic hydroxylation of an unactivated methylene C–H bond guided by molecular dynamics simulations”, *Nature Chemistry*, vol. 7, no. 8. Springer Science and Business Media LLC, pp. 653–660, Jun. 29, 2015. doi: 10.1038/nchem.2285.  
  
M. K. Narayanam, Y. Liang, K. N. Houkand J. M. Murphy, “Discovery of new mutually orthogonal bioorthogonal cycloaddition pairs through computational screening”, *Chemical Science*, vol. 7, no. 2. Royal Society of Chemistry (RSC), pp. 1257–1261, 2016. doi: 10.1039/c5sc03259h.  
  
M. K. Narayanam, G. Ma, P. A. Champagne, K. N. Houkand J. M. Murphy, “Synthesis of [18F]Fluoroarenes by Nucleophilic Radiofluorination of*N*-Arylsydnones”, *Angewandte Chemie International Edition*, vol. 56, no. 42. Wiley, pp. 13006–13010, Sep. 07, 2017. doi: 10.1002/anie.201707274.  
  
S. R. Neufeldt, G. Jiménez-Osés, D. L. Cominsand K. N. Houk, “A Twist on Facial Selectivity of Hydride Reductions of Cyclic Ketones: Twist-Boat Conformers in Cyclohexanone, Piperidone, and Tropinone Reactions”, *The Journal of Organic Chemistry*, vol. 79, no. 23. American Chemical Society (ACS), pp. 11609–11618, Nov. 24, 2014. doi: 10.1021/jo5022635.  
  
S. R. Neufeldt, G. Jiménez-Osés, J. R. Huckins, O. R. Thieland K. N. Houk, “Pyridine *N*-Oxide vs Pyridine Substrates for Rh(III)-Catalyzed Oxidative C–H Bond Functionalization”, *Journal of the American Chemical Society*, vol. 137, no. 31. American Chemical Society (ACS), pp. 9843–9854, Aug. 03, 2015. doi: 10.1021/jacs.5b03535.  
  
S. A. Newmister, “Structural basis of the Cope rearrangement and cyclization in hapalindole biogenesis”, *Nature Chemical Biology*, vol. 14, no. 4. Springer Science and Business Media LLC, pp. 345–351, Mar. 12, 2018. doi: 10.1038/s41589-018-0003-x.  
  
E. L. Noey, “Origins of Regioselectivity in the Fischer Indole Synthesis of a Selective Androgen Receptor Modulator”, *The Journal of Organic Chemistry*, vol. 82, no. 11. American Chemical Society (ACS), pp. 5904–5909, May 17, 2017. doi: 10.1021/acs.joc.7b00878.  
  
Y. Numajiri, G. Jiménez-Osés, B. Wang, K. N. Houkand B. M. Stoltz, “Enantioselective Synthesis of Dialkylated *N*-Heterocycles by Palladium-Catalyzed Allylic Alkylation”, *Organic Letters*, vol. 17, no. 5. American Chemical Society (ACS), pp. 1082–1085, Feb. 25, 2015. doi: 10.1021/ol503425t.  
  
M. Ohashi, “SAM-dependent enzyme-catalysed pericyclic reactions in natural product biosynthesis”, *Nature*, vol. 549, no. 7673. Springer Science and Business Media LLC, pp. 502–506, Sep. 2017. doi: 10.1038/nature23882.  
  
S. Osuna, G. Jiménez-Osés, E. L. Noeyand K. N. Houk, “Molecular Dynamics Explorations of Active Site Structure in Designed and Evolved Enzymes”, *Accounts of Chemical Research*, vol. 48, no. 4. American Chemical Society (ACS), pp. 1080–1089, Mar. 04, 2015. doi: 10.1021/ar500452q.  
  
J. Park, J. J. McDonald, R. C. Petterand K. N. Houk, “Molecular Dynamics Analysis of Binding of Kinase Inhibitors to WT EGFR and the T790M Mutant”, *Journal of Chemical Theory and Computation*, vol. 12, no. 4. American Chemical Society (ACS), pp. 2066–2078, Apr. 04, 2016. doi: 10.1021/acs.jctc.5b01221.  
  
A. Patel, G. A. Barcan, O. Kwonand K. N. Houk, “Origins of 1,6-Stereoinduction in Torquoselective 6π Electrocyclizations”, *Journal of the American Chemical Society*, vol. 135, no. 12. American Chemical Society (ACS), pp. 4878–4883, Mar. 18, 2013. doi: 10.1021/ja400882y.  
  
A. Patel, “Dynamically Complex [6+4] and [4+2] Cycloadditions in the Biosynthesis of Spinosyn A”, *Journal of the American Chemical Society*, vol. 138, no. 11. American Chemical Society (ACS), pp. 3631–3634, Mar. 09, 2016. doi: 10.1021/jacs.6b00017.  
  
A. Patel and K. N. Houk, “Terminal Substituent Effects on the Reactivity, Thermodynamics, and Stereoselectivity of the 8π–6π Electrocyclization Cascades of 1,3,5,7-Tetraenes”, *The Journal of Organic Chemistry*, vol. 79, no. 23. American Chemical Society (ACS), pp. 11370–11377, Nov. 17, 2014. doi: 10.1021/jo5015728.  
  
A. Patel, J. R. Vella, Z.-X. Ma, R. P. Hsungand K. N. Houk, “Transition State *Gauche* Effects Control the Torquoselectivities of the Electrocyclizations of Chiral 1-Azatrienes”, *The Journal of Organic Chemistry*, vol. 80, no. 23. American Chemical Society (ACS), pp. 11888–11894, Oct. 16, 2015. doi: 10.1021/acs.joc.5b02085.  
  
A. Patel, F. G. Westand K. N. Houk, “Reactivity and Stereoselectivity of 6π and Nazarov Electrocyclizations of Bridged Bicyclic Trienes and Divinyl Ketones”, *The Journal of Organic Chemistry*, vol. 80, no. 5. American Chemical Society (ACS), pp. 2790–2795, Feb. 24, 2015. doi: 10.1021/acs.joc.5b00070.  
  
S. Pérez-Estrada, “Thermodynamic Evaluation of Aromatic CH/π Interactions and Rotational Entropy in a Molecular Rotor”, *Journal of the American Chemical Society*, vol. 137, no. 6. American Chemical Society (ACS), pp. 2175–2178, Feb. 04, 2015. doi: 10.1021/ja512053t.  
  
H. V. Pham and K. N. Houk, “Diels–Alder Reactions of Allene with Benzene and Butadiene: Concerted, Stepwise, and Ambimodal Transition States”, *The Journal of Organic Chemistry*, vol. 79, no. 19. American Chemical Society (ACS), pp. 8968–8976, Sep. 18, 2014. doi: 10.1021/jo502041f.  
  
H. V. Pham, A. S. Karns, C. D. Vanderwaland K. N. Houk, “Computational and Experimental Investigations of the Formal Dyotropic Rearrangements of Himbert Arene/Allene Cycloadducts”, *Journal of the American Chemical Society*, vol. 137, no. 21. American Chemical Society (ACS), pp. 6956–6964, May 22, 2015. doi: 10.1021/jacs.5b03718.  
  
E. M. Phillips, “Synthesis of*ent*-Ketorfanol via a C-H Alkenylation/Torquoselective 6π Electrocyclization Cascade”, *Angewandte Chemie International Edition*, vol. 54, no. 41. Wiley, pp. 12044–12048, Aug. 17, 2015. doi: 10.1002/anie.201505604.  
  
E. Picazo, “Arynes and Cyclic Alkynes as Synthetic Building Blocks for Stereodefined Quaternary Centers”, *Journal of the American Chemical Society*, vol. 140, no. 24. American Chemical Society (ACS), pp. 7605–7610, May 01, 2018. doi: 10.1021/jacs.8b02875.  
  
K. W. Quasdorf, “Suzuki−Miyaura Cross-Coupling of Aryl Carbamates and Sulfamates: Experimental and Computational Studies”, *Journal of the American Chemical Society*, vol. 133, no. 16. American Chemical Society (ACS), pp. 6352–6363, Apr. 01, 2011. doi: 10.1021/ja200398c.  
  
E. Richmond, “An asymmetric pericyclic cascade approach to 3-alkyl-3-aryloxindoles: generality, applications and mechanistic investigations”, *Organic & Biomolecular Chemistry*, vol. 13, no. 6. Royal Society of Chemistry (RSC), pp. 1807–1817, 2015. doi: 10.1039/c4ob02526a.  
  
E. Rodríguez, M. N. Grayson, A. Asensio, P. Barrio, K. N. Houkand S. Fustero, “Chiral Brønsted Acid-Catalyzed Asymmetric Allyl(propargyl)boration Reaction of *ortho*-Alkynyl Benzaldehydes: Synthetic Applications and Factors Governing the Enantioselectivity”, *ACS Catalysis*, vol. 6, no. 4. American Chemical Society (ACS), pp. 2506–2514, Mar. 15, 2016. doi: 10.1021/acscatal.6b00209.  
  
L. E. Rosebrugh, “Probing Stereoselectivity in Ring-Opening Metathesis Polymerization Mediated by Cyclometalated Ruthenium-Based Catalysts: A Combined Experimental and Computational Study”, *Journal of the American Chemical Society*, vol. 138, no. 4. American Chemical Society (ACS), pp. 1394–1405, Jan. 13, 2016. doi: 10.1021/jacs.5b12277.  
  
T. E. Rose, B. H. Curtin, K. V. Lawson, A. Simon, K. N. Houkand P. G. Harran, “On the prevalence of bridged macrocyclic pyrroloindolines formed in regiodivergent alkylations of tryptophan”, *Chemical Science*, vol. 7, no. 7. Royal Society of Chemistry (RSC), pp. 4158–4166, 2016. doi: 10.1039/c5sc04612b.  
  
R. Saleem-Batcha, “Enzymatic control of dioxygen binding and functionalization of the flavin cofactor”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 19. Proceedings of the National Academy of Sciences, pp. 4909–4914, Apr. 23, 2018. doi: 10.1073/pnas.1801189115.  
  
M. Sato, “Involvement of Lipocalin-like CghA in Decalin-Forming Stereoselective Intramolecular [4+2] Cycloaddition”, *ChemBioChem*, vol. 16, no. 16. Wiley, pp. 2294–2298, Oct. 02, 2015. doi: 10.1002/cbic.201500386.  
  
A. Simon, Y.-. hong . Lamand K. N. Houk, “Transition States of Vicinal Diamine-Catalyzed Aldol Reactions”, *Journal of the American Chemical Society*, vol. 138, no. 2. American Chemical Society (ACS), pp. 503–506, Jan. 08, 2016. doi: 10.1021/jacs.5b12097.  
  
C. Souris, F. Frébault, A. Patel, D. Audisio, K. N. Houkand N. Maulide, “Stereoselective Synthesis of Dienyl-Carboxylate Building Blocks: Formal Synthesis of Inthomycin C”, *Organic Letters*, vol. 15, no. 13. American Chemical Society (ACS), pp. 3242–3245, Jun. 13, 2013. doi: 10.1021/ol401226y.  
  
S.-E. Suh, S. Chen, K. N. Houkand D. M. Chenoweth, “The mechanism of the triple aryne–tetrazine reaction cascade: theory and experiment”, *Chemical Science*, vol. 9, no. 39. Royal Society of Chemistry (RSC), pp. 7688–7693, 2018. doi: 10.1039/c8sc01796d.  
  
C. Thiehoff, M. C. Holland, C. Daniliuc, K. N. Houkand R. Gilmour, “Can acyclic conformational control be achieved via a sulfur–fluorine gauche effect?”, *Chemical Science*, vol. 6, no. 6. Royal Society of Chemistry (RSC), pp. 3565–3571, 2015. doi: 10.1039/c5sc00871a.  
  
L. Törk, G. Jiménez-Osés, C. Doubleday, F. Liuand K. N. Houk, “Molecular Dynamics of the Diels–Alder Reactions of Tetrazines with Alkenes and N2 Extrusions from Adducts”, *Journal of the American Chemical Society*, vol. 137, no. 14. American Chemical Society (ACS), pp. 4749–4758, Apr. 06, 2015. doi: 10.1021/jacs.5b00014.  
  
A. A. Toutov, “A potassium tert-butoxide and hydrosilane system for ultra-deep desulfurization of fuels”, *Nature Energy*, vol. 2, no. 3. Springer Science and Business Media LLC, Feb. 17, 2017. doi: 10.1038/nenergy.2017.8.  
  
A. T. Tran, P. Liu, K. N. Houkand K. M. Nicholas, “Regioselectivity in the Cu(I)-Catalyzed [4 + 2]-Cycloaddition of 2-Nitrosopyridine with Unsymmetrical Dienes”, *The Journal of Organic Chemistry*, vol. 79, no. 12. American Chemical Society (ACS), pp. 5617–5626, Jun. 09, 2014. doi: 10.1021/jo5005907.  
  
M. C. Walton, Y.-F. Yang, X. Hong, K. N. Houkand L. E. Overman, “Ligand-Controlled Diastereoselective 1,3-Dipolar Cycloadditions of Azomethine Ylides with Methacrylonitrile”, *Organic Letters*, vol. 17, no. 24. American Chemical Society (ACS), pp. 6166–6169, Nov. 25, 2015. doi: 10.1021/acs.orglett.5b03171.  
  
H. Wang, “Solvent Effects on Polymer Sorting of Carbon Nanotubes with Applications in Printed Electronics”, *Small*, vol. 11, no. 1. Wiley, pp. 126–133, Aug. 19, 2014. doi: 10.1002/smll.201401890.  
  
H. Wang, “High-Yield Sorting of Small-Diameter Carbon Nanotubes for Solar Cells and Transistors”, *ACS Nano*, vol. 8, no. 3. American Chemical Society (ACS), pp. 2609–2617, Feb. 10, 2014. doi: 10.1021/nn406256y.  
  
H. Wang, “N-Type Conjugated Polymer-Enabled Selective Dispersion of Semiconducting Carbon Nanotubes for Flexible CMOS-Like Circuits”, *Advanced Functional Materials*, vol. 25, no. 12. Wiley, pp. 1837–1844, Feb. 13, 2015. doi: 10.1002/adfm.201404126.  
  
H. Wang, “Scalable and Selective Dispersion of Semiconducting Arc-Discharged Carbon Nanotubes by Dithiafulvalene/Thiophene Copolymers for Thin Film Transistors”, *ACS Nano*, vol. 7, no. 3. American Chemical Society (ACS), pp. 2659–2668, Feb. 22, 2013. doi: 10.1021/nn4000435.  
  
X.-N. Wang, E. H. Krenske, R. C. Johnston, K. N. Houkand R. P. Hsung, “AlCl3-Catalyzed Ring Expansion Cascades of Bicyclic Cyclobutenamides Involving Highly Strained *Cis*,*Trans*-Cycloheptadienone Intermediates”, *Journal of the American Chemical Society*, vol. 137, no. 16. American Chemical Society (ACS), pp. 5596–5601, Apr. 20, 2015. doi: 10.1021/jacs.5b02561.  
  
S. Xie, S. A. Lopez, O. Ramström, M. Yanand K. N. Houk, “1,3-Dipolar Cycloaddition Reactivities of Perfluorinated Aryl Azides with Enamines and Strained Dipolarophiles”, *Journal of the American Chemical Society*, vol. 137, no. 8. American Chemical Society (ACS), pp. 2958–2966, Feb. 18, 2015. doi: 10.1021/ja511457g.  
  
X.-S. Xue, B. J. Levandowski, C. Q. Heand K. N. Houk, “Origins of Selectivities in the Stork Diels–Alder Cycloaddition for the Synthesis of (±)-4-Methylenegermine”, *Organic Letters*, vol. 20, no. 19. American Chemical Society (ACS), pp. 6108–6111, Sep. 24, 2018. doi: 10.1021/acs.orglett.8b02548.  
  
X. Xu, P. Liu, A. Lesser, L. E. Sirois, P. A. Wenderand K. N. Houk, “Ligand Effects on Rates and Regioselectivities of Rh(I)-Catalyzed (5 + 2) Cycloadditions: A Computational Study of Cyclooctadiene and Dinaphthocyclooctatetraene as Ligands”, *Journal of the American Chemical Society*, vol. 134, no. 26. American Chemical Society (ACS), pp. 11012–11025, Jun. 21, 2012. doi: 10.1021/ja3041724.  
  
X. Xu, P. Liu, X.-. zhong . Shu, W. Tangand K. N. Houk, “Rh-Catalyzed (5+2) Cycloadditions of 3-Acyloxy-1,4-enynes and Alkynes: Computational Study of Mechanism, Reactivity, and Regioselectivity”, *Journal of the American Chemical Society*, vol. 135, no. 25. American Chemical Society (ACS), pp. 9271–9274, Jun. 14, 2013. doi: 10.1021/ja4036785.  
  
T. Yang, “(2 + 2) Cycloaddition of Benzyne to Endohedral Metallofullerenes M3N@C80 (M = Sc, Y): A Rotating-Intermediate Mechanism”, *Journal of the American Chemical Society*, vol. 137, no. 21. American Chemical Society (ACS), pp. 6820–6828, May 22, 2015. doi: 10.1021/jacs.5b01444.  
  
X. Yang, “Catalytic, Enantioselective N-Acylation of Lactams and Thiolactams Using Amidine-Based Catalysts”, *Journal of the American Chemical Society*, vol. 134, no. 42. American Chemical Society (ACS), pp. 17605–17612, Oct. 12, 2012. doi: 10.1021/ja306766n.  
  
X. Yang, P. Liu, K. N. Houkand V. B. Birman, “Manifestation of Felkin-Anh Control in Enantioselective Acyl Transfer Catalysis: Kinetic Resolution of Carboxylic Acids”, *Angewandte Chemie International Edition*, vol. 51, no. 38. Wiley, pp. 9638–9642, Aug. 22, 2012. doi: 10.1002/anie.201203327.  
  
Y.-F. Yang, “Palladium-Catalyzed *Meta*-Selective C–H Bond Activation with a Nitrile-Containing Template: Computational Study on Mechanism and Origins of Selectivity”, *Journal of the American Chemical Society*, vol. 136, no. 1. American Chemical Society (ACS), pp. 344–355, Dec. 17, 2013. doi: 10.1021/ja410485g.  
  
Y.-F. Yang, G. Chen, X. Hong, J.-Q. Yuand K. N. Houk, “The Origins of Dramatic Differences in Five-Membered vs Six-Membered Chelation of Pd(II) on Efficiency of C(sp3)–H Bond Activation”, *Journal of the American Chemical Society*, vol. 139, no. 25. American Chemical Society (ACS), pp. 8514–8521, Jun. 19, 2017. doi: 10.1021/jacs.7b01801.  
  
Y.-F. Yang, K. N. Houkand Y.-D. Wu, “Computational Exploration of RhIII/RhV and RhIII/RhI Catalysis in Rhodium(III)-Catalyzed C–H Activation Reactions of *N*-Phenoxyacetamides with Alkynes”, *Journal of the American Chemical Society*, vol. 138, no. 21. American Chemical Society (ACS), pp. 6861–6868, May 23, 2016. doi: 10.1021/jacs.6b03424.  
  
Y.-F. Yang, Y. Liang, F. Liuand K. N. Houk, “Diels–Alder Reactivities of Benzene, Pyridine, and Di-, Tri-, and Tetrazines: The Roles of Geometrical Distortions and Orbital Interactions”, *Journal of the American Chemical Society*, vol. 138, no. 5. American Chemical Society (ACS), pp. 1660–1667, Feb. 02, 2016. doi: 10.1021/jacs.5b12054.  
  
Y.-F. Yang, P. Yuand K. N. Houk, “Computational Exploration of Concerted and Zwitterionic Mechanisms of Diels–Alder Reactions between 1,2,3-Triazines and Enamines and Acceleration by Hydrogen-Bonding Solvents”, *Journal of the American Chemical Society*, vol. 139, no. 50. American Chemical Society (ACS), pp. 18213–18221, Dec. 05, 2017. doi: 10.1021/jacs.7b08325.  
  
Z. Yang, “Relationships between Product Ratios in Ambimodal Pericyclic Reactions and Bond Lengths in Transition Structures”, *Journal of the American Chemical Society*, vol. 140, no. 8. American Chemical Society (ACS), pp. 3061–3067, Feb. 19, 2018. doi: 10.1021/jacs.7b13562.  
  
Z. Yang, G. Jiménez-Osés, C. J. López, M. D. Bridges, K. N. Houkand W. L. Hubbell, “Long-Range Distance Measurements in Proteins at Physiological Temperatures Using Saturation Recovery EPR Spectroscopy”, *Journal of the American Chemical Society*, vol. 136, no. 43. American Chemical Society (ACS), pp. 15356–15365, Oct. 17, 2014. doi: 10.1021/ja5083206.  
  
Z. Yang, P. Yuand K. N. Houk, “Molecular Dynamics of Dimethyldioxirane C–H Oxidation”, *Journal of the American Chemical Society*, vol. 138, no. 12. American Chemical Society (ACS), pp. 4237–4242, Mar. 22, 2016. doi: 10.1021/jacs.6b01028.  
  
Z. Yang, L. Zou, Y. Yu, F. Liu, X. Dongand K. N. Houk, “Molecular dynamics of the two-stage mechanism of cyclopentadiene dimerization: concerted or stepwise?”, *Chemical Physics*, vol. 514. Elsevier BV, pp. 120–125, Oct. 2018. doi: 10.1016/j.chemphys.2018.02.020.  
  
I. Yavuz, J. B. Linand K. N. Houk, “Impact of morphology, side-chains, and crystallinity on charge-transport properties of π-extended double helicenes”, *Physical Chemistry Chemical Physics*, vol. 21, no. 2. Royal Society of Chemistry (RSC), pp. 901–914, 2019. doi: 10.1039/c8cp06982d.  
  
I. Yavuz, B. N. Martin, J. Parkand K. N. Houk, “Theoretical Study of the Molecular Ordering, Paracrystallinity, And Charge Mobilities of Oligomers in Different Crystalline Phases”, *Journal of the American Chemical Society*, vol. 137, no. 8. American Chemical Society (ACS), pp. 2856–2866, Feb. 19, 2015. doi: 10.1021/ja5076376.  
  
P. Yu, “Mechanisms and Origins of Periselectivity of the Ambimodal [6 + 4] Cycloadditions of Tropone to Dimethylfulvene”, *Journal of the American Chemical Society*, vol. 139, no. 24. American Chemical Society (ACS), pp. 8251–8258, Jun. 07, 2017. doi: 10.1021/jacs.7b02966.  
  
P. Yu, W. Liand K. N. Houk, “Mechanisms and Origins of Selectivities of the Lewis Acid-Catalyzed Diels–Alder Reactions between Arylallenes and Acrylates”, *The Journal of Organic Chemistry*, vol. 82, no. 12. American Chemical Society (ACS), pp. 6398–6402, Jun. 02, 2017. doi: 10.1021/acs.joc.7b01132.  
  
P. Yu, A. Pateland K. N. Houk, “Transannular [6 + 4] and Ambimodal Cycloaddition in the Biosynthesis of Heronamide A”, *Journal of the American Chemical Society*, vol. 137, no. 42. American Chemical Society (ACS), pp. 13518–13523, Oct. 15, 2015. doi: 10.1021/jacs.5b06656.  
  
Y. Yu, Z. Yangand K. N. Houk, “Molecular dynamics of the intramolecular 1, 3-dipolar ene reaction of a nitrile oxide and an alkene: non-statistical behavior of a reaction involving a diradical intermediate”, *Molecular Physics*, vol. 117, no. 9–12. Informa UK Limited, pp. 1360–1366, Nov. 25, 2018. doi: 10.1080/00268976.2018.1549338.  
  
J. Zhang, “Asymmetric phosphoric acid–catalyzed four-component Ugi reaction”, *Science*, vol. 361, no. 6407. American Association for the Advancement of Science (AAAS), Sep. 14, 2018. doi: 10.1126/science.aas8707.  
  
K. Zhang, L. Cai, Z. Yang, K. N. Houkand O. Kwon, “Bridged [2.2.1] bicyclic phosphine oxide facilitates catalytic γ-umpolung addition–Wittig olefination”, *Chemical Science*, vol. 9, no. 7. Royal Society of Chemistry (RSC), pp. 1867–1872, 2018. doi: 10.1039/c7sc04381c.  
  
L. Zhang, “Unconventional, Chemically Stable, and Soluble Two-Dimensional Angular Polycyclic Aromatic Hydrocarbons: From Molecular Design to Device Applications”, *Accounts of Chemical Research*, vol. 48, no. 3. American Chemical Society (ACS), pp. 500–509, Dec. 02, 2014. doi: 10.1021/ar500278w.  
  
J. Zhao, “Intramolecular Crossed [2+2] Photocycloaddition through Visible Light-Induced Energy Transfer”, *Journal of the American Chemical Society*, vol. 139, no. 29. American Chemical Society (ACS), pp. 9807–9810, Jul. 11, 2017. doi: 10.1021/jacs.7b05277.  
  
Z. Zhou, “Catalytic Enantioselective Intramolecular C(sp 3 )−H Amination of 2‐Azidoacetamides”, *Angewandte Chemie International Edition*, vol. 58, no. 4. Wiley, pp. 1088–1093, Jan. 21, 2019. doi: 10.1002/anie.201811927.  
  
C. Zhu, “Iodoarene-Catalyzed Stereospecific Intramolecular sp3 C–H Amination: Reaction Development and Mechanistic Insights”, *Journal of the American Chemical Society*, vol. 137, no. 24. American Chemical Society (ACS), pp. 7564–7567, Jun. 11, 2015. doi: 10.1021/jacs.5b03488.  
  
I. Ugur, “1,3-Dipolar Cycloaddition Reactions of Low-Valent Rhodium and Iridium Complexes with Arylnitrile *N*-Oxides”, *The Journal of Organic Chemistry*, vol. 82, no. 10. American Chemical Society (ACS), pp. 5096–5101, Apr. 27, 2017. doi: 10.1021/acs.joc.7b00282.  
  
M. B. Griffin, A. A. Rodriguez, M. M. Montemore, J. R. Monnier, C. T. Williamsand J. W. Medlin, “The selective oxidation of ethylene glycol and 1,2-propanediol on Au, Pd, and Au–Pd bimetallic catalysts”, *Journal of Catalysis*, vol. 307. Elsevier BV, pp. 111–120, Nov. 2013. doi: 10.1016/j.jcat.2013.07.012.  
  
M. M. Montemore and J. W. Medlin, “A density functional study of C1–C4 alkyl adsorption on Cu(111)”, *The Journal of Chemical Physics*, vol. 136, no. 20. AIP Publishing, p. 204710, May 28, 2012. doi: 10.1063/1.4722102.  
  
A. J. Phares, “Coadsorption of *n* Monomer Species on Terraces and Nanotubes”, *Langmuir*, vol. 27, no. 13. American Chemical Society (ACS), pp. 8105–8119, Jun. 08, 2011. doi: 10.1021/la200583r.  
  
A. J. Phares and D. W. Grumbine Jr, “Dimer adsorption on square nanotubes with first-and second-neighbor interactions”, *Journal of Physics: Conference Series*, vol. 410. IOP Publishing, p. 012157, Feb. 08, 2013. doi: 10.1088/1742-6596/410/1/012157.  
  
A. J. Phares and D. W. Grumbine, “Dimer Adsorption on a (100) Nanotube of Arbitrary Diameter, with First- and Second-Neighbor Interactions”, *Langmuir*, vol. 30, no. 23. American Chemical Society (ACS), pp. 6831–6840, Jun. 05, 2014. doi: 10.1021/la500616t.  
  
A. J. Phares, D. W. Grumbine Jr.and F. J. Wunderlich, “Hollow Adsorption on Zigzag Single-Walled Carbon Nanotubes: Repulsive First-Neighbor Interactions”, *Langmuir*, vol. 26, no. 13. American Chemical Society (ACS), pp. 10750–10757, Apr. 08, 2010. doi: 10.1021/la1005488.  
  
A. J. Phares, D. W. Grumbine Jr.and F. J. Wunderlich, “Modeling adsorption on fcc(nnm) surfaces”, *The European Physical Journal B*, vol. 80, no. 3. Springer Science and Business Media LLC, pp. 311–319, Mar. 16, 2011. doi: 10.1140/epjb/e2011-10720-3.  
  
A. J. Phares, P. M. Pasinetti, D. W. Grumbine Jr.and F. J. Wunderlich, “Dimer adsorption on square surfaces with first- and second-neighbor interactions”, *Physica B: Condensed Matter*, vol. 406, no. 5. Elsevier BV, pp. 1096–1105, Mar. 2011. doi: 10.1016/j.physb.2010.12.053.  
  
M. E. Abbasov, B. M. Hudson, D. J. Tantilloand D. Romo, “Acylammonium Salts as Dienophiles in Diels–Alder/Lactonization Organocascades”, *Journal of the American Chemical Society*, vol. 136, no. 12. American Chemical Society (ACS), pp. 4492–4495, Mar. 12, 2014. doi: 10.1021/ja501005g.  
  
S. R. Hare, “Experimental and Computational Mechanistic Investigation of Chlorocarbene Additions to Bridgehead Carbene–Anti-Bredt Systems: Noradamantylcarbene–Adamantene and Adamantylcarbene–Homoadamantene”, *The Journal of Organic Chemistry*, vol. 80, no. 10. American Chemical Society (ACS), pp. 5049–5065, May 06, 2015. doi: 10.1021/acs.joc.5b00456.  
  
Y. J. Hong, J.-L. Ginerand D. J. Tantillo, “Bicyclobutonium Ions in Biosynthesis – Interconversion of Cyclopropyl-Containing Sterols from Orchids”, *Journal of the American Chemical Society*, vol. 137, no. 5. American Chemical Society (ACS), pp. 2085–2088, Jan. 30, 2015. doi: 10.1021/ja512901a.  
  
Y. J. Hong and D. J. Tantillo, “Biosynthetic consequences of multiple sequential post-transition-state bifurcations”, *Nature Chemistry*, vol. 6, no. 2. Springer Science and Business Media LLC, pp. 104–111, Jan. 19, 2014. doi: 10.1038/nchem.1843.  
  
Y. J. Hong and D. J. Tantillo, “Branching Out from the Bisabolyl Cation. Unifying Mechanistic Pathways to Barbatene, Bazzanene, Chamigrene, Chamipinene, Cumacrene, Cuprenene, Dunniene, Isobazzanene, Iso-γ-bisabolene, Isochamigrene, Laurene, Microbiotene, Sesquithujene, Sesquisabinene, Thujopsene, Trichodiene, and Widdradiene Sesquiterpenes”, *Journal of the American Chemical Society*, vol. 136, no. 6. American Chemical Society (ACS), pp. 2450–2463, Feb. 03, 2014. doi: 10.1021/ja4106489.  
  
Y. J. Hong and D. J. Tantillo, “How cyclobutanes are assembled in nature – insights from quantum chemistry”, *Chemical Society Reviews*, vol. 43, no. 14. Royal Society of Chemistry (RSC), p. 5042, 2014. doi: 10.1039/c3cs60452g.  
  
Y. J. Hong and D. J. Tantillo, “Viability of Nonclassical Carbocations Proposed as Intermediates in the Biosynthesis of Atiserene, Beyerene, Kaurene, and Trachylobane Diterpenes”, *Helvetica Chimica Acta*, vol. 97, no. 11. Wiley, pp. 1475–1480, Nov. 2014. doi: 10.1002/hlca.201400082.  
  
Y. J. Hong and D. J. Tantillo, “Feasibility of Intramolecular Proton Transfers in Terpene Biosynthesis – Guiding Principles”, *Journal of the American Chemical Society*, vol. 137, no. 12. American Chemical Society (ACS), pp. 4134–4140, Mar. 19, 2015. doi: 10.1021/ja512685x.  
  
M. Isegawa, S. Maeda, D. J. Tantilloand K. Morokuma, “Predicting pathways for terpene formation from first principles – routes to known and new sesquiterpenes”, *Chemical Science*, vol. 5, no. 4. Royal Society of Chemistry (RSC), p. 1555, 2014. doi: 10.1039/c3sc53293c.  
  
L. S. Kocsis, “Mechanistic Insight into the Dehydro-Diels–Alder Reaction of Styrene–Ynes”, *The Journal of Organic Chemistry*, vol. 80, no. 23. American Chemical Society (ACS), pp. 11686–11698, Mar. 02, 2015. doi: 10.1021/acs.joc.5b00200.  
  
E. V. Mercado-Marin, “Total synthesis and isolation of citrinalin and cyclopiamine congeners”, *Nature*, vol. 509, no. 7500. Springer Science and Business Media LLC, pp. 318–324, May 2014. doi: 10.1038/nature13273.  
  
A. T. Merrill and D. J. Tantillo, “Solvent optimization and conformational flexibility effects on 1 H and 13 C NMR scaling factors”, *Magnetic Resonance in Chemistry*, vol. 58, no. 6. Wiley, pp. 576–583, Jan. 14, 2020. doi: 10.1002/mrc.4986.  
  
Q. N. N. Nguyen, J. Yangand D. J. Tantillo, “Factors Controlling the Facility of Transannular Diels–Alder Reactions of Macrocyclic Bis-enones”, *The Journal of Organic Chemistry*, vol. 79, no. 15. American Chemical Society (ACS), pp. 7162–7168, Jul. 15, 2014. doi: 10.1021/jo5013064.  
  
P. P. Painter, B. M. Wongand D. J. Tantillo, “Facilitating the Cope Rearrangement by Partial Protonation: Implications for Synthesis and Biosynthesis”, *Organic Letters*, vol. 16, no. 18. American Chemical Society (ACS), pp. 4818–4821, Sep. 04, 2014. doi: 10.1021/ol5023036.  
  
D. Patra, T. A. Palazzo, N. N. Malaeb, M. J. Haddadin, D. J. Tantilloand M. J. Kurth, “Cyclic Azacyanines: Experimental and Computational Studies on Spectroscopic Properties and Unique Reactivity”, *Journal of Fluorescence*, vol. 24, no. 4. Springer Science and Business Media LLC, pp. 1285–1296, Jun. 10, 2014. doi: 10.1007/s10895-014-1413-0.  
  
R. P. Pemberton, K. C. Hoand D. J. Tantillo, “Modulation of inherent dynamical tendencies of the bisabolyl cation via preorganization in epi-isozizaene synthase”, *Chemical Science*, vol. 6, no. 4. Royal Society of Chemistry (RSC), pp. 2347–2353, 2015. doi: 10.1039/c4sc03782k.  
  
R. P. Pemberton and D. J. Tantillo, “Lifetimes of carbocations encountered along reaction coordinates for terpene formation”, *Chemical Science*, vol. 5, no. 8. Royal Society of Chemistry (RSC), p. 3301, 2014. doi: 10.1039/c4sc00674g.  
  
C. M. Rasik, Y. J. Hong, D. J. Tantilloand M. K. Brown, “Origins of Diastereoselectivity in Lewis Acid Promoted Ketene–Alkene [2 + 2] Cycloadditions”, *Organic Letters*, vol. 16, no. 19. American Chemical Society (ACS), pp. 5168–5171, Sep. 17, 2014. doi: 10.1021/ol5025184.  
  
S. Strych, G. Journot, R. P. Pemberton, S. C. Wang, D. J. Tantilloand D. Trauner, “Cover Picture: Biomimetic Total Synthesis of Santalin Y (Angew. Chem. Int. Ed. 17/2015)”, *Angewandte Chemie International Edition*, vol. 54, no. 17. Wiley, pp. 4971–4971, Apr. 02, 2015. doi: 10.1002/anie.201502755.  
  
D. R. Williams, B. A. Atwater, S. A. Bawel, P. Ke, O. Gutierrezand D. J. Tantillo, “Stereocontrol in Asymmetric SE′ Reactions of γ-Substituted α,β-Unsaturated Aldehydes”, *Organic Letters*, vol. 16, no. 2. American Chemical Society (ACS), pp. 468–471, Dec. 31, 2013. doi: 10.1021/ol403351x.  
  
S. Zaretsky, “Predicting cyclic peptide chemical shifts using quantum mechanical calculations”, *Tetrahedron*, vol. 70, no. 42. Elsevier BV, pp. 7655–7663, Oct. 2014. doi: 10.1016/j.tet.2014.07.070.  
  
J. Zi, “Biosynthesis of Lycosantalonol, a *cis*-Prenyl Derived Diterpenoid”, *Journal of the American Chemical Society*, vol. 136, no. 49. American Chemical Society (ACS), pp. 16951–16953, Nov. 21, 2014. doi: 10.1021/ja508477e.  
  
C. Saunders and D. Tantillo, “Application of Computational Chemical Shift Prediction Techniques to the Cereoanhydride Structure Problem—Carboxylate Complications”, *Marine Drugs*, vol. 15, no. 6. MDPI AG, p. 171, Jun. 12, 2017. doi: 10.3390/md15060171.  
  
F. Bartels, “Bioinspired synthesis of pentacyclic onocerane triterpenoids”, *Chemical Science*, vol. 8, no. 12. Royal Society of Chemistry (RSC), pp. 8285–8290, 2017. doi: 10.1039/c7sc03903d.  
  
M. Blümel, S. Nagasawa, K. Blackford, S. R. Hare, D. J. Tantilloand R. Sarpong, “Rearrangement of Hydroxylated Pinene Derivatives to Fenchone-Type Frameworks: Computational Evidence for Dynamically-Controlled Selectivity”, *Journal of the American Chemical Society*, vol. 140, no. 29. American Chemical Society (ACS), pp. 9291–9298, Jul. 03, 2018. doi: 10.1021/jacs.8b05804.  
  
R. B. Campos and D. J. Tantillo, “Coupled Electrocyclization/Prototropic Shift in the Biosynthesis of Crotinsulidane Diterpenoids”, *The Journal of Organic Chemistry*, vol. 83, no. 2. American Chemical Society (ACS), pp. 1073–1076, Jan. 09, 2018. doi: 10.1021/acs.joc.7b02904.  
  
L. G. Cool, K. E. Vermillion, G. R. Takeoka, S. C. Wangand D. J. Tantillo, “Biosynthesis and Conformational Properties of the Irregular Sesquiterpenoids Isothapsadiene and β-Isothapsenol”, *The Journal of Organic Chemistry*, vol. 83, no. 10. American Chemical Society (ACS), pp. 5724–5730, Apr. 23, 2018. doi: 10.1021/acs.joc.8b00800.  
  
G. S. Freund, “Elucidating Substrate Promiscuity within the FabI Enzyme Family”, *ACS Chemical Biology*, vol. 12, no. 9. American Chemical Society (ACS), pp. 2465–2473, Aug. 31, 2017. doi: 10.1021/acschembio.7b00400.  
  
Y. J. Hong and D. J. Tantillo, “A Maze of Dyotropic Rearrangements and Triple Shifts: Carbocation Rearrangements Connecting Stemarene, Stemodene, Betaerdene, Aphidicolene, and Scopadulanol”, *The Journal of Organic Chemistry*, vol. 83, no. 7. American Chemical Society (ACS), pp. 3780–3793, Mar. 01, 2018. doi: 10.1021/acs.joc.8b00138.  
  
A. C. Huang, Y. J. Hong, A. D. Bond, D. J. Tantilloand A. Osbourn, “Diverged Plant Terpene Synthases Reroute the Carbocation Cyclization Path towards the Formation of Unprecedented 6/11/5 and 6/6/7/5 Sesterterpene Scaffolds”, *Angewandte Chemie International Edition*, vol. 57, no. 5. Wiley, pp. 1291–1295, Dec. 28, 2017. doi: 10.1002/anie.201711444.  
  
A. C. Huang, “Unearthing a sesterterpene biosynthetic repertoire in the Brassicaceae through genome mining reveals convergent evolution”, *Proceedings of the National Academy of Sciences*, vol. 114, no. 29. Proceedings of the National Academy of Sciences, Jul. 03, 2017. doi: 10.1073/pnas.1705567114.  
  
R. H. Kaufman, “Oxidopyrylium-Alkene [5 + 2] Cycloaddition Conjugate Addition Cascade (C3) Sequences: Scope, Limitation, and Computational Investigations”, *The Journal of Organic Chemistry*, vol. 83, no. 17. American Chemical Society (ACS), pp. 9818–9838, Jul. 12, 2018. doi: 10.1021/acs.joc.8b01322.  
  
C. H. McCulley and D. J. Tantillo, “Secondary Carbocations in the Biosynthesis of Pupukeanane Sesquiterpenes”, *The Journal of Physical Chemistry A*, vol. 122, no. 40. American Chemical Society (ACS), pp. 8058–8061, Sep. 13, 2018. doi: 10.1021/acs.jpca.8b07961.  
  
R. Mendoza‐Sanchez, “Cyclols Revisited: Facile Synthesis of Medium‐Sized Cyclic Peptides”, *Chemistry – A European Journal*, vol. 23, no. 54. Wiley, pp. 13319–13322, Aug. 31, 2017. doi: 10.1002/chem.201703616.  
  
Q. N. N. Nguyen, J. Schwochert, D. J. Tantilloand R. S. Lokey, “Using 1H and 13C NMR chemical shifts to determine cyclic peptide conformations: a combined molecular dynamics and quantum mechanics approach”, *Physical Chemistry Chemical Physics*, vol. 20, no. 20. Royal Society of Chemistry (RSC), pp. 14003–14012, 2018. doi: 10.1039/c8cp01616j.  
  
T. E. O’Brien, S. J. Bertolani, Y. Zhang, J. B. Siegeland D. J. Tantillo, “Predicting Productive Binding Modes for Substrates and Carbocation Intermediates in Terpene Synthases—Bornyl Diphosphate Synthase As a Representative Case”, *ACS Catalysis*, vol. 8, no. 4. American Chemical Society (ACS), pp. 3322–3330, Mar. 08, 2018. doi: 10.1021/acscatal.8b00342.  
  
C. Saunders, M. B. Khaled, J. D. Weaver IIIand D. J. Tantillo, “Prediction of 19F NMR Chemical Shifts for Fluorinated Aromatic Compounds”, *The Journal of Organic Chemistry*, vol. 83, no. 6. American Chemical Society (ACS), pp. 3220–3225, Feb. 22, 2018. doi: 10.1021/acs.joc.8b00104.  
  
V. M. Schmiedel, Y. J. Hong, D. Lentz, D. J. Tantilloand M. Christmann, “Synthesis and Structure Revision of Dichrocephones A and B”, *Angewandte Chemie International Edition*, vol. 57, no. 9. Wiley, pp. 2419–2422, Jan. 16, 2018. doi: 10.1002/anie.201711766.  
  
S. M. Wilkerson-Hill, “Mechanism of a No-Metal-Added Heterocycloisomerization of Alkynylcyclopropylhydrazones: Synthesis of Cycloheptane-Fused Aminopyrroles Facilitated by Copper Salts at Trace Loadings”, *Journal of the American Chemical Society*, vol. 139, no. 30. American Chemical Society (ACS), pp. 10569–10577, Jul. 20, 2017. doi: 10.1021/jacs.7b06007.  
  
G. Xu, M. Elkin, D. J. Tantillo, T. R. Newhouseand T. J. Maimone, “Traversing Biosynthetic Carbocation Landscapes in the Total Synthesis of Andrastin and Terretonin Meroterpenes”, *Angewandte Chemie International Edition*, vol. 56, no. 41. Wiley, pp. 12498–12502, Aug. 30, 2017. doi: 10.1002/anie.201705654.  
  
M. Xu, “Premutilin Synthase: Ring Rearrangement by a Class II Diterpene Cyclase”, *Organic Letters*, vol. 20, no. 4. American Chemical Society (ACS), pp. 1200–1202, Feb. 01, 2018. doi: 10.1021/acs.orglett.8b00121.  
  
Y. Xu, Y. J. Hong, D. J. Tantilloand M. K. Brown, “Intramolecular Chirality Transfer [2 + 2] Cycloadditions of Allenoates and Alkenes”, *Organic Letters*, vol. 19, no. 14. American Chemical Society (ACS), pp. 3703–3706, Jul. 07, 2017. doi: 10.1021/acs.orglett.7b01420.  
  
J. S. Zhu, “N–N Bond Formation between Primary Amines and Nitrosos: Direct Synthesis of 2-Substituted Indazolones with Mechanistic Insights”, *Organic Letters*, vol. 20, no. 16. American Chemical Society (ACS), pp. 4736–4739, Aug. 01, 2018. doi: 10.1021/acs.orglett.8b01655.  
  
J. S. Zhu, J.-H. Son, A. P. Teuthorn, M. J. Haddadin, M. J. Kurthand D. J. Tantillo, “Diverting Reactive Intermediates Toward Unusual Chemistry: Unexpected Anthranil Products from Davis–Beirut Reaction”, *The Journal of Organic Chemistry*, vol. 82, no. 20. American Chemical Society (ACS), pp. 10875–10882, Sep. 28, 2017. doi: 10.1021/acs.joc.7b01521.  
  
W. Lee, J. Zhouand O. Gutierrez, “Mechanism of Nakamura’s Bisphosphine-Iron-Catalyzed Asymmetric C(sp2)–C(sp3) Cross-Coupling Reaction: The Role of Spin in Controlling Arylation Pathways”, *Journal of the American Chemical Society*, vol. 139, no. 45. American Chemical Society (ACS), pp. 16126–16133, Nov. 02, 2017. doi: 10.1021/jacs.7b06377.  
  
Y. Li and H. Guo, “Atomistic simulations of an antimicrobial molecule interacting with a model bacterial membrane”, *Theoretical Chemistry Accounts*, vol. 132, no. 1. Springer Science and Business Media LLC, Dec. 04, 2012. doi: 10.1007/s00214-012-1303-y.  
  
Y. Hu, L. Huang, S. Zhao, H. Liuand K. E. Gubbins, “Effect of confinement in nano-porous materials on the solubility of a supercritical gas”, *Molecular Physics*, vol. 114, no. 22. Informa UK Limited, pp. 3294–3306, Sep. 27, 2016. doi: 10.1080/00268976.2016.1229871.  
  
S. K. Jain, R. J.-M. Pellenq, K. E. Gubbinsand X. Peng, “Molecular Modeling and Adsorption Properties of Ordered Silica-Templated CMK Mesoporous Carbons”, *Langmuir*, vol. 33, no. 9. American Chemical Society (ACS), pp. 2109–2121, Feb. 20, 2017. doi: 10.1021/acs.langmuir.6b04169.  
  
D. Srivastava, C. H. Turner, E. E. Santisoand K. E. Gubbins, “The Nitric Oxide Dimer Reaction in Carbon Nanopores”, *The Journal of Physical Chemistry B*, vol. 122, no. 13. American Chemical Society (ACS), pp. 3604–3614, Dec. 14, 2017. doi: 10.1021/acs.jpcb.7b10876.  
  
M. Greschek, K. E. Gubbinsand M. Schoen, “Imprinting substrate structures onto a nematic liquid crystal”, *The Journal of Chemical Physics*, vol. 137, no. 14. AIP Publishing, p. 144703, Oct. 14, 2012. doi: 10.1063/1.4757391.  
  
L. Huang, T. Bandosz, K. L. Joshi, A. C. T. van Duinand K. E. Gubbins, “Reactive adsorption of ammonia and ammonia/water on CuBTC metal-organic framework: A ReaxFF molecular dynamics simulation”, *The Journal of Chemical Physics*, vol. 138, no. 3. AIP Publishing, p. 034102, Jan. 21, 2013. doi: 10.1063/1.4774332.  
  
L. Huang, K. L. Joshi, A. C. T. van . Duin, T. J. Bandoszand K. E. Gubbins, “ReaxFF molecular dynamics simulation of thermal stability of a Cu3(BTC)2 metal–organic framework”, *Physical Chemistry Chemical Physics*, vol. 14, no. 32. Royal Society of Chemistry (RSC), p. 11327, 2012. doi: 10.1039/c2cp41511a.  
  
L. Huang, M. Seredych, T. J. Bandosz, A. C. T. van Duin, X. Luand K. E. Gubbins, “Controllable atomistic graphene oxide model and its application in hydrogen sulfide removal”, *The Journal of Chemical Physics*, vol. 139, no. 19. AIP Publishing, p. 194707, Nov. 21, 2013. doi: 10.1063/1.4832039.  
  
Y. Long, J. C. Palmer, B. Coasne, M. Śliwinska-Bartkowiakand K. E. Gubbins, “Pressure enhancement in carbon nanopores: a major confinement effect”, *Physical Chemistry Chemical Physics*, vol. 13, no. 38. Royal Society of Chemistry (RSC), pp. 17163–17170, 2011. doi: 10.1039/c1cp21407a.  
  
J. C. Palmer, B. Coasne, M. Śliwinska-Bartkowiak, G. Jackson, E. A. Müllerand K. E. Gubbins, “On the molecular origin of high-pressure effects in nanoconfinement: The role of surface chemistry and roughness”, *The Journal of Chemical Physics*, vol. 139, no. 14. AIP Publishing, p. 144701, Oct. 14, 2013. doi: 10.1063/1.4824125.  
  
M. Miao, “Activation of water on the TiO2 (110) surface: The case of Ti adatoms”, *The Journal of Chemical Physics*, vol. 136, no. 6. AIP Publishing, p. 064703, Feb. 14, 2012. doi: 10.1063/1.3682781.  
  
C. Petit, L. Huang, J. Jagiello, J. Kenvin, K. E. Gubbinsand T. J. Bandosz, “Toward Understanding Reactive Adsorption of Ammonia on Cu-MOF/Graphite Oxide Nanocomposites”, *Langmuir*, vol. 27, no. 21. American Chemical Society (ACS), pp. 13043–13051, Oct. 04, 2011. doi: 10.1021/la202924y.  
  
G. Rosenthal, K. E. Gubbinsand S. H. L. Klapp, “Self-assembly of model amphiphilic Janus particles”, *The Journal of Chemical Physics*, vol. 136, no. 17. AIP Publishing, p. 174901, May 07, 2012. doi: 10.1063/1.4707954.  
  
M. Śliwińska-Bartkowiak, “Structural analysis of water and carbon tetrachloride adsorbed in activated carbon fibres”, *Physical Chemistry Chemical Physics*, vol. 14, no. 19. Royal Society of Chemistry (RSC), p. 7145, 2012. doi: 10.1039/c2cp22111j.  
  
M.-J. Wei, L. Zhang, L. Lu, Y. Zhu, K. E. Gubbinsand X. Lu, “Molecular behavior of water in TiO2 nano-slits with varying coverages of carbon: a molecular dynamics simulation study”, *Physical Chemistry Chemical Physics*, vol. 14, no. 48. Royal Society of Chemistry (RSC), p. 16536, 2012. doi: 10.1039/c2cp40687j.  
  
R. L. Birke, J. R. Lombardi, W. A. Saidiand P. Norman, “Surface-Enhanced Raman Scattering Due to Charge-Transfer Resonances: A Time-Dependent Density Functional Theory Study of Ag13-4-Mercaptopyridine”, *The Journal of Physical Chemistry C*, vol. 120, no. 37. American Chemical Society (ACS), pp. 20721–20735, Apr. 27, 2016. doi: 10.1021/acs.jpcc.6b01961.  
  
N. V. Bashmakova, “Design and Electronic Structure of New Styryl Dye Bases: Steady-State and Time-Resolved Spectroscopic Studies”, *The Journal of Physical Chemistry A*, vol. 118, no. 25. American Chemical Society (ACS), pp. 4502–4509, Jun. 11, 2014. doi: 10.1021/jp503263f.  
  
W. M. Berhanu and A. E. Masunov, “Atomistic mechanism of polyphenol amyloid aggregation inhibitors: molecular dynamics study of Curcumin, Exifone, and Myricetin interaction with the segment of tau peptide oligomer”, *Journal of Biomolecular Structure and Dynamics*, vol. 33, no. 7. Informa UK Limited, pp. 1399–1411, Sep. 09, 2014. doi: 10.1080/07391102.2014.951689.  
  
T. M. Inerbaev, A. S. Karakoti, S. V. N. T. Kuchibhatla, A. Kumar, A. E. Masunovand S. Seal, “Aqueous medium induced optical transitions in cerium oxide nanoparticles”, *Physical Chemistry Chemical Physics*, vol. 17, no. 9. Royal Society of Chemistry (RSC), pp. 6217–6221, 2015. doi: 10.1039/c4cp04961f.  
  
A. E. Masunov, D. Anderson, A. Y. Freidzonand A. A. Bagaturyants, “Symmetry-Breaking in Cationic Polymethine Dyes: Part 2. Shape of Electronic Absorption Bands Explained by the Thermal Fluctuations of the Solvent Reaction Field”, *The Journal of Physical Chemistry A*, vol. 119, no. 26. American Chemical Society (ACS), pp. 6807–6815, Jun. 18, 2015. doi: 10.1021/acs.jpca.5b03877.  
  
D. B. Lingerfelt, P. Ganesh, J. Jakowskiand B. G. Sumpter, “Electronically Nonadiabatic Structural Transformations Promoted by Electron Beams”, *Advanced Functional Materials*, vol. 29, no. 52. Wiley, p. 1901901, Jun. 07, 2019. doi: 10.1002/adfm.201901901.  
  
D. B. Lingerfelt, P. Ganesh, J. Jakowskiand B. G. Sumpter, “Understanding Beam-Induced Electronic Excitations in Materials”, *Journal of Chemical Theory and Computation*, vol. 16, no. 2. American Chemical Society (ACS), pp. 1200–1214, Jan. 03, 2020. doi: 10.1021/acs.jctc.9b00792.  
  
A. J. McCaskey, “Quantum chemistry as a benchmark for near-term quantum computers”, *npj Quantum Information*, vol. 5, no. 1. Springer Science and Business Media LLC, Nov. 15, 2019. doi: 10.1038/s41534-019-0209-0.  
  
I. Savchenko, B. Gu, T. Heine, J. Jakowskiand S. Garashchuk, “Nuclear quantum effects on adsorption of H2 and isotopologues on metal ions”, *Chemical Physics Letters*, vol. 670. Elsevier BV, pp. 64–70, Feb. 2017. doi: 10.1016/j.cplett.2016.12.069.  
  
G. Gao, X. Liang, N. W. Ashcroftand R. Hoffmann, “Potential Semiconducting and Superconducting Metastable Si3C Structures under Pressure”, *Chemistry of Materials*, vol. 30, no. 2. American Chemical Society (ACS), pp. 421–427, Jan. 11, 2018. doi: 10.1021/acs.chemmater.7b04243.  
  
M. Rahm, R. Hoffmannand N. W. Ashcroft, “Ternary Gold Hydrides: Routes to Stable and Potentially Superconducting Compounds”, *Journal of the American Chemical Society*, vol. 139, no. 25. American Chemical Society (ACS), pp. 8740–8751, Jun. 19, 2017. doi: 10.1021/jacs.7b04456.  
  
A. Hermann, N. W. Ashcroftand R. Hoffmann, “Lithium hydroxide, LiOH, at elevated densities”, *The Journal of Chemical Physics*, vol. 141, no. 2. AIP Publishing, p. 024505, Jul. 14, 2014. doi: 10.1063/1.4886335.  
  
A. Y. Rogachev, M.-. sheng . Miao, G. Merinoand R. Hoffmann, “Molecular CsF5and CsF2+”, *Angewandte Chemie International Edition*, vol. 54, no. 28. Wiley, pp. 8275–8278, Jun. 03, 2015. doi: 10.1002/anie.201500402.  
  
D. B. Lawson and S. Spaulding, “Non-fused polyaromatic hydrocarbons: interactions of aromatic and antiaromatic rings through a CC bond”, *Structural Chemistry*, vol. 24, no. 1. Springer Science and Business Media LLC, pp. 223–232, Jun. 08, 2012. doi: 10.1007/s11224-012-0068-1.  
  
J. He, X.-M. Lin, H. Chan, L. Vuković, P. Králand H. M. Jaeger, “Diffusion and Filtration Properties of Self-Assembled Gold Nanocrystal Membranes”, *Nano Letters*, vol. 11, no. 6. American Chemical Society (ACS), pp. 2430–2435, May 06, 2011. doi: 10.1021/nl200841a.  
  
X. Fan, “Defect-enriched iron fluoride-oxide nanoporous thin films bifunctional catalyst for water splitting”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, May 04, 2018. doi: 10.1038/s41467-018-04248-y.  
  
X. Fan, “Defect-enriched iron fluoride-oxide nanoporous thin films bifunctional catalyst for water splitting”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, May 04, 2018. doi: 10.1038/s41467-018-04248-y.  
  
J. Qian, Q. An, A. Fortunelli, R. J. Nielsenand W. A. Goddard III, “Reaction Mechanism and Kinetics for Ammonia Synthesis on the Fe(111) Surface”, *Journal of the American Chemical Society*, vol. 140, no. 20. American Chemical Society (ACS), pp. 6288–6297, Apr. 27, 2018. doi: 10.1021/jacs.7b13409.  
  
J. Qian, Q. An, A. Fortunelli, R. J. Nielsenand W. A. Goddard III, “Reaction Mechanism and Kinetics for Ammonia Synthesis on the Fe(111) Surface”, *Journal of the American Chemical Society*, vol. 140, no. 20. American Chemical Society (ACS), pp. 6288–6297, Apr. 27, 2018. doi: 10.1021/jacs.7b13409.  
  
H. Shin, H. Xiaoand W. A. Goddard III, “In Silico Discovery of New Dopants for Fe-Doped Ni Oxyhydroxide (Ni1–*x*Fe*x*OOH) Catalysts for Oxygen Evolution Reaction”, *Journal of the American Chemical Society*, vol. 140, no. 22. American Chemical Society (ACS), pp. 6745–6748, May 11, 2018. doi: 10.1021/jacs.8b02225.  
  
C. Wang, “Monolayer atomic crystal molecular superlattices”, *Nature*, vol. 555, no. 7695. Springer Science and Business Media LLC, pp. 231–236, Mar. 2018. doi: 10.1038/nature25774.  
  
C. Wang, “Monolayer atomic crystal molecular superlattices”, *Nature*, vol. 555, no. 7695. Springer Science and Business Media LLC, pp. 231–236, Mar. 2018. doi: 10.1038/nature25774.  
  
Y. Wang, “Field-effect transistors made from solution-grown two-dimensional tellurene”, *Nature Electronics*, vol. 1, no. 4. Springer Science and Business Media LLC, pp. 228–236, Apr. 17, 2018. doi: 10.1038/s41928-018-0058-4.  
  
Y. Wang, “Field-effect transistors made from solution-grown two-dimensional tellurene”, *Nature Electronics*, vol. 1, no. 4. Springer Science and Business Media LLC, pp. 228–236, Apr. 17, 2018. doi: 10.1038/s41928-018-0058-4.  
  
H. Xiao, H. Shinand W. A. Goddard III, “Synergy between Fe and Ni in the optimal performance of (Ni,Fe)OOH catalysts for the oxygen evolution reaction”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 23. Proceedings of the National Academy of Sciences, pp. 5872–5877, May 21, 2018. doi: 10.1073/pnas.1722034115.  
  
S. Yang, “Oxygen-Vacancy Abundant Ultrafine Co3 O4 /Graphene Composites for High-Rate Supercapacitor Electrodes”, *Advanced Science*, vol. 5, no. 4. Wiley, p. 1700659, Jan. 15, 2018. doi: 10.1002/advs.201700659.  
  
S. Yang, “Oxygen-Vacancy Abundant Ultrafine Co3 O4 /Graphene Composites for High-Rate Supercapacitor Electrodes”, *Advanced Science*, vol. 5, no. 4. Wiley, p. 1700659, Jan. 15, 2018. doi: 10.1002/advs.201700659.  
  
J. M. Standard, R. J. Steidl, M. C. Beecherand R. W. Quandt, “Multireference Configuration Interaction Study of Bromocarbenes”, *The Journal of Physical Chemistry A*, vol. 115, no. 7. American Chemical Society (ACS), pp. 1243–1249, Jan. 31, 2011. doi: 10.1021/jp107688v.  
  
M. O. Altman, “Human Influenza A Virus Hemagglutinin Glycan Evolution Follows a Temporal Pattern to a Glycan Limit”, *mBio*, vol. 10, no. 2. American Society for Microbiology, Apr. 30, 2019. doi: 10.1128/mbio.00204-19.  
  
R. E. Amaro and M. Bansal, “Editorial overview: Theory and simulation: Tools for solving the insolvable”, *Current Opinion in Structural Biology*, vol. 25. Elsevier BV, p. iv–v, Apr. 2014. doi: 10.1016/j.sbi.2014.04.004.  
  
R. E. Amaro, “A Computational Assay that Explores the Hemagglutinin/Neuraminidase Functional Balance Reveals the Neuraminidase Secondary Site as a Novel Anti-Influenza Target”, *ACS Central Science*, vol. 4, no. 11. American Chemical Society (ACS), pp. 1570–1577, Nov. 09, 2018. doi: 10.1021/acscentsci.8b00666.  
  
H. O. Bohl, “The substrate-binding cap of the UDP-diacylglucosamine pyrophosphatase LpxH is highly flexible, enabling facile substrate binding and product release”, *Journal of Biological Chemistry*, vol. 293, no. 21. Elsevier BV, pp. 7969–7981, May 2018. doi: 10.1074/jbc.ra118.002503.  
  
G. Castro-Falcón, “Neolymphostin A Is a Covalent Phosphoinositide 3-Kinase (PI3K)/Mammalian Target of Rapamycin (mTOR) Dual Inhibitor That Employs an Unusual Electrophilic Vinylogous Ester”, *Journal of Medicinal Chemistry*, vol. 61, no. 23. American Chemical Society (ACS), pp. 10463–10472, Oct. 31, 2018. doi: 10.1021/acs.jmedchem.8b00975.  
  
E. Chen, R. V. Swift, N. Alderson, V. A. Feher, G.-S. Fengand R. E. Amaro, “Computation-Guided Discovery of Influenza Endonuclease Inhibitors”, *ACS Medicinal Chemistry Letters*, vol. 5, no. 1. American Chemical Society (ACS), pp. 61–64, Nov. 06, 2013. doi: 10.1021/ml4003474.  
  
K. Cheng, Ö. Demirand R. Amaro, “A Comparative Study of the Structural Dynamics of Four Terminal Uridylyl Transferases”, *Genes*, vol. 8, no. 6. MDPI AG, p. 166, Jun. 20, 2017. doi: 10.3390/genes8060166.  
  
Ö. Demir and R. E. Amaro, “Designing Novel Inhibitors of Trypanosoma brucei”, *Methods in Molecular Biology*. Humana Press, pp. 231–243, 2013. doi: 10.1007/978-1-62703-342-8\_15.  
  
Ö. Demir, P. U. Ieongand R. E. Amaro, “Full-length p53 tetramer bound to DNA and its quaternary dynamics”, *Oncogene*, vol. 36, no. 10. Springer Science and Business Media LLC, pp. 1451–1460, Sep. 19, 2016. doi: 10.1038/onc.2016.321.  
  
Ö. Demir, M. Labaied, C. Merritt, K. Stuartand R. E. Amaro, “Computer-Aided Discovery of*Trypanosoma brucei*RNA-Editing Terminal Uridylyl Transferase 2 Inhibitors”, *Chemical Biology & Drug Design*, vol. 84, no. 2. Wiley, pp. 131–139, Jun. 05, 2014. doi: 10.1111/cbdd.12302.  
  
J. D. Durrant and R. E. Amaro, “LipidWrapper: An Algorithm for Generating Large-Scale Membrane Models of Arbitrary Geometry”, *PLoS Computational Biology*, vol. 10, no. 7. Public Library of Science (PLoS), p. e1003720, Jul. 17, 2014. doi: 10.1371/journal.pcbi.1003720.  
  
J. D. Durrant and R. E. Amaro, “WebChem Viewer: a tool for the easy dissemination of chemical and structural data sets”, *BMC Bioinformatics*, vol. 15, no. 1. Springer Science and Business Media LLC, May 23, 2014. doi: 10.1186/1471-2105-15-159.  
  
J. D. Durrant, L. Votapka, J. Sørensenand R. E. Amaro, “POVME 2.0: An Enhanced Tool for Determining Pocket Shape and Volume Characteristics”, *Journal of Chemical Theory and Computation*, vol. 10, no. 11. American Chemical Society (ACS), pp. 5047–5056, Oct. 15, 2014. doi: 10.1021/ct500381c.  
  
V. A. Feher, J. D. Durrant, A. T. Van Wartand R. E. Amaro, “Computational approaches to mapping allosteric pathways”, *Current Opinion in Structural Biology*, vol. 25. Elsevier BV, pp. 98–103, Apr. 2014. doi: 10.1016/j.sbi.2014.02.004.  
  
V. A. Feher, “Mechanisms for Benzene Dissociation through the Excited State of T4 Lysozyme L99A Mutant”, *Biophysical Journal*, vol. 116, no. 2. Elsevier BV, pp. 205–214, Jan. 2019. doi: 10.1016/j.bpj.2018.09.035.  
  
F. Grogan, M. Holst, L. Lindblomand R. Amaro, “Reliability assessment for large-scale molecular dynamics approximations”, *The Journal of Chemical Physics*, vol. 147, no. 23. AIP Publishing, p. 234106, Dec. 21, 2017. doi: 10.1063/1.5009431.  
  
S. P. Hirakis, R. D. Malmstromand R. E. Amaro, “Molecular Simulations Reveal an Unresolved Conformation of the Type IA Protein Kinase A Regulatory Subunit and Suggest Its Role in the cAMP Regulatory Mechanism”, *Biochemistry*, vol. 56, no. 30. American Chemical Society (ACS), pp. 3885–3888, Jul. 17, 2017. doi: 10.1021/acs.biochem.7b00461.  
  
P. U. Ieong, “Progress towards Automated Kepler Scientific Workflows for Computer-aided Drug Discovery and Molecular Simulations”, *Procedia Computer Science*, vol. 29. Elsevier BV, pp. 1745–1755, 2014. doi: 10.1016/j.procs.2014.05.159.  
  
B. R. Jagger, C. T. Leeand R. E. Amaro, “Quantitative Ranking of Ligand Binding Kinetics with a Multiscale Milestoning Simulation Approach”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 17. American Chemical Society (ACS), pp. 4941–4948, Aug. 02, 2018. doi: 10.1021/acs.jpclett.8b02047.  
  
R. D. Malmstrom, C. T. Lee, A. T. Van Wartand R. E. Amaro, “Application of Molecular-Dynamics Based Markov State Models to Functional Proteins”, *Journal of Chemical Theory and Computation*, vol. 10, no. 7. American Chemical Society (ACS), pp. 2648–2657, Jun. 11, 2014. doi: 10.1021/ct5002363.  
  
M. C. Mulero, “Protein Cofactors Are Essential for High-Affinity DNA Binding by the Nuclear Factor κB RelA Subunit”, *Biochemistry*, vol. 57, no. 20. American Chemical Society (ACS), pp. 2943–2957, Apr. 30, 2018. doi: 10.1021/acs.biochem.8b00158.  
  
T. L. Offutt, P. U. Ieong, Ö. Demirand R. E. Amaro, “Dynamics and Molecular Mechanisms of p53 Transcriptional Activation”, *Biochemistry*, vol. 57, no. 46. American Chemical Society (ACS), pp. 6528–6537, Nov. 02, 2018. doi: 10.1021/acs.biochem.8b01005.  
  
E. P. Barros, “Electrostatic Interactions as Mediators in the Allosteric Activation of Protein Kinase A RIα”, *Biochemistry*, vol. 56, no. 10. American Chemical Society (ACS), pp. 1536–1545, Mar. 06, 2017. doi: 10.1021/acs.biochem.6b01152.  
  
L. Prabhu, “Development of an AlphaLISA high throughput technique to screen for small molecule inhibitors targeting protein arginine methyltransferases”, *Molecular BioSystems*, vol. 13, no. 12. Royal Society of Chemistry (RSC), pp. 2509–2520, 2017. doi: 10.1039/c7mb00391a.  
  
L. Prabhu, “Adapting AlphaLISA high throughput screen to discover a novel small-molecule inhibitor targeting protein arginine methyltransferase 5 in pancreatic and colorectal cancers”, *Oncotarget*, vol. 8, no. 25. Impact Journals, LLC, pp. 39963–39977, May 23, 2017. doi: 10.18632/oncotarget.18102.  
  
S. Purawat, “A Kepler Workflow Tool for Reproducible AMBER GPU Molecular Dynamics”, *Biophysical Journal*, vol. 112, no. 12. Elsevier BV, pp. 2469–2474, Jun. 2017. doi: 10.1016/j.bpj.2017.04.055.  
  
A. Rathore, “The Local Dinucleotide Preference of APOBEC3G Can Be Altered from 5′-CC to 5′-TC by a Single Amino Acid Substitution”, *Journal of Molecular Biology*, vol. 425, no. 22. Elsevier BV, pp. 4442–4454, Nov. 2013. doi: 10.1016/j.jmb.2013.07.040.  
  
D. J. Salamango, “APOBEC3H Subcellular Localization Determinants Define Zipcode for Targeting HIV-1 for Restriction”, *Molecular and Cellular Biology*, vol. 38, no. 23. Informa UK Limited, Dec. 2018. doi: 10.1128/mcb.00356-18.  
  
D. J. Salamango, J. L. McCann, Ö. Demir, W. L. Brown, R. E. Amaroand R. S. Harris, “APOBEC3B Nuclear Localization Requires Two Distinct N-Terminal Domain Surfaces”, *Journal of Molecular Biology*, vol. 430, no. 17. Elsevier BV, pp. 2695–2708, Aug. 2018. doi: 10.1016/j.jmb.2018.04.044.  
  
J. M. Schiffer, “Impacts of Lipase Enzyme on the Surface Properties of Marine Aerosols”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 14. American Chemical Society (ACS), pp. 3839–3849, Jun. 19, 2018. doi: 10.1021/acs.jpclett.8b01363.  
  
J. M. Schiffer, L. E. Mael, K. A. Prather, R. E. Amaroand V. H. Grassian, “Sea Spray Aerosol: Where Marine Biology Meets Atmospheric Chemistry”, *ACS Central Science*, vol. 4, no. 12. American Chemical Society (ACS), pp. 1617–1623, Dec. 14, 2018. doi: 10.1021/acscentsci.8b00674.  
  
C. Seitz, L. Casalino, R. Konecny, G. Huber, R. E. Amaroand J. A. McCammon, “Multiscale Simulations Examining Glycan Shield Effects on Drug Binding to Influenza Neuraminidase”, *Biophysical Journal*, vol. 119, no. 11. Elsevier BV, pp. 2275–2289, Dec. 2020. doi: 10.1016/j.bpj.2020.10.024.  
  
K. Shi, “Conformational Switch Regulates the DNA Cytosine Deaminase Activity of Human APOBEC3B”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Dec. 12, 2017. doi: 10.1038/s41598-017-17694-3.  
  
A. T. Van Wart, J. Durrant, L. Votapkaand R. E. Amaro, “Weighted Implementation of Suboptimal Paths (WISP): An Optimized Algorithm and Tool for Dynamical Network Analysis”, *Journal of Chemical Theory and Computation*, vol. 10, no. 2. American Chemical Society (ACS), pp. 511–517, Jan. 31, 2014. doi: 10.1021/ct4008603.  
  
L. Votapka and R. E. Amaro, “Multistructural hot spot characterization with FTProd”, *Bioinformatics*, vol. 29, no. 3. Oxford University Press (OUP), pp. 393–394, Nov. 29, 2012. doi: 10.1093/bioinformatics/bts689.  
  
L. W. Votapka, B. R. Jagger, A. L. Heynemanand R. E. Amaro, “SEEKR: Simulation Enabled Estimation of Kinetic Rates, A Computational Tool to Estimate Molecular Kinetics and Its Application to Trypsin–Benzamidine Binding”, *The Journal of Physical Chemistry B*, vol. 121, no. 15. American Chemical Society (ACS), pp. 3597–3606, Mar. 03, 2017. doi: 10.1021/acs.jpcb.6b09388.  
  
J. R. Wagner, “Determinants of Oligonucleotide Selectivity of APOBEC3B”, *Journal of Chemical Information and Modeling*, vol. 59, no. 5. American Chemical Society (ACS), pp. 2264–2273, Aug. 21, 2018. doi: 10.1021/acs.jcim.8b00427.  
  
J. R. Wagner, “POVME 3.0: Software for Mapping Binding Pocket Flexibility”, *Journal of Chemical Theory and Computation*, vol. 13, no. 9. American Chemical Society (ACS), pp. 4584–4592, Aug. 30, 2017. doi: 10.1021/acs.jctc.7b00500.  
  
C. D. Wassman, “Computational identification of a transiently open L1/S3 pocket for reactivation of mutant p53”, *Nature Communications*, vol. 4, no. 1. Springer Science and Business Media LLC, Jan. 29, 2013. doi: 10.1038/ncomms2361.  
  
L. Andrews, X. Wang, Y. Gong, B. Vlaisavljevichand L. Gagliardi, “Infrared Spectra and Electronic Structure Calculations for the NUN(NN)1–5 and NU(NN)1–6 Complexes in Solid Argon”, *Inorganic Chemistry*, vol. 52, no. 17. American Chemical Society (ACS), pp. 9989–9993, Aug. 15, 2013. doi: 10.1021/ic401857u.  
  
R. D. Bach and H. B. Schlegel, “Bond Dissociation Energy of Peroxides Revisited”, *The Journal of Physical Chemistry A*, vol. 124, no. 23. American Chemical Society (ACS), pp. 4742–4751, May 12, 2020. doi: 10.1021/acs.jpca.0c02859.  
  
D. Q. Dao, “Insight into Antioxidant and Photoprotective Properties of Natural Compounds from Marine Fungus”, *Journal of Chemical Information and Modeling*, vol. 60, no. 3. American Chemical Society (ACS), pp. 1329–1351, Jan. 30, 2020. doi: 10.1021/acs.jcim.9b00964.  
  
D. Dumett Torres, S. Pamidighantamand P. K. Jain, “Crystal Symmetry, Strain, and Facet-Dependent Nature of Topological Surface States in Mercury Selenide”, *The Journal of Physical Chemistry C*, vol. 124, no. 19. American Chemical Society (ACS), pp. 10344–10352, Apr. 21, 2020. doi: 10.1021/acs.jpcc.0c01663.  
  
S. A. Emambocus, L. Rhymanand P. Ramasami, “Theoretical Study of the Microhydration the Chemical Warfare Agent Sulfur Mustard”, *ACS Omega*, vol. 5, no. 4. American Chemical Society (ACS), pp. 1822–1831, Jan. 22, 2020. doi: 10.1021/acsomega.9b03061.  
  
G. Ernouf, E. Chirkin, L. Rhyman, P. Ramasamiand J.-C. Cintrat, “Photochemical Strain-Release Driven Cyclobutylation of C(sp3)-Centered Radicals”, *[]*. American Chemical Society (ACS), Jun. 26, 2019. doi: 10.26434/chemrxiv.8323406.v1.  
  
A. J. Fairhall, M. M. Orlandoand J. A. Bartz, “355 nm Photodissociation of N2O3 Revealed by Velocity-Mapped Ion Imaging”, *The Journal of Physical Chemistry A*, vol. 124, no. 3. American Chemical Society (ACS), pp. 472–478, Dec. 28, 2019. doi: 10.1021/acs.jpca.9b08688.  
  
D. Hallooman, M. Ríos-Gutiérrez, L. Rhyman, I. A. Alswaidan, L. R. Domingoand P. Ramasami, “A molecular electron density theory study of the [3 + 2] cycloaddition reaction of 1,4-diphosphorinium-3-olates with methyl acrylate and methyl methacrylate”, *Theoretical Chemistry Accounts*, vol. 139, no. 7. Springer Science and Business Media LLC, Jun. 27, 2020. doi: 10.1007/s00214-020-02637-5.  
  
S. I. Hassan, “Thioxanthone-based organic probe with aggregation enhanced emission and exceptional mineral acids sensing abilities”, *Journal of Molecular Structure*, vol. 1224. Elsevier BV, p. 129004, Jan. 2021. doi: 10.1016/j.molstruc.2020.129004.  
  
Y. A. Imrit, “A theoretical study of the hydrolysis mechanism of A-234; the suspected novichok agent in the Skripal attack”, *RSC Advances*, vol. 10, no. 47. Royal Society of Chemistry (RSC), pp. 27884–27893, 2020. doi: 10.1039/d0ra05086e.  
  
S. Nakandala, “Anatomy of the SEAGrid Science Gateway”, *Proceedings of the XSEDE16 Conference on Diversity, Big Data, and Science at Scale*. ACM, Jul. 17, 2016. doi: 10.1145/2949550.2949591.  
  
T. C. Ngo, “SERS Spectra of the Pesticide Chlorpyrifos Adsorbed on Silver Nanosurface: The Ag20 Cluster Model”, *The Journal of Physical Chemistry C*, vol. 124, no. 39. American Chemical Society (ACS), pp. 21702–21716, Sep. 03, 2020. doi: 10.1021/acs.jpcc.0c06078.  
  
L. Rhyman, M. Ríos-Gutiérrez, L. R. Domingoand P. Ramasami, “Unveiling the high reactivity of benzyne in the formal [3+2] cycloaddition reactions towards thioamides through the Molecular Electron Density Theory”, *Tetrahedron*, vol. 76, no. 39. Elsevier BV, p. 131458, Sep. 2020. doi: 10.1016/j.tet.2020.131458.  
  
N. Savoo, J. Z. A. Laloo, L. Rhyman, P. Ramasami, F. M. Bickelhauptand J. Poater, “Activation Strain Analyses of Counterion and Solvent Effects on the Ion‐Pair S N 2 Reaction of and CH 3 Cl”, *Journal of Computational Chemistry*, vol. 41, no. 4. Wiley, pp. 317–327, Nov. 11, 2019. doi: 10.1002/jcc.26104.  
  
E. Talla, “Density functional theory studies of Hypaphorine from Erythrina mildbraedii and Erythrina addisoniae: structural and biological properties”, *SN Applied Sciences*, vol. 2, no. 3. Springer Science and Business Media LLC, Feb. 17, 2020. doi: 10.1007/s42452-020-2228-z.  
  
H. L. Abbott, “CO Adsorption on Monometallic and Bimetallic Au−Pd Nanoparticles Supported on Oxide Thin Films”, *The Journal of Physical Chemistry C*, vol. 114, no. 40. American Chemical Society (ACS), pp. 17099–17104, Jul. 19, 2010. doi: 10.1021/jp1038333.  
  
J. Jelic and R. J. Meyer, “A density functional theory study of water gas shift over pseudomorphic monolayer alloy catalysts: Comparison with NO oxidation”, *Journal of Catalysis*, vol. 272, no. 1. Elsevier BV, pp. 151–157, May 25, 2010. doi: 10.1016/j.jcat.2010.03.002.  
  
Y. Lei, J. Jelic, L. C. Nitsche, R. Meyerand J. Miller, “Effect of Particle Size and Adsorbates on the L3, L2 and L1 X-ray Absorption Near Edge Structure of Supported Pt Nanoparticles”, *Topics in Catalysis*, vol. 54, no. 5–7. Springer Science and Business Media LLC, pp. 334–348, Feb. 15, 2011. doi: 10.1007/s11244-011-9662-5.  
  
R. Todorovic and R. J. Meyer, “A comparative density functional theory study of the direct synthesis of H2O2 on Pd, Pt and Au surfaces”, *Catalysis Today*, vol. 160, no. 1. Elsevier BV, pp. 242–248, Feb. 02, 2011. doi: 10.1016/j.cattod.2010.07.011.  
  
H. Wei, C. Gomezand R. J. Meyer, “A Comparative Density Functional Theory Study of Water Gas Shift Over PdZn(111) and NiZn(111)”, *Topics in Catalysis*, vol. 55, no. 5–6. Springer Science and Business Media LLC, pp. 313–321, Apr. 21, 2012. doi: 10.1007/s11244-012-9799-x.  
  
T. Wu, “General Method for Determination of the Surface Composition in Bimetallic Nanoparticle Catalysts from the L Edge X-ray Absorption Near-Edge Spectra”, *ACS Catalysis*, vol. 2, no. 11. American Chemical Society (ACS), pp. 2433–2443, Oct. 19, 2012. doi: 10.1021/cs3004566.  
  
C. K. Addington, J. M. Manselland K. E. Gubbins, “Computer simulation of conductive linear sulfur chains confined in carbon nanotubes”, *Molecular Simulation*, vol. 43, no. 7. Informa UK Limited, pp. 519–525, Jan. 23, 2017. doi: 10.1080/08927022.2016.1269259.  
  
R. An, L. Huang, Y. Long, B. Kalanyan, X. Luand K. E. Gubbins, “Liquid–Solid Nanofriction and Interfacial Wetting”, *Langmuir*, vol. 32, no. 3. American Chemical Society (ACS), pp. 743–750, Jan. 13, 2016. doi: 10.1021/acs.langmuir.5b04115.  
  
B. Coasne, Y. Longand K. E. Gubbins, “Pressure effects in confined nanophases”, *Molecular Simulation*, vol. 40, no. 7–9. Informa UK Limited, pp. 721–730, Feb. 05, 2014. doi: 10.1080/08927022.2013.829227.  
  
K. E. Gubbins, “Perturbation theories of the thermodynamics of polar and associating liquids: A historical perspective”, *Fluid Phase Equilibria*, vol. 416. Elsevier BV, pp. 3–17, May 2016. doi: 10.1016/j.fluid.2015.12.043.  
  
K. E. Gubbins, Y. Longand M. Śliwinska-Bartkowiak, “Thermodynamics of confined nano-phases”, *The Journal of Chemical Thermodynamics*, vol. 74. Elsevier BV, pp. 169–183, Jul. 2014. doi: 10.1016/j.jct.2014.01.024.  
  
L. Huang and K. E. Gubbins, “Ammonia Dissociation on Graphene Oxide: An Ab Initio Density Functional Theory Calculation”, *Zeitschrift für Physikalische Chemie*, vol. 229, no. 7–8. Walter de Gruyter GmbH, pp. 1211–1223, Mar. 27, 2015. doi: 10.1515/zpch-2014-0621.  
  
L. Huang, K. E. Gubbins, L. Liand X. Lu, “Water on Titanium Dioxide Surface: A Revisiting by Reactive Molecular Dynamics Simulations”, *Langmuir*, vol. 30, no. 49. American Chemical Society (ACS), pp. 14832–14840, Dec. 03, 2014. doi: 10.1021/la5037426.  
  
Y. Long, “High pressure effect in nanoporous carbon materials: Effects of pore geometry”, *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, vol. 437. Elsevier BV, pp. 33–41, Nov. 2013. doi: 10.1016/j.colsurfa.2012.11.024.  
  
M. Sliwinska-Bartkowiak, M. Jazdzewska, M. Trafas, M. Kaczmarek-Klinowskaand K. E. Gubbins, “Melting of Eutectic Mixtures in Silica and Carbon Nanopores”, *Journal of Chemical & Engineering Data*, vol. 60, no. 11. American Chemical Society (ACS), pp. 3093–3100, Sep. 15, 2015. doi: 10.1021/acs.jced.5b00131.  
  
R. Alfieri, S. Arezzini, A. Ciampa, R. De Pietriand E. Mazzoni, “HPC on the Grid: The Theophys Experience”, *Journal of Grid Computing*, vol. 11, no. 2. Springer Science and Business Media LLC, pp. 265–280, Aug. 05, 2012. doi: 10.1007/s10723-012-9223-6.  
  
S. Katariya, L. Rhyman, I. A. Alswaidan, P. Ramasamiand N. Sekar, “Triphenylamine-Based Fluorescent Styryl Dyes: DFT, TD-DFT and Non-Linear Optical Property Study”, *Journal of Fluorescence*, vol. 27, no. 3. Springer Science and Business Media LLC, pp. 993–1007, Jan. 31, 2017. doi: 10.1007/s10895-017-2034-1.  
  
M. M. Jadhav, L. Rhyman, P. Ramasamiand N. Sekar, “Unfolding ESIPT in Bis-2,5-(2-benzoxazolyl) Hydroquinone and 2,5-Bis(benzo[d]oxazol-2-yl)-4-methoxyphenol: a Comprehensive Computational Approach”, *Journal of Fluorescence*, vol. 26, no. 4. Springer Science and Business Media LLC, pp. 1295–1307, May 04, 2016. doi: 10.1007/s10895-016-1816-1.  
  
R. D. Bach, “The Rate-Limiting Step in P450 Hydroxylation of Hydrocarbons A Direct Comparison of the “Somersault” versus the “Consensus” Mechanism Involving Compound I”, *The Journal of Physical Chemistry A*, vol. 114, no. 34. American Chemical Society (ACS), pp. 9319–9332, Aug. 06, 2010. doi: 10.1021/jp1045518.  
  
R. D. Bach, “Role of the Somersault Rearrangement in the Oxidation Step for Flavin Monooxygenases (FMO). A Comparison between FMO and Conventional Xenobiotic Oxidation with Hydroperoxides”, *The Journal of Physical Chemistry A*, vol. 115, no. 40. American Chemical Society (ACS), pp. 11087–11100, Sep. 20, 2011. doi: 10.1021/jp208087u.  
  
R. D. Bach, “The Role of Acid Catalysis in the Baeyer–Villiger Reaction. A Theoretical Study”, *The Journal of Organic Chemistry*, vol. 77, no. 16. American Chemical Society (ACS), pp. 6801–6815, Aug. 09, 2012. doi: 10.1021/jo300727w.  
  
R. D. Bach, “The DMDO Hydroxylation of Hydrocarbons via the Oxygen Rebound Mechanism”, *The Journal of Physical Chemistry A*, vol. 120, no. 5. American Chemical Society (ACS), pp. 840–850, Feb. 02, 2016. doi: 10.1021/acs.jpca.5b12086.  
  
R. D. Bach and O. Dmitrenko, “Transient Inverted Metastable Iron Hydroperoxides in Fenton Chemistry. A Nonenzymatic Model for Cytochrome P450 Hydroxylation”, *The Journal of Organic Chemistry*, vol. 75, no. 11. American Chemical Society (ACS), pp. 3705–3714, Apr. 30, 2010. doi: 10.1021/jo1004668.  
  
R. D. Bach and A. Mattevi, “Mechanistic Aspects Regarding the Elimination of H2O2 from C(4a)-Hydroperoxyflavin. The Role of a Proton Shuttle Required for H2O2 Elimination”, *The Journal of Organic Chemistry*, vol. 78, no. 17. American Chemical Society (ACS), pp. 8585–8593, Aug. 12, 2013. doi: 10.1021/jo401274u.  
  
R. Barbera, G. La Rocca, R. Rotondo, A. Falzone, P. Maggiand N. Venuti, “Conjugating science gateways and grid portals into e-collaboration environments”, *Proceedings of the 2010 TeraGrid Conference*. ACM, Aug. 02, 2010. doi: 10.1145/1838574.1838575.  
  
J. Basney, R. Dooley, J. Gaynor, S. Marruand M. Pierce, “Distributed web security for science gateways”, *Proceedings of the 2011 ACM workshop on Gateway computing environments*. ACM, Nov. 18, 2011. doi: 10.1145/2110486.2110489.  
  
M. Bencivenni, “Accessing Grid and Cloud Services Through a Scientific Web Portal”, *Journal of Grid Computing*, vol. 13, no. 2. Springer Science and Business Media LLC, pp. 159–175, Sep. 23, 2014. doi: 10.1007/s10723-014-9310-y.  
  
H. Bhakhoa, L. Rhyman, E. P. F. Lee, P. Ramasamiand J. M. Dyke, “Can Cyclen Bind Alkali Metal Azides? A DFT Study as a Precursor to Synthesis”, *Chemistry - A European Journal*, vol. 22, no. 13. Wiley, pp. 4469–4482, Feb. 16, 2016. doi: 10.1002/chem.201504607.  
  
H. Bhakhoa, L. Rhymanand P. Ramasami, “Theoretical study of the molecular aspect of the suspected novichok agent A234 of the Skripal poisoning”, *Royal Society Open Science*, vol. 6, no. 2. The Royal Society, p. 181831, Feb. 2019. doi: 10.1098/rsos.181831.  
  
M. G. Bhowon, S. Jhaumeer Laulloo, E. C. Hosten, M. M. Khodabaccus, L. Rhymanand P. Ramasami, “Synthesis, spectroscopic, biological and DFT studies of new t-butyl substituted salicylaldimines having disulfide moiety”, *Journal of Molecular Structure*, vol. 1175. Elsevier BV, pp. 13–23, Jan. 2019. doi: 10.1016/j.molstruc.2018.07.086.  
  
J. J. Biswakarma, V. Ciocoiand R. Q. Topper, “Energetics, Thermodynamics, and Hydrogen Bonding Diversity in Ammonium Halide Clusters”, *The Journal of Physical Chemistry A*, vol. 120, no. 40. American Chemical Society (ACS), pp. 7924–7934, Oct. 04, 2016. doi: 10.1021/acs.jpca.6b06788.  
  
I. N. Booysen, V. Ngwenya, A. Mambanda, M. Simelane, L. Rhymanand P. Ramasami, “Synthesis, characterization, biological and DFT studies of new 4-substituted phthalonitriles”, *Journal of Molecular Structure*, vol. 1191. Elsevier BV, pp. 244–252, Sep. 2019. doi: 10.1016/j.molstruc.2019.04.104.  
  
D. H. Brouwer, S. Cadars, J. Eckert, Z. Liu, O. Terasakiand B. F. Chmelka, “A General Protocol for Determining the Structures of Molecularly Ordered but Noncrystalline Silicate Frameworks”, *Journal of the American Chemical Society*, vol. 135, no. 15. American Chemical Society (ACS), pp. 5641–5655, Apr. 05, 2013. doi: 10.1021/ja311649m.  
  
S. P. Coleman, S. Pamidighantam, M. Van Moer, Y. Wang, L. Koesterkeand D. E. Spearot, “Performance Improvement and Workflow Development of Virtual Diffraction Calculations”, *Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment*. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616552.  
  
A. Direm, M. Tursun, C. Parlakand N. Benali-Cherif, “Trans-dichlorotetrakis(1H-pyrazole-κN2)copper(II): Synthesis, crystal structure, hydrogen bonding graph-sets, vibrational and DFT studies”, *Journal of Molecular Structure*, vol. 1093. Elsevier BV, pp. 208–218, Aug. 2015. doi: 10.1016/j.molstruc.2015.03.068.  
  
R. Dooley and M. R. Hanlon, “Recipes 2.0: building for today and tomorrow”, *Concurrency and Computation: Practice and Experience*, vol. 27, no. 2. Wiley, pp. 258–270, Apr. 29, 2014. doi: 10.1002/cpe.3285.  
  
Q. Duan, Z. Jin, Q. Liuand X. Chi, “An Integrated and Grid Based Solution of Chemical Applications”, *Communications in Computer and Information Science*. Springer Berlin Heidelberg, pp. 40–47, 2010. doi: 10.1007/978-3-642-16339-5\_6.  
  
J. C. Ezeorah, “Synthesis, characterization and computational studies of 3-{(E)-[(2-hydroxyphenyl)imino]methyl}benzene-1,2-diol and molecular structure of its zwitterionic form”, *Journal of Molecular Structure*, vol. 1152. Elsevier BV, pp. 21–28, Jan. 2018. doi: 10.1016/j.molstruc.2017.09.083.  
  
Y. Gawale, L. Rhyman, M. I. Elzagheid, P. Ramasamiand N. Sekar, “Excited State and Non-linear Optical Properties of NIR Absorbing β-Thiophene-Fused BF2-Azadipyrromethene Dyes—Computational Investigation”, *Journal of Fluorescence*, vol. 28, no. 1. Springer Science and Business Media LLC, pp. 243–250, Nov. 21, 2017. doi: 10.1007/s10895-017-2186-z.  
  
K. Ghebreyessus and S. M. Cooper Jr., “Photoswitchable Arylazopyrazole-Based Ruthenium(II) Arene Complexes”, *Organometallics*, vol. 36, no. 17. American Chemical Society (ACS), pp. 3360–3370, Aug. 29, 2017. doi: 10.1021/acs.organomet.7b00493.  
  
K. Gör, “Novel Cyanide-Bridged Heterometallic Two-Dimensional Complex of 3-Methylpyridazine: Synthesis, Crystallographical, Vibrational, Thermal and DFT Studies”, *Journal of Inorganic and Organometallic Polymers and Materials*, vol. 25, no. 5. Springer Science and Business Media LLC, pp. 1205–1217, May 14, 2015. doi: 10.1007/s10904-015-0229-y.  
  
R. Guha, K. Gilbert, G. Fox, M. Pierce, D. Wildand H. Yuan, “Advances in Cheminformatics Methodologies and Infrastructure to Support the Data Mining of Large, Heterogeneous Chemical Datasets”, *Current Computer Aided-Drug Design*, vol. 6, no. 1. Bentham Science Publishers Ltd., pp. 50–67, Mar. 01, 2010. doi: 10.2174/157340910790980115.  
  
D. Hallooman, “Copper(I)-catalysed regioselective synthesis of pyrazolo[5,1-c]-1,2,4-triazoles: A DFT mechanistic study”, *Tetrahedron*, vol. 73, no. 31. Elsevier BV, pp. 4653–4662, Aug. 2017. doi: 10.1016/j.tet.2017.06.040.  
  
D. Hallooman, M. Ríos-Gutiérrez, L. Rhyman, I. A. Alswaidan, L. R. Domingoand P. Ramasami, “DFT exploration of [3 + 2] cycloaddition reaction of 1*H*-phosphorinium-3-olate and 1-methylphosphorinium-3-olate with methyl methacrylate”, *RSC Advances*, vol. 8, no. 48. Royal Society of Chemistry (RSC), pp. 27406–27416, 2018. doi: 10.1039/c8ra04703k.  
  
D. Hallooman, “[3+2] Cycloaddition reaction of 1H-phosphorinium-3-olate and 1-methylphosphorinium-3-olate with methyl acrylate: A DFT study”, *Computational and Theoretical Chemistry*, vol. 1087. Elsevier BV, pp. 36–47, Jul. 2016. doi: 10.1016/j.comptc.2016.04.015.  
  
D. E. Hudak, “OSC OnDemand”, *Proceedings of the Conference on Extreme Science and Engineering Discovery Environment: Gateway to Discovery*. ACM, Jul. 22, 2013. doi: 10.1145/2484762.2484780.  
  
H. T. Pham, N. M. Tam, Y. A. Jeilaniand M. T. Nguyen, “Structural evolution and bonding of phosphorus-doped silicon clusters SinPm−/0/+ with n = 1–10, m = 1, 2”, *Computational and Theoretical Chemistry*, vol. 1107. Elsevier BV, pp. 115–126, May 2017. doi: 10.1016/j.comptc.2017.01.032.  
  
A. G. Jadhav, L. Rhyman, I. A. Alswaidan, P. Ramasamiand N. Sekar, “Spectroscopic and DFT approach for structure property relationship of red emitting rhodamine analogues: A study of linear and nonlinear optical properties”, *Computational and Theoretical Chemistry*, vol. 1131. Elsevier BV, pp. 1–12, May 2018. doi: 10.1016/j.comptc.2018.03.029.  
  
B. Jadoo, I. N. Booysen, M. P. Akerman, L. Rhymanand P. Ramasami, “Novel coumarin rhenium(I) and -(V) complexes: Formation, DFT and DNA binding studies”, *Polyhedron*, vol. 144. Elsevier BV, pp. 107–118, Apr. 2018. doi: 10.1016/j.poly.2018.01.017.  
  
W. H. James III, E. E. Baquero, S. H. Choi, S. H. Gellmanand T. S. Zwier, “Laser Spectroscopy of Conformationally Constrained α/β-Peptides: Ac-ACPC-Phe-NHMe and Ac-Phe-ACPC-NHMe”, *The Journal of Physical Chemistry A*, vol. 114, no. 3. American Chemical Society (ACS), pp. 1581–1591, Dec. 29, 2009. doi: 10.1021/jp9090975.  
  
Y. A. Jeilani, C. Fearceand M. T. Nguyen, “Acetylene as an essential building block for prebiotic formation of pyrimidine bases on Titan”, *Physical Chemistry Chemical Physics*, vol. 17, no. 37. Royal Society of Chemistry (RSC), pp. 24294–24303, 2015. doi: 10.1039/c5cp03247d.  
  
Y. A. Jeilani, B. Ross, N. Aweis, C. Fearce, H. Minh Hungand M. T. Nguyen, “Reaction Routes for Experimentally Observed Intermediates in the Prebiotic Formation of Nucleobases under High-Temperature Conditions”, *The Journal of Physical Chemistry A*, vol. 122, no. 11. American Chemical Society (ACS), pp. 2992–3003, Feb. 23, 2018. doi: 10.1021/acs.jpca.7b11466.  
  
J. C. Ezeorah, “Synthesis, characterization and computational studies of 3-{(E)-[(2-hydroxyphenyl)imino]methyl}benzene-1,2-diol and molecular structure of its zwitterionic form”, *Journal of Molecular Structure*, vol. 1152. Elsevier BV, pp. 21–28, Jan. 2018. doi: 10.1016/j.molstruc.2017.09.083.  
  
M. A. Kabeshov, “Development of a web-based platform for studying lithiation reactions in silico”, *Chemical Communications*, vol. 51, no. 33. Royal Society of Chemistry (RSC), pp. 7172–7175, 2015. doi: 10.1039/c5cc00782h.  
  
S. B. Katariya, D. Patil, L. Rhyman, I. A. Alswaidan, P. Ramasamiand N. Sekar, “Triphenylamine-based fluorescent NLO phores with ICT characteristics: Solvatochromic and theoretical study”, *Journal of Molecular Structure*, vol. 1150. Elsevier BV, pp. 493–506, Dec. 2017. doi: 10.1016/j.molstruc.2017.08.084.  
  
D. Kodi Ramanah, “Ab initio studies on cyanoacetylenes of astrochemical interest: [Y(CC)CN, Y  C2H5, C3H7, C4H9, F, Cl, Br and CN]”, *New Astronomy*, vol. 42. Elsevier BV, pp. 42–48, Jan. 2016. doi: 10.1016/j.newast.2015.07.001.  
  
D. Kodi Ramanah, “Ab initio studies on cyanoacetylenes of astrochemical interest: [Y(CC)CN, Y  C2H5, C3H7, C4H9, F, Cl, Br and CN]”, *New Astronomy*, vol. 42. Elsevier BV, pp. 42–48, Jan. 2016. doi: 10.1016/j.newast.2015.07.001.  
  
J. Krüger, “The MoSGrid Science Gateway – A Complete Solution for Molecular Simulations”, *Journal of Chemical Theory and Computation*, vol. 10, no. 6. American Chemical Society (ACS), pp. 2232–2245, May 19, 2014. doi: 10.1021/ct500159h.  
  
C. S. C. Kumar, “3-Iodobenzaldehyde: XRD, FT-IR, Raman and DFT studies”, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 145. Elsevier BV, pp. 90–97, Jun. 2015. doi: 10.1016/j.saa.2015.02.079.  
  
J. Z. A. Laloo, L. Rhyman, O. Larrañaga, P. Ramasami, F. M. Bickelhauptand A. de Cózar, “Ion-Pair SN 2 Reaction of OH− and CH3 Cl: Activation Strain Analyses of Counterion and Solvent Effects”, *Chemistry - An Asian Journal*, vol. 13, no. 9. Wiley, pp. 1138–1147, Apr. 06, 2018. doi: 10.1002/asia.201800082.  
  
J. Z. A. Laloo, L. Rhyman, P. Ramasami, F. M. Bickelhauptand A. de Cózar, “Ion-Pair SN 2 Substitution: Activation Strain Analyses of Counter-Ion and Solvent Effects”, *Chemistry - A European Journal*, vol. 22, no. 13. Wiley, pp. 4431–4439, Feb. 16, 2016. doi: 10.1002/chem.201504456.  
  
J. Z. A. Laloo, N. Savoo, N. Laloo, L. Rhymanand P. Ramasami, “ExcelAutomat 1.3: Fragment analysis based on the distortion/interaction-activation strain model”, *Journal of Computational Chemistry*, vol. 40, no. 3. Wiley, pp. 619–624, Aug. 24, 2018. doi: 10.1002/jcc.25546.  
  
S. Mandal, “Synthesis, characterization, DFT and antimicrobial studies of transition metal ion complexes of a new schiff base ligand, 5-methylpyrazole-3yl-N-(2́-hydroxyphenylamine)methyleneimine, (MPzOAP)”, *Journal of Molecular Structure*, vol. 1178. Elsevier BV, pp. 100–111, Feb. 2019. doi: 10.1016/j.molstruc.2018.09.095.  
  
S. N. Margar, L. Rhyman, P. Ramasamiand N. Sekar, “Fluorescent difluoroboron-curcumin analogs: An investigation of the electronic structures and photophysical properties”, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 152. Elsevier BV, pp. 241–251, Jan. 2016. doi: 10.1016/j.saa.2015.07.064.  
  
L. Marini, R. Kooper, J. Myersand P. Bajcsy, “Dynamic publishing in digital catchments”, *Proceedings of the Institution of Civil Engineers - Water Management*, vol. 163, no. 1. Thomas Telford Ltd., pp. 27–38, Jan. 2010. doi: 10.1680/wama.2010.163.1.27.  
  
S. Marru, “Apache airavata”, *Proceedings of the 2011 ACM workshop on Gateway computing environments*. ACM, Nov. 18, 2011. doi: 10.1145/2110486.2110490.  
  
M. A. Miller, W. Pfeifferand T. Schwartz, “The CIPRES science gateway”, *Proceedings of the 2011 TeraGrid Conference: Extreme Digital Discovery*. ACM, Jul. 18, 2011. doi: 10.1145/2016741.2016785.  
  
M. A. Miller, W. Pfeifferand T. Schwartz, “The CIPRES science gateway”, *Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment: Bridging from the eXtreme to the campus and beyond*. ACM, Jul. 16, 2012. doi: 10.1145/2335755.2335836.  
  
M. A. Miller, T. Schwartzand W. Pfeiffer, “Embedding CIPRES science gateway capabilities in phylogenetics software environments”, *Proceedings of the Conference on Extreme Science and Engineering Discovery Environment: Gateway to Discovery*. ACM, Jul. 22, 2013. doi: 10.1145/2484762.2484806.  
  
R. L. Moore, “Gateways to Discovery”, *Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment*. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616540.  
  
M. Mphahlele, H. Paumo, L. Rhymanand P. Ramasami, “Synthesis and Photophysical Properties of Polycarbo-Substituted Quinazolines Derived from the 2-Aryl-4-chloro-6-iodoquinazolines”, *Molecules*, vol. 20, no. 8. MDPI AG, pp. 14656–14683, Aug. 13, 2015. doi: 10.3390/molecules200814656.  
  
T. C. Ngo, T. H. Nguyenand D. Q. Dao, “Radical Scavenging Activity of Natural-Based Cassaine Diterpenoid Amides and Amines”, *Journal of Chemical Information and Modeling*, vol. 59, no. 2. American Chemical Society (ACS), pp. 766–776, Jan. 25, 2019. doi: 10.1021/acs.jcim.8b00847.  
  
H. T. Nguyen, T. D. Hangand M. T. Nguyen, “Theoretical Study of Silicon Monoxide Reactions with Ammonia and Methane”, *The Journal of Physical Chemistry A*, vol. 121, no. 5. American Chemical Society (ACS), pp. 1032–1040, Jan. 27, 2017. doi: 10.1021/acs.jpca.6b11665.  
  
L. N. Obasi, “Structural, computational and in silico studies of Schiff bases derived from 2,3-dihydroxybenzaldehyde and molecular structure of their zwitterionic forms”, *Journal of Molecular Structure*, vol. 1188. Elsevier BV, pp. 69–75, Jul. 2019. doi: 10.1016/j.molstruc.2019.03.081.  
  
L. N. Obasi, G. U. Kaior, L. Rhyman, I. A. Alswaidan, H.-K. Funand P. Ramasami, “Synthesis, characterization, antimicrobial screening and computational studies of 4-[3-(4-methoxy-phenyl)-allylideneamino]-1,5-dimethyl-2-phenyl-1,2-dihydro-pyrazol-3-one”, *Journal of Molecular Structure*, vol. 1120. Elsevier BV, pp. 180–186, Sep. 2016. doi: 10.1016/j.molstruc.2016.05.037.  
  
N. L. Obasi, “Synthesis, characterization, antimicrobial screening and in silico studies of Schiff bases derived from trans-para-methoxycinnamaldehyde”, *Journal of Molecular Structure*, vol. 1149. Elsevier BV, pp. 8–16, Dec. 2017. doi: 10.1016/j.molstruc.2017.07.097.  
  
U. S. Oruma, “Synthesis, Characterization, Antimicrobial Screening, and Computational Studies of a Tripodal Schiff Base Containing Pyrimidine Unit”, *Journal of Heterocyclic Chemistry*, vol. 55, no. 5. Wiley, pp. 1119–1129, Mar. 14, 2018. doi: 10.1002/jhet.3142.  
  
S. Pamidighantam, “Community Science Exemplars in SEAGrid Science Gateway: Apache Airavata Based Implementation of Advanced Infrastructure”, *Procedia Computer Science*, vol. 80. Elsevier BV, pp. 1927–1939, 2016. doi: 10.1016/j.procs.2016.05.535.  
  
S. Paramasivam, “Solid-State NMR and Density Functional Theory Studies of Ionization States of Thiamin”, *The Journal of Physical Chemistry B*, vol. 115, no. 4. American Chemical Society (ACS), pp. 730–736, Dec. 22, 2010. doi: 10.1021/jp109765b.  
  
G. B. Peleyeju, “Crystal structure and antibacterial activity of scandenone (warangalone) from Erythrina plants”, *Journal of Molecular Structure*, vol. 1191. Elsevier BV, pp. 43–51, Sep. 2019. doi: 10.1016/j.molstruc.2019.04.070.  
  
M. Pierce, S. Marru, R. Singh, A. Kulshresthaand K. Muthuraman, “Open grid computing environments”, *Proceedings of the 2010 TeraGrid Conference*. ACM, Aug. 02, 2010. doi: 10.1145/1838574.1838590.  
  
P. Ramasami and N. B. Jaufeerally, “First Principle Attempt towards the Thermodynamic Stability of Telluroformaldehyde and its Heavier Analogs: H(2-n)X(n)A=Te (X=H, F, Cl and Br; A=C, Si and Ge; n=0-2)”, *Procedia Computer Science*, vol. 18. Elsevier BV, pp. 806–815, 2013. doi: 10.1016/j.procs.2013.05.245.  
  
C. Redwood, “Four-Component Fluorescence of *trans*-1,2-Di(1-methyl-2-naphthyl)ethene at 77 K in Glassy Media. Conformational Subtleties Revealed”, *The Journal of Physical Chemistry A*, vol. 118, no. 45. American Chemical Society (ACS), pp. 10575–10586, Aug. 27, 2014. doi: 10.1021/jp5056478.  
  
C. Redwood, “Photoisomerization of*cis*-1,2-di(1-Methyl-2-naphthyl)ethene at 77 K in Glassy Media”, *Photochemistry and Photobiology*, vol. 91, no. 3. Wiley, pp. 607–615, Nov. 21, 2014. doi: 10.1111/php.12367.  
  
L. Rhyman, I. A. Alswaidan, H.-K. Fun, J. A. Jouleand P. Ramasami, “Theoretical insight into the effect of fluorine substituents on the rearrangement step in Fischer indolisations”, *Tetrahedron*, vol. 71, no. 39. Elsevier BV, pp. 7199–7203, Sep. 2015. doi: 10.1016/j.tet.2015.02.012.  
  
L. Rhyman, “Theoretical investigation of the derivatives of favipiravir (T-705) as potential drugs for Ebola virus”, *Physical Sciences Reviews*, vol. 3, no. 9. Walter de Gruyter GmbH, Jun. 23, 2018. doi: 10.1515/psr-2017-0198.  
  
V. M. Rosas-García, I. del Carmen Sáenz-Tavera, V. J. Rodríguez-Herreraand B. R. Garza-Campos, “Microsolvation and hydration enthalpies of CaC2O4(H2O) n (n = 0-16) and C2O4 2-(H2O) n (n = 0-14): an ab initio study”, *Journal of Molecular Modeling*, vol. 19, no. 4. Springer Science and Business Media LLC, pp. 1459–1471, Dec. 12, 2012. doi: 10.1007/s00894-012-1707-6.  
  
J. Saltiel, S. R. Hutchinson, K. Chitwoodand O. Dmitrenko, “Photoisomerization of *cis*-1-(3-Methyl-2-naphthyl)-2-phenylethene in Glassy Methylcyclohexane at 77 K”, *The Journal of Physical Chemistry A*, vol. 116, no. 22. American Chemical Society (ACS), pp. 5293–5298, May 29, 2012. doi: 10.1021/jp3017198.  
  
J. Saltiel, R. Klima, L. J. van de Burgt, S. Wangand O. Dmitrenko, “Temperature Dependence of the 1,6-Diphenyl-1,3,5-hexatriene Triplet Lifetime in Solution and Theoretical Evaluation of Triplet Conformer Interconversion”, *The Journal of Physical Chemistry B*, vol. 114, no. 45. American Chemical Society (ACS), pp. 14480–14486, May 07, 2010. doi: 10.1021/jp101754h.  
  
C. Sarkar, “Interface Engineering of Graphene-Supported Cu Nanoparticles Encapsulated by Mesoporous Silica for Size-Dependent Catalytic Oxidative Coupling of Aromatic Amines”, *ACS Applied Materials & Interfaces*, vol. 11, no. 12. American Chemical Society (ACS), pp. 11722–11735, Mar. 06, 2019. doi: 10.1021/acsami.8b18675.  
  
X. Schoultz, T. I. A. Gerber, E. Hosten, R. Betz, L. Rhymanand P. Ramasami, “The reaction of [ReIIICl3(t-BuNC)(PPh3)2] with aniline derivatives: Isolation of imido-Re(V) complexes and a Re(III) complex containing iminobenzoquinonate as ligand”, *Polyhedron*, vol. 96. Elsevier BV, pp. 6–15, Aug. 2015. doi: 10.1016/j.poly.2015.04.023.  
  
N. Seeburrun, I. A. Alswaidan, H.-K. Fun, E. F. Archibongand P. Ramasami, “Probing the structural and electronic properties of doped gallium oxide and sulfide, M(GaX2)2 where M = alkali or coinage metal; X = O, S”, *RSC Advances*, vol. 5, no. 128. Royal Society of Chemistry (RSC), pp. 106141–106150, 2015. doi: 10.1039/c5ra19970k.  
  
N. Seeburrun, E. F. Archibongand P. Ramasami, “Mono and digallium selenide clusters as potential superhalogens”, *Journal of Molecular Modeling*, vol. 21, no. 3. Springer Science and Business Media LLC, Feb. 13, 2015. doi: 10.1007/s00894-014-2555-3.  
  
N. Sekar, S. Katariya, L. Rhyman, I. A. Alswaidanand P. Ramasami, “Molecular and NLO Properties of Red Fluorescent Coumarins – DFT Computations Using Long-Range Separated and Conventional Functionals”, *Journal of Fluorescence*, vol. 29, no. 1. Springer Science and Business Media LLC, pp. 241–253, Dec. 15, 2018. doi: 10.1007/s10895-018-2333-1.  
  
K. Singh, B. Chandra, L. Rhymanand P. Ramasami, “Effective adsorption of pyridine (Py)—onto mesoporous silica derived from de-oiled mustard cake (DOMC): Experimental and theoretical study”, *Journal of Environmental Chemical Engineering*, vol. 4, no. 1. Elsevier BV, pp. 1383–1392, Mar. 2016. doi: 10.1016/j.jece.2016.01.033.  
  
P. Surajbali, “Density Functional Theory Study of Cyanoetheneselenol: A Molecule of Astrobiological Interest”, *Origins of Life and Evolution of Biospheres*, vol. 45, no. 4. Springer Science and Business Media LLC, pp. 455–468, Jun. 20, 2015. doi: 10.1007/s11084-015-9436-3.  
  
L. Tabrizi, D. Q. Daoand T. A. Vu, “Experimental and theoretical evaluation on the antioxidant activity of a copper(ii) complex based on lidocaine and ibuprofen amide-phenanthroline agents”, *RSC Advances*, vol. 9, no. 6. Royal Society of Chemistry (RSC), pp. 3320–3335, 2019. doi: 10.1039/c8ra09763a.  
  
A. B. Tathe, L. Rhyman, P. Ramasamiand N. Sekar, “Red Emitting Coumarins: Insights of Photophysical Properties with DFT Methods”, *Journal of Fluorescence*, vol. 25, no. 4. Springer Science and Business Media LLC, pp. 1117–1126, Jul. 2015. doi: 10.1007/s10895-015-1602-5.  
  
N. Toorabally, “Structural and spectroscopic parameters of C n F 2 + (n = 1–5): Insights using MP2/CBS method”, *Journal of Fluorine Chemistry*, vol. 200. Elsevier BV, pp. 96–101, Aug. 2017. doi: 10.1016/j.jfluchem.2017.06.008.  
  
V. Uahengo, “Photophysical, electrochemical, and DFT studies of the novel azacrown-bridged dinuclear ruthenium dye sensitizers for solar cells”, *Polyhedron*, vol. 173. Elsevier BV, p. 114106, Nov. 2019. doi: 10.1016/j.poly.2019.114106.  
  
E. H. Umukoro, “Photoelectrocatalytic application of palladium decorated zinc oxide-expanded graphite electrode for the removal of 4-nitrophenol: experimental and computational studies”, *RSC Advances*, vol. 8, no. 19. Royal Society of Chemistry (RSC), pp. 10255–10266, 2018. doi: 10.1039/c8ra00180d.  
  
J. Wang, “Theoretical enzyme design using the Kepler scientific workflows on the Grid”, *Procedia Computer Science*, vol. 1, no. 1. Elsevier BV, pp. 1175–1184, May 2010. doi: 10.1016/j.procs.2010.04.131.  
  
U. Warde, L. Rhyman, P. Ramasamiand N. Sekar, “DFT Studies of the Photophysical Properties of Fluorescent and Semiconductor Polycyclic Benzimidazole Derivatives”, *Journal of Fluorescence*, vol. 25, no. 3. Springer Science and Business Media LLC, pp. 685–694, Mar. 26, 2015. doi: 10.1007/s10895-015-1554-9.  
  
S. P. Coleman, M. M. Sichaniand D. E. Spearot, “A Computational Algorithm to Produce Virtual X-ray and Electron Diffraction Patterns from Atomistic Simulations”, *JOM*, vol. 66, no. 3. Springer Science and Business Media LLC, pp. 408–416, Jan. 01, 2014. doi: 10.1007/s11837-013-0829-3.  
  
A. S. Eisenberg, I. V. Likhtina, V. S. Znamenskiyand R. L. Birke, “Electronic Spectroscopy and Computational Studies of Glutathionylco(III)balamin”, *The Journal of Physical Chemistry A*, vol. 116, no. 25. American Chemical Society (ACS), pp. 6851–6869, Jun. 07, 2012. doi: 10.1021/jp301294x.  
  
T. A. Manz and D. S. Sholl, “A dimensionless reaction coordinate for quantifying the lateness of transition states”, *Journal of Computational Chemistry*. Wiley, p. NA–NA, 2009. doi: 10.1002/jcc.21440.  
  
T. A. Manz, “Structure–Activity Correlation for Relative Chain Initiation to Propagation Rates in Single-Site Olefin Polymerization Catalysis”, *Organometallics*, vol. 31, no. 2. American Chemical Society (ACS), pp. 602–618, Jan. 10, 2012. doi: 10.1021/om200884x.  
  
T. A. Manz, “Deactivation of Ti and Zr half-metallocene complexes activated with B(C6F5)3: a case study in constructing DFT-based QSARs to predict unimolecular rate constants”, *RSC Advances*, vol. 5, no. 60. Royal Society of Chemistry (RSC), pp. 48246–48254, 2015. doi: 10.1039/c5ra00546a.  
  
R. L. Birke and J. R. Lombardi, “Relative contributions of Franck–Condon to Herzberg–Teller terms in charge transfer surface-enhanced Raman scattering spectroscopy”, *The Journal of Chemical Physics*, vol. 152, no. 22. AIP Publishing, p. 224107, Jun. 14, 2020. doi: 10.1063/5.0005012.  
  
S. K. Islam, Y. P. Cheng, R. L. Birke, M. V. Cañamares, C. Muehlethalerand J. R. Lombardi, “An analysis of tetrahydrocannabinol (THC) and its analogs using surface enhanced Raman Scattering (SERS)”, *Chemical Physics*, vol. 536. Elsevier BV, p. 110812, Aug. 2020. doi: 10.1016/j.chemphys.2020.110812.  
  
J. Leonard, “SERS , Raman , and DFT analyses of fentanyl and carfentanil: Toward detection of trace samples”, *Journal of Raman Spectroscopy*, vol. 48, no. 10. Wiley, pp. 1323–1329, Aug. 24, 2017. doi: 10.1002/jrs.5220.  
  
A. Sajan and R. L. Birke, “The Reductive Cleavage Mechanism and Complex Stability of Glutathionyl-Cobalamin in Acidic Media”, *Electroanalysis*, vol. 28, no. 11. Wiley, pp. 2743–2753, Jun. 28, 2016. doi: 10.1002/elan.201600341.  
  
E. Choi, J. G. McDaniel, J. R. Schmidtand A. Yethiraj, “First-Principles, Physically Motivated Force Field for the Ionic Liquid [BMIM][BF4]”, *The Journal of Physical Chemistry Letters*, vol. 5, no. 15. American Chemical Society (ACS), pp. 2670–2674, Jul. 24, 2014. doi: 10.1021/jz5010945.  
  
E. Choi, J. Mondaland A. Yethiraj, “Coarse-Grained Models for Aqueous Polyethylene Glycol Solutions”, *The Journal of Physical Chemistry B*, vol. 118, no. 1. American Chemical Society (ACS), pp. 323–329, Dec. 30, 2013. doi: 10.1021/jp408392b.  
  
E. Choi and A. Yethiraj, “Entropic Mechanism for the Lower Critical Solution Temperature of Poly(ethylene oxide) in a Room Temperature Ionic Liquid”, *ACS Macro Letters*, vol. 4, no. 7. American Chemical Society (ACS), pp. 799–803, Jul. 13, 2015. doi: 10.1021/acsmacrolett.5b00355.  
  
E. Choi and A. Yethiraj, “Conformational Properties of a Polymer in an Ionic Liquid: Computer Simulations and Integral Equation Theory of a Coarse-Grained Model”, *The Journal of Physical Chemistry B*, vol. 119, no. 29. American Chemical Society (ACS), pp. 9091–9097, Oct. 24, 2014. doi: 10.1021/jp508876q.  
  
S. Mantha and A. Yethiraj, “Conformational Properties of Sodium Polystyrenesulfonate in Water: Insights from a Coarse-Grained Model with Explicit Solvent”, *The Journal of Physical Chemistry B*, vol. 119, no. 34. American Chemical Society (ACS), pp. 11010–11018, Jun. 22, 2015. doi: 10.1021/acs.jpcb.5b01700.  
  
J. G. McDaniel, E. Choi, C.-Y. Son, J. R. Schmidtand A. Yethiraj, “Conformational and Dynamic Properties of Poly(ethylene oxide) in an Ionic Liquid: Development and Implementation of a First-Principles Force Field”, *The Journal of Physical Chemistry B*, vol. 120, no. 1. American Chemical Society (ACS), pp. 231–243, Jan. 05, 2016. doi: 10.1021/acs.jpcb.5b10065.  
  
J. Mondal, E. Choiand A. Yethiraj, “Atomistic Simulations of Poly(ethylene oxide) in Water and an Ionic Liquid at Room Temperature”, *Macromolecules*, vol. 47, no. 1. American Chemical Society (ACS), pp. 438–446, Dec. 23, 2013. doi: 10.1021/ma4016714.  
  
J. Mondal, M. Mahanthappaand A. Yethiraj, “Self-Assembly of Gemini Surfactants: A Computer Simulation Study”, *The Journal of Physical Chemistry B*, vol. 117, no. 16. American Chemical Society (ACS), pp. 4254–4262, Sep. 21, 2012. doi: 10.1021/jp304933k.  
  
J. Mondal and A. Yethiraj, “Driving Force for the Association of Amphiphilic Molecules”, *The Journal of Physical Chemistry Letters*, vol. 2, no. 19. American Chemical Society (ACS), pp. 2391–2395, Sep. 06, 2011. doi: 10.1021/jz201046x.  
  
J. Mondal and A. Yethiraj, “Effect of secondary structure on the self-assembly of amphiphilic molecules: A multiscale simulation study”, *The Journal of Chemical Physics*, vol. 136, no. 8. AIP Publishing, p. 084902, Feb. 28, 2012. doi: 10.1063/1.3689298.  
  
K. Black, P. Liu, L. Xu, C. Doubledayand K. N. Houk, “Dynamics, transition states, and timing of bond formation in Diels–Alder reactions”, *Proceedings of the National Academy of Sciences*, vol. 109, no. 32. Proceedings of the National Academy of Sciences, pp. 12860–12865, Jul. 02, 2012. doi: 10.1073/pnas.1209316109.  
  
L. Cheng, C. Doubledayand R. Breslow, “Evidence for tunneling in base-catalyzed isomerization of glyceraldehyde to dihydroxyacetone by hydride shift under formose conditions”, *Proceedings of the National Academy of Sciences*, vol. 112, no. 14. Proceedings of the National Academy of Sciences, pp. 4218–4220, Mar. 23, 2015. doi: 10.1073/pnas.1503739112.  
  
D. Devarajan, C. E. Doubledayand D. H. Ess, “Theory of Divalent Main Group H2 Activation: Electronics and Quasiclassical Trajectories”, *Inorganic Chemistry*, vol. 52, no. 15. American Chemical Society (ACS), pp. 8820–8833, Jul. 09, 2013. doi: 10.1021/ic4010399.  
  
C. Doubleday, R. Armas, D. Walker, C. V. Cosgriffand E. M. Greer, “Heavy‐Atom Tunneling Calculations in Thirteen Organic Reactions: Tunneling Contributions are Substantial, and Bell’s Formula Closely Approximates Multidimensional Tunneling at ≥250 K”, *Angewandte Chemie International Edition*, vol. 56, no. 42. Wiley, pp. 13099–13102, Sep. 18, 2017. doi: 10.1002/anie.201708489.  
  
C. Doubleday, M. Boguslav, C. Howell, S. D. Korotkinand D. Shaked, “Trajectory Calculations for Bergman Cyclization Predict H/D Kinetic Isotope Effects Due to Nonstatistical Dynamics in the Product”, *Journal of the American Chemical Society*, vol. 138, no. 24. American Chemical Society (ACS), pp. 7476–7479, Jun. 13, 2016. doi: 10.1021/jacs.6b03466.  
  
E. M. Greer, C. V. Cosgriffand C. Doubleday, “Computational Evidence for Heavy-Atom Tunneling in the Bergman Cyclization of a 10-Membered-Ring Enediyne”, *Journal of the American Chemical Society*, vol. 135, no. 28. American Chemical Society (ACS), pp. 10194–10197, Jul. 02, 2013. doi: 10.1021/ja402445a.  
  
E. M. Greer, K. Kwon, A. Greerand C. Doubleday, “Thermally activated tunneling in organic reactions”, *Tetrahedron*, vol. 72, no. 47. Elsevier BV, pp. 7357–7373, Nov. 2016. doi: 10.1016/j.tet.2016.09.029.  
  
Z. Yang, C. Doubledayand K. N. Houk, “QM/MM Protocol for Direct Molecular Dynamics of Chemical Reactions in Solution: The Water-Accelerated Diels–Alder Reaction”, *Journal of Chemical Theory and Computation*, vol. 11, no. 12. American Chemical Society (ACS), pp. 5606–5612, Nov. 17, 2015. doi: 10.1021/acs.jctc.5b01029.  
  
Z. Yang, “Influence of water and enzyme SpnF on the dynamics and energetics of the ambimodal [6+4]/[4+2] cycloaddition”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 5. Proceedings of the National Academy of Sciences, Jan. 18, 2018. doi: 10.1073/pnas.1719368115.  
  
A. Han, T. Spataru, J. Hartung, G. Liand J. R. Norton, “Effect of Double-Bond Substituents on the Rate of Cyclization of α-Carbomethoxyhex-5-enyl Radicals”, *The Journal of Organic Chemistry*, vol. 79, no. 5. American Chemical Society (ACS), pp. 1938–1946, Feb. 18, 2014. doi: 10.1021/jo402499w.  
  
J. R. Norton, “Kinetics and Mechanism of the Hydrogenation of the CpCr(CO)3•/[CpCr(CO)3]2 Equilibrium to CpCr(CO)3H”, *Organometallics*, vol. 33, no. 10. American Chemical Society (ACS), pp. 2496–2502, May 12, 2014. doi: 10.1021/om4012399.  
  
R. M. Shields, B. Temelso, K. A. Archer, T. E. Morrelland G. C. Shields, “Accurate Predictions of Water Cluster Formation, (H2O)*n*=2−10”, *The Journal of Physical Chemistry A*, vol. 114, no. 43. American Chemical Society (ACS), pp. 11725–11737, Sep. 30, 2010. doi: 10.1021/jp104865w.  
  
B. Temelso and G. C. Shields, “The Role of Anharmonicity in Hydrogen-Bonded Systems: The Case of Water Clusters”, *Journal of Chemical Theory and Computation*, vol. 7, no. 9. American Chemical Society (ACS), pp. 2804–2817, Aug. 05, 2011. doi: 10.1021/ct2003308.  
  
B. Temelso, K. A. Alser, A. Gauthier, A. K. Palmerand G. C. Shields, “Structural Analysis of α-Fetoprotein (AFP)-like Peptides with Anti-Breast-Cancer Properties”, *The Journal of Physical Chemistry B*, vol. 118, no. 17. American Chemical Society (ACS), pp. 4514–4526, Apr. 22, 2014. doi: 10.1021/jp500017b.  
  
D. E. Husar, B. Temelso, A. L. Ashworthand G. C. Shields, “Hydration of the Bisulfate Ion: Atmospheric Implications”, *The Journal of Physical Chemistry A*, vol. 116, no. 21. American Chemical Society (ACS), pp. 5151–5163, May 18, 2012. doi: 10.1021/jp300717j.  
  
J. S. Swan, P. M. Findeis, S. Hilton, K. M. Lebold, B. Temelsoand G. C. Shields, “Formation of deprotonated 2-imidazoline-4(5)-one product ions in the collision-induced dissociation of some serine-containing dipeptides”, *International Journal of Mass Spectrometry*, vol. 381–382. Elsevier BV, pp. 25–32, May 2015. doi: 10.1016/j.ijms.2015.03.005.  
  
B. Temelso, K. A. Archerand G. C. Shields, “Benchmark Structures and Binding Energies of Small Water Clusters with Anharmonicity Corrections”, *The Journal of Physical Chemistry A*, vol. 115, no. 43. American Chemical Society (ACS), pp. 12034–12046, Oct. 07, 2011. doi: 10.1021/jp2069489.  
  
B. Temelso, “Quantum Mechanical Study of Sulfuric Acid Hydration: Atmospheric Implications”, *The Journal of Physical Chemistry A*, vol. 116, no. 9. American Chemical Society (ACS), pp. 2209–2224, Feb. 22, 2012. doi: 10.1021/jp2119026.  
  
B. Temelso, T. N. Phanand G. C. Shields, “Computational Study of the Hydration of Sulfuric Acid Dimers: Implications for Acid Dissociation and Aerosol Formation”, *The Journal of Physical Chemistry A*, vol. 116, no. 39. American Chemical Society (ACS), pp. 9745–9758, Sep. 25, 2012. doi: 10.1021/jp3054394.  
  
B. Temelso, C. R. Rennerand G. C. Shields, “Importance and Reliability of Small Basis Set CCSD(T) Corrections to MP2 Binding and Relative Energies of Water Clusters”, *Journal of Chemical Theory and Computation*, vol. 11, no. 4. American Chemical Society (ACS), pp. 1439–1448, Mar. 23, 2015. doi: 10.1021/ct500944v.  
  
J. Wang, “Development of Polarizable Models for Molecular Mechanical Calculations. 3. Polarizable Water Models Conforming to Thole Polarization Screening Schemes”, *The Journal of Physical Chemistry B*, vol. 116, no. 28. American Chemical Society (ACS), pp. 7999–8008, Jul. 05, 2012. doi: 10.1021/jp212117d.  
  
J. Wang, “Development of Polarizable Models for Molecular Mechanical Calculations. 4. van der Waals Parametrization”, *The Journal of Physical Chemistry B*, vol. 116, no. 24. American Chemical Society (ACS), pp. 7088–7101, Jun. 06, 2012. doi: 10.1021/jp3019759.  
  
J. Wang, P. Cieplak, J. Li, T. Hou, R. Luoand Y. Duan, “Development of Polarizable Models for Molecular Mechanical Calculations I: Parameterization of Atomic Polarizability”, *The Journal of Physical Chemistry B*, vol. 115, no. 12. American Chemical Society (ACS), pp. 3091–3099, Mar. 10, 2011. doi: 10.1021/jp112133g.  
  
J. Wang, “Development of Polarizable Models for Molecular Mechanical Calculations II: Induced Dipole Models Significantly Improve Accuracy of Intermolecular Interaction Energies”, *The Journal of Physical Chemistry B*, vol. 115, no. 12. American Chemical Society (ACS), pp. 3100–3111, Mar. 10, 2011. doi: 10.1021/jp1121382.  
  
J. Wang and T. Hou, “Application of Molecular Dynamics Simulations in Molecular Property Prediction. 1. Density and Heat of Vaporization”, *Journal of Chemical Theory and Computation*, vol. 7, no. 7. American Chemical Society (ACS), pp. 2151–2165, Jun. 08, 2011. doi: 10.1021/ct200142z.  
  
J. Wang and T. Hou, “Application of molecular dynamics simulations in molecular property prediction II: Diffusion coefficient”, *Journal of Computational Chemistry*, vol. 32, no. 16. Wiley, pp. 3505–3519, Sep. 22, 2011. doi: 10.1002/jcc.21939.  
  
J. Wang and T. Hou, “Develop and Test a Solvent Accessible Surface Area-Based Model in Conformational Entropy Calculations”, *Journal of Chemical Information and Modeling*, vol. 52, no. 5. American Chemical Society (ACS), pp. 1199–1212, Apr. 24, 2012. doi: 10.1021/ci300064d.  
  
T. V. Esipova, M. J. P. Barrett, E. Erlebach, A. E. Masunov, B. Weberand S. A. Vinogradov, “Oxyphor 2P: A High-Performance Probe for Deep-Tissue Longitudinal Oxygen Imaging”, *Cell Metabolism*, vol. 29, no. 3. Elsevier BV, pp. 736–744.e7, Mar. 2019. doi: 10.1016/j.cmet.2018.12.022.  
  
C. A. Cole, N. J. Demarais, Z. Yang, T. P. Snowand V. M. Bierbaum, “HETEROCYCLIC ANIONS OF ASTROBIOLOGICAL INTEREST”, *The Astrophysical Journal*, vol. 779, no. 2. American Astronomical Society, p. 181, Dec. 04, 2013. doi: 10.1088/0004-637x/779/2/181.  
  
C. A. Cole, Z.-C. Wang, T. P. Snowand V. M. Bierbaum, “Anionic derivatives of uracil: fragmentation and reactivity”, *Phys. Chem. Chem. Phys.*, vol. 16, no. 33. Royal Society of Chemistry (RSC), pp. 17835–17844, 2014. doi: 10.1039/c4cp02277g.  
  
C. A. Cole, Z.-C. Wang, T. P. Snowand V. M. Bierbaum, “Deprotonated Purine Dissociation: Experiments, Computations, and Astrobiological Implications”, *The Journal of Physical Chemistry A*, vol. 119, no. 2. American Chemical Society (ACS), pp. 334–343, Jan. 05, 2015. doi: 10.1021/jp509012s.  
  
C. A. Cole, N. Wehres, Z. Yang, D. L. Thomsen, T. P. Snowand V. M. Bierbaum, “A GAS-PHASE FORMATION ROUTE TO INTERSTELLAR TRANS-METHYL FORMATE”, *The Astrophysical Journal*, vol. 754, no. 1. American Astronomical Society, p. L5, Jul. 02, 2012. doi: 10.1088/2041-8205/754/1/l5.  
  
Z. Lin, “CAN INTERSTELLAR PROPENE (CH3CHCH2) BE FORMED VIA GAS-PHASE REACTIONS?”, *The Astrophysical Journal*, vol. 765, no. 2. American Astronomical Society, p. 80, Feb. 19, 2013. doi: 10.1088/0004-637x/765/2/80.  
  
Z.-C. Wang, C. A. Cole, T. P. Snowand V. M. Bierbaum, “EXPERIMENTAL AND COMPUTATIONAL STUDIES OF THE FORMATION MECHANISM OF PROTONATED INTERSTELLAR DIAZINES”, *The Astrophysical Journal*, vol. 798, no. 2. American Astronomical Society, p. 102, Jan. 05, 2015. doi: 10.1088/0004-637x/798/2/102.  
  
Z. Yang, C. A. Cole, O. Martinez, Jr., M. Y. Carpenter, T. P. Snowand V. M. Bierbaum, “EXPERIMENTAL AND THEORETICAL STUDIES OF REACTIONS BETWEEN H ATOMS AND NITROGEN-CONTAINING CARBANIONS”, *The Astrophysical Journal*, vol. 739, no. 1. American Astronomical Society, p. 19, Aug. 30, 2011. doi: 10.1088/0004-637x/739/1/19.  
  
D. B. Lawson and A. Walker, “Cycloaddition of ethene on a series of single-walled carbon nanotubes”, *Computational and Theoretical Chemistry*, vol. 981. Elsevier BV, pp. 31–37, Feb. 2012. doi: 10.1016/j.comptc.2011.11.040.  
  
K. Park, W. Linand F. Paesani, “A Refined MS-EVB Model for Proton Transport in Aqueous Environments”, *The Journal of Physical Chemistry B*, vol. 116, no. 1. American Chemical Society (ACS), pp. 343–352, Dec. 12, 2011. doi: 10.1021/jp208946p.  
  
J. E. Stevens, L. D. Macomberand L. W. Davis, “IR Spectra and Vibrational Modes of the Hydrofluoroethers CF3OCH3, CF3OCF2H, and CF3OCF2CF2H and Corresponding Alkanes CF3CH3, CF3CF2H, and CF3CF2CF2H!2010-03-11!2010-05-19!2010-08-06!”, *The Open Physical Chemistry Journal*, vol. 4, no. 1. Bentham Science Publishers Ltd., pp. 17–27, Aug. 19, 2010. doi: 10.2174/1874067701004010017.  
  
E. B. Guidez and C. M. Aikens, “Diameter Dependence of the Excitation Spectra of Silver and Gold Nanorods”, *The Journal of Physical Chemistry C*, vol. 117, no. 23. American Chemical Society (ACS), pp. 12325–12336, May 31, 2013. doi: 10.1021/jp4023103.  
  
W. Wang, J. Li, K. Wang, T. I. Smirnovaand E. Oldfield, “Pyridine Inhibitor Binding to the 4Fe-4S Protein *A. aeolicus* IspH (LytB): A HYSCORE Investigation”, *Journal of the American Chemical Society*, vol. 133, no. 17. American Chemical Society (ACS), pp. 6525–6528, Apr. 12, 2011. doi: 10.1021/ja2008455.  
  
M. C. Haibach, “Olefin Hydroaryloxylation Catalyzed by Pincer–Iridium Complexes”, *Journal of the American Chemical Society*, vol. 135, no. 40. American Chemical Society (ACS), pp. 15062–15070, Sep. 27, 2013. doi: 10.1021/ja404566v.  
  
F. Hasanayn, P. Achord, P. Braunstein, H. J. Magnier, K. Krogh-Jespersenand A. S. Goldman, “Theoretical Structure–Reactivity Study of Ethylene Insertion into Nickel–Alkyl Bonds. A Kinetically Significant and Unanticipated Role of*trans*Influence in Determining Agostic Bond Strengths”, *Organometallics*, vol. 31, no. 13. American Chemical Society (ACS), pp. 4680–4692, Jun. 25, 2012. doi: 10.1021/om300001n.  
  
S. Kundu, “Cleavage of Ether, Ester, and Tosylate C(sp3)–O Bonds by an Iridium Complex, Initiated by Oxidative Addition of C–H Bonds. Experimental and Computational Studies”, *Journal of the American Chemical Society*, vol. 135, no. 13. American Chemical Society (ACS), pp. 5127–5143, Mar. 21, 2013. doi: 10.1021/ja312464b.  
  
D. A. Laviska, “Addition of C–C and C–H bonds by pincer-iridium complexes: a combined experimental and computational study”, *Dalton Trans.*, vol. 43, no. 43. Royal Society of Chemistry (RSC), pp. 16354–16365, Sep. 12, 2014. doi: 10.1039/c4dt02043j.  
  
G.-T. Bae and C. M. Aikens, “Improved ReaxFF Force Field Parameters for Au–S–C–H Systems”, *The Journal of Physical Chemistry A*, vol. 117, no. 40. American Chemical Society (ACS), pp. 10438–10446, Sep. 27, 2013. doi: 10.1021/jp405992m.  
  
C. Lee and C. M. Aikens, “Water Splitting Processes on Mn4O4 and CaMn3O4 Model Cubane Systems”, *The Journal of Physical Chemistry A*, vol. 119, no. 35. American Chemical Society (ACS), pp. 9325–9337, Aug. 25, 2015. doi: 10.1021/acs.jpca.5b03170.  
  
X. Li, D. M. Yorkand M. P. Meyer, “Quantum Suppression of Intramolecular Deuterium Kinetic Isotope Effects in a Pericyclic Hydrogen Transfer Reaction”, *The Journal of Physical Chemistry A*, vol. 123, no. 17. American Chemical Society (ACS), pp. 3647–3654, Mar. 11, 2019. doi: 10.1021/acs.jpca.9b00172.  
  
H. Chen, T. J. Giese, M. Huang, K.-Y. Wong, M. E. Harrisand D. M. York, “Mechanistic Insights into RNA Transphosphorylation from Kinetic Isotope Effects and Linear Free Energy Relationships of Model Reactions”, *Chemistry - A European Journal*, vol. 20, no. 44. Wiley, pp. 14336–14343, Sep. 15, 2014. doi: 10.1002/chem.201403862.  
  
H. Chen, J. A. Piccirilli, M. E. Harrisand D. M. York, “Effect of Zn2+ binding and enzyme active site on the transition state for RNA 2′-O-transphosphorylation interpreted through kinetic isotope effects”, *Biochimica et Biophysica Acta (BBA) - Proteins and Proteomics*, vol. 1854, no. 11. Elsevier BV, pp. 1795–1800, Nov. 2015. doi: 10.1016/j.bbapap.2015.02.022.  
  
T. Dissanayake, J. M. Swails, M. E. Harris, A. E. Roitbergand D. M. York, “Interpretation of pH–Activity Profiles for Acid–Base Catalysis from Molecular Simulations”, *Biochemistry*, vol. 54, no. 6. American Chemical Society (ACS), pp. 1307–1313, Feb. 06, 2015. doi: 10.1021/bi5012833.  
  
G. M. Giambaşu, T. Luchko, D. Herschlag, D. M. Yorkand D. A. Case, “Ion Counting from Explicit-Solvent Simulations and 3D-RISM”, *Biophysical Journal*, vol. 106, no. 4. Elsevier BV, pp. 883–894, Feb. 2014. doi: 10.1016/j.bpj.2014.01.021.  
  
G. M. Giambaşu, D. M. Yorkand D. A. Case, “Structural fidelity and NMR relaxation analysis in a prototype RNA hairpin”, *RNA*, vol. 21, no. 5. Cold Spring Harbor Laboratory, pp. 963–974, Mar. 24, 2015. doi: 10.1261/rna.047357.114.  
  
T. J. Giese, H. Chen, M. Huangand D. M. York, “Parametrization of an Orbital-Based Linear-Scaling Quantum Force Field for Noncovalent Interactions”, *Journal of Chemical Theory and Computation*, vol. 10, no. 3. American Chemical Society (ACS), pp. 1086–1098, Feb. 24, 2014. doi: 10.1021/ct401035t.  
  
T. J. Giese, M. Huang, H. Chenand D. M. York, “Recent Advances toward a General Purpose Linear-Scaling Quantum Force Field”, *Accounts of Chemical Research*, vol. 47, no. 9. American Chemical Society (ACS), pp. 2812–2820, Jun. 17, 2014. doi: 10.1021/ar500103g.  
  
T. J. Giese, M. T. Panteva, H. Chenand D. M. York, “Multipolar Ewald Methods, 1: Theory, Accuracy, and Performance”, *Journal of Chemical Theory and Computation*, vol. 11, no. 2. American Chemical Society (ACS), pp. 436–450, Jan. 14, 2015. doi: 10.1021/ct5007983.  
  
T. J. Giese, M. T. Panteva, H. Chenand D. M. York, “Multipolar Ewald Methods, 2: Applications Using a Quantum Mechanical Force Field”, *Journal of Chemical Theory and Computation*, vol. 11, no. 2. American Chemical Society (ACS), pp. 451–461, Jan. 13, 2015. doi: 10.1021/ct500799g.  
  
H. Heldenbrand, P. A. Janowski, G. Giambaşu, T. J. Giese, J. E. Wedekindand D. M. York, “Evidence for the Role of Active Site Residues in the Hairpin Ribozyme from Molecular Simulations along the Reaction Path”, *Journal of the American Chemical Society*, vol. 136, no. 22. American Chemical Society (ACS), pp. 7789–7792, May 23, 2014. doi: 10.1021/ja500180q.  
  
M. Huang, T. J. Giese, T.-S. Leeand D. M. York, “Improvement of DNA and RNA Sugar Pucker Profiles from Semiempirical Quantum Methods”, *Journal of Chemical Theory and Computation*, vol. 10, no. 4. American Chemical Society (ACS), pp. 1538–1545, Mar. 14, 2014. doi: 10.1021/ct401013s.  
  
M. Huang and D. M. York, “Linear free energy relationships in RNA transesterification: theoretical models to aid experimental interpretations”, *Phys. Chem. Chem. Phys.*, vol. 16, no. 30. Royal Society of Chemistry (RSC), pp. 15846–15855, 2014. doi: 10.1039/c4cp01050g.  
  
P. A. Janowski, D. S. Cerutti, J. Holtonand D. A. Case, “Peptide Crystal Simulations Reveal Hidden Dynamics”, *Journal of the American Chemical Society*, vol. 135, no. 21. American Chemical Society (ACS), pp. 7938–7948, May 16, 2013. doi: 10.1021/ja401382y.  
  
D. L. Kellerman, D. M. York, J. A. Piccirilliand M. E. Harris, “Altered (transition) states: mechanisms of solution and enzyme catalyzed RNA 2′-O-transphosphorylation”, *Current Opinion in Chemical Biology*, vol. 21. Elsevier BV, pp. 96–102, Aug. 2014. doi: 10.1016/j.cbpa.2014.06.010.  
  
E. R. Kuechler and D. M. York, “Quantum mechanical study of solvent effects in a prototype S*N*2 reaction in solution: Cl− attack on CH3Cl”, *The Journal of Chemical Physics*, vol. 140, no. 5. AIP Publishing, p. 054109, Feb. 07, 2014. doi: 10.1063/1.4863344.  
  
T.-S. Lee, B. K. Radak, M. Huang, K.-Y. Wongand D. M. York, “Roadmaps through Free Energy Landscapes Calculated Using the Multidimensional vFEP Approach”, *Journal of Chemical Theory and Computation*, vol. 10, no. 1. American Chemical Society (ACS), pp. 24–34, Dec. 09, 2013. doi: 10.1021/ct400691f.  
  
A. Pabis, I. Geronimo, D. M. Yorkand P. Paneth, “Molecular Dynamics Simulation of Nitrobenzene Dioxygenase Using AMBER Force Field”, *Journal of Chemical Theory and Computation*, vol. 10, no. 6. American Chemical Society (ACS), pp. 2246–2254, May 08, 2014. doi: 10.1021/ct500205z.  
  
M. T. Panteva, “Multiscale Methods for Computational RNA Enzymology”, *Methods in Enzymology*. Elsevier, pp. 335–374, 2015. doi: 10.1016/bs.mie.2014.10.064.  
  
M. T. Panteva, G. M. Giambaşuand D. M. York, “Comparison of structural, thermodynamic, kinetic and mass transport properties of Mg2+ion models commonly used in biomolecular simulations”, *Journal of Computational Chemistry*, vol. 36, no. 13. Wiley, pp. 970–982, Mar. 04, 2015. doi: 10.1002/jcc.23881.  
  
B. K. Radak, “Characterization of the Three-Dimensional Free Energy Manifold for the Uracil Ribonucleoside from Asynchronous Replica Exchange Simulations”, *Journal of Chemical Theory and Computation*, vol. 11, no. 2. American Chemical Society (ACS), pp. 373–377, Jan. 26, 2015. doi: 10.1021/ct500776j.  
  
J. M. Swails, D. M. Yorkand A. E. Roitberg, “Constant pH Replica Exchange Molecular Dynamics in Explicit Solvent Using Discrete Protonation States: Implementation, Testing, and Validation”, *Journal of Chemical Theory and Computation*, vol. 10, no. 3. American Chemical Society (ACS), pp. 1341–1352, Feb. 25, 2014. doi: 10.1021/ct401042b.  
  
K.-Y. Wong, Y. Xuand D. M. York, “*Ab initio*path-integral calculations of kinetic and equilibrium isotope effects on base-catalyzed RNA transphosphorylation models”, *Journal of Computational Chemistry*, vol. 35, no. 17. Wiley, pp. 1302–1316, May 20, 2014. doi: 10.1002/jcc.23628.  
  
E. R. Beyerle and M. G. Guenza, “Kinetics analysis of ubiquitin local fluctuations with Markov state modeling of the LE4PD normal modes”, *The Journal of Chemical Physics*, vol. 151, no. 16. AIP Publishing, p. 164119, Oct. 28, 2019. doi: 10.1063/1.5123513.  
  
J. Copperman, M. Dinpajooh, E. R. Beyerleand M. G. Guenza, “Universality and Specificity in Protein Fluctuation Dynamics”, *Physical Review Letters*, vol. 119, no. 15. American Physical Society (APS), Oct. 11, 2017. doi: 10.1103/physrevlett.119.158101.  
  
J. Copperman and M. G. Guenza, “Coarse-Grained Langevin Equation for Protein Dynamics: Global Anisotropy and a Mode Approach to Local Complexity”, *The Journal of Physical Chemistry B*, vol. 119, no. 29. American Chemical Society (ACS), pp. 9195–9211, Nov. 20, 2014. doi: 10.1021/jp509473z.  
  
J. Copperman and M. G. Guenza, “Mode localization in the cooperative dynamics of protein recognition”, *The Journal of Chemical Physics*, vol. 145, no. 1. AIP Publishing, p. 015101, Jul. 07, 2016. doi: 10.1063/1.4954506.  
  
E. deLorimier, “Modifications to toxic CUG RNAs induce structural stability, rescue mis-splicing in a myotonic dystrophy cell model and reduce toxicity in a myotonic dystrophy zebrafish model”, *Nucleic Acids Research*, vol. 42, no. 20. Oxford University Press (OUP), pp. 12768–12778, Oct. 10, 2014. doi: 10.1093/nar/gku941.  
  
E. deLorimier, M. N. Hinman, J. Copperman, K. Datta, M. Guenzaand J. A. Berglund, “Pseudouridine Modification Inhibits Muscleblind-like 1 (MBNL1) Binding to CCUG Repeats and Minimally Structured RNA through Reduced RNA Flexibility”, *Journal of Biological Chemistry*, vol. 292, no. 10. Elsevier BV, pp. 4350–4357, Mar. 2017. doi: 10.1074/jbc.m116.770768.  
  
M. Dinpajooh and M. G. Guenza, “Thermodynamic consistency in the structure-based integral equation coarse-grained method”, *Polymer*, vol. 117. Elsevier BV, pp. 282–286, May 2017. doi: 10.1016/j.polymer.2017.04.025.  
  
M. Dinpajooh and M. G. Guenza, “On the Density Dependence of the Integral Equation Coarse-Graining Effective Potential”, *The Journal of Physical Chemistry B*, vol. 122, no. 13. American Chemical Society (ACS), pp. 3426–3440, Nov. 16, 2017. doi: 10.1021/acs.jpcb.7b10494.  
  
M. Dinpajooh and M. G. Guenza, “Coarse-graining simulation approaches for polymer melts: the effect of potential range on computational efficiency”, *Soft Matter*, vol. 14, no. 35. Royal Society of Chemistry (RSC), pp. 7126–7144, 2018. doi: 10.1039/c8sm00868j.  
  
M. Dinpajooh and M. G. Guenza, “Can pure polymer liquids be represented at two different resolutions simultaneously?”, *The Journal of Chemical Physics*, vol. 151, no. 6. AIP Publishing, p. 061102, Aug. 14, 2019. doi: 10.1063/1.5115791.  
  
D. Ozog, A. D. Malonyand M. Guenza, “The UA?CG Workflow: High Performance Molecular Dynamics of Coarse-Grained Polymers”, *2016 24th Euromicro International Conference on Parallel, Distributed, and Network-Based Processing (PDP)*. IEEE, Feb. 2016. doi: 10.1109/pdp.2016.127.  
  
P. G. Romano and M. G. Guenza, “GRadient Adaptive Decomposition (GRAD) Method: Optimized Refinement Along Macrostate Borders in Markov State Models”, *Journal of Chemical Information and Modeling*, vol. 57, no. 11. American Chemical Society (ACS), pp. 2729–2740, Oct. 31, 2017. doi: 10.1021/acs.jcim.7b00261.  
  
A. J. Clark and M. G. Guenza, “Mapping of polymer melts onto liquids of soft-colloidal chains”, *The Journal of Chemical Physics*, vol. 132, no. 4. AIP Publishing, p. 044902, Jan. 28, 2010. doi: 10.1063/1.3292013.  
  
A. J. Clark and M. G. Guenza, “Mapping of polymer melts onto liquids of soft-colloidal chains”, *The Journal of Chemical Physics*, vol. 132, no. 4. AIP Publishing, p. 044902, Jan. 28, 2010. doi: 10.1063/1.3292013.  
  
A. J. Clark, J. McCarty, I. Y. Lyubimovand M. G. Guenza, “Thermodynamic Consistency in Variable-Level Coarse Graining of Polymeric Liquids”, *Physical Review Letters*, vol. 109, no. 16. American Physical Society (APS), Oct. 15, 2012. doi: 10.1103/physrevlett.109.168301.  
  
A. J. Clark, J. McCarty, I. Y. Lyubimovand M. G. Guenza, “Thermodynamic Consistency in Variable-Level Coarse Graining of Polymeric Liquids”, *Physical Review Letters*, vol. 109, no. 16. American Physical Society (APS), Oct. 15, 2012. doi: 10.1103/physrevlett.109.168301.  
  
J. Copperman and M. G. Guenza, “Predicting protein dynamics from structural ensembles”, *The Journal of Chemical Physics*, vol. 143, no. 24. AIP Publishing, p. 243131, Dec. 28, 2015. doi: 10.1063/1.4935575.  
  
M. G. Guenza, “Localization of chain dynamics in entangled polymer melts”, *Physical Review E*, vol. 89, no. 5. American Physical Society (APS), May 27, 2014. doi: 10.1103/physreve.89.052603.  
  
I. Lyubimov and M. G. Guenza, “First-principle approach to rescale the dynamics of simulated coarse-grained macromolecular liquids”, *Physical Review E*, vol. 84, no. 3. American Physical Society (APS), Sep. 13, 2011. doi: 10.1103/physreve.84.031801.  
  
I. Y. Lyubimov and M. G. Guenza, “Theoretical reconstruction of realistic dynamics of highly coarse-grained *cis*-1,4-polybutadiene melts”, *The Journal of Chemical Physics*, vol. 138, no. 12. AIP Publishing, pp. 12A546, Mar. 28, 2013. doi: 10.1063/1.4792367.  
  
I. Y. Lyubimov and M. G. Guenza, “Theoretical reconstruction of realistic dynamics of highly coarse-grained *cis*-1,4-polybutadiene melts”, *The Journal of Chemical Physics*, vol. 138, no. 12. AIP Publishing, pp. 12A546, Mar. 28, 2013. doi: 10.1063/1.4792367.  
  
I. Y. Lyubimov, J. McCarty, A. Clarkand M. G. Guenza, “Analytical rescaling of polymer dynamics from mesoscale simulations”, *The Journal of Chemical Physics*, vol. 132, no. 22. AIP Publishing, p. 224903, Jun. 14, 2010. doi: 10.1063/1.3450301.  
  
I. Y. Lyubimov, J. McCarty, A. Clarkand M. G. Guenza, “Analytical rescaling of polymer dynamics from mesoscale simulations”, *The Journal of Chemical Physics*, vol. 132, no. 22. AIP Publishing, p. 224903, Jun. 14, 2010. doi: 10.1063/1.3450301.  
  
J. McCarty, A. J. Clark, J. Coppermanand M. G. Guenza, “An analytical coarse-graining method which preserves the free energy, structural correlations, and thermodynamic state of polymer melts from the atomistic to the mesoscale”, *The Journal of Chemical Physics*, vol. 140, no. 20. AIP Publishing, p. 204913, May 28, 2014. doi: 10.1063/1.4875923.  
  
J. McCarty and M. G. Guenza, “Multiscale modeling of binary polymer mixtures: Scale bridging in the athermal and thermal regime”, *The Journal of Chemical Physics*, vol. 133, no. 9. AIP Publishing, p. 094904, Sep. 07, 2010. doi: 10.1063/1.3483236.  
  
S. Nekkanti and C. B. Martin, “Theoretical study on the relative energies of cationic pterin tautomers”, *Pteridines*, vol. 26, no. 1. Walter de Gruyter GmbH, pp. 13–22, Jan. 30, 2015. doi: 10.1515/pterid-2014-0011.  
  
H. Li and M. N. Kobrak, “Instantaneous Normal Mode Analysis of a Series of Model Molten Salts”, *ChemPhysChem*, vol. 13, no. 7. Wiley, pp. 1934–1941, Jan. 12, 2012. doi: 10.1002/cphc.201100727.  
  
H. Li and M. N. Kobrak, “The Influence of Charge Distribution on Ion Diffusion in Molten Salts: A Model Study”, *ECS Transactions*, vol. 41, no. 36. The Electrochemical Society, pp. 13–21, May 04, 2012. doi: 10.1149/1.4703918.  
  
B. R. Meher and Y. Wang, “Interaction of I50V Mutant and I50L/A71V Double Mutant HIV-Protease with Inhibitor TMC114 (Darunavir): Molecular Dynamics Simulation and Binding Free Energy Studies”, *The Journal of Physical Chemistry B*, vol. 116, no. 6. American Chemical Society (ACS), pp. 1884–1900, Feb. 03, 2012. doi: 10.1021/jp2074804.  
  
B. R. Meher and Y. Wang, “Binding of single walled carbon nanotube to WT and mutant HIV-1 proteases: Analysis of flap dynamics and binding mechanism”, *Journal of Molecular Graphics and Modelling*, vol. 38. Elsevier BV, pp. 430–445, Sep. 2012. doi: 10.1016/j.jmgm.2012.10.001.  
  
D. M. Driscoll, “Binding Sites, Geometry, and Energetics of Propene at Nanoparticulate Au/TiO2”, *The Journal of Physical Chemistry C*, vol. 121, no. 3. American Chemical Society (ACS), pp. 1683–1689, Jan. 10, 2017. doi: 10.1021/acs.jpcc.6b10997.  
  
I. X. Green, M. McEntee, W. Tang, M. Neurockand J. T. Yates Jr., “Direct Formation of Acetate from the Partial Oxidation of Ethylene on a Au/TiO2 Catalyst”, *Topics in Catalysis*, vol. 56, no. 15–17. Springer Science and Business Media LLC, pp. 1512–1524, Aug. 20, 2013. doi: 10.1007/s11244-013-0154-7.  
  
I. X. Green, W. Tang, M. McEntee, M. Neurockand J. T. Yates Jr., “Inhibition at Perimeter Sites of Au/TiO2 Oxidation Catalyst by Reactant Oxygen”, *Journal of the American Chemical Society*, vol. 134, no. 30. American Chemical Society (ACS), pp. 12717–12723, Jul. 17, 2012. doi: 10.1021/ja304426b.  
  
I. X. Green, W. Tang, M. Neurockand J. T. Yates Jr., “Low-Temperature Catalytic H2 Oxidation over Au Nanoparticle/TiO2 Dual Perimeter Sites”, *Angewandte Chemie International Edition*, vol. 50, no. 43. Wiley, pp. 10186–10189, May 31, 2011. doi: 10.1002/anie.201101612.  
  
I. X. Green, W. Tang, M. Neurockand J. T. Yates Jr., “Spectroscopic Observation of Dual Catalytic Sites During Oxidation of CO on a Au/TiO 2 Catalyst”, *Science*, vol. 333, no. 6043. American Association for the Advancement of Science (AAAS), pp. 736–739, Aug. 05, 2011. doi: 10.1126/science.1207272.  
  
I. X. Green, W. Tang, M. Neurockand J. T. Yates Jr., “Localized Partial Oxidation of Acetic Acid at the Dual Perimeter Sites of the Au/TiO2 Catalyst—Formation of Gold Ketenylidene”, *Journal of the American Chemical Society*, vol. 134, no. 33. American Chemical Society (ACS), pp. 13569–13572, Aug. 13, 2012. doi: 10.1021/ja305911e.  
  
I. X. Green, W. Tang, M. Neurockand J. T. Yates Jr., “Insights into Catalytic Oxidation at the Au/TiO2 Dual Perimeter Sites”, *Accounts of Chemical Research*, vol. 47, no. 3. American Chemical Society (ACS), pp. 805–815, Dec. 30, 2013. doi: 10.1021/ar400196f.  
  
M. McEntee, A. Stevanovic, W. Tang, M. Neurockand J. T. Yates Jr., “Electric Field Changes on Au Nanoparticles on Semiconductor Supports – The Molecular Voltmeter and Other Methods to Observe Adsorbate-Induced Charge-Transfer Effects in Au/TiO2 Nanocatalysts”, *Journal of the American Chemical Society*, vol. 137, no. 5. American Chemical Society (ACS), pp. 1972–1982, Feb. 03, 2015. doi: 10.1021/ja511982n.  
  
M. McEntee, W. Tang, M. Neurockand J. T. Yates Jr, “Selective Catalytic Oxidative-Dehydrogenation of Carboxylic Acids—Acrylate and Crotonate Formation at the Au/TiO2 Interface”, *Journal of the American Chemical Society*, vol. 136, no. 13. American Chemical Society (ACS), pp. 5116–5120, Mar. 19, 2014. doi: 10.1021/ja500928h.  
  
M. McEntee, W. Tang, M. Neurockand J. T. Yates Jr., “Mechanistic Insights into the Catalytic Oxidation of Carboxylic Acids on Au/TiO2: Partial Oxidation of Propionic and Butyric Acid to Gold Ketenylidene through Unsaturated Acids”, *ACS Catalysis*, vol. 5, no. 2. American Chemical Society (ACS), pp. 744–753, Dec. 29, 2014. doi: 10.1021/cs5014255.  
  
P. Nandi, “Catalytic consequences of open and closed grafted Al(III)-calix[4]arene complexes for hydride and oxo transfer reactions”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 7. Proceedings of the National Academy of Sciences, pp. 2484–2489, Jan. 28, 2013. doi: 10.1073/pnas.1211158110.  
  
D. Panayotov, “Infrared studies of propene and propene oxide adsorption on nanoparticulate Au/TiO2”, *Surface Science*, vol. 652. Elsevier BV, pp. 172–182, Oct. 2016. doi: 10.1016/j.susc.2016.03.033.  
  
J. Wang, “Formation, Migration, and Reactivity of Au–CO Complexes on Gold Surfaces”, *Journal of the American Chemical Society*, vol. 138, no. 5. American Chemical Society (ACS), pp. 1518–1526, Jan. 28, 2016. doi: 10.1021/jacs.5b09052.  
  
Z. Zhang, W. Tang, M. Neurockand J. T. Yates Jr., “Electric Charge of Single Au Atoms Adsorbed on TiO2(110) and Associated Band Bending”, *The Journal of Physical Chemistry C*, vol. 115, no. 48. American Chemical Society (ACS), pp. 23848–23853, Nov. 15, 2011. doi: 10.1021/jp2067809.  
  
H. Cui, E. Lymanand G. A. Voth, “Mechanism of Membrane Curvature Sensing by Amphipathic Helix Containing Proteins”, *Biophysical Journal*, vol. 100, no. 5. Elsevier BV, pp. 1271–1279, Mar. 2011. doi: 10.1016/j.bpj.2011.01.036.  
  
H. Cui, C. Mim, F. X. Vázquez, E. Lyman, V. M. Ungerand G. A. Voth, “Understanding the Role of Amphipathic Helices in N-BAR Domain Driven Membrane Remodeling”, *Biophysical Journal*, vol. 104, no. 2. Elsevier BV, pp. 404–411, Jan. 2013. doi: 10.1016/j.bpj.2012.12.006.  
  
C. J. McGill and P. R. Westmoreland, “Monosaccharide Isomer Interconversions Become Significant at High Temperatures”, *The Journal of Physical Chemistry A*, vol. 123, no. 1. American Chemical Society (ACS), pp. 120–131, Nov. 28, 2018. doi: 10.1021/acs.jpca.8b07217.  
  
V. Seshadri and P. R. Westmoreland, “Concerted Reactions and Mechanism of Glucose Pyrolysis and Implications for Cellulose Kinetics”, *The Journal of Physical Chemistry A*, vol. 116, no. 49. American Chemical Society (ACS), pp. 11997–12013, Nov. 09, 2012. doi: 10.1021/jp3085099.  
  
V. Seshadri and P. R. Westmoreland, “Roles of hydroxyls in the noncatalytic and catalyzed formation of levoglucosan from glucose”, *Catalysis Today*, vol. 269. Elsevier BV, pp. 110–121, Jul. 2016. doi: 10.1016/j.cattod.2015.10.033.  
  
J. Wereszczynski and J. A. McCammon, “Nucleotide-dependent mechanism of Get3 as elucidated from free energy calculations”, *Proceedings of the National Academy of Sciences*, vol. 109, no. 20. Proceedings of the National Academy of Sciences, pp. 7759–7764, Apr. 30, 2012. doi: 10.1073/pnas.1117441109.  
  
D. C. Merrer and C. Doubleday, “Dynamic control of dichlorocarbene addition to cyclopropene”, *Journal of Physical Organic Chemistry*, vol. 24, no. 10. Wiley, pp. 947–951, Jul. 07, 2011. doi: 10.1002/poc.1883.  
  
C. D. Daub, D. Bratkoand A. Luzar, “Nanoscale Wetting Under Electric Field from Molecular Simulations”, *Multiscale Molecular Methods in Applied Chemistry*. Springer Berlin Heidelberg, pp. 155–179, 2011. doi: 10.1007/128\_2011\_188.  
  
C. D. Daub, D. Bratkoand A. Luzar, “Electric Control of Wetting by Salty Nanodrops: Molecular Dynamics Simulations”, *The Journal of Physical Chemistry C*, vol. 115, no. 45. American Chemical Society (ACS), pp. 22393–22399, Oct. 26, 2011. doi: 10.1021/jp206242n.  
  
C. D. Daub, J. Wang, S. Kudesia, D. Bratkoand A. Luzar, “The influence of molecular-scale roughness on the surface spreading of an aqueous nanodrop”, *Faraday Discussions*, vol. 146. Royal Society of Chemistry (RSC), p. 67, 2010. doi: 10.1039/b927061m.  
  
J. Wang, D. Bratkoand A. Luzar, “Probing surface tension additivity on chemically heterogeneous surfaces by a molecular approach”, *Proceedings of the National Academy of Sciences*, vol. 108, no. 16. Proceedings of the National Academy of Sciences, pp. 6374–6379, Apr. 2011. doi: 10.1073/pnas.1014970108.  
  
J. Wang, D. Bratkoand A. Luzar, “Length-Scale Dependence of Hydration Free Energy: Effect of Solute Charge”, *Journal of Statistical Physics*, vol. 145, no. 2. Springer Science and Business Media LLC, pp. 253–264, Sep. 13, 2011. doi: 10.1007/s10955-011-0337-1.  
  
J. Wang, S. Kudesia, D. Bratkoand A. Luzar, “Computational probe of cavitation events in protein systems”, *Physical Chemistry Chemical Physics*, vol. 13, no. 44. Royal Society of Chemistry (RSC), p. 19902, 2011. doi: 10.1039/c1cp22082a.  
  
C. D. Daub, N. M. Cann, D. Bratkoand A. Luzar, “Electrokinetic flow of an aqueous electrolyte in amorphous silica nanotubes”, *Physical Chemistry Chemical Physics*, vol. 20, no. 44. Royal Society of Chemistry (RSC), pp. 27838–27848, 2018. doi: 10.1039/c8cp03791d.  
  
B. S. Jabes, D. Bratkoand A. Luzar, “Curvature dependence of the effect of ionic functionalization on the attraction among nanoparticles in dispersion”, *The Journal of Chemical Physics*, vol. 148, no. 22. AIP Publishing, p. 222815, Jun. 14, 2018. doi: 10.1063/1.5017525.  
  
A. W. Götz, M. A. Clarkand R. C. Walker, “An extensible interface for QM/MM molecular dynamics simulations with AMBER”, *Journal of Computational Chemistry*, vol. 35, no. 2. Wiley, pp. 95–108, Oct. 09, 2013. doi: 10.1002/jcc.23444.  
  
S. L. Fiedler and J. Eloranta, “Interaction of Helium Rydberg State Atoms with Superfluid Helium”, *Journal of Low Temperature Physics*, vol. 174, no. 5–6. Springer Science and Business Media LLC, pp. 269–283, Dec. 15, 2013. doi: 10.1007/s10909-013-0991-6.  
  
S. L. Fiedler, D. Mateo, T. Aleksanyanand J. Eloranta, “Theoretical modeling of ion mobility in superfluidHe”, *Physical Review B*, vol. 86, no. 14. American Physical Society (APS), Oct. 19, 2012. doi: 10.1103/physrevb.86.144522.  
  
G. M. Hocky, L. Berthier, W. Koband D. R. Reichman, “Crossovers in the dynamics of supercooled liquids probed by an amorphous wall”, *Physical Review E*, vol. 89, no. 5. American Physical Society (APS), May 23, 2014. doi: 10.1103/physreve.89.052311.  
  
G. M. Hocky, T. E. Marklandand D. R. Reichman, “Growing Point-to-Set Length Scale Correlates with Growing Relaxation Times in Model Supercooled Liquids”, *Physical Review Letters*, vol. 108, no. 22. American Physical Society (APS), Jun. 01, 2012. doi: 10.1103/physrevlett.108.225506.  
  
G. M. Hocky and D. R. Reichman, “A small subset of normal modes mimics the properties of dynamical heterogeneity in a model supercooled liquid”, *The Journal of Chemical Physics*, vol. 138, no. 12. AIP Publishing, pp. 12A537, Mar. 28, 2013. doi: 10.1063/1.4790799.  
  
Z. A. Piazza, W.-L. Li, C. Romanescu, A. P. Sergeeva, L.-S. Wangand A. I. Boldyrev, “A photoelectron spectroscopy and *ab initio* study of B21−: Negatively charged boron clusters continue to be planar at 21”, *The Journal of Chemical Physics*, vol. 136, no. 10. AIP Publishing, p. 104310, Mar. 14, 2012. doi: 10.1063/1.3692967.  
  
A. P. Sergeeva, Z. A. Piazza, C. Romanescu, W.-L. Li, A. I. Boldyrevand L.-S. Wang, “B22– and B23–: All-Boron Analogues of Anthracene and Phenanthrene”, *Journal of the American Chemical Society*, vol. 134, no. 43. American Chemical Society (ACS), pp. 18065–18073, Oct. 17, 2012. doi: 10.1021/ja307605t.  
  
D. J. Arismendi-Arrieta, M. Riera, P. Bajaj, R. Prosmitiand F. Paesani, “i-TTM Model for Ab Initio-Based Ion–Water Interaction Potentials. 1. Halide–Water Potential Energy Functions”, *The Journal of Physical Chemistry B*, vol. 120, no. 8. American Chemical Society (ACS), pp. 1822–1832, Nov. 24, 2015. doi: 10.1021/acs.jpcb.5b09562.  
  
V. Babin, C. Leforestierand F. Paesani, “Development of a “First Principles” Water Potential with Flexible Monomers: Dimer Potential Energy Surface, VRT Spectrum, and Second Virial Coefficient”, *Journal of Chemical Theory and Computation*, vol. 9, no. 12. American Chemical Society (ACS), pp. 5395–5403, Nov. 25, 2013. doi: 10.1021/ct400863t.  
  
V. Babin, G. R. Meddersand F. Paesani, “Toward a Universal Water Model: First Principles Simulations from the Dimer to the Liquid Phase”, *The Journal of Physical Chemistry Letters*, vol. 3, no. 24. American Chemical Society (ACS), pp. 3765–3769, Dec. 06, 2012. doi: 10.1021/jz3017733.  
  
V. Babin, G. R. Meddersand F. Paesani, “Development of a “First Principles” Water Potential with Flexible Monomers. II: Trimer Potential Energy Surface, Third Virial Coefficient, and Small Clusters”, *Journal of Chemical Theory and Computation*, vol. 10, no. 4. American Chemical Society (ACS), pp. 1599–1607, Mar. 21, 2014. doi: 10.1021/ct500079y.  
  
V. Babin and F. Paesani, “The curious case of the water hexamer: Cage vs. Prism”, *Chemical Physics Letters*, vol. 580. Elsevier BV, pp. 1–8, Aug. 2013. doi: 10.1016/j.cplett.2013.06.041.  
  
P. Bajaj, A. W. Götzand F. Paesani, “Toward Chemical Accuracy in the Description of Ion–Water Interactions through Many-Body Representations. I. Halide–Water Dimer Potential Energy Surfaces”, *Journal of Chemical Theory and Computation*, vol. 12, no. 6. American Chemical Society (ACS), pp. 2698–2705, May 12, 2016. doi: 10.1021/acs.jctc.6b00302.  
  
P. Bajaj, X.-G. Wang, T. Carrington Jr.and F. Paesani, “Vibrational spectra of halide-water dimers: Insights on ion hydration from full-dimensional quantum calculations on many-body potential energy surfaces”, *The Journal of Chemical Physics*, vol. 148, no. 10. AIP Publishing, p. 102321, Mar. 14, 2018. doi: 10.1063/1.5005540.  
  
P. Bajaj, D. Zhuangand F. Paesani, “Specific Ion Effects on Hydrogen-Bond Rearrangements in the Halide–Dihydrate Complexes”, *The Journal of Physical Chemistry Letters*, vol. 10, no. 11. American Chemical Society (ACS), pp. 2823–2828, May 13, 2019. doi: 10.1021/acs.jpclett.9b00899.  
  
G. A. Cisneros, “Modeling Molecular Interactions in Water: From Pairwise to Many-Body Potential Energy Functions”, *Chemical Reviews*, vol. 116, no. 13. American Chemical Society (ACS), pp. 7501–7528, May 17, 2016. doi: 10.1021/acs.chemrev.5b00644.  
  
C. K. Egan, B. B. Bizzarro, M. Rieraand F. Paesani, “Nature of Alkali Ion–Water Interactions: Insights from Many-Body Representations and Density Functional Theory. II”, *Journal of Chemical Theory and Computation*, vol. 16, no. 5. American Chemical Society (ACS), pp. 3055–3072, Apr. 06, 2020. doi: 10.1021/acs.jctc.0c00082.  
  
C. K. Egan and F. Paesani, “Assessing Many-Body Effects of Water Self-Ions. I: OH–(H2O)*n* Clusters”, *Journal of Chemical Theory and Computation*, vol. 14, no. 4. American Chemical Society (ACS), pp. 1982–1997, Mar. 15, 2018. doi: 10.1021/acs.jctc.7b01273.  
  
C. K. Egan and F. Paesani, “Assessing Many-Body Effects of Water Self-Ions. II: H3O+(H2O)*n* Clusters”, *Journal of Chemical Theory and Computation*, vol. 15, no. 9. American Chemical Society (ACS), pp. 4816–4833, Jul. 25, 2019. doi: 10.1021/acs.jctc.9b00418.  
  
A. P. Gaiduk, T. A. Pham, M. Govoni, F. Paesaniand G. Galli, “Electron affinity of liquid water”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Jan. 16, 2018. doi: 10.1038/s41467-017-02673-z.  
  
G.-L. Hou, “Negative Ion Photoelectron Spectroscopy Reveals Thermodynamic Advantage of Organic Acids in Facilitating Formation of Bisulfate Ion Clusters: Atmospheric Implications”, *The Journal of Physical Chemistry Letters*, vol. 4, no. 5. American Chemical Society (ACS), pp. 779–785, Feb. 19, 2013. doi: 10.1021/jz400108y.  
  
W. Lin and F. Paesani, “Systematic Study of Structural and Thermodynamic Properties of HCl(H2O)*n* Clusters from Semiempirical Replica Exchange Simulations”, *The Journal of Physical Chemistry A*, vol. 117, no. 32. American Chemical Society (ACS), pp. 7131–7141, Apr. 16, 2013. doi: 10.1021/jp400629t.  
  
W. Lin and F. Paesani, “Infrared Spectra of HCl(H2O)*n* Clusters from Semiempirical Born–Oppenheimer Molecular Dynamics Simulations”, *The Journal of Physical Chemistry A*, vol. 119, no. 19. American Chemical Society (ACS), pp. 4450–4456, Nov. 25, 2014. doi: 10.1021/jp509791n.  
  
G. R. Medders, V. Babinand F. Paesani, “A Critical Assessment of Two-Body and Three-Body Interactions in Water”, *Journal of Chemical Theory and Computation*, vol. 9, no. 2. American Chemical Society (ACS), pp. 1103–1114, Jan. 16, 2013. doi: 10.1021/ct300913g.  
  
G. R. Medders, V. Babinand F. Paesani, “Development of a “First-Principles” Water Potential with Flexible Monomers. III. Liquid Phase Properties”, *Journal of Chemical Theory and Computation*, vol. 10, no. 8. American Chemical Society (ACS), pp. 2906–2910, Jul. 08, 2014. doi: 10.1021/ct5004115.  
  
G. R. Medders, A. W. Götz, M. A. Morales, P. Bajajand F. Paesani, “On the representation of many-body interactions in water”, *The Journal of Chemical Physics*, vol. 143, no. 10. AIP Publishing, p. 104102, Sep. 14, 2015. doi: 10.1063/1.4930194.  
  
G. R. Medders and F. Paesani, “Many-Body Convergence of the Electrostatic Properties of Water”, *Journal of Chemical Theory and Computation*, vol. 9, no. 11. American Chemical Society (ACS), pp. 4844–4852, Oct. 01, 2013. doi: 10.1021/ct400696d.  
  
G. R. Medders and F. Paesani, “Water Dynamics in Metal–Organic Frameworks: Effects of Heterogeneous Confinement Predicted by Computational Spectroscopy”, *The Journal of Physical Chemistry Letters*, vol. 5, no. 16. American Chemical Society (ACS), pp. 2897–2902, Aug. 11, 2014. doi: 10.1021/jz5013998.  
  
G. R. Medders and F. Paesani, “Infrared and Raman Spectroscopy of Liquid Water through “First-Principles” Many-Body Molecular Dynamics”, *Journal of Chemical Theory and Computation*, vol. 11, no. 3. American Chemical Society (ACS), pp. 1145–1154, Feb. 25, 2015. doi: 10.1021/ct501131j.  
  
G. R. Medders and F. Paesani, “On the interplay of the potential energy and dipole moment surfaces in controlling the infrared activity of liquid water”, *The Journal of Chemical Physics*, vol. 142, no. 21. AIP Publishing, p. 212411, Jun. 07, 2015. doi: 10.1063/1.4916629.  
  
G. R. Medders and F. Paesani, “Dissecting the Molecular Structure of the Air/Water Interface from Quantum Simulations of the Sum-Frequency Generation Spectrum”, *Journal of the American Chemical Society*, vol. 138, no. 11. American Chemical Society (ACS), pp. 3912–3919, Mar. 15, 2016. doi: 10.1021/jacs.6b00893.  
  
D. R. Moberg, “The end of ice I”, *Proceedings of the National Academy of Sciences*, vol. 116, no. 49. Proceedings of the National Academy of Sciences, pp. 24413–24419, Nov. 04, 2019. doi: 10.1073/pnas.1914254116.  
  
D. R. Moberg, S. C. Straight, C. Knightand F. Paesani, “Molecular Origin of the Vibrational Structure of Ice Ih”, *The Journal of Physical Chemistry Letters*, vol. 8, no. 12. American Chemical Society (ACS), pp. 2579–2583, May 26, 2017. doi: 10.1021/acs.jpclett.7b01106.  
  
D. R. Moberg, S. C. Straightand F. Paesani, “Temperature Dependence of the Air/Water Interface Revealed by Polarization Sensitive Sum-Frequency Generation Spectroscopy”, *The Journal of Physical Chemistry B*, vol. 122, no. 15. American Chemical Society (ACS), pp. 4356–4365, Apr. 03, 2018. doi: 10.1021/acs.jpcb.8b01726.  
  
V. O. Özçelik, Y. Li, W. Xiongand F. Paesani, “Modeling Spontaneous Charge Transfer at Metal/Organic Hybrid Heterostructures”, *The Journal of Physical Chemistry C*, vol. 124, no. 8. American Chemical Society (ACS), pp. 4802–4809, Jan. 30, 2020. doi: 10.1021/acs.jpcc.9b10055.  
  
F. Paesani, “Molecular Mechanisms of Water-Mediated Proton Transport in MIL-53 Metal–Organic Frameworks”, *The Journal of Physical Chemistry C*, vol. 117, no. 38. American Chemical Society (ACS), pp. 19508–19516, Sep. 26, 2013. doi: 10.1021/jp406163q.  
  
F. Paesani, “Getting the Right Answers for the Right Reasons: Toward Predictive Molecular Simulations of Water with Many-Body Potential Energy Functions”, *Accounts of Chemical Research*, vol. 49, no. 9. American Chemical Society (ACS), pp. 1844–1851, Aug. 22, 2016. doi: 10.1021/acs.accounts.6b00285.  
  
F. Paesani, P. Bajajand M. Riera, “Chemical accuracy in modeling halide ion hydration from many-body representations”, *Advances in Physics: X*, vol. 4, no. 1. Informa UK Limited, p. 1631212, Jan. 01, 2019. doi: 10.1080/23746149.2019.1631212.  
  
K. Park, W. Linand F. Paesani, “Fast and Slow Proton Transfer in Ice: The Role of the Quasi-Liquid Layer and Hydrogen-Bond Network”, *The Journal of Physical Chemistry B*, vol. 118, no. 28. American Chemical Society (ACS), pp. 8081–8089, Apr. 15, 2014. doi: 10.1021/jp501116d.  
  
C. H. Pham and F. Paesani, “Spin Crossover in the {Fe(pz)[Pt(CN)4]} Metal–Organic Framework upon Pyrazine Adsorption”, *The Journal of Physical Chemistry Letters*, vol. 7, no. 19. American Chemical Society (ACS), pp. 4022–4026, Sep. 28, 2016. doi: 10.1021/acs.jpclett.6b01788.  
  
K. L. Rallapalli, A. C. Komorand F. Paesani, “Computer simulations explain mutation-induced effects on the DNA editing by adenine base editors”, *Science Advances*, vol. 6, no. 10. American Association for the Advancement of Science (AAAS), Mar. 06, 2020. doi: 10.1126/sciadv.aaz2309.  
  
S. K. Reddy, D. R. Moberg, S. C. Straightand F. Paesani, “Temperature-dependent vibrational spectra and structure of liquid water from classical and quantum simulations with the MB-pol potential energy function”, *The Journal of Chemical Physics*, vol. 147, no. 24. AIP Publishing, p. 244504, Dec. 28, 2017. doi: 10.1063/1.5006480.  
  
M. Riera, A. W. Götzand F. Paesani, “The i-TTM model for ab initio-based ion–water interaction potentials. II. Alkali metal ion–water potential energy functions”, *Physical Chemistry Chemical Physics*, vol. 18, no. 44. Royal Society of Chemistry (RSC), pp. 30334–30343, 2016. doi: 10.1039/c6cp02553f.  
  
M. Riera, E. Lambros, T. T. Nguyen, A. W. Götzand F. Paesani, “Low-order many-body interactions determine the local structure of liquid water”, *Chemical Science*, vol. 10, no. 35. Royal Society of Chemistry (RSC), pp. 8211–8218, 2019. doi: 10.1039/c9sc03291f.  
  
M. Riera, N. Mardirossian, P. Bajaj, A. W. Götzand F. Paesani, “Toward chemical accuracy in the description of ion–water interactions through many-body representations. Alkali-water dimer potential energy surfaces”, *The Journal of Chemical Physics*, vol. 147, no. 16. AIP Publishing, p. 161715, Oct. 28, 2017. doi: 10.1063/1.4993213.  
  
M. Riera, E. P. Yehand F. Paesani, “Data-Driven Many-Body Models for Molecular Fluids: CO2/H2O Mixtures as a Case Study”, *Journal of Chemical Theory and Computation*, vol. 16, no. 4. American Chemical Society (ACS), pp. 2246–2257, Mar. 04, 2020. doi: 10.1021/acs.jctc.9b01175.  
  
A. Rieth, K. M. Hunter, M. Dincaand P. Lab, “Neither Solid Nor Liquid Nor Vapor: Hydrogen Bonding Structure of Water Confined in Metal-Organic Frameworks with Open Metal Sites”, *[]*. American Chemical Society (ACS), May 02, 2019. doi: 10.26434/chemrxiv.8059625.v1.  
  
A. J. Rieth, K. M. Hunter, M. Dincăand F. Paesani, “Hydrogen bonding structure of confined water templated by a metal-organic framework with open metal sites”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Oct. 18, 2019. doi: 10.1038/s41467-019-12751-z.  
  
M. Rossi, H. Liu, F. Paesani, J. Bowmanand M. Ceriotti, “Communication: On the consistency of approximate quantum dynamics simulation methods for vibrational spectra in the condensed phase”, *The Journal of Chemical Physics*, vol. 141, no. 18. AIP Publishing, p. 181101, Nov. 14, 2014. doi: 10.1063/1.4901214.  
  
J. Shin, “MIL-101(Fe) as a lithium-ion battery electrode material: a relaxation and intercalation mechanism during lithium insertion”, *Journal of Materials Chemistry A*, vol. 3, no. 8. Royal Society of Chemistry (RSC), pp. 4738–4744, 2015. doi: 10.1039/c4ta06694d.  
  
S. C. Straight and F. Paesani, “Exploring Electrostatic Effects on the Hydrogen Bond Network of Liquid Water through Many-Body Molecular Dynamics”, *The Journal of Physical Chemistry B*, vol. 120, no. 33. American Chemical Society (ACS), pp. 8539–8546, May 02, 2016. doi: 10.1021/acs.jpcb.6b02366.  
  
Z. L. Terranova, M. M. Ageeand F. Paesani, “Water Structure and Dynamics in Homochiral [Zn(*l*-L)(X)] Metal–Organic Frameworks”, *The Journal of Physical Chemistry C*, vol. 119, no. 32. American Chemical Society (ACS), pp. 18239–18247, Aug. 05, 2015. doi: 10.1021/acs.jpcc.5b04242.  
  
Y. Wang, V. Babin, J. M. Bowmanand F. Paesani, “The Water Hexamer: Cage, Prism, or Both. Full Dimensional Quantum Simulations Say Both”, *Journal of the American Chemical Society*, vol. 134, no. 27. American Chemical Society (ACS), pp. 11116–11119, Jun. 28, 2012. doi: 10.1021/ja304528m.  
  
Y. Zhai, A. Caruso, S. Gaoand F. Paesani, “Active learning of many-body configuration space: Application to the Cs+–water MB-nrg potential energy function as a case study”, *The Journal of Chemical Physics*, vol. 152, no. 14. AIP Publishing, p. 144103, Apr. 14, 2020. doi: 10.1063/5.0002162.  
  
T. T. Nguyen, “Comparison of permutationally invariant polynomials, neural networks, and Gaussian approximation potentials in representing water interactions through many-body expansions”, *The Journal of Chemical Physics*, vol. 148, no. 24. AIP Publishing, p. 241725, Jun. 28, 2018. doi: 10.1063/1.5024577.  
  
A. J. Bendelsmith, K. T. Kuwataand T. D. Varberg, “Hyperfine structure in the electronic spectrum of TaS”, *Journal of Molecular Spectroscopy*, vol. 276–277. Elsevier BV, pp. 14–18, Jun. 2012. doi: 10.1016/j.jms.2012.06.009.  
  
J. Hang, “Generation of Singlet Oxygen from Fragmentation of Monoactivated 1,1-Dihydroperoxides”, *The Journal of Organic Chemistry*, vol. 77, no. 3. American Chemical Society (ACS), pp. 1233–1243, Jan. 23, 2012. doi: 10.1021/jo202265j.  
  
J. Bame, C. Hoeck, M. J. Carrington, C. P. Butts, C. M. Jägerand A. K. Croft, “Improved NOE fitting for flexible molecules based on molecular mechanics data – a case study with *S*-adenosylmethionine”, *Physical Chemistry Chemical Physics*, vol. 20, no. 11. Royal Society of Chemistry (RSC), pp. 7523–7531, 2018. doi: 10.1039/c7cp07265a.  
  
C. J. Cadman and A. K. Croft, “Anion–π interactions influence p*K*a values”, *Beilstein Journal of Organic Chemistry*, vol. 7. Beilstein Institut, pp. 320–328, Mar. 17, 2011. doi: 10.3762/bjoc.7.42.  
  
A. K. Croft, H. M. Howard-Jones, C. E. Skatesand C. C. Wood, “Controlling the action of chlorine radical: from lab to environment”, *Organic & Biomolecular Chemistry*, vol. 9, no. 21. Royal Society of Chemistry (RSC), p. 7439, 2011. doi: 10.1039/c1ob00001b.  
  
D. P. Dowling, A. K. Croftand C. L. Drennan, “Radical Use of Rossmann and TIM Barrel Architectures for Controlling Coenzyme B12Chemistry”, *Annual Review of Biophysics*, vol. 41, no. 1. Annual Reviews, pp. 403–427, Jun. 09, 2012. doi: 10.1146/annurev-biophys-050511-102225.  
  
D. P. Dowling, “Structural elements of an NRPS cyclization domain and its intermodule docking domain”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 44. Proceedings of the National Academy of Sciences, pp. 12432–12437, Oct. 17, 2016. doi: 10.1073/pnas.1608615113.  
  
D. P. Dowling, J. L. Vey, A. K. Croftand C. L. Drennan, “Structural diversity in the AdoMet radical enzyme superfamily”, *Biochimica et Biophysica Acta (BBA) - Proteins and Proteomics*, vol. 1824, no. 11. Elsevier BV, pp. 1178–1195, Nov. 2012. doi: 10.1016/j.bbapap.2012.04.006.  
  
C. M. Jäger and A. K. Croft, “Radical Reaction Control in the AdoMet Radical Enzyme CDG Synthase (QueE): Consolidate, Destabilize, Accelerate”, *Chemistry - A European Journal*, vol. 23, no. 4. Wiley, pp. 953–962, Dec. 13, 2016. doi: 10.1002/chem.201604719.  
  
C. M. Jäger and A. K. Croft, “Anaerobic Radical Enzymes for Biotechnology”, *ChemBioEng Reviews*, vol. 5, no. 3. Wiley, pp. 143–162, Apr. 26, 2018. doi: 10.1002/cben.201800003.  
  
P. Deria, C. D. Von Bargen, J.-H. Olivier, A. S. Kumbhar, J. G. Savenand M. J. Therien, “Single-Handed Helical Wrapping of Single-Walled Carbon Nanotubes by Chiral, Ionic, Semiconducting Polymers”, *Journal of the American Chemical Society*, vol. 135, no. 43. American Chemical Society (ACS), pp. 16220–16234, Oct. 21, 2013. doi: 10.1021/ja408430v.  
  
M. J. Eibling, C. M. MacDermaid, Z. Qian, C. J. Lanci, S.-J. Parkand J. G. Saven, “Controlling Association and Separation of Gold Nanoparticles with Computationally Designed Zinc-Coordinating Proteins”, *Journal of the American Chemical Society*, vol. 139, no. 49. American Chemical Society (ACS), pp. 17811–17823, Nov. 30, 2017. doi: 10.1021/jacs.7b04786.  
  
L. Gao, W. Liu, O.-S. Lee, I. J. Dmochowskiand J. G. Saven, “Xe affinities of water-soluble cryptophanes and the role of confined water”, *Chemical Science*, vol. 6, no. 12. Royal Society of Chemistry (RSC), pp. 7238–7248, 2015. doi: 10.1039/c5sc02401c.  
  
M. J. Haider, “Self-assembly and soluble aggregate behavior of computationally designed coiled-coil peptide bundles”, *Soft Matter*, vol. 14, no. 26. Royal Society of Chemistry (RSC), pp. 5488–5496, 2018. doi: 10.1039/c8sm00435h.  
  
J. Ho, J. M. Perez-Aguilar, L. Gao, J. G. Saven, H. Matsunamiand R. G. Eckenhoff, “Molecular recognition of ketamine by a subset of olfactory G protein–coupled receptors”, *Science Signaling*, vol. 8, no. 370. American Association for the Advancement of Science (AAAS), Mar. 31, 2015. doi: 10.1126/scisignal.2005912.  
  
K. W. Pulsipher, J. A. Bulos, J. A. Villegas, J. G. Savenand I. J. Dmochowski, “A protein–protein host–guest complex: Thermostable ferritin encapsulating positively supercharged green fluorescent protein”, *Protein Science*, vol. 27, no. 10. Wiley, pp. 1755–1766, Oct. 2018. doi: 10.1002/pro.3483.  
  
K. W. Pulsipher, “Thermophilic Ferritin 24mer Assembly and Nanoparticle Encapsulation Modulated by Interdimer Electrostatic Repulsion”, *Biochemistry*, vol. 56, no. 28. American Chemical Society (ACS), pp. 3596–3606, Jul. 06, 2017. doi: 10.1021/acs.biochem.7b00296.  
  
S. Sathaye, “Engineering Complementary Hydrophobic Interactions to Control β-Hairpin Peptide Self-Assembly, Network Branching, and Hydrogel Properties”, *Biomacromolecules*, vol. 15, no. 11. American Chemical Society (ACS), pp. 3891–3900, Oct. 17, 2014. doi: 10.1021/bm500874t.  
  
Y. Tian, F. B. Polzer, H. V. Zhang, K. L. Kiick, J. G. Savenand D. J. Pochan, “Nanotubes, Plates, and Needles: Pathway-Dependent Self-Assembly of Computationally Designed Peptides”, *Biomacromolecules*, vol. 19, no. 11. American Chemical Society (ACS), pp. 4286–4298, Oct. 09, 2018. doi: 10.1021/acs.biomac.8b01163.  
  
Y. Tian, H. V. Zhang, K. L. Kiick, J. G. Savenand D. J. Pochan, “Fabrication of One- and Two-Dimensional Gold Nanoparticle Arrays on Computationally Designed Self-Assembled Peptide Templates”, *Chemistry of Materials*, vol. 30, no. 23. American Chemical Society (ACS), pp. 8510–8520, Nov. 12, 2018. doi: 10.1021/acs.chemmater.8b03206.  
  
C. D. Von Bargen, C. M. MacDermaid, O.-S. Lee, P. Deria, M. J. Therienand J. G. Saven, “Origins of the Helical Wrapping of Phenyleneethynylene Polymers about Single-Walled Carbon Nanotubes”, *The Journal of Physical Chemistry B*, vol. 117, no. 42. American Chemical Society (ACS), pp. 12953–12965, Aug. 14, 2013. doi: 10.1021/jp402140t.  
  
H. V. Zhang, “Computationally designed peptides for self-assembly of nanostructured lattices”, *Science Advances*, vol. 2, no. 9. American Association for the Advancement of Science (AAAS), Sep. 02, 2016. doi: 10.1126/sciadv.1600307.  
  
J. Ping, “pH Sensing Properties of Flexible, Bias‐Free Graphene Microelectrodes in Complex Fluids: From Phosphate Buffer Solution to Human Serum”, *Small*, vol. 13, no. 30. Wiley, p. 1700564, Jun. 14, 2017. doi: 10.1002/smll.201700564.  
  
Y. Tian, H. V. Zhang, K. L. Kiick, J. G. Savenand D. J. Pochan, “Transition from disordered aggregates to ordered lattices: kinetic control of the assembly of a computationally designed peptide”, *Organic & Biomolecular Chemistry*, vol. 15, no. 29. Royal Society of Chemistry (RSC), pp. 6109–6118, 2017. doi: 10.1039/c7ob01197k.  
  
C. A. Brosey, “Functional Dynamics in Replication Protein A DNA Binding and Protein Recruitment Domains”, *Structure*, vol. 23, no. 6. Elsevier BV, pp. 1028–1038, Jun. 2015. doi: 10.1016/j.str.2015.04.008.  
  
C. A. Brosey, “A new structural framework for integrating replication protein A into DNA processing machinery”, *Nucleic Acids Research*, vol. 41, no. 4. Oxford University Press (OUP), pp. 2313–2327, Jan. 07, 2013. doi: 10.1093/nar/gks1332.  
  
E. K. Carter, S. Laughlin-Toth, T. Dodd, W. D. Wilsonand I. Ivanov, “Small molecule binders recognize DNA microstructural variations *via* an induced fit mechanism”, *Physical Chemistry Chemical Physics*, vol. 21, no. 4. Royal Society of Chemistry (RSC), pp. 1841–1851, 2019. doi: 10.1039/c8cp05537h.  
  
T. Dodd, C. Yan, B. R. Kossmann, K. Martinand I. Ivanov, “Uncovering universal rules governing the selectivity of the archetypal DNA glycosylase TDG”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 23. Proceedings of the National Academy of Sciences, pp. 5974–5979, May 21, 2018. doi: 10.1073/pnas.1803323115.  
  
S. Fritsch, I. Ivanov, H. Wangand X. Cheng, “Ion Selectivity Mechanism in a Bacterial Pentameric Ligand-Gated Ion Channel”, *Biophysical Journal*, vol. 100, no. 2. Elsevier BV, pp. 390–398, Jan. 2011. doi: 10.1016/j.bpj.2010.11.077.  
  
Y. Han, C. Yan, S. Fishbain, I. Ivanovand Y. He, “Structural visualization of RNA polymerase III transcription machineries”, *Cell Discovery*, vol. 4, no. 1. Springer Science and Business Media LLC, Jul. 31, 2018. doi: 10.1038/s41421-018-0044-z.  
  
Y. Han, “Structural mechanism of ATP-independent transcription initiation by RNA polymerase I”, *eLife*, vol. 6. eLife Sciences Publications, Ltd, Jun. 17, 2017. doi: 10.7554/elife.27414.  
  
Y. He, “Near-atomic resolution visualization of human transcription promoter opening”, *Nature*, vol. 533, no. 7603. Springer Science and Business Media LLC, pp. 359–365, May 11, 2016. doi: 10.1038/nature17970.  
  
W. H. Hudson, “Distal substitutions drive divergent DNA specificity among paralogous transcription factors through subdivision of conformational space”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 2. Proceedings of the National Academy of Sciences, pp. 326–331, Dec. 29, 2015. doi: 10.1073/pnas.1518960113.  
  
B. R. Kossmann, “Discovery of selective inhibitors of tyrosyl-DNA phosphodiesterase 2 by targeting the enzyme DNA-binding cleft”, *Bioorganic & Medicinal Chemistry Letters*, vol. 26, no. 14. Elsevier BV, pp. 3232–3236, Jul. 2016. doi: 10.1016/j.bmcl.2016.05.065.  
  
B. Kossmann and I. Ivanov, “Alkylpurine Glycosylase D Employs DNA Sculpting as a Strategy to Extrude and Excise Damaged Bases”, *PLoS Computational Biology*, vol. 10, no. 7. Public Library of Science (PLoS), p. e1003704, Jul. 03, 2014. doi: 10.1371/journal.pcbi.1003704.  
  
S. Laughlin-Toth, E. K. Carter, I. Ivanovand W. D. Wilson, “DNA microstructure influences selective binding of small molecules designed to target mixed-site DNA sequences”, *Nucleic Acids Research*, vol. 45, no. 3. Oxford University Press (OUP), pp. 1297–1306, Dec. 09, 2016. doi: 10.1093/nar/gkw1232.  
  
J. Li, “Natural Product Micheliolide (MCL) Irreversibly Activates Pyruvate Kinase M2 and Suppresses Leukemia”, *Journal of Medicinal Chemistry*, vol. 61, no. 9. American Chemical Society (ACS), pp. 4155–4164, Apr. 11, 2018. doi: 10.1021/acs.jmedchem.8b00241.  
  
P. M. Musille, B. R. Kossmann, J. A. Kohn, I. Ivanovand E. A. Ortlund, “Unexpected Allosteric Network Contributes to LRH-1 Co-regulator Selectivity”, *Journal of Biological Chemistry*, vol. 291, no. 3. Elsevier BV, pp. 1411–1426, Jan. 2016. doi: 10.1074/jbc.m115.662874.  
  
S. K. Perumal, X. Xu, C. Yan, I. Ivanovand S. J. Benkovic, “Recognition of a Key Anchor Residue by a Conserved Hydrophobic Pocket Ensures Subunit Interface Integrity in DNA Clamps”, *Journal of Molecular Biology*, vol. 431, no. 14. Elsevier BV, pp. 2493–2510, Jun. 2019. doi: 10.1016/j.jmb.2019.04.035.  
  
J. Querol-Audí, “Repair complexes of FEN1 endonuclease, DNA, and Rad9-Hus1-Rad1 are distinguished from their PCNA counterparts by functionally important stability”, *Proceedings of the National Academy of Sciences*, vol. 109, no. 22. Proceedings of the National Academy of Sciences, pp. 8528–8533, May 14, 2012. doi: 10.1073/pnas.1121116109.  
  
F. Rashid, “Single-molecule FRET unveils induced-fit mechanism for substrate selectivity in flap endonuclease 1”, *eLife*, vol. 6. eLife Sciences Publications, Ltd, Feb. 23, 2017. doi: 10.7554/elife.21884.  
  
T. Sander, B. Frølund, A. T. Bruun, I. Ivanov, J. A. McCammonand T. Balle, “New insights into the GABAAreceptor structure and orthosteric ligand binding: Receptor modeling guided by experimental data”, *Proteins: Structure, Function, and Bioinformatics*, vol. 79, no. 5. Wiley, pp. 1458–1477, Mar. 01, 2011. doi: 10.1002/prot.22975.  
  
J. A. Tainer, J. A. McCammonand I. Ivanov, “Recognition of the Ring-Opened State of Proliferating Cell Nuclear Antigen by Replication Factor C Promotes Eukaryotic Clamp-Loading”, *Journal of the American Chemical Society*, vol. 132, no. 21. American Chemical Society (ACS), pp. 7372–7378, May 10, 2010. doi: 10.1021/ja100365x.  
  
S. E. Tsutakawa, “Solution X-ray scattering combined with computational modeling reveals multiple conformations of covalently bound ubiquitin on PCNA”, *Proceedings of the National Academy of Sciences*, vol. 108, no. 43. Proceedings of the National Academy of Sciences, pp. 17672–17677, Oct. 17, 2011. doi: 10.1073/pnas.1110480108.  
  
S. E. Tsutakawa, “Structurally Distinct Ubiquitin- and Sumo-Modified PCNA: Implications for Their Distinct Roles in the DNA Damage Response”, *Structure*, vol. 23, no. 4. Elsevier BV, pp. 724–733, Apr. 2015. doi: 10.1016/j.str.2015.02.008.  
  
R. C. Turaga, “Rational design of a protein that binds integrin αvβ3 outside the ligand binding site”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, May 31, 2016. doi: 10.1038/ncomms11675.  
  
L. Wang, “Probing DNA clamps with single-molecule force spectroscopy”, *Nucleic Acids Research*, vol. 41, no. 16. Oxford University Press (OUP), pp. 7804–7814, Jun. 19, 2013. doi: 10.1093/nar/gkt487.  
  
X. Xu, C. Guardiani, C. Yanand I. Ivanov, “Opening pathways of the DNA clamps proliferating cell nuclear antigen and Rad9-Rad1-Hus1”, *Nucleic Acids Research*, vol. 41, no. 22. Oxford University Press (OUP), pp. 10020–10031, Sep. 12, 2013. doi: 10.1093/nar/gkt810.  
  
X. Xu, C. Yan, B. R. Kossmannand I. Ivanov, “Secondary Interaction Interfaces with PCNA Control Conformational Switching of DNA Polymerase PolB from Polymerization to Editing”, *The Journal of Physical Chemistry B*, vol. 120, no. 33. American Chemical Society (ACS), pp. 8379–8388, May 04, 2016. doi: 10.1021/acs.jpcb.6b02082.  
  
X. Xu, C. Yan, R. Wohlhueterand I. Ivanov, “Integrative Modeling of Macromolecular Assemblies from Low to Near-Atomic Resolution”, *Computational and Structural Biotechnology Journal*, vol. 13. Elsevier BV, pp. 492–503, 2015. doi: 10.1016/j.csbj.2015.08.005.  
  
C. Yan, T. Dodd, Y. He, J. A. Tainer, S. E. Tsutakawaand I. Ivanov, “Transcription preinitiation complex structure and dynamics provide insight into genetic diseases”, *Nature Structural & Molecular Biology*, vol. 26, no. 6. Springer Science and Business Media LLC, pp. 397–406, May 20, 2019. doi: 10.1038/s41594-019-0220-3.  
  
L. Yan, “Diamidine Compounds for Selective Inhibition of Protein Arginine Methyltransferase 1”, *Journal of Medicinal Chemistry*, vol. 57, no. 6. American Chemical Society (ACS), pp. 2611–2622, Mar. 06, 2014. doi: 10.1021/jm401884z.  
  
J. Zhang, “Discovery of decamidine as a new and potent PRMT1 inhibitor”, *MedChemComm*, vol. 8, no. 2. Royal Society of Chemistry (RSC), pp. 440–444, 2017. doi: 10.1039/c6md00573j.  
  
S. Er, C. Suh, M. P. Marshakand A. Aspuru-Guzik, “Computational design of molecules for an all-quinone redox flow battery”, *Chemical Science*, vol. 6, no. 2. Royal Society of Chemistry (RSC), pp. 885–893, 2015. doi: 10.1039/c4sc03030c.  
  
J. Hachmann, “Lead candidates for high-performance organic photovoltaics from high-throughput quantum chemistry – the Harvard Clean Energy Project”, *Energy Environ. Sci.*, vol. 7, no. 2. Royal Society of Chemistry (RSC), pp. 698–704, 2014. doi: 10.1039/c3ee42756k.  
  
B. Huskinson, “A metal-free organic–inorganic aqueous flow battery”, *Nature*, vol. 505, no. 7482. Springer Science and Business Media LLC, pp. 195–198, Jan. 2014. doi: 10.1038/nature12909.  
  
A. Jinich, “Quantum Chemical Approach to Estimating the Thermodynamics of Metabolic Reactions”, *Scientific Reports*, vol. 4, no. 1. Springer Science and Business Media LLC, Nov. 12, 2014. doi: 10.1038/srep07022.  
  
L. T. Sein Jr. and L. J. Forsyth, “Adsorption of quinonediimines on aluminum(100): A computational and FT-IR study”, *Synthetic Metals*, vol. 162, no. 24. Elsevier BV, pp. 2390–2400, Dec. 2012. doi: 10.1016/j.synthmet.2012.11.020.  
  
D. Bao, “Dipole-Mediated Rectification of Intramolecular Photoinduced Charge Separation and Charge Recombination”, *Journal of the American Chemical Society*, vol. 136, no. 37. American Chemical Society (ACS), pp. 12966–12973, Sep. 08, 2014. doi: 10.1021/ja505618n.  
  
G. J. O. Beran, “Solid state photodimerization of 9-*tert*-butyl anthracene ester produces an exceptionally metastable polymorph according to first-principles calculations”, *CrystEngComm*, vol. 21, no. 4. Royal Society of Chemistry (RSC), pp. 758–764, 2019. doi: 10.1039/c8ce01985a.  
  
P. M. Bogie, “A Springloaded Metal-Ligand Mesocate Allows Access to Trapped Intermediates of Self-Assembly”, *Inorganic Chemistry*, vol. 57, no. 7. American Chemical Society (ACS), pp. 4155–4163, Mar. 21, 2018. doi: 10.1021/acs.inorgchem.8b00370.  
  
C. Červinka and G. J. O. Beran, “*Ab initio*prediction of the polymorph phase diagram for crystalline methanol”, *Chemical Science*, vol. 9, no. 20. Royal Society of Chemistry (RSC), pp. 4622–4629, 2018. doi: 10.1039/c8sc01237g.  
  
C. Červinka and G. J. O. Beran, “Towards reliable *ab initio* sublimation pressures for organic molecular crystals – are we there yet?”, *Physical Chemistry Chemical Physics*, vol. 21, no. 27. Royal Society of Chemistry (RSC), pp. 14799–14810, 2019. doi: 10.1039/c9cp01572h.  
  
M. Dračínský, P. Unzuetaand G. J. O. Beran, “Improving the accuracy of solid-state nuclear magnetic resonance chemical shift prediction with a simple molecular correction”, *Physical Chemistry Chemical Physics*, vol. 21, no. 27. Royal Society of Chemistry (RSC), pp. 14992–15000, 2019. doi: 10.1039/c9cp01666j.  
  
C. Greenwell, “Overcoming the difficulties of predicting conformational polymorph energetics in molecular crystals *via* correlated wavefunction methods”, *Chemical Science*, vol. 11, no. 8. Royal Society of Chemistry (RSC), pp. 2200–2214, 2020. doi: 10.1039/c9sc05689k.  
  
J. D. Hartman, A. Balajiand G. J. O. Beran, “Improved Electrostatic Embedding for Fragment-Based Chemical Shift Calculations in Molecular Crystals”, *Journal of Chemical Theory and Computation*, vol. 13, no. 12. American Chemical Society (ACS), pp. 6043–6051, Nov. 15, 2017. doi: 10.1021/acs.jctc.7b00677.  
  
J. D. Hartman and G. J. O. Beran, “Fragment-Based Electronic Structure Approach for Computing Nuclear Magnetic Resonance Chemical Shifts in Molecular Crystals”, *Journal of Chemical Theory and Computation*, vol. 10, no. 11. American Chemical Society (ACS), pp. 4862–4872, Oct. 24, 2014. doi: 10.1021/ct500749h.  
  
J. D. Hartman and G. J. O. Beran, “Accurate 13-C and 15-N molecular crystal chemical shielding tensors from fragment-based electronic structure theory”, *Solid State Nuclear Magnetic Resonance*, vol. 96. Elsevier BV, pp. 10–18, Dec. 2018. doi: 10.1016/j.ssnmr.2018.09.003.  
  
J. D. Hartman, G. M. Dayand G. J. O. Beran, “Enhanced NMR Discrimination of Pharmaceutically Relevant Molecular Crystal Forms through Fragment-Based Ab Initio Chemical Shift Predictions”, *Crystal Growth & Design*, vol. 16, no. 11. American Chemical Society (ACS), pp. 6479–6493, Oct. 04, 2016. doi: 10.1021/acs.cgd.6b01157.  
  
J. D. Hartman, R. A. Kudla, G. M. Day, L. J. Muellerand G. J. O. Beran, “Benchmark fragment-based1H,13C,15N and17O chemical shift predictions in molecular crystals”, *Physical Chemistry Chemical Physics*, vol. 18, no. 31. Royal Society of Chemistry (RSC), pp. 21686–21709, 2016. doi: 10.1039/c6cp01831a.  
  
Y. Heit and G. J. O. Beran, “Exploiting space-group symmetry in fragment-based molecular crystal calculations”, *Journal of Computational Chemistry*, vol. 35, no. 30. Wiley, pp. 2205–2214, Oct. 01, 2014. doi: 10.1002/jcc.23737.  
  
Y. N. Heit and G. J. O. Beran, “How important is thermal expansion for predicting molecular crystal structures and thermochemistry at finite temperatures?”, *Acta Crystallographica Section B Structural Science, Crystal Engineering and Materials*, vol. 72, no. 4. International Union of Crystallography (IUCr), pp. 514–529, Jul. 16, 2016. doi: 10.1107/s2052520616005382.  
  
Y. N. Heit, K. D. Nandaand G. J. O. Beran, “Predicting finite-temperature properties of crystalline carbon dioxide from first principles with quantitative accuracy”, *Chemical Science*, vol. 7, no. 1. Royal Society of Chemistry (RSC), pp. 246–255, 2016. doi: 10.1039/c5sc03014e.  
  
L. R. Holloway, H. H. McGarraugh, M. C. Young, W. Sontising, G. J. O. Beranand R. J. Hooley, “Structural switching in self-assembled metal–ligand helicate complexes via ligand-centered reactions”, *Chemical Science*, vol. 7, no. 7. Royal Society of Chemistry (RSC), pp. 4423–4427, 2016. doi: 10.1039/c6sc01038e.  
  
Y. Huang and G. J. O. Beran, “Reliable prediction of three-body intermolecular interactions using dispersion-corrected second-order Møller-Plesset perturbation theory”, *The Journal of Chemical Physics*, vol. 143, no. 4. AIP Publishing, p. 044113, Jul. 28, 2015. doi: 10.1063/1.4927304.  
  
M. Krzeszewski, “Dipole Effects on Electron Transfer are Enormous”, *Angewandte Chemie International Edition*, vol. 57, no. 38. Wiley, pp. 12365–12369, Jun. 14, 2018. doi: 10.1002/anie.201802637.  
  
J. L. McKinley and G. J. O. Beran, “Identifying pragmatic quasi-harmonic electronic structure approaches for modeling molecular crystal thermal expansion”, *Faraday Discussions*, vol. 211. Royal Society of Chemistry (RSC), pp. 181–207, 2018. doi: 10.1039/c8fd00048d.  
  
J. L. McKinley and G. J. O. Beran, “Improving Predicted Nuclear Magnetic Resonance Chemical Shifts Using the Quasi-Harmonic Approximation”, *Journal of Chemical Theory and Computation*, vol. 15, no. 10. American Chemical Society (ACS), pp. 5259–5274, Aug. 23, 2019. doi: 10.1021/acs.jctc.9b00481.  
  
T. F. Miller, “Small Structural Variations Have Large Effects on the Assembly Properties and Spin State of Room Temperature High Spin Fe(II) Iminopyridine Cages”, *Inorganic Chemistry*, vol. 57, no. 21. American Chemical Society (ACS), pp. 13386–13396, Oct. 05, 2018. doi: 10.1021/acs.inorgchem.8b01973.  
  
D. Nocito and G. J. O. Beran, “Averaged Condensed Phase Model for Simulating Molecules in Complex Environments”, *Journal of Chemical Theory and Computation*, vol. 13, no. 3. American Chemical Society (ACS), pp. 1117–1129, Feb. 07, 2017. doi: 10.1021/acs.jctc.6b00890.  
  
D. Nocito and G. J. O. Beran, “Fast divide-and-conquer algorithm for evaluating polarization in classical force fields”, *The Journal of Chemical Physics*, vol. 146, no. 11. AIP Publishing, p. 114103, Mar. 21, 2017. doi: 10.1063/1.4977981.  
  
D. Nocito and G. J. O. Beran, “Massively Parallel Implementation of Divide-and-Conquer Jacobi Iterations Using Particle-Mesh Ewald for Force Field Polarization”, *Journal of Chemical Theory and Computation*, vol. 14, no. 7. American Chemical Society (ACS), pp. 3633–3642, May 30, 2018. doi: 10.1021/acs.jctc.8b00328.  
  
D. Nocito and G. J. O. Beran, “Reduced computational cost of polarizable force fields by a modification of the always stable predictor-corrector”, *The Journal of Chemical Physics*, vol. 150, no. 15. AIP Publishing, p. 151103, Apr. 21, 2019. doi: 10.1063/1.5092133.  
  
J. Řezáč, C. Greenwelland G. J. O. Beran, “Accurate Noncovalent Interactions via Dispersion-Corrected Second-Order Møller–Plesset Perturbation Theory”, *Journal of Chemical Theory and Computation*, vol. 14, no. 9. American Chemical Society (ACS), pp. 4711–4721, Aug. 07, 2018. doi: 10.1021/acs.jctc.8b00548.  
  
W. Sontising and G. J. O. Beran, “Theoretical assessment of the structure and stability of the phase of nitrogen”, *Physical Review Materials*, vol. 3, no. 9. American Physical Society (APS), Sep. 13, 2019. doi: 10.1103/physrevmaterials.3.095002.  
  
W. Sontising, Y. N. Heit, J. L. McKinleyand G. J. O. Beran, “Theoretical predictions suggest carbon dioxide phases III and VII are identical”, *Chem. Sci.*, vol. 8, no. 11. Royal Society of Chemistry (RSC), pp. 7374–7382, 2017. doi: 10.1039/c7sc03267f.  
  
C. Yang, “Crystal structure of the meta-stable intermediate in the photomechanical, crystal-to-crystal reaction of 9-tert-butyl anthracene ester”, *CrystEngComm*, vol. 18, no. 38. Royal Society of Chemistry (RSC), pp. 7319–7329, 2016. doi: 10.1039/c6ce00742b.  
  
E. M. Curtis, X. Xiao, S. Sofouand C. K. Hall, “Phase Separation Behavior of Mixed Lipid Systems at Neutral and Low pH: Coarse-Grained Simulations with DMD/LIME”, *Langmuir*, vol. 31, no. 3. American Chemical Society (ACS), pp. 1086–1094, Jan. 15, 2015. doi: 10.1021/la504082x.  
  
Q. Shao and C. K. Hall, “A Discontinuous Potential Model for Protein–Protein Interactions”, *Foundations of Molecular Modeling and Simulation*. Springer Singapore, pp. 1–20, 2016. doi: 10.1007/978-981-10-1128-3\_1.  
  
Q. Shao and C. K. Hall, “Allosteric effects of gold nanoparticles on human serum albumin”, *Nanoscale*, vol. 9, no. 1. Royal Society of Chemistry (RSC), pp. 380–390, 2017. doi: 10.1039/c6nr07665c.  
  
J. L. Spears, X. Xiao, C. K. Halland P. F. Agris, “Amino Acid Signature Enables Proteins to Recognize Modified tRNA”, *Biochemistry*, vol. 53, no. 7. American Chemical Society (ACS), pp. 1125–1133, Feb. 14, 2014. doi: 10.1021/bi401174h.  
  
X. Xiao, P. F. Agrisand C. K. Hall, “Molecular recognition mechanism of peptide chain bound to the tRNALys3anticodon loop*in silico*”, *Journal of Biomolecular Structure and Dynamics*, vol. 33, no. 1. Informa UK Limited, pp. 14–27, Jan. 13, 2014. doi: 10.1080/07391102.2013.869660.  
  
X. Xiao, P. F. Agrisand C. K. Hall, “Designing Peptide Sequences in Flexible Chain Conformations to Bind RNA: A Search Algorithm Combining Monte Carlo, Self-Consistent Mean Field and Concerted Rotation Techniques”, *Journal of Chemical Theory and Computation*, vol. 11, no. 2. American Chemical Society (ACS), pp. 740–752, Feb. 02, 2015. doi: 10.1021/ct5008247.  
  
X. Xiao, C. K. Halland P. F. Agris, “The design of a peptide sequence to inhibit HIV replication: a search algorithm combining Monte Carlo and self-consistent mean field techniques”, *Journal of Biomolecular Structure and Dynamics*, vol. 32, no. 10. Informa UK Limited, pp. 1523–1536, Oct. 23, 2013. doi: 10.1080/07391102.2013.825757.  
  
X. Xiao, Y. Wang, J. N. Leonardand C. K. Hall, “Extended Concerted Rotation Technique Enhances the Sampling Efficiency of the Computational Peptide-Design Algorithm”, *Journal of Chemical Theory and Computation*, vol. 13, no. 11. American Chemical Society (ACS), pp. 5709–5720, Oct. 27, 2017. doi: 10.1021/acs.jctc.7b00714.  
  
X. Xiao, B. Zhao, P. F. Agrisand C. K. Hall, “Simulation study of the ability of a computationally‐designed peptide to recognize target tRNA Lys3 and other decoy tRNAs”, *Protein Science*, vol. 25, no. 12. Wiley, pp. 2243–2255, Oct. 07, 2016. doi: 10.1002/pro.3056.  
  
B. Zhao, M. A. Cohen Stuartand C. K. Hall, “Dock ‘n roll: folding of a silk-inspired polypeptide into an amyloid-like beta solenoid”, *Soft Matter*, vol. 12, no. 16. Royal Society of Chemistry (RSC), pp. 3721–3729, 2016. doi: 10.1039/c6sm00169f.  
  
B. Zhao, N. K. Li, Y. G. Yinglingand C. K. Hall, “LCST Behavior is Manifested in a Single Molecule: Elastin-Like polypeptide (VPGVG)*n*”, *Biomacromolecules*, vol. 17, no. 1. American Chemical Society (ACS), pp. 111–118, Dec. 07, 2015. doi: 10.1021/acs.biomac.5b01235.  
  
C. L. Muhich, Y. Zhou, A. M. Holder, A. W. Weimerand C. B. Musgrave, “Effect of Surface Deposited Pt on the Photoactivity of TiO2”, *The Journal of Physical Chemistry C*, vol. 116, no. 18. American Chemical Society (ACS), pp. 10138–10149, Apr. 30, 2012. doi: 10.1021/jp301862m.  
  
Y. Zhou, C. L. Muhich, B. T. Neltner, A. W. Weimerand C. B. Musgrave, “Growth of Pt Particles on the Anatase TiO2 (101) Surface”, *The Journal of Physical Chemistry C*, vol. 116, no. 22. American Chemical Society (ACS), pp. 12114–12123, May 29, 2012. doi: 10.1021/jp302273m.  
  
G. Li, “Transition-metal-free formal cross-coupling of aryl methyl sulfoxides and alcohols via nucleophilic activation of C-S bond”, *Nature Communications*, vol. 11, no. 1. Springer Science and Business Media LLC, Jun. 08, 2020. doi: 10.1038/s41467-020-16713-8.  
  
B. Qu, “Rational Design of New Dihydrobenzooxophosphole-Based Lewis Base Organocatalysts”, *Synlett*, vol. 31, no. 6. Georg Thieme Verlag KG, pp. 587–591, Mar. 12, 2020. doi: 10.1055/s-0039-1690851.  
  
S. Tcyrulnikov and M. C. Kozlowski, “Accounting for Strong Ligand Sensitivity in Pd-Catalyzed α-Arylation of Enolates from Ketones, Esters, and Nitroalkanes”, *The Journal of Organic Chemistry*, vol. 85, no. 5. American Chemical Society (ACS), pp. 3465–3472, Jan. 29, 2020. doi: 10.1021/acs.joc.9b03203.  
  
S. E. Allen, S.-Y. Hsieh, O. Gutierrez, J. W. Bodeand M. C. Kozlowski, “Concerted Amidation of Activated Esters: Reaction Path and Origins of Selectivity in the Kinetic Resolution of Cyclic Amines via N-Heterocyclic Carbenes and Hydroxamic Acid Cocatalyzed Acyl Transfer”, *Journal of the American Chemical Society*, vol. 136, no. 33. American Chemical Society (ACS), pp. 11783–11791, Aug. 08, 2014. doi: 10.1021/ja505784w.  
  
B. Yuan, J.-W. Shinand E. R. Bernstein, “Dynamics and fragmentation of van der Waals and hydrogen bonded cluster cations: (NH3)n and (NH3BH3)n ionized at 10.51 eV”, *The Journal of Chemical Physics*, vol. 144, no. 14. AIP Publishing, p. 144315, Apr. 14, 2016. doi: 10.1063/1.4945624.  
  
T. E. Morrell, I. U. Rafalska-Metcalf, J.-W. Chuand H. Yang, “Coupling between Protein Conformation and Local Unfolding Highlights the Role of Disorder in Protein Function and Suggests a New Target for Tuberculosis Treatment”, *Biophysical Journal*, vol. 106, no. 2. Elsevier BV, p. 257a, Jan. 2014. doi: 10.1016/j.bpj.2013.11.1509.  
  
J. Ahn, T. Kent, E. Chagarov, K. Tang, A. C. Kummeland P. C. McIntyre, “Arsenic decapping and pre-atomic layer deposition trimethylaluminum passivation of Al2O3/InGaAs(100) interfaces”, *Applied Physics Letters*, vol. 103, no. 7. AIP Publishing, p. 071602, Aug. 12, 2013. doi: 10.1063/1.4818330.  
  
S. R. Bishop, J. B. Clemens, E. A. Chagarov, J. Shenand A. C. Kummel, “Theoretical analysis of initial adsorption of high-κ metal oxides on InxGa1−xAs(0 0 1)-(4×2) surfaces”, *The Journal of Chemical Physics*, vol. 133, no. 19. AIP Publishing, p. 194702, Nov. 21, 2010. doi: 10.1063/1.3501371.  
  
E. A. Chagarov and A. C. Kummel, “Density Functional Theory Simulations of High-k Oxides on III-V Semiconductors”, *Fundamentals of III-V Semiconductor MOSFETs*. Springer US, pp. 93–130, 2010. doi: 10.1007/978-1-4419-1547-4\_5.  
  
E. A. Chagarov and A. C. Kummel, “Density functional theory simulations of amorphous high-κ oxides on a compound semiconductor alloy: a-Al2O3/InGaAs(100)-(4×2), a-HfO2/InGaAs(100)-(4×2), and a-ZrO2/InGaAs(100)-(4×2)”, *The Journal of Chemical Physics*, vol. 135, no. 24. AIP Publishing, p. 244705, Dec. 28, 2011. doi: 10.1063/1.3657439.  
  
E. A. Chagarov, L. Porterand A. C. Kummel, “Density-functional theory molecular dynamics simulations of a-HfO2/Ge(100)(2 × 1) and a-ZrO2/Ge(100)(2 × 1) interface passivation”, *The Journal of Chemical Physics*, vol. 144, no. 8. AIP Publishing, p. 084704, Feb. 28, 2016. doi: 10.1063/1.4941947.  
  
E. Chagarov, K. Sardashti, M. Edmonds, M. Clemonsand A. Kummel, “Density functional theory simulations and experimental measurements of a-HfO<inf>2</inf>/a-Si<inf>3</inf>N<inf>4</inf>/SiGe, a-HfO<inf>2</inf>/SiO<inf>0.8</inf>N<inf>0.8</inf>/SiGe and a-HfO<inf>2</inf>/a-SiO/SiGe interfaces”, *2016 IEEE International Electron Devices Meeting (IEDM)*. IEEE, Dec. 2016. doi: 10.1109/iedm.2016.7838554.  
  
E. Chagarov, K. Sardashti, R. Haight, D. B. Mitziand A. C. Kummel, “Density-functional theory computer simulations of CZTS0.25Se0.75 alloy phase diagrams”, *The Journal of Chemical Physics*, vol. 145, no. 6. AIP Publishing, p. 064704, Aug. 09, 2016. doi: 10.1063/1.4959591.  
  
E. Chagarov, “Density-Functional Theory Molecular Dynamics Simulations and Experimental Characterization of a-Al2O3/SiGe Interfaces”, *ACS Applied Materials & Interfaces*, vol. 7, no. 47. American Chemical Society (ACS), pp. 26275–26283, Nov. 17, 2015. doi: 10.1021/acsami.5b08727.  
  
E. Chagarov, K. Sardashti, A. C. Kummel, Y. S. Lee, R. Haightand T. S. Gershon, “Ag2ZnSn(S,Se)4: A highly promising absorber for thin film photovoltaics”, *The Journal of Chemical Physics*, vol. 144, no. 10. AIP Publishing, p. 104704, Mar. 14, 2016. doi: 10.1063/1.4943270.  
  
J. B. Clemens, E. A. Chagarov, M. Holland, R. Droopad, J. Shenand A. C. Kummel, “Atomic imaging of the monolayer nucleation and unpinning of a compound semiconductor surface during atomic layer deposition”, *The Journal of Chemical Physics*, vol. 133, no. 15. AIP Publishing, p. 154704, Oct. 21, 2010. doi: 10.1063/1.3487737.  
  
M. Edmonds, “Passivation of InGaAs(001)-(2 × 4) by Self-Limiting Chemical Vapor Deposition of a Silicon Hydride Control Layer”, *Journal of the American Chemical Society*, vol. 137, no. 26. American Chemical Society (ACS), pp. 8526–8533, Jun. 23, 2015. doi: 10.1021/jacs.5b03660.  
  
M. Edmonds, “Passivation of surface defects on InGaAs (001) and (110) surfaces in preparation for subsequent gate oxide ALD”, *2015 International Symposium on VLSI Technology, Systems and Applications*. IEEE, Apr. 2015. doi: 10.1109/vlsi-tsa.2015.7117580.  
  
M. Edmonds, W. Melitz, T. J. Kent, E. Chagarovand A. C. Kummel, “(Invited) Surface Preparation and In/Ga Alloying Effects on InGaAs(001)-(2x4) Surfaces For ALD Gate Oxide Deposition”, *ECS Transactions*, vol. 50, no. 4. The Electrochemical Society, pp. 129–140, Mar. 15, 2013. doi: 10.1149/05004.0129ecst.  
  
M. Edmonds, “Low temperature thermal ALD of a SiNx interfacial diffusion barrier and interface passivation layer on SixGe1− x(001) and SixGe1− x(110)”, *The Journal of Chemical Physics*, vol. 146, no. 5. AIP Publishing, p. 052820, Feb. 07, 2017. doi: 10.1063/1.4975081.  
  
M. Edmonds, “Self-limiting CVD of a passivating SiO x control layer on InGaAs(001)-(2x4) with the prevention of III-V oxidation”, *Surface Science*, vol. 660. Elsevier BV, pp. 31–38, Jun. 2017. doi: 10.1016/j.susc.2017.02.006.  
  
S. Gu, “Characterization of interface and border traps in ALD Al2O3/GaN MOS capacitors with two-step surface pretreatments on Ga-polar GaN”, *Applied Surface Science*, vol. 317. Elsevier BV, pp. 1022–1027, Oct. 2014. doi: 10.1016/j.apsusc.2014.09.028.  
  
R. Haight, “Industrial perspectives on earth abundant, multinary thin film photovoltaics”, *Semiconductor Science and Technology*, vol. 32, no. 3. IOP Publishing, p. 033004, Feb. 28, 2017. doi: 10.1088/1361-6641/aa5c18.  
  
T. Kaufman-Osborn, E. A. Chagarovand A. C. Kummel, “Atomic imaging and modeling of H2O2(g) surface passivation, functionalization, and atomic layer deposition nucleation on the Ge(100) surface”, *The Journal of Chemical Physics*, vol. 140, no. 20. AIP Publishing, p. 204708, May 28, 2014. doi: 10.1063/1.4878496.  
  
T. Kaufman-Osborn, E. A. Chagarov, S. W. Park, B. Sahu, S. Siddiquiand A. C. Kummel, “Atomic imaging and modeling of passivation, functionalization, and atomic layer deposition nucleation of the SiGe(001) surface via H2O2(g) and trimethylaluminum dosing”, *Surface Science*, vol. 630. Elsevier BV, pp. 273–279, Dec. 2014. doi: 10.1016/j.susc.2014.08.027.  
  
T. Kent, E. Chagarov, M. Edmonds, R. Droopadand A. C. Kummel, “Dual Passivation of Intrinsic Defects at the Compound Semiconductor/Oxide Interface Using an Oxidant and a Reductant”, *ACS Nano*, vol. 9, no. 5. American Chemical Society (ACS), pp. 4843–4849, Apr. 21, 2015. doi: 10.1021/nn5063003.  
  
T. J. Kent, M. Edmonds, E. Chagarov, R. Droopadand A. C. Kummel, “Dual passivation of GaAs (110) surfaces using O2/H2O and trimethylaluminum”, *The Journal of Chemical Physics*, vol. 139, no. 24. AIP Publishing, p. 244706, Dec. 28, 2013. doi: 10.1063/1.4852155.  
  
A. J. Kerr, “Preparation of gallium nitride surfaces for atomic layer deposition of aluminum oxide”, *The Journal of Chemical Physics*, vol. 141, no. 10. AIP Publishing, p. 104702, Sep. 14, 2014. doi: 10.1063/1.4894541.  
  
J. S. Lee, S. R. Bishop, T. Kaufman-Osborn, E. Chagarovand A. C. Kummel, “Monolayer Passivation of Ge(100) Surface via Nitridation and Oxidation”, *ECS Transactions*, vol. 33, no. 6. The Electrochemical Society, pp. 447–454, Oct. 01, 2010. doi: 10.1149/1.3487575.  
  
W. Melitz, “Mechanism of dangling bond elimination on As-rich InGaAs surface”, *2012 International Electron Devices Meeting*. IEEE, Dec. 2012. doi: 10.1109/iedm.2012.6479152.  
  
W. Melitz, “Scanning Probe Microscopy Imaging before and after Atomic Layer Oxide Deposition on a Compound Semiconductor Surface”, *Solid State Phenomena*, vol. 187. Trans Tech Publications, Ltd., pp. 9–10, Apr. 2012. doi: 10.4028/www.scientific.net/ssp.187.9.  
  
J. H. Park, “Atomic Imaging of the Irreversible Sensing Mechanism of NO2 Adsorption on Copper Phthalocyanine”, *Journal of the American Chemical Society*, vol. 135, no. 39. American Chemical Society (ACS), pp. 14600–14609, Sep. 17, 2013. doi: 10.1021/ja403752r.  
  
S. W. Park, “Combined wet and dry cleaning of SiGe(001)”, *Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films*, vol. 33, no. 4. American Vacuum Society, p. 041403, Jul. 2015. doi: 10.1116/1.4922282.  
  
S. W. Park, “Chemically selective formation of Si–O–Al on SiGe(110) and (001) for ALD nucleation using H2O2(g)”, *Surface Science*, vol. 652. Elsevier BV, pp. 322–333, Oct. 2016. doi: 10.1016/j.susc.2016.01.009.  
  
M. Rodwell, “III&#x2013;V FET channel designs for high current densities and thin inversion layers”, *68th Device Research Conference*. IEEE, Jun. 2010. doi: 10.1109/drc.2010.5551882.  
  
M. J. W. Rodwell, “III-V MOSFETs: Scaling laws, scaling limits, fabrication processes”, *2010 22nd International Conference on Indium Phosphide and Related Materials (IPRM)*. IEEE, May 2010. doi: 10.1109/iciprm.2010.5515914.  
  
K. Sardashti, “Nanoscale Characterization of Back Surfaces and Interfaces in Thin-Film Kesterite Solar Cells”, *ACS Applied Materials & Interfaces*, vol. 9, no. 20. American Chemical Society (ACS), pp. 17024–17033, May 09, 2017. doi: 10.1021/acsami.7b01838.  
  
K. Sardashti, “Impact of Nanoscale Elemental Distribution in High-Performance Kesterite Solar Cells”, *Advanced Energy Materials*, vol. 5, no. 10. Wiley, p. 1402180, Mar. 13, 2015. doi: 10.1002/aenm.201402180.  
  
J. Shen, “Scanning tunneling microscopy/spectroscopy study of atomic and electronic structures of In2O on InAs and In0.53Ga0.47As(001)-(4×2) surfaces”, *The Journal of Chemical Physics*, vol. 133, no. 16. AIP Publishing, p. 164704, Oct. 28, 2010. doi: 10.1063/1.3497040.  
  
J. Shen, “Structural and electronic properties of group III Rich In0.53Ga0.47As(001)”, *Surface Science*, vol. 604, no. 19–20. Elsevier BV, pp. 1757–1766, Sep. 2010. doi: 10.1016/j.susc.2010.07.001.  
  
G. A. Cisneros, “Application of Gaussian Electrostatic Model (GEM) Distributed Multipoles in the AMOEBA Force Field”, *Journal of Chemical Theory and Computation*, vol. 8, no. 12. American Chemical Society (ACS), pp. 5072–5080, Sep. 06, 2012. doi: 10.1021/ct300630u.  
  
G. A. Cisneros, M. Karttunen, P. Renand C. Sagui, “Classical Electrostatics for Biomolecular Simulations”, *Chemical Reviews*, vol. 114, no. 1. American Chemical Society (ACS), pp. 779–814, Aug. 27, 2013. doi: 10.1021/cr300461d.  
  
D. Fang, R. E. Dukeand G. A. Cisneros, “A new smoothing function to introduce long-range electrostatic effects in QM/MM calculations”, *The Journal of Chemical Physics*, vol. 143, no. 4. AIP Publishing, p. 044103, Jul. 28, 2015. doi: 10.1063/1.4926652.  
  
D. Fang, R. L. Lordand G. A. Cisneros, “*Ab Initio* QM/MM Calculations Show an Intersystem Crossing in the Hydrogen Abstraction Step in Dealkylation Catalyzed by AlkB”, *The Journal of Physical Chemistry B*, vol. 117, no. 21. American Chemical Society (ACS), pp. 6410–6420, May 16, 2013. doi: 10.1021/jp403116e.  
  
E. G. Kratz, R. E. Dukeand G. A. Cisneros, “Long-range electrostatic corrections in multipolar/polarizable QM/MM simulations”, *Theoretical Chemistry Accounts*, vol. 135, no. 7. Springer Science and Business Media LLC, Jun. 17, 2016. doi: 10.1007/s00214-016-1923-8.  
  
M. Y. Liu, “Mutations along a TET2 active site scaffold stall oxidation at 5-hydroxymethylcytosine”, *Nature Chemical Biology*, vol. 13, no. 2. Springer Science and Business Media LLC, pp. 181–187, Dec. 05, 2016. doi: 10.1038/nchembio.2250.  
  
Y.-J. Tu, M. J. Allenand G. A. Cisneros, “Simulations of the water exchange dynamics of lanthanide ions in 1-ethyl-3-methylimidazolium ethyl sulfate ([EMIm][EtSO4]) and water”, *Physical Chemistry Chemical Physics*, vol. 18, no. 44. Royal Society of Chemistry (RSC), pp. 30323–30333, 2016. doi: 10.1039/c6cp04957e.  
  
W. A. Alexander, J. Zhang, V. J. Murray, G. M. Nathansonand T. K. Minton, “Kinematics and dynamics of atomic-beam scattering on liquid and self-assembled monolayer surfaces”, *Faraday Discussions*, vol. 157. Royal Society of Chemistry (RSC), p. 355, 2012. doi: 10.1039/c2fd20034a.  
  
G. R. Jenness and J. R. Schmidt, “Unraveling the Role of Metal–Support Interactions in Heterogeneous Catalysis: Oxygenate Selectivity in Fischer–Tropsch Synthesis”, *ACS Catalysis*, vol. 3, no. 12. American Chemical Society (ACS), pp. 2881–2890, Nov. 08, 2013. doi: 10.1021/cs4006277.  
  
A. S. Jalilov, “Structure and Electronic Spectra of Purine–Methyl Viologen Charge Transfer Complexes”, *The Journal of Physical Chemistry B*, vol. 118, no. 1. American Chemical Society (ACS), pp. 125–133, Dec. 23, 2013. doi: 10.1021/jp410348b.  
  
A. P. Sergeeva, Z. A. Piazza, C. Romanescu, W.-L. Li, A. I. Boldyrevand L.-S. Wang, “B22– and B23–: All-Boron Analogues of Anthracene and Phenanthrene”, *Journal of the American Chemical Society*, vol. 134, no. 43. American Chemical Society (ACS), pp. 18065–18073, Oct. 17, 2012. doi: 10.1021/ja307605t.  
  
J. R. Choudhuri, D. Vanzo, P. A. Madden, M. Salanne, D. Bratkoand A. Luzar, “Dynamic Response in Nanoelectrowetting on a Dielectric”, *ACS Nano*, vol. 10, no. 9. American Chemical Society (ACS), pp. 8536–8544, Aug. 29, 2016. doi: 10.1021/acsnano.6b03753.  
  
J. Driskill, D. Vanzo, D. Bratkoand A. Luzar, “Wetting transparency of graphene in water”, *The Journal of Chemical Physics*, vol. 141, no. 18. AIP Publishing, pp. 18C517, Nov. 14, 2014. doi: 10.1063/1.4895541.  
  
B. S. Jabes, D. Bratkoand A. Luzar, “Extent of Surface Force Additivity on Chemically Heterogeneous Substrates at Varied Orientations”, *The Journal of Physical Chemistry B*, vol. 122, no. 13. American Chemical Society (ACS), pp. 3596–3603, Nov. 29, 2017. doi: 10.1021/acs.jpcb.7b10790.  
  
B. S. Jabes, J. Driskill, D. Vanzo, D. Bratkoand A. Luzar, “Metastable Vapor in a Janus Nanoconfinement”, *The Journal of Physical Chemistry C*, vol. 121, no. 24. American Chemical Society (ACS), pp. 13144–13150, Jun. 07, 2017. doi: 10.1021/acs.jpcc.7b02147.  
  
F. Moučka, S. Zamfir, D. Bratkoand A. Luzar, “Molecular polarizability in open ensemble simulations of aqueous nanoconfinements under electric field”, *The Journal of Chemical Physics*, vol. 150, no. 16. AIP Publishing, p. 164702, Apr. 28, 2019. doi: 10.1063/1.5094170.  
  
N. Ojaghlou, H. V. Tafreshi, D. Bratkoand A. Luzar, “Dynamical insights into the mechanism of a droplet detachment from a fiber”, *Soft Matter*, vol. 14, no. 44. Royal Society of Chemistry (RSC), pp. 8924–8934, 2018. doi: 10.1039/c8sm01257a.  
  
J. A. Ritchie, J. S. Yazdi, D. Bratkoand A. Luzar, “Metastable Sessile Nanodroplets on Nanopatterned Surfaces”, *The Journal of Physical Chemistry C*, vol. 116, no. 15. American Chemical Society (ACS), pp. 8634–8641, Apr. 10, 2012. doi: 10.1021/jp300166h.  
  
M. Shafiei, N. Ojaghlou, S. G. Zamfir, D. Bratkoand A. Luzar, “Modulation of structure and dynamics of water under alternating electric field and the role of hydrogen bonding”, *Molecular Physics*, vol. 117, no. 22. Informa UK Limited, pp. 3282–3296, Aug. 09, 2019. doi: 10.1080/00268976.2019.1651919.  
  
M. Shafiei, M. von Domaros, D. Bratkoand A. Luzar, “Anisotropic structure and dynamics of water under static electric fields”, *The Journal of Chemical Physics*, vol. 150, no. 7. AIP Publishing, p. 074505, Feb. 21, 2019. doi: 10.1063/1.5079393.  
  
D. Vanzo, D. Bratkoand A. Luzar, “Wettability of pristine and alkyl-functionalized graphane”, *The Journal of Chemical Physics*, vol. 137, no. 3. AIP Publishing, p. 034707, Jul. 21, 2012. doi: 10.1063/1.4732520.  
  
D. Vanzo, D. Bratkoand A. Luzar, “Tunable Wetting of Surfaces with Ionic Functionalities”, *The Journal of Physical Chemistry C*, vol. 116, no. 29. American Chemical Society (ACS), pp. 15467–15473, Jul. 13, 2012. doi: 10.1021/jp3044384.  
  
D. Vanzo, D. Bratkoand A. Luzar, “Nanoconfined water under electric field at constant chemical potential undergoes electrostriction”, *The Journal of Chemical Physics*, vol. 140, no. 7. AIP Publishing, p. 074710, Feb. 21, 2014. doi: 10.1063/1.4865126.  
  
D. Vanzo, D. Bratkoand A. Luzar, “Dynamic Control of Nanopore Wetting in Water and Saline Solutions under an Electric Field”, *The Journal of Physical Chemistry B*, vol. 119, no. 29. American Chemical Society (ACS), pp. 8890–8899, Oct. 15, 2014. doi: 10.1021/jp506389p.  
  
M. von Domaros, D. Bratko, B. Kirchner, G. Hummerand A. Luzar, “Multifaceted Water Dynamics in Spherical Nanocages”, *The Journal of Physical Chemistry C*, vol. 123, no. 10. American Chemical Society (ACS), pp. 5989–5998, Feb. 15, 2019. doi: 10.1021/acs.jpcc.8b11567.  
  
M. von Domaros, D. Bratko, B. Kirchnerand A. Luzar, “Dynamics at a Janus Interface”, *The Journal of Physical Chemistry C*, vol. 117, no. 9. American Chemical Society (ACS), pp. 4561–4567, Feb. 20, 2013. doi: 10.1021/jp3111259.  
  
D. J. Bustos, B. Temelsoand G. C. Shields, “Hydration of the Sulfuric Acid–Methylamine Complex and Implications for Aerosol Formation”, *The Journal of Physical Chemistry A*, vol. 118, no. 35. American Chemical Society (ACS), pp. 7430–7441, Apr. 28, 2014. doi: 10.1021/jp500015t.  
  
C. Pérez, “Broadband Fourier transform rotational spectroscopy for structure determination: The water heptamer”, *Chemical Physics Letters*, vol. 571. Elsevier BV, pp. 1–15, May 2013. doi: 10.1016/j.cplett.2013.04.014.  
  
C. Pérez, “Structures of Cage, Prism, and Book Isomers of Water Hexamer from Broadband Rotational Spectroscopy”, *Science*, vol. 336, no. 6083. American Association for the Advancement of Science (AAAS), pp. 897–901, May 18, 2012. doi: 10.1126/science.1220574.  
  
C. Pérez, “Corannulene and its complex with water: a tiny cup of water”, *Physical Chemistry Chemical Physics*, vol. 19, no. 22. Royal Society of Chemistry (RSC), pp. 14214–14223, 2017. doi: 10.1039/c7cp01506b.  
  
C. Pérez, “Hydrogen Bond Cooperativity and the Three-Dimensional Structures of Water Nonamers and Decamers”, *Angewandte Chemie International Edition*, vol. 53, no. 52. Wiley, pp. 14368–14372, Oct. 27, 2014. doi: 10.1002/anie.201407447.  
  
J. O. Richardson, “Concerted hydrogen-bond breaking by quantum tunneling in the water hexamer prism”, *Science*, vol. 351, no. 6279. American Association for the Advancement of Science (AAAS), pp. 1310–1313, Mar. 18, 2016. doi: 10.1126/science.aae0012.  
  
A. L. Steber, “Capturing the Elusive Water Trimer from the Stepwise Growth of Water on the Surface of the Polycyclic Aromatic Hydrocarbon Acenaphthene”, *The Journal of Physical Chemistry Letters*, vol. 8, no. 23. American Chemical Society (ACS), pp. 5744–5750, Nov. 13, 2017. doi: 10.1021/acs.jpclett.7b02695.  
  
B. Temelso, T. Köddermann, K. N. Kirschner, K. Kleinand G. C. Shields, “Structure and thermodynamics of H3O+(H2O)8 clusters: A combined molecular dynamics and quantum mechanics approach”, *Computational and Theoretical Chemistry*, vol. 1021. Elsevier BV, pp. 240–248, Oct. 2013. doi: 10.1016/j.comptc.2013.07.039.  
  
R. Baron and N. A. Vellore, “LSD1/CoREST is an allosteric nanoscale clamp regulated by H3-histone-tail molecular recognition”, *Proceedings of the National Academy of Sciences*, vol. 109, no. 31. Proceedings of the National Academy of Sciences, pp. 12509–12514, Jul. 16, 2012. doi: 10.1073/pnas.1207892109.  
  
M. B. Tsinberg, R. Chindamand J. D. Gough, “Structural and charge-transfer properties of indolylfulgides”, *International Journal of Quantum Chemistry*, vol. 113, no. 15. Wiley, pp. 1949–1955, Mar. 05, 2013. doi: 10.1002/qua.24421.  
  
M. Z. Chen, O. Gutierrezand A. B. Smith III, “Through-Bond/Through-Space Anion Relay Chemistry Exploiting Vinylepoxides as Bifunctional Linchpins”, *Angewandte Chemie International Edition*, vol. 53, no. 5. Wiley, pp. 1279–1282, Dec. 16, 2013. doi: 10.1002/anie.201309270.  
  
J.-N. Desrosiers, “Nickel-catalyzed C-3 direct arylation of pyridinium ions for the synthesis of 1-azafluorenes”, *Chemical Science*, vol. 7, no. 8. Royal Society of Chemistry (RSC), pp. 5581–5586, 2016. doi: 10.1039/c6sc01457g.  
  
J.-N. Desrosiers, “Enantioselective Nickel-Catalyzed Mizoroki–Heck Cyclizations To Generate Quaternary Stereocenters”, *Organic Letters*, vol. 19, no. 13. American Chemical Society (ACS), pp. 3338–3341, Jun. 12, 2017. doi: 10.1021/acs.orglett.7b01054.  
  
J. S. Dickstein, J. M. Curto, O. Gutierrez, C. A. Mulrooneyand M. C. Kozlowski, “Mild Aromatic Palladium-Catalyzed Protodecarboxylation: Kinetic Assessment of the Decarboxylative Palladation and the Protodepalladation Steps”, *The Journal of Organic Chemistry*, vol. 78, no. 10. American Chemical Society (ACS), pp. 4744–4761, Apr. 29, 2013. doi: 10.1021/jo400222c.  
  
O. Gutierrez, “Practical, Asymmetric Route to Sitagliptin and Derivatives: Development and Origin of Diastereoselectivity”, *Organic Letters*, vol. 17, no. 7. American Chemical Society (ACS), pp. 1742–1745, Mar. 23, 2015. doi: 10.1021/acs.orglett.5b00520.  
  
O. Gutierrez, J. C. Tellis, D. N. Primer, G. A. Molanderand M. C. Kozlowski, “Nickel-Catalyzed Cross-Coupling of Photoredox-Generated Radicals: Uncovering a General Manifold for Stereoconvergence in Nickel-Catalyzed Cross-Couplings”, *Journal of the American Chemical Society*, vol. 137, no. 15. American Chemical Society (ACS), pp. 4896–4899, Apr. 08, 2015. doi: 10.1021/ja513079r.  
  
M. Li, “Transition-metal-free chemo- and regioselective vinylation of azaallyls”, *Nature Chemistry*, vol. 9, no. 10. Springer Science and Business Media LLC, pp. 997–1004, Apr. 17, 2017. doi: 10.1038/nchem.2760.  
  
A. E. Metz, K. Ramalingamand M. C. Kozlowski, “Xanthene-4,5-diamine derivatives: a study of anion-binding catalysis”, *Tetrahedron Letters*, vol. 56, no. 37. Elsevier BV, pp. 5180–5184, Sep. 2015. doi: 10.1016/j.tetlet.2015.07.058.  
  
N. D. Patel, “Computationally Assisted Mechanistic Investigation and Development of Pd-Catalyzed Asymmetric Suzuki–Miyaura and Negishi Cross-Coupling Reactions for Tetra-*ortho*-Substituted Biaryl Synthesis”, *ACS Catalysis*, vol. 8, no. 11. American Chemical Society (ACS), pp. 10190–10209, Sep. 20, 2018. doi: 10.1021/acscatal.8b02509.  
  
B. Qu, “Enantioselective Synthesis of α-(Hetero)aryl Piperidines through Asymmetric Hydrogenation of Pyridinium Salts and Its Mechanistic Insights”, *Organic Letters*, vol. 20, no. 5. American Chemical Society (ACS), pp. 1333–1337, Feb. 20, 2018. doi: 10.1021/acs.orglett.8b00067.  
  
L. Raffier, O. Gutierrez, G. R. Stanton, M. C. Kozlowskiand P. J. Walsh, “Alkenes as Chelating Groups in Diastereoselective Additions of Organometallics to Ketones”, *Organometallics*, vol. 33, no. 19. American Chemical Society (ACS), pp. 5371–5377, Sep. 09, 2014. doi: 10.1021/om5007006.  
  
S.-C. Sha, “Cation−π Interactions in the Benzylic Arylation of Toluenes with Bimetallic Catalysts”, *Journal of the American Chemical Society*, vol. 140, no. 39. American Chemical Society (ACS), pp. 12415–12423, Sep. 05, 2018. doi: 10.1021/jacs.8b05143.  
  
B. Wanner, I. Kreituss, O. Gutierrez, M. C. Kozlowskiand J. W. Bode, “Catalytic Kinetic Resolution of Disubstituted Piperidines by Enantioselective Acylation: Synthetic Utility and Mechanistic Insights”, *Journal of the American Chemical Society*, vol. 137, no. 35. American Chemical Society (ACS), pp. 11491–11497, Aug. 26, 2015. doi: 10.1021/jacs.5b07201.  
  
X. Wei, “Sequential C–H Arylation and Enantioselective Hydrogenation Enables Ideal Asymmetric Entry to the Indenopiperidine Core of an 11β-HSD-1 Inhibitor”, *Journal of the American Chemical Society*, vol. 138, no. 47. American Chemical Society (ACS), pp. 15473–15481, Nov. 17, 2016. doi: 10.1021/jacs.6b09764.  
  
O. V. Zatolochnaya, “Copper-catalyzed asymmetric hydrogenation of 2-substituted ketones *via* dynamic kinetic resolution”, *Chemical Science*, vol. 9, no. 19. Royal Society of Chemistry (RSC), pp. 4505–4510, 2018. doi: 10.1039/c8sc00434j.  
  
Y. Zou, “A Computational Investigation of the Ligand-Controlled Cu-Catalyzed Site-Selective Propargylation and Allenylation of Carbonyl Compounds”, *Organic Letters*, vol. 19, no. 22. American Chemical Society (ACS), pp. 6064–6067, Nov. 02, 2017. doi: 10.1021/acs.orglett.7b02845.  
  
A. W. Götz, D. Bucher, S. Lindertand J. A. McCammon, “Dipeptide Aggregation in Aqueous Solution from Fixed Point-Charge Force Fields”, *Journal of Chemical Theory and Computation*, vol. 10, no. 4. American Chemical Society (ACS), pp. 1631–1637, Mar. 19, 2014. doi: 10.1021/ct401049q.  
  
S. Gozem, F. Melaccio, H. L. Luk, S. Rinaldiand M. Olivucci, “Learning from photobiology how to design molecular devices using a computer”, *Chem. Soc. Rev.*, vol. 43, no. 12. Royal Society of Chemistry (RSC), pp. 4019–4036, 2014. doi: 10.1039/c4cs00037d.  
  
S. Gozem, “Shape of Multireference, Equation-of-Motion Coupled-Cluster, and Density Functional Theory Potential Energy Surfaces at a Conical Intersection”, *Journal of Chemical Theory and Computation*, vol. 10, no. 8. American Chemical Society (ACS), pp. 3074–3084, Jun. 11, 2014. doi: 10.1021/ct500154k.  
  
S. Gozem, E. Mirzakulova, I. Schapiro, F. Melaccio, K. D. Glusacand M. Olivucci, “A Conical Intersection Controls the Deactivation of the Bacterial Luciferase Fluorophore”, *Angewandte Chemie International Edition*, vol. 53, no. 37. Wiley, pp. 9870–9875, Jul. 14, 2014. doi: 10.1002/anie.201404011.  
  
S. Rinaldi, F. Melaccio, S. Gozem, F. Fanelliand M. Olivucci, “Comparison of the isomerization mechanisms of human melanopsin and invertebrate and vertebrate rhodopsins”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 5. Proceedings of the National Academy of Sciences, pp. 1714–1719, Jan. 21, 2014. doi: 10.1073/pnas.1309508111.  
  
I. Schapiro, S. Fusi, M. Olivucci, T. Andruniów, S. Sasidharanpillaiand G. R. Loppnow, “Initial Excited-State Dynamics of an*N*-Alkylated Indanylidene–Pyrroline (NAIP) Rhodopsin Analog”, *The Journal of Physical Chemistry B*, vol. 118, no. 42. American Chemical Society (ACS), pp. 12243–12250, Oct. 10, 2014. doi: 10.1021/jp508060z.  
  
J. A. Bogart, “Homoleptic Cerium(III) and Cerium(IV) Nitroxide Complexes: Significant Stabilization of the 4+ Oxidation State”, *Inorganic Chemistry*, vol. 52, no. 19. American Chemical Society (ACS), pp. 11600–11607, Sep. 11, 2013. doi: 10.1021/ic401974t.  
  
A. J. Lewis, P. J. Carrolland E. J. Schelter, “Reductive Cleavage of Nitrite to Form Terminal Uranium Mono-Oxo Complexes”, *Journal of the American Chemical Society*, vol. 135, no. 1. American Chemical Society (ACS), pp. 511–518, Dec. 18, 2012. doi: 10.1021/ja311057y.  
  
A. J. Lewis, P. J. Carrolland E. J. Schelter, “Stable Uranium(VI) Methyl and Acetylide Complexes and the Elucidation of an Inverse Trans Influence Ligand Series”, *Journal of the American Chemical Society*, vol. 135, no. 35. American Chemical Society (ACS), pp. 13185–13192, Aug. 22, 2013. doi: 10.1021/ja406610r.  
  
A. J. Lewis, U. J. Williams, P. J. Carrolland E. J. Schelter, “Tetrakis(bis(trimethylsilyl)amido)uranium(IV): Synthesis and Reactivity”, *Inorganic Chemistry*, vol. 52, no. 13. American Chemical Society (ACS), pp. 7326–7328, Jun. 07, 2013. doi: 10.1021/ic401181j.  
  
V. Thakore and J. J. Hickman, “Charge Relaxation Dynamics of an Electrolytic Nanocapacitor”, *The Journal of Physical Chemistry C*, vol. 119, no. 4. American Chemical Society (ACS), pp. 2121–2132, Jan. 14, 2015. doi: 10.1021/jp508677g.  
  
D. W. Rogers and A. A. Zavitsas, “Using only the very accurately known experimental enthalpy of hydrogenation of ethylene as a reference standard in the atomization method”, *Structural Chemistry*, vol. 24, no. 6. Springer Science and Business Media LLC, pp. 1909–1921, Apr. 06, 2013. doi: 10.1007/s11224-013-0250-0.  
  
D. W. Rogers and A. A. Zavitsas, “Enthalpies of reaction, formation, and hydrogenation among long chain alkanes, monoalkenes, acids, alcohols, and amines: G4 computed and experimental results”, *The Journal of Chemical Thermodynamics*, vol. 79. Elsevier BV, pp. 258–265, Dec. 2014. doi: 10.1016/j.jct.2014.05.002.  
  
D. W. Rogers and A. A. Zavitsas, “Long Chain Saturated and Unsaturated Carboxylic Acids: Filling a Large Gap of Knowledge in Their Enthalpies of Formation”, *The Journal of Organic Chemistry*, vol. 82, no. 1. American Chemical Society (ACS), pp. 673–679, Dec. 28, 2016. doi: 10.1021/acs.joc.6b02674.  
  
W. F. K. Schnatter, D. W. Rogersand A. A. Zavitsas, “Electrophilic Aromatic Substitution: Enthalpies of Hydrogenation of the Ring Determine Reactivities of C6H5X. The Direction of the C6H5–X Bond Dipole Determines Orientation of the Substitution”, *The Journal of Physical Chemistry A*, vol. 117, no. 49. American Chemical Society (ACS), pp. 13079–13088, Dec. 03, 2013. doi: 10.1021/jp409623j.  
  
W. F. K. Schnatter, D. W. Rogersand A. A. Zavitsas, “Teaching Electrophilic Aromatic Substitution: Enthalpies of Hydrogenation of the Rings of C6H5X Predict Relative Reactivities; 13C NMR Shifts Predict Directing Effects of X”, *Journal of Chemical Education*, vol. 92, no. 3. American Chemical Society (ACS), pp. 586–588, Oct. 31, 2014. doi: 10.1021/ed3007742.  
  
W. F. K. Schnatter, D. W. Rogersand A. A. Zavitsas, “Electrophilic Addition to Alkenes: The Relation between Reactivity and Enthalpy of Hydrogenation: Regioselectivity is Determined by the Stability of the Two Conceivable Products”, *Chemistry - A European Journal*, vol. 21, no. 29. Wiley, pp. 10348–10361, May 08, 2015. doi: 10.1002/chem.201500314.  
  
R. Baron and V. Molinero, “Water-Driven Cavity–Ligand Binding: Comparison of Thermodynamic Signatures from Coarse-Grained and Atomic-Level Simulations”, *Journal of Chemical Theory and Computation*, vol. 8, no. 10. American Chemical Society (ACS), pp. 3696–3704, Jun. 14, 2012. doi: 10.1021/ct300121r.  
  
R. Baron, P. Setnyand F. Paesani, “Water Structure, Dynamics, and Spectral Signatures: Changes Upon Model Cavity–Ligand Recognition”, *The Journal of Physical Chemistry B*, vol. 116, no. 46. American Chemical Society (ACS), pp. 13774–13780, Nov. 07, 2012. doi: 10.1021/jp309373q.  
  
J. C. Robertson, “Expanding the Druggable Space of the LSD1/CoREST Epigenetic Target: New Potential Binding Regions for Drug-Like Molecules, Peptides, Protein Partners, and Chromatin”, *PLoS Computational Biology*, vol. 9, no. 7. Public Library of Science (PLoS), p. e1003158, Jul. 18, 2013. doi: 10.1371/journal.pcbi.1003158.  
  
A. M. Eiring, “Combined STAT3 and BCR-ABL1 inhibition induces synthetic lethality in therapy-resistant chronic myeloid leukemia”, *Leukemia*, vol. 29, no. 3. Springer Science and Business Media LLC, pp. 586–597, Aug. 19, 2014. doi: 10.1038/leu.2014.245.  
  
R. A. Kulkarni, “Thiuram Disulfides as Pseudo‐irreversible Inhibitors of Lymphoid Tyrosine Phosphatase”, *ChemMedChem*, vol. 8, no. 9. Wiley, pp. 1561–1568, Jul. 19, 2013. doi: 10.1002/cmdc.201300215.  
  
P. Setny, R. Baronand J. A. McCammon, “Comment on ‘Molecular driving forces of the pocket-ligand hydrophobic association’ by G. Graziano, Chem. Phys. Lett. 533 (2012) 95”, *Chemical Physics Letters*, vol. 555. Elsevier BV, pp. 306–309, Jan. 2013. doi: 10.1016/j.cplett.2012.11.004.  
  
P. Setny, R. Baron, P. Michael Kekenes-Huskey, J. A. McCammonand J. Dzubiella, “Solvent fluctuations in hydrophobic cavity–ligand binding kinetics”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 4. Proceedings of the National Academy of Sciences, pp. 1197–1202, Jan. 07, 2013. doi: 10.1073/pnas.1221231110.  
  
M. Tortorici, “Protein Recognition by Short Peptide Reversible Inhibitors of the Chromatin-Modifying LSD1/CoREST Lysine Demethylase”, *ACS Chemical Biology*, vol. 8, no. 8. American Chemical Society (ACS), pp. 1677–1682, Jun. 11, 2013. doi: 10.1021/cb4001926.  
  
N. A. Vellore and R. Baron, “Molecular dynamics simulations indicate an induced-fit mechanism for LSD1/CoREST-H3-histone molecular recognition”, *BMC Biophysics*, vol. 6, no. 1. Springer Science and Business Media LLC, Nov. 25, 2013. doi: 10.1186/2046-1682-6-15.  
  
N. A. Vellore and R. Baron, “Epigenetic Molecular Recognition: A Biomolecular Modeling Perspective”, *ChemMedChem*, vol. 9, no. 3. Wiley, pp. 484–494, Feb. 12, 2014. doi: 10.1002/cmdc.201300510.  
  
M. S. Zabriskie, “BCR-ABL1 Compound Mutations Combining Key Kinase Domain Positions Confer Clinical Resistance to Ponatinib in Ph Chromosome-Positive Leukemia”, *Cancer Cell*, vol. 26, no. 3. Elsevier BV, pp. 428–442, Sep. 2014. doi: 10.1016/j.ccr.2014.07.006.  
  
R. Han, N. Tymińska, J. R. Schmidtand D. S. Sholl, “Propagation of Degradation-Induced Defects in Zeolitic Imidazolate Frameworks”, *The Journal of Physical Chemistry C*, vol. 123, no. 11. American Chemical Society (ACS), pp. 6655–6666, Feb. 26, 2019. doi: 10.1021/acs.jpcc.9b00304.  
  
E. D. Hermes, A. N. Janesand J. R. Schmidt, “Micki: A python-based object-oriented microkinetic modeling code”, *The Journal of Chemical Physics*, vol. 151, no. 1. AIP Publishing, p. 014112, Jul. 07, 2019. doi: 10.1063/1.5109116.  
  
E. D. Hermes, G. R. Jennessand J. R. Schmidt, “Decoupling the electronic, geometric and interfacial contributions to support effects in heterogeneous catalysis”, *Molecular Simulation*, vol. 41, no. 1–3. Informa UK Limited, pp. 123–133, Jun. 16, 2014. doi: 10.1080/08927022.2014.926549.  
  
Y. Guan, “Catalytic Asymmetric Synthesis of Alkynyl Aziridines: Both Enantiomers of *cis* ‐Aziridines from One Enantiomer of the Catalyst”, *Chemistry – A European Journal*, vol. 20, no. 43. Wiley, pp. 13894–13900, Sep. 09, 2014. doi: 10.1002/chem.201404587.  
  
M. J. Vetticatt and D. A. Singleton, “Isotope Effects and Heavy-Atom Tunneling in the Roush Allylboration of Aldehydes”, *Organic Letters*, vol. 14, no. 9. American Chemical Society (ACS), pp. 2370–2373, Apr. 16, 2012. doi: 10.1021/ol300789a.  
  
J. Chen, M. Zhao, F. Feng, A. Sizovsand J. Wang, “Tunable Thioesters as “Reduction” Responsive Functionality for Traceless Reversible Protein PEGylation”, *Journal of the American Chemical Society*, vol. 135, no. 30. American Chemical Society (ACS), pp. 10938–10941, Jul. 16, 2013. doi: 10.1021/ja405261u.  
  
R. P. Bora, M. J. L. Mills, M. P. Frushichevaand A. Warshel, “On the Challenge of Exploring the Evolutionary Trajectory from Phosphotriesterase to Arylesterase Using Computer Simulations”, *The Journal of Physical Chemistry B*, vol. 119, no. 8. American Chemical Society (ACS), pp. 3434–3445, Feb. 13, 2015. doi: 10.1021/jp5124025.  
  
M. P. Frushicheva, M. J. Mills, P. Schopf, M. K. Singh, R. B. Prasadand A. Warshel, “Computer aided enzyme design and catalytic concepts”, *Current Opinion in Chemical Biology*, vol. 21. Elsevier BV, pp. 56–62, Aug. 2014. doi: 10.1016/j.cbpa.2014.03.022.  
  
S. C. L. Kamerlin, P. K. Sharma, R. B. Prasadand A. Warshel, “Why nature really chose phosphate”, *Quarterly Reviews of Biophysics*, vol. 46, no. 1. Cambridge University Press (CUP), pp. 1–132, Jan. 15, 2013. doi: 10.1017/s0033583512000157.  
  
B. R. Prasad, N. V. Plotnikovand A. Warshel, “Addressing Open Questions about Phosphate Hydrolysis Pathways by Careful Free Energy Mapping”, *The Journal of Physical Chemistry B*, vol. 117, no. 1. American Chemical Society (ACS), pp. 153–163, Dec. 28, 2012. doi: 10.1021/jp309778n.  
  
P. Schopf, M. J. L. Millsand A. Warshel, “The entropic contributions in vitamin B 12 enzymes still reflect the electrostatic paradigm”, *Proceedings of the National Academy of Sciences*, vol. 112, no. 14. Proceedings of the National Academy of Sciences, pp. 4328–4333, Mar. 24, 2015. doi: 10.1073/pnas.1503828112.  
  
Y. Li, J. T. Lyon, A. P. Woodham, A. Fielickeand E. Janssens, “The Geometric Structure of Silver-Doped Silicon Clusters”, *ChemPhysChem*, vol. 15, no. 2. Wiley, pp. 328–336, Jan. 08, 2014. doi: 10.1002/cphc.201300944.  
  
J. T. Lyon, H.-G. Choand L. Andrews, “Matrix Infrared Spectroscopic and Quantum Chemical Investigations of the Group 5 Transition Metal Atom and CX4 Molecule (X = H, F, and Cl) Reaction Products”, *The Journal of Physical Chemistry A*, vol. 119, no. 51. American Chemical Society (ACS), pp. 12742–12755, Dec. 11, 2015. doi: 10.1021/acs.jpca.5b10992.  
  
M. Kang, P. Zhang, H. Cuiand S. M. Loverde, “π–π Stacking Mediated Chirality in Functional Supramolecular Filaments”, *Macromolecules*, vol. 49, no. 3. American Chemical Society (ACS), pp. 994–1001, Jan. 26, 2016. doi: 10.1021/acs.macromol.5b02148.  
  
S. M. Loverde, “Computer simulation of polymer and biopolymer self-assembly for drug delivery”, *Molecular Simulation*, vol. 40, no. 10–11. Informa UK Limited, pp. 794–801, Mar. 19, 2014. doi: 10.1080/08927022.2014.898118.  
  
S. M. Loverde, “Molecular Simulation of the Transport of Drugs across Model Membranes”, *The Journal of Physical Chemistry Letters*, vol. 5, no. 10. American Chemical Society (ACS), pp. 1659–1665, Apr. 25, 2014. doi: 10.1021/jz500321d.  
  
A. Geragotelis and G. L. Barnes, “Surface Deposition Resulting from Collisions between Diglycine and Chemically Modified Alkylthiolate Self-Assembled Monolayer Surfaces”, *The Journal of Physical Chemistry C*, vol. 117, no. 25. American Chemical Society (ACS), pp. 13087–13093, Jun. 17, 2013. doi: 10.1021/jp402424z.  
  
Z. Gregg, W. Ijaz, S. Jannettiand G. L. Barnes, “The Role of Proton Transfer in Surface-Induced Dissociation”, *The Journal of Physical Chemistry C*, vol. 118, no. 38. American Chemical Society (ACS), pp. 22149–22155, Sep. 10, 2014. doi: 10.1021/jp507069x.  
  
W. Ijaz, Z. Greggand G. L. Barnes, “Complex Formation during SID and Its Effect on Proton Mobility”, *The Journal of Physical Chemistry Letters*, vol. 4, no. 22. American Chemical Society (ACS), pp. 3935–3939, Nov. 07, 2013. doi: 10.1021/jz402093q.  
  
P. Z. El-Khoury, E. J. Bylaskaand W. P. Hess, “Time domain simulations of chemical bonding effects in surface-enhanced spectroscopy”, *The Journal of Chemical Physics*, vol. 139, no. 17. AIP Publishing, p. 174303, Nov. 07, 2013. doi: 10.1063/1.4827455.  
  
P. Z. El-Khoury, “Tip-Enhanced Raman Nanographs: Mapping Topography and Local Electric Fields”, *Nano Letters*, vol. 15, no. 4. American Chemical Society (ACS), pp. 2385–2390, Mar. 09, 2015. doi: 10.1021/acs.nanolett.5b00609.  
  
P. Z. El-Khoury and W. P. Hess, “Raman scattering from 1,3-propanedithiol at a hot spot: Theory meets experiment”, *Chemical Physics Letters*, vol. 581. Elsevier BV, pp. 57–63, Aug. 2013. doi: 10.1016/j.cplett.2013.05.066.  
  
P. Z. El-Khoury and W. P. Hess, “Vibronic Raman Scattering at the Quantum Limit of Plasmons”, *Nano Letters*, vol. 14, no. 7. American Chemical Society (ACS), pp. 4114–4118, Jun. 17, 2014. doi: 10.1021/nl501690u.  
  
P. Z. El-Khoury, K. Honkalaand W. P. Hess, “Electronic and Vibrational Properties of *meso*-Tetraphenylporphyrin on Silver Substrates”, *The Journal of Physical Chemistry A*, vol. 118, no. 37. American Chemical Society (ACS), pp. 8115–8123, Mar. 12, 2014. doi: 10.1021/jp412360b.  
  
P. Z. El-Khoury, D. Hu, V. A. Apkarianand W. P. Hess, “Raman Scattering at Plasmonic Junctions Shorted by Conductive Molecular Bridges”, *Nano Letters*, vol. 13, no. 4. American Chemical Society (ACS), pp. 1858–1861, Mar. 29, 2013. doi: 10.1021/nl400733r.  
  
P. Z. El-Khoury, D. Huand W. P. Hess, “Junction Plasmon-Induced Molecular Reorientation”, *The Journal of Physical Chemistry Letters*, vol. 4, no. 20. American Chemical Society (ACS), pp. 3435–3439, Sep. 30, 2013. doi: 10.1021/jz401838b.  
  
P. Z. El-Khoury, S. Joseph, I. Schapiro, S. Gozem, M. Olivucciand A. N. Tarnovsky, “Probing Vibrationally Mediated Ultrafast Excited-State Reaction Dynamics with Multireference (CASPT2) Trajectories”, *The Journal of Physical Chemistry A*, vol. 117, no. 44. American Chemical Society (ACS), pp. 11271–11275, Oct. 23, 2013. doi: 10.1021/jp408441w.  
  
P. Z. El-Khoury, “Electric field enhancement in a self-assembled 2D array of silver nanospheres”, *The Journal of Chemical Physics*, vol. 141, no. 21. AIP Publishing, p. 214308, Dec. 04, 2014. doi: 10.1063/1.4902905.  
  
P. Z. El-Khoury, S. J. Peppernick, D. Hu, A. G. Jolyand W. P. Hess, “The Origin of Surface-Enhanced Raman Scattering of 4,4′-Biphenyldicarboxylate on Silver Substrates”, *The Journal of Physical Chemistry C*, vol. 117, no. 14. American Chemical Society (ACS), pp. 7260–7268, Mar. 28, 2013. doi: 10.1021/jp401026x.  
  
P. Z. El-Khoury, T. W. Ueltschi, A. L. Mifflin, D. Huand W. P. Hess, “Frequency-Resolved Nanoscale Chemical Imaging of 4,4′-Dimercaptostilbene on Silver”, *The Journal of Physical Chemistry C*, vol. 118, no. 47. American Chemical Society (ACS), pp. 27525–27530, Nov. 12, 2014. doi: 10.1021/jp509082c.  
  
J. Lee, S. M. Perdue, A. R. Perez, P. Z. El-Khoury, K. Honkalaand V. A. Apkarian, “Orbiting Orbitals: Visualization of Vibronic Motion at a Conical Intersection”, *The Journal of Physical Chemistry A*, vol. 117, no. 46. American Chemical Society (ACS), pp. 11655–11664, Mar. 18, 2013. doi: 10.1021/jp311894n.  
  
A. Bacolla, X. Zhu, H. Chen, K. Howells, D. N. Cooperand K. M. Vasquez, “Local DNA dynamics shape mutational patterns of mononucleotide repeats in human genomes”, *Nucleic Acids Research*, vol. 43, no. 10. Oxford University Press (OUP), pp. 5065–5080, Apr. 20, 2015. doi: 10.1093/nar/gkv364.  
  
L. Yan and H. Chen, “Migration of Holstein Polarons in Anatase TiO2”, *Journal of Chemical Theory and Computation*, vol. 10, no. 11. American Chemical Society (ACS), pp. 4995–5001, Oct. 14, 2014. doi: 10.1021/ct500873s.  
  
G.-H. Deng, “Vibronic fingerprint of singlet fission in hexacene”, *The Journal of Chemical Physics*, vol. 151, no. 5. AIP Publishing, p. 054703, Aug. 07, 2019. doi: 10.1063/1.5110263.  
  
J. E. Elenewski, J. Y. Cai, W. Jiangand H. Chen, “Functional Mode Hot Electron Transfer Theory”, *The Journal of Physical Chemistry C*, vol. 120, no. 37. American Chemical Society (ACS), pp. 20579–20587, Mar. 07, 2016. doi: 10.1021/acs.jpcc.6b00099.  
  
J. E. Elenewski, U. S. Cubeta, E. Koand H. Chen, “Computer Simulation of Singlet Fission in Single Crystalline Pentacene by Functional Mode Vibronic Theory”, *The Journal of Physical Chemistry C*, vol. 121, no. 21. American Chemical Society (ACS), pp. 11159–11165, May 18, 2017. doi: 10.1021/acs.jpcc.7b03107.  
  
J. E. Elenewski, U. S. Cubeta, E. Koand H. Chen, “Functional Mode Singlet Fission Theory”, *The Journal of Physical Chemistry C*, vol. 121, no. 8. American Chemical Society (ACS), pp. 4130–4138, Feb. 15, 2017. doi: 10.1021/acs.jpcc.6b11722.  
  
D. Sun, “Anisotropic Singlet Fission in Single Crystalline Hexacene”, *iScience*, vol. 19. Elsevier BV, pp. 1079–1089, Sep. 2019. doi: 10.1016/j.isci.2019.08.053.  
  
P. J. Whiteman, J. F. Schultz, Z. D. Porach, H. Chenand N. Jiang, “Dual Binding Configurations of Subphthalocyanine on Ag(100) Substrate Characterized by Scanning Tunneling Microscopy, Tip-Enhanced Raman Spectroscopy, and Density Functional Theory”, *The Journal of Physical Chemistry C*, vol. 122, no. 10. American Chemical Society (ACS), pp. 5489–5495, Feb. 22, 2018. doi: 10.1021/acs.jpcc.7b12068.  
  
L. Yan, J. E. Elenewski, W. Jiangand H. Chen, “Computational modeling of self-trapped electrons in rutile TiO2”, *Physical Chemistry Chemical Physics*, vol. 17, no. 44. Royal Society of Chemistry (RSC), pp. 29949–29957, 2015. doi: 10.1039/c5cp05271h.  
  
Q. Zheng, “Visible-Light-Responsive Graphitic Carbon Nitride: Rational Design and Photocatalytic Applications for Water Treatment”, *Environmental Science & Technology*, vol. 50, no. 23. American Chemical Society (ACS), pp. 12938–12948, Nov. 17, 2016. doi: 10.1021/acs.est.6b02579.  
  
H. Chen, “Functional Mode Electron-Transfer Theory”, *The Journal of Physical Chemistry B*, vol. 118, no. 27. American Chemical Society (ACS), pp. 7586–7593, Jun. 25, 2014. doi: 10.1021/jp504418c.  
  
W. Chen, L. Sun, Z. Tang, Z. Ali, B. Wongand C.-. en . Chang, “An MM and QM Study of Biomimetic Catalysis of Diels-Alder Reactions Using Cyclodextrins”, *Catalysts*, vol. 8, no. 2. MDPI AG, p. 51, Jan. 29, 2018. doi: 10.3390/catal8020051.  
  
T. Cholko, W. Chen, Z. Tangand C.-. en A. Chang, “A molecular dynamics investigation of CDK8/CycC and ligand binding: conformational flexibility and implication in drug discovery”, *Journal of Computer-Aided Molecular Design*, vol. 32, no. 6. Springer Science and Business Media LLC, pp. 671–685, May 08, 2018. doi: 10.1007/s10822-018-0120-3.  
  
E. Hilario, “Visualizing the tunnel in tryptophan synthase with crystallography: Insights into a selective filter for accommodating indole and rejecting water”, *Biochimica et Biophysica Acta (BBA) - Proteins and Proteomics*, vol. 1864, no. 3. Elsevier BV, pp. 268–279, Mar. 2016. doi: 10.1016/j.bbapap.2015.12.006.  
  
Y.-. ming M. Huang, W. You, B. G. Caulkins, M. F. Dunn, L. J. Muellerand C.-. en A. Chang, “Protonation states and catalysis: Molecular dynamics studies of intermediates in tryptophan synthase”, *Protein Science*, vol. 25, no. 1. Wiley, pp. 166–183, Sep. 22, 2015. doi: 10.1002/pro.2709.  
  
C. C. Roberts and C.-. en A. Chang, “Analysis of Ligand–Receptor Association and Intermediate Transfer Rates in Multienzyme Nanostructures with All-Atom Brownian Dynamics Simulations”, *The Journal of Physical Chemistry B*, vol. 120, no. 33. American Chemical Society (ACS), pp. 8518–8531, Jun. 24, 2016. doi: 10.1021/acs.jpcb.6b02236.  
  
Z. Tang and C.-. en A. Chang, “Systematic Dissociation Pathway Searches Guided by Principal Component Modes”, *Journal of Chemical Theory and Computation*, vol. 13, no. 5. American Chemical Society (ACS), pp. 2230–2244, May 01, 2017. doi: 10.1021/acs.jctc.6b01204.  
  
Z. Tang and C.-. en A. Chang, “Binding Thermodynamics and Kinetics Calculations Using Chemical Host and Guest: A Comprehensive Picture of Molecular Recognition”, *Journal of Chemical Theory and Computation*, vol. 14, no. 1. American Chemical Society (ACS), pp. 303–318, Dec. 14, 2017. doi: 10.1021/acs.jctc.7b00899.  
  
W. You and C.-. en A. Chang, “Role of Molecular Interactions and Protein Rearrangement in the Dissociation Kinetics of p38α MAP Kinase Type-I/II/III Inhibitors”, *Journal of Chemical Information and Modeling*, vol. 58, no. 5. American Chemical Society (ACS), pp. 968–981, Apr. 05, 2018. doi: 10.1021/acs.jcim.7b00640.  
  
B. G. Caulkins, “Protonation States of the Tryptophan Synthase Internal Aldimine Active Site from Solid-State NMR Spectroscopy: Direct Observation of the Protonated Schiff Base Linkage to Pyridoxal-5′-Phosphate”, *Journal of the American Chemical Society*, vol. 136, no. 37. American Chemical Society (ACS), pp. 12824–12827, Sep. 03, 2014. doi: 10.1021/ja506267d.  
  
Y.-. ming M. Huang and C.-. en A. Chang, “Achieving Peptide Binding Specificity and Promiscuity by Loops: Case of the Forkhead-Associated Domain”, *PLoS ONE*, vol. 9, no. 5. Public Library of Science (PLoS), p. e98291, May 28, 2014. doi: 10.1371/journal.pone.0098291.  
  
Y.-. ming M. Huang, M. Kangand C.-. en A. Chang, “Switches of hydrogen bonds during ligand-protein association processes determine binding kinetics”, *Journal of Molecular Recognition*, vol. 27, no. 9. Wiley, pp. 537–548, Jun. 24, 2014. doi: 10.1002/jmr.2377.  
  
C. C. Roberts and C.-. en A. Chang, “Modeling of Enhanced Catalysis in Multienzyme Nanostructures: Effect of Molecular Scaffolds, Spatial Organization, and Concentration”, *Journal of Chemical Theory and Computation*, vol. 11, no. 1. American Chemical Society (ACS), pp. 286–292, Dec. 18, 2014. doi: 10.1021/ct5007482.  
  
J. S. M. Anderson, J. I. Rodríguez, P. W. Ayersand A. W. Götz, “Relativistic (SR‐ZORA) quantum theory of atoms in molecules properties”, *Journal of Computational Chemistry*, vol. 38, no. 2. Wiley, pp. 81–86, Nov. 10, 2016. doi: 10.1002/jcc.24520.  
  
W.-G. H. Du, A. W. Götzand L. Noodleman, “DFT Fea3–O/O–O Vibrational Frequency Calculations over Catalytic Reaction Cycle States in the Dinuclear Center of Cytochrome *c* Oxidase”, *Inorganic Chemistry*, vol. 58, no. 20. American Chemical Society (ACS), pp. 13933–13944, Sep. 30, 2019. doi: 10.1021/acs.inorgchem.9b01840.  
  
A. W. Götz, J. I. Rodríguez, F. L. Castillo‐Alvaradoand D. E. Trujillo‐González, “Van der Waals effects on structure and optical properties in organic photovoltaics”, *International Journal of Quantum Chemistry*, vol. 119, no. 14. Wiley, Jan. 03, 2019. doi: 10.1002/qua.25883.  
  
I. Gutiérrez-González, B. Molina-Brito, A. W. Götz, F. L. Castillo-Alvaradoand J. I. Rodríguez, “Structural and electronic properties of the P3HT–PCBM dimer: A theoretical Study”, *Chemical Physics Letters*, vol. 612. Elsevier BV, pp. 234–239, Sep. 2014. doi: 10.1016/j.cplett.2014.08.030.  
  
W.-G. Han Du, A. W. Götzand L. Noodleman, “A Water Dimer Shift Activates a Proton Pumping Pathway in the **PR** → **F** Transition of *ba3* Cytochrome *c* Oxidase”, *Inorganic Chemistry*, vol. 57, no. 3. American Chemical Society (ACS), pp. 1048–1059, Jan. 08, 2018. doi: 10.1021/acs.inorgchem.7b02461.  
  
W.-G. Han Du, A. W. Götz, L. Yang, R. C. Walkerand L. Noodleman, “A broken-symmetry density functional study of structures, energies, and protonation states along the catalytic O–O bond cleavage pathway in ba3cytochrome c oxidase from Thermus thermophilus”, *Physical Chemistry Chemical Physics*, vol. 18, no. 31. Royal Society of Chemistry (RSC), pp. 21162–21171, 2016. doi: 10.1039/c6cp00349d.  
  
W.-G. Han Du, D. McRee, A. W. Götzand L. Noodleman, “A Water Molecule Residing in the Fea33+···CuB2+ Dinuclear Center of the Resting Oxidized as-Isolated Cytochrome *c* Oxidase: A Density Functional Study”, *Inorganic Chemistry*, vol. 59, no. 13. American Chemical Society (ACS), pp. 8906–8915, Jun. 11, 2020. doi: 10.1021/acs.inorgchem.0c00724.  
  
M. Manathunga, Y. Miao, D. Mu, A. W. Götzand K. M. Merz Jr., “Parallel Implementation of Density Functional Theory Methods in the Quantum Interaction Computational Kernel Program”, *Journal of Chemical Theory and Computation*, vol. 16, no. 7. American Chemical Society (ACS), pp. 4315–4326, Jun. 08, 2020. doi: 10.1021/acs.jctc.0c00290.  
  
J. P. Martínez, D. E. Trujillo-González, A. W. Götz, F. L. Castillo-Alvaradoand J. I. Rodríguez, “Effects of Dispersion Forces on Structure and Photoinduced Charge Separation in Organic Photovoltaics”, *The Journal of Physical Chemistry C*, vol. 121, no. 37. American Chemical Society (ACS), pp. 20134–20140, Sep. 07, 2017. doi: 10.1021/acs.jpcc.7b05107.  
  
L. Mones, “The adaptive buffered force QM/MM method in the CP2K and AMBER software packages”, *Journal of Computational Chemistry*, vol. 36, no. 9. Wiley, pp. 633–648, Feb. 03, 2015. doi: 10.1002/jcc.23839.  
  
L. Noodleman, W.-G. Han Du, J. A. Fee, A. W. Götzand R. C. Walker, “Linking Chemical Electron–Proton Transfer to Proton Pumping in Cytochrome *c* Oxidase: Broken-Symmetry DFT Exploration of Intermediates along the Catalytic Reaction Pathway of the Iron–Copper Dinuclear Complex”, *Inorganic Chemistry*, vol. 53, no. 13. American Chemical Society (ACS), pp. 6458–6472, Jun. 24, 2014. doi: 10.1021/ic500363h.  
  
J. I. Rodríguez, C. F. Matta, E. A. Uribe, A. W. Götz, F. L. Castillo-Alvaradoand B. Molina-Brito, “A QTAIM topological analysis of the P3HT⿿PCBM dimer”, *Chemical Physics Letters*, vol. 644. Elsevier BV, pp. 157–162, Jan. 2016. doi: 10.1016/j.cplett.2015.11.052.  
  
S. N. Steinmann, “Force Field for Water over Pt(111): Development, Assessment, and Comparison”, *Journal of Chemical Theory and Computation*, vol. 14, no. 6. American Chemical Society (ACS), pp. 3238–3251, Apr. 16, 2018. doi: 10.1021/acs.jctc.7b01177.  
  
S. N. Steinmann, P. Fleurat‐Lessard, A. W. Götz, C. Michel, R. Ferreira de Moraisand P. Sautet, “Molecular mechanics models for the image charge, a comment on “including image charge effects in the molecular dynamics simulations of molecules on metal surfaces””, *Journal of Computational Chemistry*, vol. 38, no. 24. Wiley, pp. 2127–2129, Jul. 04, 2017. doi: 10.1002/jcc.24861.  
  
L. Yang, Å. A. Skjevik, W.-G. Han Du, L. Noodleman, R. C. Walkerand A. W. Götz, “Water exit pathways and proton pumping mechanism in B-type cytochrome c oxidase from molecular dynamics simulations”, *Biochimica et Biophysica Acta (BBA) - Bioenergetics*, vol. 1857, no. 9. Elsevier BV, pp. 1594–1606, Sep. 2016. doi: 10.1016/j.bbabio.2016.06.005.  
  
S. A. Yao, “Electronic Structure of Ni2E2 Complexes (E = S, Se, Te) and a Global Analysis of M2E2 Compounds: A Case for Quantized E2*n*– Oxidation Levels with *n* = 2, 3, or 4”, *Journal of the American Chemical Society*, vol. 137, no. 15. American Chemical Society (ACS), pp. 4993–5011, Apr. 08, 2015. doi: 10.1021/ja511607j.  
  
B. Hirshberg, “N2O5at water surfaces: binding forces, charge separation, energy accommodation and atmospheric implications”, *Physical Chemistry Chemical Physics*, vol. 20, no. 26. Royal Society of Chemistry (RSC), pp. 17961–17976, 2018. doi: 10.1039/c8cp03022g.  
  
T. M. Simeon, M. A. Ratnerand G. C. Schatz, “Nature of Noncovalent Interactions in Catenane Supramolecular Complexes: Calibrating the MM3 Force Field with ab Initio, DFT, and SAPT Methods”, *The Journal of Physical Chemistry A*, vol. 117, no. 33. American Chemical Society (ACS), pp. 7918–7927, Aug. 13, 2013. doi: 10.1021/jp400051b.  
  
S. R. Dalton, A. R. Vienneau, S. R. Burstein, R. J. Xu, S. Linseand C. H. Londergan, “Cyanylated Cysteine Reports Site-Specific Changes at Protein–Protein-Binding Interfaces Without Perturbation”, *Biochemistry*, vol. 57, no. 26. American Chemical Society (ACS), pp. 3702–3712, May 22, 2018. doi: 10.1021/acs.biochem.8b00283.  
  
S. B. Donald, J. K. Navinand I. Harrison, “Methane dissociative chemisorption and detailed balance on Pt(111): Dynamical constraints and the modest influence of tunneling”, *The Journal of Chemical Physics*, vol. 139, no. 21. AIP Publishing, p. 214707, Dec. 07, 2013. doi: 10.1063/1.4837697.  
  
E. T. Baxter, M.-A. Ha, A. C. Cass, H. Zhai, A. N. Alexandrovaand S. L. Anderson, “Diborane Interactions with Pt7/Alumina: Preparation of Size-Controlled Borated Pt Model Catalysts”, *The Journal of Physical Chemistry C*, vol. 122, no. 3. American Chemical Society (ACS), pp. 1631–1644, Jan. 16, 2018. doi: 10.1021/acs.jpcc.7b10423.  
  
M.-A. Ha, E. T. Baxter, A. C. Cass, S. L. Andersonand A. N. Alexandrova, “Boron Switch for Selectivity of Catalytic Dehydrogenation on Size-Selected Pt Clusters on Al2O3”, *Journal of the American Chemical Society*, vol. 139, no. 33. American Chemical Society (ACS), pp. 11568–11575, Aug. 11, 2017. doi: 10.1021/jacs.7b05894.  
  
H. Zhai and A. N. Alexandrova, “Local Fluxionality of Surface-Deposited Cluster Catalysts: The Case of Pt7 on Al2O3”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 7. American Chemical Society (ACS), pp. 1696–1702, Mar. 18, 2018. doi: 10.1021/acs.jpclett.8b00379.  
  
A. Ajaz, A. C. Voukides, K. J. Cahill, R. Thamatam, S. L. Skraba-Joinerand R. P. Johnson, “Microwave Flash Pyrolysis: C9H8 Interconversions and Dimerisations”, *Australian Journal of Chemistry*, vol. 67, no. 9. CSIRO Publishing, p. 1301, 2014. doi: 10.1071/ch14238.  
  
R. Thamatam, S. L. Skrabaand R. P. Johnson, “Scalable synthesis of quaterrylene: solution-phase 1H NMR spectroscopy of its oxidative dication”, *Chemical Communications*, vol. 49, no. 80. Royal Society of Chemistry (RSC), p. 9122, 2013. doi: 10.1039/c3cc46270f.  
  
A. C. Voukides, K. J. Cahilland R. P. Johnson, “Computational Studies on a Carbenoid Mechanism for the Doering–Moore–Skattebøl Reaction”, *The Journal of Organic Chemistry*, vol. 78, no. 23. American Chemical Society (ACS), pp. 11815–11823, Nov. 13, 2013. doi: 10.1021/jo401847v.  
  
S. Kal, A. S. Filatovand P. H. Dinolfo, “Structural, Electrochemical, and Spectroscopic Investigation of Acetate Bridged Dinuclear Tetrakis-Schiff Base Macrocycles of Mn and Zn”, *Inorganic Chemistry*, vol. 52, no. 24. American Chemical Society (ACS), pp. 13963–13973, Nov. 21, 2013. doi: 10.1021/ic401631e.  
  
J. R. Buchwald, S. Kaland P. H. Dinolfo, “Determination of the Mechanism of Electrocatalytic Water Oxidation by a Dimanganese Tetrakis-Schiff Base Complex: Comparison of Density Functional Theory Calculations with Experiment”, *The Journal of Physical Chemistry C*, vol. 118, no. 45. American Chemical Society (ACS), pp. 25869–25877, Nov. 05, 2014. doi: 10.1021/jp505774h.  
  
T. Avanesian and P. Christopher, “Adsorbate Specificity in Hot Electron Driven Photochemistry on Catalytic Metal Surfaces”, *The Journal of Physical Chemistry C*, vol. 118, no. 48. American Chemical Society (ACS), pp. 28017–28031, Nov. 20, 2014. doi: 10.1021/jp509555m.  
  
T. Avanesian, S. Dai, M. J. Kale, G. W. Graham, X. Panand P. Christopher, “Quantitative and Atomic-Scale View of CO-Induced Pt Nanoparticle Surface Reconstruction at Saturation Coverage via DFT Calculations Coupled with *in Situ* TEM and IR”, *Journal of the American Chemical Society*, vol. 139, no. 12. American Chemical Society (ACS), pp. 4551–4558, Mar. 20, 2017. doi: 10.1021/jacs.7b01081.  
  
T. Avanesian, G. S. Gusmãoand P. Christopher, “Mechanism of CO2 reduction by H2 on Ru(0 0 0 1) and general selectivity descriptors for late-transition metal catalysts”, *Journal of Catalysis*, vol. 343. Elsevier BV, pp. 86–96, Nov. 2016. doi: 10.1016/j.jcat.2016.03.016.  
  
M. J. Kale, T. Avanesian, H. Xin, J. Yanand P. Christopher, “Controlling Catalytic Selectivity on Metal Nanoparticles by Direct Photoexcitation of Adsorbate–Metal Bonds”, *Nano Letters*, vol. 14, no. 9. American Chemical Society (ACS), pp. 5405–5412, Aug. 14, 2014. doi: 10.1021/nl502571b.  
  
T. Avanesian and P. Christopher, “Scaled Degree of Rate Control: Identifying Elementary Steps That Control Differences in Performance of Transition-Metal Catalysts”, *ACS Catalysis*, vol. 6, no. 8. American Chemical Society (ACS), pp. 5268–5272, Jul. 13, 2016. doi: 10.1021/acscatal.6b01547.  
  
G. Ali, P. E. VanNatta, D. A. Ramirez, K. M. Lightand M. T. Kieber-Emmons, “Thermodynamics of a μ-oxo Dicopper(II) Complex for Hydrogen Atom Abstraction”, *Journal of the American Chemical Society*, vol. 139, no. 51. American Chemical Society (ACS), pp. 18448–18451, Dec. 15, 2017. doi: 10.1021/jacs.7b10833.  
  
N. D. Staudaher, A. M. Arifand J. Louie, “Synergy between Experimental and Computational Chemistry Reveals the Mechanism of Decomposition of Nickel–Ketene Complexes”, *Journal of the American Chemical Society*, vol. 138, no. 42. American Chemical Society (ACS), pp. 14083–14091, Oct. 14, 2016. doi: 10.1021/jacs.6b08897.  
  
R. Cao, “Peroxo and Superoxo Moieties Bound to Copper Ion: Electron-Transfer Equilibrium with a Small Reorganization Energy”, *Journal of the American Chemical Society*, vol. 138, no. 22. American Chemical Society (ACS), pp. 7055–7066, May 26, 2016. doi: 10.1021/jacs.6b02404.  
  
S. J. Koepke, K. M. Light, P. E. VanNatta, K. M. Wileyand M. T. Kieber-Emmons, “Electrocatalytic Water Oxidation by a Homogeneous Copper Catalyst Disfavors Single-Site Mechanisms”, *Journal of the American Chemical Society*, vol. 139, no. 25. American Chemical Society (ACS), pp. 8586–8600, Jun. 15, 2017. doi: 10.1021/jacs.7b03278.  
  
A. W. Schaefer, M. T. Kieber-Emmons, S. M. Adam, K. D. Karlinand E. I. Solomon, “Phenol-Induced O–O Bond Cleavage in a Low-Spin Heme–Peroxo–Copper Complex: Implications for O2 Reduction in Heme–Copper Oxidases”, *Journal of the American Chemical Society*, vol. 139, no. 23. American Chemical Society (ACS), pp. 7958–7973, Jun. 06, 2017. doi: 10.1021/jacs.7b03292.  
  
J.-W. Shin and E. R. Bernstein, “Vacuum ultraviolet photoionization of carbohydrates and nucleotides”, *The Journal of Chemical Physics*, vol. 140, no. 4. AIP Publishing, p. 044330, Jan. 28, 2014. doi: 10.1063/1.4862829.  
  
T. S. Dibble and A. C. Schwid, “Thermodynamics limits the reactivity of radical with volatile organic compounds”, *Chemical Physics Letters*, vol. 659. Elsevier BV, pp. 289–294, Aug. 2016. doi: 10.1016/j.cplett.2016.07.065.  
  
T. S. Dibble, Y. Sha, W. F. Thorntonand F. Zhang, “Cis–Trans Isomerization of Chemically Activated 1-Methylallyl Radical and Fate of the Resulting 2-Buten-1-peroxy Radical”, *The Journal of Physical Chemistry A*, vol. 116, no. 29. American Chemical Society (ACS), pp. 7603–7614, Jul. 12, 2012. doi: 10.1021/jp303652x.  
  
H. Hu and T. S. Dibble, “Quantum Chemistry, Reaction Kinetics, and Tunneling Effects in the Reaction of Methoxy Radicals with O2”, *The Journal of Physical Chemistry A*, vol. 117, no. 51. American Chemical Society (ACS), pp. 14230–14242, Dec. 09, 2013. doi: 10.1021/jp409105q.  
  
Y. Jiao and T. S. Dibble, “First kinetic study of the atmospherically important reactions BrHg˙ + NO2and BrHg˙ + HOO”, *Physical Chemistry Chemical Physics*, vol. 19, no. 3. Royal Society of Chemistry (RSC), pp. 1826–1838, 2017. doi: 10.1039/c6cp06276h.  
  
Y. Jiao, F. Zhangand T. S. Dibble, “Quantum Chemical Study of Autoignition of Methyl Butanoate”, *The Journal of Physical Chemistry A*, vol. 119, no. 28. American Chemical Society (ACS), pp. 7282–7292, Mar. 27, 2015. doi: 10.1021/jp5122118.  
  
K. A. A. Belfon and J. D. Gough, “Theoretical analysis of an all-photonic multifunctional molecular logic device: Using TD-DFT//DFT to assess photochromic activity of multimeric photochrome”, *Chemical Physics Letters*, vol. 585. Elsevier BV, pp. 63–68, Oct. 2013. doi: 10.1016/j.cplett.2013.08.099.  
  
K. A. A. Belfon and J. D. Gough, “Geometry deformation and mesomeric effect at the minimal-energy conical intersections and their relationship to the photoreactivity of indolylfulgides: A TD-DFT study”, *Chemical Physics Letters*, vol. 593. Elsevier BV, pp. 174–180, Feb. 2014. doi: 10.1016/j.cplett.2014.01.011.  
  
R. Chindam, H. M. Hoque, A. S. Ali, F. Z. Rafiqueand J. D. Gough, “Theoretical assessment of indolylfulgimides and novel asymmetric di-indolylfulgimide photochromes”, *Journal of Photochemistry and Photobiology A: Chemistry*, vol. 279. Elsevier BV, pp. 38–46, Apr. 2014. doi: 10.1016/j.jphotochem.2014.01.007.  
  
A. Aguirre-Soto, C.-H. Lim, A. T. Hwang, C. B. Musgraveand J. W. Stansbury, “Visible-Light Organic Photocatalysis for Latent Radical-Initiated Polymerization via 2e–/1H+ Transfers: Initiation with Parallels to Photosynthesis”, *Journal of the American Chemical Society*, vol. 136, no. 20. American Chemical Society (ACS), pp. 7418–7427, May 08, 2014. doi: 10.1021/ja502441d.  
  
C.-H. Lim, A. M. Holder, J. T. Hynesand C. B. Musgrave, “Roles of the Lewis Acid and Base in the Chemical Reduction of CO2 Catalyzed by Frustrated Lewis Pairs”, *Inorganic Chemistry*, vol. 52, no. 17. American Chemical Society (ACS), pp. 10062–10066, Aug. 13, 2013. doi: 10.1021/ic4013729.  
  
C.-H. Lim, A. M. Holderand C. B. Musgrave, “Mechanism of Homogeneous Reduction of CO2 by Pyridine: Proton Relay in Aqueous Solvent and Aromatic Stabilization”, *Journal of the American Chemical Society*, vol. 135, no. 1. American Chemical Society (ACS), pp. 142–154, Dec. 21, 2012. doi: 10.1021/ja3064809.  
  
C.-H. Lim, A. M. Holder, J. T. Hynesand C. B. Musgrave, “Reduction of CO2 to Methanol Catalyzed by a Biomimetic Organo-Hydride Produced from Pyridine”, *Journal of the American Chemical Society*, vol. 136, no. 45. American Chemical Society (ACS), pp. 16081–16095, Nov. 04, 2014. doi: 10.1021/ja510131a.  
  
S. Fatehi and R. P. Steele, “Multiple-Time Step Ab Initio Molecular Dynamics Based on Two-Electron Integral Screening”, *Journal of Chemical Theory and Computation*, vol. 11, no. 3. American Chemical Society (ACS), pp. 884–898, Feb. 04, 2015. doi: 10.1021/ct500904x.  
  
P. K. Jha and R. G. Larson, “Assessing the Efficiency of Polymeric Excipients by Atomistic Molecular Dynamics Simulations”, *Molecular Pharmaceutics*, vol. 11, no. 5. American Chemical Society (ACS), pp. 1676–1686, Apr. 16, 2014. doi: 10.1021/mp500068w.  
  
R. F. Pauszek III, G. Kodaliand R. J. Stanley, “Excited State Electronic Structures of 5,10-Methenyltetrahydrofolate and 5,10-Methylenetetrahydrofolate Determined by Stark Spectroscopy”, *The Journal of Physical Chemistry A*, vol. 118, no. 37. American Chemical Society (ACS), pp. 8320–8328, May 21, 2014. doi: 10.1021/jp501143u.  
  
I. Abramova, B. Rudshteyn, J. F. Liebmanand A. Greer, “Computed Regioselectivity and Conjectured Biological Activity of Ene Reactions of Singlet Oxygen with the Natural Product Hyperforin”, *Photochemistry and Photobiology*, vol. 93, no. 2. Wiley, pp. 626–631, Feb. 16, 2017. doi: 10.1111/php.12706.  
  
B. Rudshteyn, Á. Castillo, A. A. Ghogare, J. F. Liebmanand A. Greer, “Theoretical Study of the Reaction Formalhydrazone with Singlet Oxygen. Fragmentation of the C=N Bond, Ene Reaction and Other Processes”, *Photochemistry and Photobiology*, vol. 90, no. 2. Wiley, pp. 431–438, Dec. 02, 2013. doi: 10.1111/php.12199.  
  
J. Church, S. Pezeshki, C. Davisand H. Lin, “Charge Transfer and Polarization for Chloride Ions Bound in ClC Transport Proteins: Natural Bond Orbital and Energy Decomposition Analyses”, *The Journal of Physical Chemistry B*, vol. 117, no. 50. American Chemical Society (ACS), pp. 16029–16043, Nov. 27, 2013. doi: 10.1021/jp409306x.  
  
R. Damrauer, H. Linand N. H. Damrauer, “Computational Studies of Carbodiimide Rings”, *The Journal of Organic Chemistry*, vol. 79, no. 9. American Chemical Society (ACS), pp. 3781–3788, Apr. 21, 2014. doi: 10.1021/jo4026435.  
  
S. Pezeshki and H. Lin, “Recent developments in QM/MM methods towards open-boundary multi-scale simulations”, *Molecular Simulation*, vol. 41, no. 1–3. Informa UK Limited, pp. 168–189, May 08, 2014. doi: 10.1080/08927022.2014.911870.  
  
E. M. Dore and J. T. Lyon, “The Structures of Silicon Clusters Doped with Two Gold Atoms, Si n Au2 (n = 1–10)”, *Journal of Cluster Science*, vol. 27, no. 4. Springer Science and Business Media LLC, pp. 1365–1381, Mar. 28, 2016. doi: 10.1007/s10876-016-1006-y.  
  
Y. Li, J. T. Lyon, A. P. Woodham, P. Lievens, A. Fielickeand E. Janssens, “Structural Identification of Gold-Doped Silicon Clusters via Far-Infrared Spectroscopy”, *The Journal of Physical Chemistry C*, vol. 119, no. 20. American Chemical Society (ACS), pp. 10896–10903, Dec. 23, 2014. doi: 10.1021/jp5107795.  
  
K. Chakraborty, M. Kangand S. M. Loverde, “Molecular Mechanism for the Role of the H2A and H2B Histone Tails in Nucleosome Repositioning”, *The Journal of Physical Chemistry B*, vol. 122, no. 50. American Chemical Society (ACS), pp. 11827–11840, Nov. 27, 2018. doi: 10.1021/acs.jpcb.8b07881.  
  
K. Chakraborty and S. M. Loverde, “Asymmetric breathing motions of nucleosomal DNA and the role of histone tails”, *The Journal of Chemical Physics*, vol. 147, no. 6. AIP Publishing, p. 065101, Aug. 14, 2017. doi: 10.1063/1.4997573.  
  
K. Chakraborty, K. Vijayan, A. E. X. Brown, D. E. Discherand S. M. Loverde, “Glassy worm-like micelles in solvent and shear mediated shape transitions”, *Soft Matter*, vol. 14, no. 20. Royal Society of Chemistry (RSC), pp. 4194–4203, 2018. doi: 10.1039/c8sm00080h.  
  
M. Drenscko and S. M. Loverde, “Characterisation of the hydrophobic collapse of polystyrene in water using free energy techniques”, *Molecular Simulation*, vol. 43, no. 3. Informa UK Limited, pp. 234–241, Nov. 21, 2016. doi: 10.1080/08927022.2016.1253840.  
  
M. Kang, K. Chakrabortyand S. M. Loverde, “Molecular Dynamics Simulations of Supramolecular Anticancer Nanotubes”, *Journal of Chemical Information and Modeling*, vol. 58, no. 6. American Chemical Society (ACS), pp. 1164–1168, Jun. 01, 2018. doi: 10.1021/acs.jcim.8b00193.  
  
M. Kang, H. Cuiand S. M. Loverde, “Coarse-grained molecular dynamics studies of the structure and stability of peptide-based drug amphiphile filaments”, *Soft Matter*, vol. 13, no. 42. Royal Society of Chemistry (RSC), pp. 7721–7730, 2017. doi: 10.1039/c7sm00943g.  
  
Y.-A. Lin, “Isomeric control of the mechanical properties of supramolecular filament hydrogels”, *Biomaterials Science*, vol. 6, no. 1. Royal Society of Chemistry (RSC), pp. 216–224, 2018. doi: 10.1039/c7bm00722a.  
  
A. Manandhar, M. Kang, K. Chakrabortyand S. M. Loverde, “Effect of Nucleotide State on the Protofilament Conformation of Tubulin Octamers”, *The Journal of Physical Chemistry B*, vol. 122, no. 23. American Chemical Society (ACS), pp. 6164–6178, May 16, 2018. doi: 10.1021/acs.jpcb.8b02193.  
  
A. Manandhar, M. Kang, K. Chakraborty, P. K. Tangand S. M. Loverde, “Molecular simulations of peptide amphiphiles”, *Organic & Biomolecular Chemistry*, vol. 15, no. 38. Royal Society of Chemistry (RSC), pp. 7993–8005, 2017. doi: 10.1039/c7ob01290j.  
  
M. Kang and S. M. Loverde, “Molecular Simulation of the Concentration-Dependent Interaction of Hydrophobic Drugs with Model Cellular Membranes”, *The Journal of Physical Chemistry B*, vol. 118, no. 41. American Chemical Society (ACS), pp. 11965–11972, Oct. 01, 2014. doi: 10.1021/jp5047613.  
  
Z. Ma, “TCR Triggering by pMHC Ligands Tethered on Surfaces via Poly(Ethylene Glycol) Depends on Polymer Length”, *PLoS ONE*, vol. 9, no. 11. Public Library of Science (PLoS), p. e112292, Nov. 10, 2014. doi: 10.1371/journal.pone.0112292.  
  
M. V. Ivanov, V. J. Chebny, M. R. Talipovand R. Rathore, “Poly-*p*-hydroquinone Ethers: Isoenergetic Molecular Wires with Length-Invariant Oxidation Potentials and Cation Radical Excitation Energies”, *Journal of the American Chemical Society*, vol. 139, no. 12. American Chemical Society (ACS), pp. 4334–4337, Mar. 16, 2017. doi: 10.1021/jacs.7b01226.  
  
M. V. Ivanov, K. Thakur, A. Bhatnagarand R. Rathore, “Isolation of a chiral anthracene cation radical: X-ray crystallography and computational interrogation of its racemization”, *Chemical Communications*, vol. 53, no. 18. Royal Society of Chemistry (RSC), pp. 2748–2751, 2017. doi: 10.1039/c6cc10307c.  
  
M. V. Ivanov, K. Thakur, A. Boddeda, D. Wangand R. Rathore, “Nodal Arrangement of HOMO Controls the Turning On/Off the Electronic Coupling in Isomeric Polypyrene Wires”, *The Journal of Physical Chemistry C*, vol. 121, no. 17. American Chemical Society (ACS), pp. 9202–9208, Apr. 20, 2017. doi: 10.1021/acs.jpcc.7b02264.  
  
F. A. Khan, D. Wang, B. Pemberton, M. R. Talipovand R. Rathore, “Toroidal delocalization of a single electron through circularly-arrayed benzophenone chromophores in hexakis(4-benzoylphenyl)benzene”, *Journal of Photochemistry and Photobiology A: Chemistry*, vol. 331. Elsevier BV, pp. 153–159, Dec. 2016. doi: 10.1016/j.jphotochem.2016.05.002.  
  
N. Reilly, M. Ivanov, B. Uhler, M. Talipov, R. Rathoreand S. A. Reid, “First Experimental Evidence for the Diverse Requirements of Excimer vs Hole Stabilization in π-Stacked Assemblies”, *The Journal of Physical Chemistry Letters*, vol. 7, no. 15. American Chemical Society (ACS), pp. 3042–3045, Jul. 27, 2016. doi: 10.1021/acs.jpclett.6b01201.  
  
M. R. Talipov, S. H. Abdelwahed, K. Thakur, S. A. Reidand R. Rathore, “From Wires to Cables: Attempted Synthesis of 1,3,5-Trifluorenylcyclohexane as a Platform for Molecular Cables”, *The Journal of Organic Chemistry*, vol. 81, no. 4. American Chemical Society (ACS), pp. 1627–1634, Jan. 29, 2016. doi: 10.1021/acs.joc.5b02792.  
  
M. R. Talipov, A. Boddeda, S. V. Lindemanand R. Rathore, “Does Koopmans’ Paradigm for 1-Electron Oxidation Always Hold? Breakdown of IP/*E*ox Relationship for *p*-Hydroquinone Ethers and the Role of Methoxy Group Rotation”, *The Journal of Physical Chemistry Letters*, vol. 6, no. 17. American Chemical Society (ACS), pp. 3373–3378, Aug. 14, 2015. doi: 10.1021/acs.jpclett.5b01532.  
  
M. R. Talipov, M. M. Hossain, A. Boddeda, K. Thakurand R. Rathore, “A search for blues brothers: X-ray crystallographic/spectroscopic characterization of the tetraarylbenzidine cation radical as a product of aging of solid magic blue”, *Organic & Biomolecular Chemistry*, vol. 14, no. 10. Royal Society of Chemistry (RSC), pp. 2961–2968, 2016. doi: 10.1039/c6ob00140h.  
  
M. R. Talipov, M. V. Ivanovand R. Rathore, “Inclusion of Asymptotic Dependence of Reorganization Energy in the Modified Marcus-Based Multistate Model Accurately Predicts Hole Distribution in Poly-*p*-phenylene Wires”, *The Journal of Physical Chemistry C*, vol. 120, no. 12. American Chemical Society (ACS), pp. 6402–6408, Mar. 18, 2016. doi: 10.1021/acs.jpcc.6b00514.  
  
M. R. Talipov, R. Jastiand R. Rathore, “A Circle Has No End: Role of Cyclic Topology and Accompanying Structural Reorganization on the Hole Distribution in Cyclic and Linear Poly-*p*-phenylene Molecular Wires”, *Journal of the American Chemical Society*, vol. 137, no. 47. American Chemical Society (ACS), pp. 14999–15006, Nov. 18, 2015. doi: 10.1021/jacs.5b09596.  
  
M. R. Talipov, T. S. Navale, M. M. Hossain, R. Shukla, M. V. Ivanovand R. Rathore, “Dihedral-Angle-Controlled Crossover from Static Hole Delocalization to Dynamic Hopping in Biaryl Cation Radicals”, *Angewandte Chemie International Edition*, vol. 56, no. 1. Wiley, pp. 266–269, Nov. 29, 2016. doi: 10.1002/anie.201609695.  
  
M. R. Talipov, T. S. Navaleand R. Rathore, “The HOMO Nodal Arrangement in Polychromophoric Molecules and Assemblies Controls the Interchromophoric Electronic Coupling”, *Angewandte Chemie International Edition*, vol. 54, no. 48. Wiley, pp. 14468–14472, Oct. 2015. doi: 10.1002/anie.201506402.  
  
M. R. Talipov, “Critical Role of the Secondary Binding Pocket in Modulating the Enzymatic Activity of DUSP5 toward Phosphorylated ERKs”, *Biochemistry*, vol. 55, no. 44. American Chemical Society (ACS), pp. 6187–6195, Oct. 26, 2016. doi: 10.1021/acs.biochem.6b00498.  
  
M. R. Talipov, A. Boddeda, Q. K. Timerghazinand R. Rathore, “Key Role of End-Capping Groups in Optoelectronic Properties of Poly-*p*-phenylene Cation Radicals”, *The Journal of Physical Chemistry C*, vol. 118, no. 37. American Chemical Society (ACS), pp. 21400–21408, Sep. 04, 2014. doi: 10.1021/jp5082752.  
  
B. Uhler, M. V. Ivanov, D. Kokkin, N. Reilly, R. Rathoreand S. A. Reid, “Effect of Facial Encumbrance on Excimer Formation and Charge Resonance Stabilization in Model Bichromophoric Assemblies”, *The Journal of Physical Chemistry C*, vol. 121, no. 29. American Chemical Society (ACS), pp. 15580–15588, Jul. 13, 2017. doi: 10.1021/acs.jpcc.7b04255.  
  
D. Wang, M. R. Talipov, M. V. Ivanovand R. Rathore, “Energy Gap between the Poly-*p*-phenylene Bridge and Donor Groups Controls the Hole Delocalization in Donor–Bridge–Donor Wires”, *Journal of the American Chemical Society*, vol. 138, no. 50. American Chemical Society (ACS), pp. 16337–16344, Dec. 07, 2016. doi: 10.1021/jacs.6b09209.  
  
T. L. Einstein and A. Pimpinelli, “Dynamical Scaling Implications of Ferrari, Prähofer, and Spohn’s Remarkable Spatial Scaling Results for Facet-Edge Fluctuations”, *Journal of Statistical Physics*, vol. 155, no. 6. Springer Science and Business Media LLC, pp. 1178–1190, Apr. 22, 2014. doi: 10.1007/s10955-014-0981-3.  
  
T. L. Einstein, A. Pimpinelliand D. Luis González, “Analyzing capture zone distributions (CZD) in growth: Theory and applications”, *Journal of Crystal Growth*, vol. 401. Elsevier BV, pp. 67–71, Sep. 2014. doi: 10.1016/j.jcrysgro.2014.01.053.  
  
D. F. Jaramillo, G. Téllez, D. L. Gonzálezand T. L. Einstein, “Interacting steps with finite-range interactions: Analytical approximation and numerical results”, *Physical Review E*, vol. 87, no. 5. American Physical Society (APS), May 24, 2013. doi: 10.1103/physreve.87.052405.  
  
J. R. Morales-Cifuentes, T. L. Einsteinand A. Pimpinelli, “How “Hot Precursors” Modify Island Nucleation: A Rate-Equation Model”, *Physical Review Letters*, vol. 113, no. 24. American Physical Society (APS), Dec. 10, 2014. doi: 10.1103/physrevlett.113.246101.  
  
P. N. Patrone, T. L. Einsteinand D. Margetis, “From atoms to steps: The microscopic origins of crystal evolution”, *Surface Science*, vol. 625. Elsevier BV, pp. 37–43, Jul. 2014. doi: 10.1016/j.susc.2014.02.015.  
  
J. Wyrick, T. L. Einsteinand L. Bartels, “Chemical insight from density functional modeling of molecular adsorption: Tracking the bonding and diffusion of anthracene derivatives on Cu(111) with molecular orbitals”, *The Journal of Chemical Physics*, vol. 142, no. 10. AIP Publishing, p. 101907, Jan. 29, 2015. doi: 10.1063/1.4906048.  
  
M. Yamamoto, T. L. Einstein, M. S. Fuhrerand W. G. Cullen, “Anisotropic Etching of Atomically Thin MoS2”, *The Journal of Physical Chemistry C*, vol. 117, no. 48. American Chemical Society (ACS), pp. 25643–25649, Nov. 20, 2013. doi: 10.1021/jp410893e.  
  
J. R. Buchwald, S. Kal, M. R. Civic, I. M. deJoode, A. S. Filatovand P. H. Dinolfo, “Spin modulation and electrochemical behavior of a five-coordinate cobalt(III) salen complex”, *Journal of Coordination Chemistry*, vol. 69, no. 11–13. Informa UK Limited, pp. 1695–1708, Apr. 28, 2016. doi: 10.1080/00958972.2016.1175001.  
  
J. M. Elward and A. Chakraborty, “Effect of Heterojunction on Exciton Binding Energy and Electron–Hole Recombination Probability in CdSe/ZnS Quantum Dots”, *Journal of Chemical Theory and Computation*, vol. 11, no. 2. American Chemical Society (ACS), pp. 462–471, Jan. 21, 2015. doi: 10.1021/ct500548x.  
  
J. M. Elward, F. J. Irudayanathan, S. Nangiaand A. Chakraborty, “Optical Signature of Formation of Protein Corona in the Firefly Luciferase-CdSe Quantum Dot Complex”, *Journal of Chemical Theory and Computation*, vol. 10, no. 12. American Chemical Society (ACS), pp. 5224–5228, Nov. 24, 2014. doi: 10.1021/ct500681m.  
  
G. Fu, H. Zheng, Y. He, W. Li, X. Lüand H. He, “Efficient near-infrared (NIR) polymer light-emitting diodes (PLEDs) based on heteroleptic iridium(iii) complexes with post-modification effects of intramolecular hydrogen bonding or BF2-chelation”, *Journal of Materials Chemistry C*, vol. 6, no. 39. Royal Society of Chemistry (RSC), pp. 10589–10596, 2018. doi: 10.1039/c8tc03432j.  
  
W. Li, Z. Liu, H. Wu, Y.-B. Cheng, Z. Zhaoand H. He, “Thiophene-Functionalized Porphyrins: Synthesis, Photophysical Properties, and Photovoltaic Performance in Dye-Sensitized Solar Cells”, *The Journal of Physical Chemistry C*, vol. 119, no. 10. American Chemical Society (ACS), pp. 5265–5273, Feb. 27, 2015. doi: 10.1021/jp509842p.  
  
P. J. Dagdigian and J. Kłos, “The effect of nonadiabaticity on the C+ + HF reaction”, *The Journal of Chemical Physics*, vol. 149, no. 20. AIP Publishing, p. 204309, Nov. 28, 2018. doi: 10.1063/1.5056312.  
  
J. Kłos, M. H. Alexanderand P. J. Dagdigian, “The interaction of NO(X2Π) with H2: *Ab initio* potential energy surfaces and bound states”, *The Journal of Chemical Physics*, vol. 146, no. 11. AIP Publishing, p. 114301, Mar. 21, 2017. doi: 10.1063/1.4977992.  
  
T. V. Tscherbul and J. Kłos, “Magnetic tuning of ultracold barrierless chemical reactions”, *Physical Review Research*, vol. 2, no. 1. American Physical Society (APS), Feb. 03, 2020. doi: 10.1103/physrevresearch.2.013117.  
  
J. Harder, S. A. Mallory, C. Tung, C. Valerianiand A. Cacciuto, “The role of particle shape in active depletion”, *The Journal of Chemical Physics*, vol. 141, no. 19. AIP Publishing, p. 194901, Nov. 21, 2014. doi: 10.1063/1.4900720.  
  
S. A. Mallory, A. Šarić, C. Valerianiand A. Cacciuto, “Anomalous thermomechanical properties of a self-propelled colloidal fluid”, *Physical Review E*, vol. 89, no. 5. American Physical Society (APS), May 06, 2014. doi: 10.1103/physreve.89.052303.  
  
S. A. Mallory, C. Valerianiand A. Cacciuto, “Curvature-induced activation of a passive tracer in an active bath”, *Physical Review E*, vol. 90, no. 3. American Physical Society (APS), Sep. 25, 2014. doi: 10.1103/physreve.90.032309.  
  
S. A. Mallory, C. Valerianiand A. Cacciuto, “Anomalous dynamics of an elastic membrane in an active fluid”, *Physical Review E*, vol. 92, no. 1. American Physical Society (APS), Jul. 20, 2015. doi: 10.1103/physreve.92.012314.  
  
K. R. Jorgensen and M. Cadena, “Theoretical study of bromine halocarbons: Accurate enthalpies of formation”, *Computational and Theoretical Chemistry*, vol. 1141. Elsevier BV, pp. 66–73, Oct. 2018. doi: 10.1016/j.comptc.2018.08.016.  
  
A. Sharma and K. Hammerton, “Comparative Study of Heavy Water Models: Solvation of Trp-Cage”, *Journal of Computational and Theoretical Nanoscience*, vol. 12, no. 1. American Scientific Publishers, pp. 113–118, Jan. 01, 2015. doi: 10.1166/jctn.2015.3706.  
  
G. M. Hocky, L. Berthierand D. R. Reichman, “Equilibrium ultrastable glasses produced by random pinning”, *The Journal of Chemical Physics*, vol. 141, no. 22. AIP Publishing, p. 224503, Dec. 14, 2014. doi: 10.1063/1.4903200.  
  
L. Ahmed, B. Rasulev, S. Kar, P. Krupa, M. A. Mozolewskaand J. Leszczynski, “Inhibitors or toxins? Large library target-specific screening of fullerene-based nanoparticles for drug design purpose”, *Nanoscale*, vol. 9, no. 29. Royal Society of Chemistry (RSC), pp. 10263–10276, 2017. doi: 10.1039/c7nr00770a.  
  
A. Gooch, N. Sizochenko, B. Rasulev, L. Gorband J. Leszczynski, “In vivo toxicity of nitroaromatics: A comprehensive quantitative structure–activity relationship study”, *Environmental Toxicology and Chemistry*, vol. 36, no. 8. Wiley, pp. 2227–2233, Mar. 21, 2017. doi: 10.1002/etc.3761.  
  
H. Yilmaz, L. Ahmed, B. Rasulevand J. Leszczynski, “Application of ligand- and receptor-based approaches for prediction of the HIV-RT inhibitory activity of fullerene derivatives”, *Journal of Nanoparticle Research*, vol. 18, no. 5. Springer Science and Business Media LLC, May 2016. doi: 10.1007/s11051-016-3429-7.  
  
V. V. Ginzburg, R. L. Sammler, W. Huangand R. G. Larson, “Anisotropic self-assembly and gelation in aqueous methylcellulose-theory and modeling”, *Journal of Polymer Science Part B: Polymer Physics*, vol. 54, no. 16. Wiley, pp. 1624–1636, Apr. 19, 2016. doi: 10.1002/polb.24065.  
  
V. V. Ginzburg, A. K. Van Dyk, T. Chatterjee, A. I. Nakatani, S. Wangand R. G. Larson, “Modeling the Adsorption of Rheology Modifiers onto Latex Particles Using Coarse-Grained Molecular Dynamics (CG-MD) and Self-Consistent Field Theory (SCFT)”, *Macromolecules*, vol. 48, no. 21. American Chemical Society (ACS), pp. 8045–8054, Nov. 02, 2015. doi: 10.1021/acs.macromol.5b02080.  
  
W. Huang, T. Mandaland R. G. Larson, “Multiscale Computational Modeling of the Nanostructure of Solid Dispersions of Hydroxypropyl Methylcellulose Acetate Succinate (HPMCAS) and Phenytoin”, *Molecular Pharmaceutics*, vol. 14, no. 10. American Chemical Society (ACS), pp. 3422–3435, Sep. 05, 2017. doi: 10.1021/acs.molpharmaceut.7b00441.  
  
W. Huang, T. Mandaland R. G. Larson, “Computational Modeling of Hydroxypropyl-Methylcellulose Acetate Succinate (HPMCAS) and Phenytoin Interactions: A Systematic Coarse-Graining Approach”, *Molecular Pharmaceutics*, vol. 14, no. 3. American Chemical Society (ACS), pp. 733–745, Feb. 13, 2017. doi: 10.1021/acs.molpharmaceut.6b01013.  
  
W. Huang, R. Ramesh, P. K. Jhaand R. G. Larson, “A Systematic Coarse-Grained Model for Methylcellulose Polymers: Spontaneous Ring Formation at Elevated Temperature”, *Macromolecules*, vol. 49, no. 4. American Chemical Society (ACS), pp. 1490–1503, Feb. 11, 2016. doi: 10.1021/acs.macromol.5b02373.  
  
K. J. Huston and R. G. Larson, “Reversible and Irreversible Adsorption Energetics of Poly(ethylene glycol) and Sorbitan Poly(ethoxylate) at a Water/Alkane Interface”, *Langmuir*, vol. 31, no. 27. American Chemical Society (ACS), pp. 7503–7511, Jul. 01, 2015. doi: 10.1021/acs.langmuir.5b00398.  
  
Z. Li, F. Yuan, K. A. Fichthorn, S. T. Milnerand R. G. Larson, “Molecular View of Polymer/Water Interfaces in Latex Paint”, *Macromolecules*, vol. 47, no. 18. American Chemical Society (ACS), pp. 6441–6452, Sep. 08, 2014. doi: 10.1021/ma500866f.  
  
T. Mandal, W. Huang, J. M. Mecca, A. Getchell, W. W. Porterand R. G. Larson, “A framework for multi-scale simulation of crystal growth in the presence of polymers”, *Soft Matter*, vol. 13, no. 9. Royal Society of Chemistry (RSC), pp. 1904–1913, 2017. doi: 10.1039/c6sm02893d.  
  
T. Mandal and R. G. Larson, “Nucleation of urea from aqueous solution: Structure, critical size, and rate”, *The Journal of Chemical Physics*, vol. 146, no. 13. AIP Publishing, p. 134501, Apr. 07, 2017. doi: 10.1063/1.4979141.  
  
T. Mandal and R. G. Larson, “Stretch and Breakage of Wormlike Micelles under Uniaxial Strain: A Simulation Study and Comparison with Experimental Results”, *Langmuir*, vol. 34, no. 42. American Chemical Society (ACS), pp. 12600–12608, Sep. 25, 2018. doi: 10.1021/acs.langmuir.8b02421.  
  
R. L. Marson, Y. Huang, M. Huang, T. Fuand R. G. Larson, “Inertio-capillary cross-streamline drift of droplets in Poiseuille flow using dissipative particle dynamics simulations”, *Soft Matter*, vol. 14, no. 12. Royal Society of Chemistry (RSC), pp. 2267–2280, 2018. doi: 10.1039/c7sm02294h.  
  
S. Wang and R. G. Larson, “Coarse-Grained Molecular Dynamics Simulation of Self-Assembly and Surface Adsorption of Ionic Surfactants Using an Implicit Water Model”, *Langmuir*, vol. 31, no. 4. American Chemical Society (ACS), pp. 1262–1271, Jan. 21, 2015. doi: 10.1021/la503700c.  
  
F. Yuan and R. G. Larson, “Multiscale Molecular Dynamics Simulations of Model Hydrophobically Modified Ethylene Oxide Urethane Micelles”, *The Journal of Physical Chemistry B*, vol. 119, no. 38. American Chemical Society (ACS), pp. 12540–12551, Sep. 15, 2015. doi: 10.1021/acs.jpcb.5b04895.  
  
F. Yuan, S. Wangand R. G. Larson, “Potentials of Mean Force and Escape Times of Surfactants from Micelles and Hydrophobic Surfaces Using Molecular Dynamics Simulations”, *Langmuir*, vol. 31, no. 4. American Chemical Society (ACS), pp. 1336–1343, Jan. 21, 2015. doi: 10.1021/la5044393.  
  
W. Zhang and R. G. Larson, “Direct All-Atom Molecular Dynamics Simulations of the Effects of Short Chain Branching on Polyethylene Oligomer Crystal Nucleation”, *Macromolecules*, vol. 51, no. 13. American Chemical Society (ACS), pp. 4762–4769, Jun. 25, 2018. doi: 10.1021/acs.macromol.8b00958.  
  
W. Zhang and R. G. Larson, “A metastable nematic precursor accelerates polyethylene oligomer crystallization as determined by atomistic simulations and self-consistent field theory”, *The Journal of Chemical Physics*, vol. 150, no. 24. AIP Publishing, p. 244903, Jun. 28, 2019. doi: 10.1063/1.5110681.  
  
W. Zhang, A. Travitzand R. G. Larson, “Modeling Intercolloidal Interactions Induced by Adsorption of Mobile Telechelic Polymers onto Particle Surfaces”, *Macromolecules*, vol. 52, no. 14. American Chemical Society (ACS), pp. 5357–5365, Jul. 10, 2019. doi: 10.1021/acs.macromol.9b00775.  
  
J. A. Bogart, “A Ligand Field Series for the 4f-Block from Experimental and DFT Computed Ce(IV/III) Electrochemical Potentials”, *Inorganic Chemistry*, vol. 54, no. 6. American Chemical Society (ACS), pp. 2830–2837, Feb. 24, 2015. doi: 10.1021/ic503000z.  
  
J. A. Bogart, A. J. Lewisand E. J. Schelter, “DFT Study of the Active Site of the XoxF-Type Natural, Cerium-Dependent Methanol Dehydrogenase Enzyme”, *Chemistry - A European Journal*, vol. 21, no. 4. Wiley, pp. 1743–1748, Nov. 24, 2014. doi: 10.1002/chem.201405159.  
  
J. A. Bogart, C. A. Lippincott, P. J. Carroll, C. H. Boothand E. J. Schelter, “Controlled Redox Chemistry at Cerium within a Tripodal Nitroxide Ligand Framework”, *Chemistry - A European Journal*, vol. 21, no. 49. Wiley, pp. 17850–17859, Oct. 27, 2015. doi: 10.1002/chem.201502952.  
  
M. A. Boreen, J. A. Bogart, P. J. Carrolland E. J. Schelter, “Rearrangement in a Tripodal Nitroxide Ligand To Modulate the Reactivity of a Ti–F Bond”, *Inorganic Chemistry*, vol. 54, no. 19. American Chemical Society (ACS), pp. 9588–9593, Sep. 23, 2015. doi: 10.1021/acs.inorgchem.5b01687.  
  
T. Cheisson, L. A. Solola, M. R. Gau, P. J. Carrolland E. J. Schelter, “Silyl Transfer Pathway to a Ce(IV) Imido Complex”, *Organometallics*, vol. 37, no. 23. American Chemical Society (ACS), pp. 4332–4335, Sep. 04, 2018. doi: 10.1021/acs.organomet.8b00366.  
  
H. Fang, “Electro‐kinetic Separation of Rare Earth Elements Using a Redox‐Active Ligand”, *Angewandte Chemie International Edition*, vol. 56, no. 43. Wiley, pp. 13450–13454, Sep. 25, 2017. doi: 10.1002/anie.201706894.  
  
J. E. Kim, P. J. Carrolland E. J. Schelter, “Bidentate nitroxide ligands stable toward oxidative redox cycling and their complexes with cerium and lanthanum”, *Chemical Communications*, vol. 51, no. 81. Royal Society of Chemistry (RSC), pp. 15047–15050, 2015. doi: 10.1039/c5cc06052d.  
  
J. R. Levin, W. L. Dorfner, P. J. Carrolland E. J. Schelter, “Control of cerium oxidation state through metal complex secondary structures”, *Chemical Science*, vol. 6, no. 12. Royal Society of Chemistry (RSC), pp. 6925–6934, 2015. doi: 10.1039/c5sc02607e.  
  
A. J. Lewis, K. C. Mullane, E. Nakamaru-Ogiso, P. J. Carrolland E. J. Schelter, “The Inverse Trans Influence in a Family of Pentavalent Uranium Complexes”, *Inorganic Chemistry*, vol. 53, no. 13. American Chemical Society (ACS), pp. 6944–6953, Jun. 10, 2014. doi: 10.1021/ic500833s.  
  
A. McSkimming, T. Cheisson, P. J. Carrolland E. J. Schelter, “Functional Synthetic Model for the Lanthanide-Dependent Quinoid Alcohol Dehydrogenase Active Site”, *Journal of the American Chemical Society*, vol. 140, no. 4. American Chemical Society (ACS), pp. 1223–1226, Jan. 18, 2018. doi: 10.1021/jacs.7b12318.  
  
K. C. Mullane, T. Cheisson, E. Nakamaru‐Ogiso, B. C. Manor, P. J. Carrolland E. J. Schelter, “Reduction of Carbonyl Groups by Uranium(III) and Formation of a Stable Amide Radical Anion”, *Chemistry – A European Journal*, vol. 24, no. 4. Wiley, pp. 826–837, Dec. 06, 2017. doi: 10.1002/chem.201703396.  
  
K. C. Mullane, A. J. Lewis, H. Yin, P. J. Carrolland E. J. Schelter, “Anomalous One-Electron Processes in the Chemistry of Uranium Nitrogen Multiple Bonds”, *Inorganic Chemistry*, vol. 53, no. 17. American Chemical Society (ACS), pp. 9129–9139, Aug. 11, 2014. doi: 10.1021/ic501149u.  
  
L. A. Solola, A. V. Zabula, W. L. Dorfner, B. C. Manor, P. J. Carrolland E. J. Schelter, “An Alkali Metal-Capped Cerium(IV) Imido Complex”, *Journal of the American Chemical Society*, vol. 138, no. 22. American Chemical Society (ACS), pp. 6928–6931, May 26, 2016. doi: 10.1021/jacs.6b03293.  
  
L. A. Solola, A. V. Zabula, W. L. Dorfner, B. C. Manor, P. J. Carrolland E. J. Schelter, “Cerium(IV) Imido Complexes: Structural, Computational, and Reactivity Studies”, *Journal of the American Chemical Society*, vol. 139, no. 6. American Chemical Society (ACS), pp. 2435–2442, Feb. 06, 2017. doi: 10.1021/jacs.6b12369.  
  
U. J. Williams, J. R. Robinson, A. J. Lewis, P. J. Carroll, P. J. Walshand E. J. Schelter, “Synthesis, Bonding, and Reactivity of a Cerium(IV) Fluoride Complex”, *Inorganic Chemistry*, vol. 53, no. 1. American Chemical Society (ACS), pp. 27–29, Dec. 06, 2013. doi: 10.1021/ic402769u.  
  
H. Yin, P. J. Carroll, J. M. Annaand E. J. Schelter, “Luminescent Ce(III) Complexes as Stoichiometric and Catalytic Photoreductants for Halogen Atom Abstraction Reactions”, *Journal of the American Chemical Society*, vol. 137, no. 29. American Chemical Society (ACS), pp. 9234–9237, Jul. 20, 2015. doi: 10.1021/jacs.5b05411.  
  
H. Yin, P. J. Carroll, B. C. Manor, J. M. Annaand E. J. Schelter, “Cerium Photosensitizers: Structure–Function Relationships and Applications in Photocatalytic Aryl Coupling Reactions”, *Journal of the American Chemical Society*, vol. 138, no. 18. American Chemical Society (ACS), pp. 5984–5993, May 02, 2016. doi: 10.1021/jacs.6b02248.  
  
H. Yin, P. J. Carrolland E. J. Schelter, “Cerium(III) and Uranium(IV) Complexes of the 2-Fluorophenyl Trimethylsilyl Amide Ligand: C–F → Ln/An Interactions that Modulate the Coordination Spheres of f-Block Elements”, *Inorganic Chemistry*, vol. 55, no. 11. American Chemical Society (ACS), pp. 5684–5692, May 26, 2016. doi: 10.1021/acs.inorgchem.6b00785.  
  
H. Yin, “The Hexachlorocerate(III) Anion: A Potent, Benchtop Stable, and Readily Available Ultraviolet A Photosensitizer for Aryl Chlorides”, *Journal of the American Chemical Society*, vol. 138, no. 50. American Chemical Society (ACS), pp. 16266–16273, Dec. 12, 2016. doi: 10.1021/jacs.6b05712.  
  
H. Yin, A. V. Zabulaand E. J. Schelter, “C–F→Ln/An interactions in synthetic f-element chemistry”, *Dalton Transactions*, vol. 45, no. 15. Royal Society of Chemistry (RSC), pp. 6313–6323, 2016. doi: 10.1039/c6dt00108d.  
  
L. Wang, M. Ceriottiand T. E. Markland, “Quantum fluctuations and isotope effects in *ab initio* descriptions of water”, *The Journal of Chemical Physics*, vol. 141, no. 10. AIP Publishing, p. 104502, Sep. 14, 2014. doi: 10.1063/1.4894287.  
  
L. Wang, S. D. Fried, S. G. Boxerand T. E. Markland, “Quantum delocalization of protons in the hydrogen-bond network of an enzyme active site”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 52. Proceedings of the National Academy of Sciences, pp. 18454–18459, Dec. 12, 2014. doi: 10.1073/pnas.1417923111.  
  
L. Wang, C. M. Isbornand T. E. Markland, “Simulating Nuclear and Electronic Quantum Effects in Enzymes”, *Methods in Enzymology*. Elsevier, pp. 389–418, 2016. doi: 10.1016/bs.mie.2016.05.047.  
  
X. Liang, “Design, Synthesis, and Antitumor Evaluation of 4-Amino-(1*H*)-pyrazole Derivatives as JAKs Inhibitors”, *ACS Medicinal Chemistry Letters*, vol. 7, no. 10. American Chemical Society (ACS), pp. 950–955, Aug. 24, 2016. doi: 10.1021/acsmedchemlett.6b00247.  
  
J. W. Nelson, L. M. Grundy, Y. Dang, Z.-X. Wangand X. Wang, “Mechanism of *Z*-Selective Olefin Metathesis Catalyzed by a Ruthenium Monothiolate Carbene Complex: A DFT Study”, *Organometallics*, vol. 33, no. 16. American Chemical Society (ACS), pp. 4290–4294, Aug. 01, 2014. doi: 10.1021/om500612r.  
  
M. A. Ashley, J. S. Hirschi, J. A. Izzoand M. J. Vetticatt, “Isotope Effects Reveal the Mechanism of Enamine Formation in l-Proline-Catalyzed α-Amination of Aldehydes”, *Journal of the American Chemical Society*, vol. 138, no. 6. American Chemical Society (ACS), pp. 1756–1759, Feb. 04, 2016. doi: 10.1021/jacs.5b10876.  
  
H. Rabaâ, H. Khaledi, M. M. Olmsteadand D. Sundholm, “Computational Studies of a Paramagnetic Planar Dibenzotetraaza[14]annulene Ni(II) Complex”, *The Journal of Physical Chemistry A*, vol. 119, no. 21. American Chemical Society (ACS), pp. 5189–5196, Jan. 05, 2015. doi: 10.1021/jp509824z.  
  
W. J. Morgan and R. C. Fortenberry, “Additional diffuse functions in basis sets for dipole-bound excited states of anions”, *Theoretical Chemistry Accounts*, vol. 134, no. 4. Springer Science and Business Media LLC, Apr. 2015. doi: 10.1007/s00214-015-1647-1.  
  
W. J. Morgan and R. C. Fortenberry, “Theoretical Rovibronic Treatment of the X̃ 2Σ+ and Ã 2Π States of C2H and the X̃ 1Σ+ State of C2H– from Quartic Force Fields”, *The Journal of Physical Chemistry A*, vol. 119, no. 27. American Chemical Society (ACS), pp. 7013–7025, Jun. 29, 2015. doi: 10.1021/acs.jpca.5b03489.  
  
M. M. Gianetti, A. Haji-Akbari, M. Paula Longinottiand P. G. Debenedetti, “Computational investigation of structure, dynamics and nucleation kinetics of a family of modified Stillinger–Weber model fluids in bulk and free-standing thin films”, *Physical Chemistry Chemical Physics*, vol. 18, no. 5. Royal Society of Chemistry (RSC), pp. 4102–4111, 2016. doi: 10.1039/c5cp06535f.  
  
J. S. Bandar, G. S. Sauer, W. D. Wulff, T. H. Lambertand M. J. Vetticatt, “Transition State Analysis of Enantioselective Brønsted Base Catalysis by Chiral Cyclopropenimines”, *Journal of the American Chemical Society*, vol. 136, no. 30. American Chemical Society (ACS), pp. 10700–10707, Jul. 16, 2014. doi: 10.1021/ja504532d.  
  
S. Akbulatov, Y. Tian, Z. Huang, T. J. Kucharski, Q.-Z. Yangand R. Boulatov, “Experimentally realized mechanochemistry distinct from force-accelerated scission of loaded bonds”, *Science*, vol. 357, no. 6348. American Association for the Advancement of Science (AAAS), pp. 299–303, Jul. 21, 2017. doi: 10.1126/science.aan1026.  
  
Z. S. Kean, S. Akbulatov, Y. Tian, R. A. Widenhoefer, R. Boulatovand S. L. Craig, “Photomechanical Actuation of Ligand Geometry in Enantioselective Catalysis”, *Angewandte Chemie*, vol. 126, no. 52. Wiley, pp. 14736–14739, Oct. 30, 2014. doi: 10.1002/ange.201407494.  
  
J. Wang, T. B. Kouznetsova, R. Boulatovand S. L. Craig, “Mechanical gating of a mechanochemical reaction cascade”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Nov. 16, 2016. doi: 10.1038/ncomms13433.  
  
L. Wang, “Mechanochemical Regulation of Oxidative Addition to a Palladium(0) Bisphosphine Complex”, *Journal of the American Chemical Society*, vol. 142, no. 41. American Chemical Society (ACS), pp. 17714–17720, Sep. 22, 2020. doi: 10.1021/jacs.0c08506.  
  
Y. Yu, “Force-Modulated Reductive Elimination from Platinum(II) Diaryl Complexes”, *[]*. American Chemical Society (ACS), Sep. 21, 2020. doi: 10.26434/chemrxiv.12977678.v1.  
  
A. Haji-Akbari and P. G. Debenedetti, “Direct calculation of ice homogeneous nucleation rate for a molecular model of water”, *Proceedings of the National Academy of Sciences*, vol. 112, no. 34. Proceedings of the National Academy of Sciences, pp. 10582–10588, Aug. 03, 2015. doi: 10.1073/pnas.1509267112.  
  
A. Haji-Akbari and P. G. Debenedetti, “Computational investigation of surface freezing in a molecular model of water”, *Proceedings of the National Academy of Sciences*, vol. 114, no. 13. Proceedings of the National Academy of Sciences, pp. 3316–3321, Mar. 14, 2017. doi: 10.1073/pnas.1620999114.  
  
S. B. Kim, J. C. Palmerand P. G. Debenedetti, “A Computational Study of the Effect of Matrix Structural Order on Water Sorption by Trp-Cage Miniproteins”, *The Journal of Physical Chemistry B*, vol. 119, no. 5. American Chemical Society (ACS), pp. 1847–1856, Jan. 23, 2015. doi: 10.1021/jp510172w.  
  
C. S. Ewing, “Structural and Electronic Properties of Pt13 Nanoclusters on Amorphous Silica Supports”, *The Journal of Physical Chemistry C*, vol. 119, no. 5. American Chemical Society (ACS), pp. 2503–2512, Jan. 26, 2015. doi: 10.1021/jp5105104.  
  
J. Ye and J. K. Johnson, “Design of Lewis Pair-Functionalized Metal Organic Frameworks for CO2 Hydrogenation”, *ACS Catalysis*, vol. 5, no. 5. American Chemical Society (ACS), pp. 2921–2928, Apr. 09, 2015. doi: 10.1021/acscatal.5b00396.  
  
J. Ye and J. K. Johnson, “Screening Lewis Pair Moieties for Catalytic Hydrogenation of CO2 in Functionalized UiO-66”, *ACS Catalysis*, vol. 5, no. 10. American Chemical Society (ACS), pp. 6219–6229, Sep. 23, 2015. doi: 10.1021/acscatal.5b01191.  
  
J. Ye and J. K. Johnson, “Catalytic hydrogenation of CO2 to methanol in a Lewis pair functionalized MOF”, *Catalysis Science & Technology*, vol. 6, no. 24. Royal Society of Chemistry (RSC), pp. 8392–8405, 2016. doi: 10.1039/c6cy01245k.  
  
C. S. Ewing, A. Bagusetty, E. G. Patriarca, D. S. Lambrecht, G. Veserand J. K. Johnson, “Impact of Support Interactions for Single-Atom Molybdenum Catalysts on Amorphous Silica”, *Industrial & Engineering Chemistry Research*, vol. 55, no. 48. American Chemical Society (ACS), pp. 12350–12357, Nov. 22, 2016. doi: 10.1021/acs.iecr.6b03558.  
  
C. S. Ewing, G. Veser, J. J. McCarthy, D. S. Lambrechtand J. K. Johnson, “Predicting catalyst-support interactions between metal nanoparticles and amorphous silica supports”, *Surface Science*, vol. 652. Elsevier BV, pp. 278–285, Oct. 2016. doi: 10.1016/j.susc.2016.03.004.  
  
J. Oomens, G. Berdenand T. H. Morton, “Negative Hyperconjugation versus Electronegativity: Vibrational Spectra of Free Fluorinated Alkoxide Ions in the Gas Phase”, *ChemPhysChem*, vol. 16, no. 9. Wiley, pp. 1992–1995, Apr. 17, 2015. doi: 10.1002/cphc.201500177.  
  
L. J. Fischer, A. S. Duttonand A. H. Winter, “Anomalous effect of non-alternant hydrocarbons on carbocation and carbanion electronic configurations”, *Chemical Science*, vol. 8, no. 6. Royal Society of Chemistry (RSC), pp. 4231–4241, 2017. doi: 10.1039/c7sc01047h.  
  
M. R. Geraskina, A. S. Dutton, M. J. Juetten, S. A. Woodand A. H. Winter, “The Viologen Cation Radical Pimer: A Case of Dispersion‐Driven Bonding”, *Angewandte Chemie International Edition*, vol. 56, no. 32. Wiley, pp. 9435–9439, Jul. 07, 2017. doi: 10.1002/anie.201704959.  
  
Z. Liu, Y. Lei, C. Grayand G. Wang, “Examination of Solid-Solution Phase Formation Rules for High Entropy Alloys from Atomistic Monte Carlo Simulations”, *JOM*, vol. 67, no. 10. Springer Science and Business Media LLC, pp. 2364–2374, Jun. 23, 2015. doi: 10.1007/s11837-015-1508-3.  
  
C. André Ohlin, J. R. Rustadand W. H. Casey, “The energetics of isomerisation in Keggin-series aluminate cations”, *Dalton Trans.*, vol. 43, no. 39. Royal Society of Chemistry (RSC), pp. 14533–14536, 2014. doi: 10.1039/c4dt01763c.  
  
R. Qi, L.-P. Wang, Q. Wang, V. S. Pandeand P. Ren, “United polarizable multipole water model for molecular mechanics simulation”, *The Journal of Chemical Physics*, vol. 143, no. 1. AIP Publishing, p. 014504, Jul. 07, 2015. doi: 10.1063/1.4923338.  
  
S. Herrmann and E. Iglesia, “Elementary steps in acetone condensation reactions catalyzed by aluminosilicates with diverse void structures”, *Journal of Catalysis*, vol. 346. Elsevier BV, pp. 134–153, Feb. 2017. doi: 10.1016/j.jcat.2016.12.011.  
  
A. J. Jones and E. Iglesia, “Kinetic, Spectroscopic, and Theoretical Assessment of Associative and Dissociative Methanol Dehydration Routes in Zeolites”, *Angewandte Chemie International Edition*, vol. 53, no. 45. Wiley, pp. 12177–12181, Sep. 11, 2014. doi: 10.1002/anie.201406823.  
  
A. J. Jones and E. Iglesia, “The Strength of Brønsted Acid Sites in Microporous Aluminosilicates”, *ACS Catalysis*, vol. 5, no. 10. American Chemical Society (ACS), pp. 5741–5755, Aug. 31, 2015. doi: 10.1021/acscatal.5b01133.  
  
A. J. Jones, S. I. Zonesand E. Iglesia, “Implications of Transition State Confinement within Small Voids for Acid Catalysis”, *The Journal of Physical Chemistry C*, vol. 118, no. 31. American Chemical Society (ACS), pp. 17787–17800, Jul. 18, 2014. doi: 10.1021/jp5050095.  
  
W. Knaeble and E. Iglesia, “Kinetic and Theoretical Insights into the Mechanism of Alkanol Dehydration on Solid Brønsted Acid Catalysts”, *The Journal of Physical Chemistry C*, vol. 120, no. 6. American Chemical Society (ACS), pp. 3371–3389, Feb. 05, 2016. doi: 10.1021/acs.jpcc.5b11127.  
  
W. Knaeble and E. Iglesia, “Acid strength and metal-acid proximity effects on methylcyclohexane ring contraction turnover rates and selectivities”, *Journal of Catalysis*, vol. 344. Elsevier BV, pp. 817–830, Dec. 2016. doi: 10.1016/j.jcat.2016.08.007.  
  
M. L. Sarazen, E. Doskociland E. Iglesia, “Catalysis on solid acids: Mechanism and catalyst descriptors in oligomerization reactions of light alkenes”, *Journal of Catalysis*, vol. 344. Elsevier BV, pp. 553–569, Dec. 2016. doi: 10.1016/j.jcat.2016.10.010.  
  
M. L. Sarazen, E. Doskociland E. Iglesia, “Effects of Void Environment and Acid Strength on Alkene Oligomerization Selectivity”, *ACS Catalysis*, vol. 6, no. 10. American Chemical Society (ACS), pp. 7059–7070, Sep. 21, 2016. doi: 10.1021/acscatal.6b02128.  
  
L. Annamalai, Y. Liu, S. Ezenwa, Y. Dang, S. L. Suiband P. Deshlahra, “Influence of Tight Confinement on Selective Oxidative Dehydrogenation of Ethane on MoVTeNb Mixed Oxides”, *ACS Catalysis*, vol. 8, no. 8. American Chemical Society (ACS), pp. 7051–7067, Jul. 05, 2018. doi: 10.1021/acscatal.8b01586.  
  
R. S. Bhatta and M. Tsige, “Effect of Fluorination on Electronic Properties of Polythienothiophene-*co*-benzodithiophenes and Their Fullerene Complexes”, *ACS Applied Materials & Interfaces*, vol. 6, no. 18. American Chemical Society (ACS), pp. 15889–15896, Aug. 29, 2014. doi: 10.1021/am5035126.  
  
R. S. Bhatta and M. Tsige, “Chain length and torsional dependence of exciton binding energies in P3HT and PTB7 conjugated polymers: A first-principles study”, *Polymer*, vol. 55, no. 11. Elsevier BV, pp. 2667–2672, May 2014. doi: 10.1016/j.polymer.2014.04.022.  
  
R. S. Bhatta and M. Tsige, “Understanding the effect of heteroatoms on structural and electronic properties of conjugated polymers”, *Polymer*, vol. 56. Elsevier BV, pp. 293–299, Jan. 2015. doi: 10.1016/j.polymer.2014.11.050.  
  
M. Bendahmane, “The synaptotagmin C2B domain calcium-binding loops modulate the rate of fusion pore expansion”, *Molecular Biology of the Cell*, vol. 29, no. 7. American Society for Cell Biology (ASCB), pp. 834–845, Apr. 2018. doi: 10.1091/mbc.e17-11-0623.  
  
N. L. Chon, “Membrane Docking of the Synaptotagmin 7 C2A Domain: Computation Reveals Interplay between Electrostatic and Hydrophobic Contributions”, *Biochemistry*, vol. 54, no. 37. American Chemical Society (ACS), pp. 5696–5711, Sep. 10, 2015. doi: 10.1021/acs.biochem.5b00422.  
  
A. W. Duster, C. M. Garza, B. O. Aydintug, M. B. Negussieand H. Lin, “Adaptive Partitioning QM/MM for Molecular Dynamics Simulations: 6. Proton Transport through a Biological Channel”, *Journal of Chemical Theory and Computation*, vol. 15, no. 2. American Chemical Society (ACS), pp. 892–905, Jan. 14, 2019. doi: 10.1021/acs.jctc.8b01128.  
  
A. Duster, C. Garzaand H. Lin, “Adaptive Partitioning QM/MM Dynamics Simulations for Substrate Uptake, Product Release, and Solvent Exchange”, *Methods in Enzymology*. Elsevier, pp. 341–357, 2016. doi: 10.1016/bs.mie.2016.05.019.  
  
A. W. Duster and H. Lin, “Restrained Proton Indicator in Combined Quantum-Mechanics/Molecular-Mechanics Dynamics Simulations of Proton Transfer through a Carbon Nanotube”, *The Journal of Physical Chemistry B*, vol. 121, no. 36. American Chemical Society (ACS), pp. 8585–8592, Aug. 30, 2017. doi: 10.1021/acs.jpcb.7b06657.  
  
A. W. Duster and H. Lin, “Tracking Proton Transfer through Titratable Amino Acid Side Chains in Adaptive QM/MM Simulations”, *Journal of Chemical Theory and Computation*, vol. 15, no. 11. American Chemical Society (ACS), pp. 5794–5809, Sep. 25, 2019. doi: 10.1021/acs.jctc.9b00649.  
  
A. W. Duster, C. Wang, C. M. Garza, D. E. Millerand H. Lin, “Adaptive quantum/molecular mechanics: what have we learned, where are we, and where do we go from here?”, *WIREs Computational Molecular Science*, vol. 7, no. 5. Wiley, Apr. 17, 2017. doi: 10.1002/wcms.1310.  
  
A. Duster, C.-H. Wangand H. Lin, “Adaptive QM/MM for Molecular Dynamics Simulations: 5. On the Energy-Conserved Permuted Adaptive-Partitioning Schemes”, *Molecules*, vol. 23, no. 9. MDPI AG, p. 2170, Aug. 28, 2018. doi: 10.3390/molecules23092170.  
  
D. D. MacDougall, “The high-affinity calcium sensor synaptotagmin-7 serves multiple roles in regulated exocytosis”, *Journal of General Physiology*, vol. 150, no. 6. Rockefeller University Press, pp. 783–807, May 24, 2018. doi: 10.1085/jgp.201711944.  
  
J. R. Osterberg, N. L. Chon, A. Boo, F. A. Maynard, H. Linand J. D. Knight, “Membrane Docking of the Synaptotagmin 7 C2A Domain: Electron Paramagnetic Resonance Measurements Show Contributions from Two Membrane Binding Loops”, *Biochemistry*, vol. 54, no. 37. American Chemical Society (ACS), pp. 5684–5695, Sep. 10, 2015. doi: 10.1021/acs.biochem.5b00421.  
  
S. Pezeshki, C. Davis, A. Heydenand H. Lin, “Adaptive-Partitioning QM/MM Dynamics Simulations: 3. Solvent Molecules Entering and Leaving Protein Binding Sites”, *Journal of Chemical Theory and Computation*, vol. 10, no. 11. American Chemical Society (ACS), pp. 4765–4776, Oct. 10, 2014. doi: 10.1021/ct500553x.  
  
S. Pezeshki and H. Lin, “Molecular dynamics simulations of ion solvation by flexible-boundary QM/MM: On-the-fly partial charge transfer between QM and MM subsystems”, *Journal of Computational Chemistry*, vol. 35, no. 24. Wiley, pp. 1778–1788, Jul. 23, 2014. doi: 10.1002/jcc.23685.  
  
S. Pezeshki and H. Lin, “Adaptive-Partitioning QM/MM for Molecular Dynamics Simulations: 4. Proton Hopping in Bulk Water”, *Journal of Chemical Theory and Computation*, vol. 11, no. 6. American Chemical Society (ACS), pp. 2398–2411, May 22, 2015. doi: 10.1021/ct501019y.  
  
S. Pezeshki and H. Lin, “Recent Progress in Adaptive-Partitioning QM/MM Methods for Born-Oppenheimer Molecular Dynamics”, *Challenges and Advances in Computational Chemistry and Physics*. Springer International Publishing, pp. 93–113, 2015. doi: 10.1007/978-3-319-21626-3\_3.  
  
C.-H. Wang, A. W. Duster, B. O. Aydintug, M. G. Zareckiand H. Lin, “Chloride Ion Transport by the E. coli CLC Cl−/H+ Antiporter: A Combined Quantum-Mechanical and Molecular-Mechanical Study”, *Frontiers in Chemistry*, vol. 6. Frontiers Media SA, Mar. 13, 2018. doi: 10.3389/fchem.2018.00062.  
  
C. Gray, Y. Leiand G. Wang, “Charged vacancy diffusion in chromium oxide crystal: DFT and DFT+U predictions”, *Journal of Applied Physics*, vol. 120, no. 21. AIP Publishing, p. 215101, Dec. 07, 2016. doi: 10.1063/1.4970882.  
  
N. He, “Mordant inspired wet-spinning of graphene fibers for high performance flexible supercapacitors”, *Journal of Materials Chemistry A*, vol. 7, no. 12. Royal Society of Chemistry (RSC), pp. 6869–6876, 2019. doi: 10.1039/c8ta12337c.  
  
S. Kattel and G. Wang, “Beneficial compressive strain for oxygen reduction reaction on Pt (111) surface”, *The Journal of Chemical Physics*, vol. 141, no. 12. AIP Publishing, p. 124713, Sep. 28, 2014. doi: 10.1063/1.4896604.  
  
J. Li, G. Wangand G. Zhou, “Surface segregation phenomena in extended and nanoparticle surfaces of Cu–Au alloys”, *Surface Science*, vol. 649. Elsevier BV, pp. 39–45, Jul. 2016. doi: 10.1016/j.susc.2016.01.013.  
  
J. Li, “Thermally Driven Structure and Performance Evolution of Atomically Dispersed FeN 4 Sites for Oxygen Reduction”, *Angewandte Chemie International Edition*, vol. 58, no. 52. Wiley, pp. 18971–18980, Nov. 11, 2019. doi: 10.1002/anie.201909312.  
  
J. Li, “Thermally Driven Structure and Performance Evolution of Atomically Dispersed FeN 4 Sites for Oxygen Reduction”, *Angewandte Chemie International Edition*, vol. 58, no. 52. Wiley, pp. 18971–18980, Nov. 11, 2019. doi: 10.1002/anie.201909312.  
  
K. Liu, S. Kattel, V. Maoand G. Wang, “Electrochemical and Computational Study of Oxygen Reduction Reaction on Nonprecious Transition Metal/Nitrogen Doped Carbon Nanofibers in Acid Medium”, *The Journal of Physical Chemistry C*, vol. 120, no. 3. American Chemical Society (ACS), pp. 1586–1596, Jan. 15, 2016. doi: 10.1021/acs.jpcc.5b10334.  
  
K. Liu, “Mn- and N- doped carbon as promising catalysts for oxygen reduction reaction: Theoretical prediction and experimental validation”, *Applied Catalysis B: Environmental*, vol. 243. Elsevier BV, pp. 195–203, Apr. 2019. doi: 10.1016/j.apcatb.2018.10.034.  
  
K. Liu, G. Wuand G. Wang, “Role of Local Carbon Structure Surrounding FeN4 Sites in Boosting the Catalytic Activity for Oxygen Reduction”, *The Journal of Physical Chemistry C*, vol. 121, no. 21. American Chemical Society (ACS), pp. 11319–11324, May 11, 2017. doi: 10.1021/acs.jpcc.7b00913.  
  
Z. Liu, Y. Leiand G. Wang, “First-principles computation of surface segregation in L10CoPt magnetic nanoparticles”, *Journal of Physics: Condensed Matter*, vol. 28, no. 26. IOP Publishing, p. 266002, May 19, 2016. doi: 10.1088/0953-8984/28/26/266002.  
  
Z. Liu, R. O. Olivares, Y. Lei, C. I. Garciaand G. Wang, “Microstructural characterization and recrystallization kinetics modeling of annealing cold-rolled vanadium microalloyed HSLA steels”, *Journal of Alloys and Compounds*, vol. 679. Elsevier BV, pp. 293–301, Sep. 2016. doi: 10.1016/j.jallcom.2016.04.057.  
  
Z. Liu and G. Wang, “Surface magnetism of L10CoPt alloy: first principles predictions”, *Journal of Physics: Condensed Matter*, vol. 29, no. 35. IOP Publishing, p. 355801, Jul. 31, 2017. doi: 10.1088/1361-648x/aa7b5b.  
  
Z. Liu and G. Wang, “Shape-dependent surface magnetism of Co-Pt and Fe-Pt nanoparticles from first principles”, *Physical Review B*, vol. 96, no. 22. American Physical Society (APS), Dec. 08, 2017. doi: 10.1103/physrevb.96.224412.  
  
Y. Li, “In Situ “Chainmail Catalyst” Assembly in Low‐Tortuosity, Hierarchical Carbon Frameworks for Efficient and Stable Hydrogen Generation”, *Advanced Energy Materials*, vol. 8, no. 25. Wiley, p. 1801289, Jul. 29, 2018. doi: 10.1002/aenm.201801289.  
  
S. Mukherjee, “Metal-organic framework-derived nitrogen-doped highly disordered carbon for electrochemical ammonia synthesis using N2 and H2O in alkaline electrolytes”, *Nano Energy*, vol. 48. Elsevier BV, pp. 217–226, Jun. 2018. doi: 10.1016/j.nanoen.2018.03.059.  
  
F. Pan, “Promoting electrocatalytic CO2 reduction on nitrogen-doped carbon with sulfur addition”, *Applied Catalysis B: Environmental*, vol. 252. Elsevier BV, pp. 240–249, Sep. 2019. doi: 10.1016/j.apcatb.2019.04.025.  
  
F. Pan, B. Li, X. Xiang, G. Wangand Y. Li, “Efficient CO2 Electroreduction by Highly Dense and Active Pyridinic Nitrogen on Holey Carbon Layers with Fluorine Engineering”, *ACS Catalysis*, vol. 9, no. 3. American Chemical Society (ACS), pp. 2124–2133, Jan. 25, 2019. doi: 10.1021/acscatal.9b00016.  
  
F. Pan, “Atomic-level active sites of efficient imidazolate framework-derived nickel catalysts for CO2 reduction”, *Journal of Materials Chemistry A*, vol. 7, no. 46. Royal Society of Chemistry (RSC), pp. 26231–26237, 2019. doi: 10.1039/c9ta08862h.  
  
Z. Qiao, “3D porous graphitic nanocarbon for enhancing the performance and durability of Pt catalysts: a balance between graphitization and hierarchical porosity”, *Energy & Environmental Science*, vol. 12, no. 9. Royal Society of Chemistry (RSC), pp. 2830–2841, 2019. doi: 10.1039/c9ee01899a.  
  
X. Shan, “Bivalence Mn5O8 with hydroxylated interphase for high-voltage aqueous sodium-ion storage”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Nov. 15, 2016. doi: 10.1038/ncomms13370.  
  
C. Stecker, “Surface Defect Dynamics in Organic–Inorganic Hybrid Perovskites: From Mechanism to Interfacial Properties”, *ACS Nano*, vol. 13, no. 10. American Chemical Society (ACS), pp. 12127–12136, Sep. 30, 2019. doi: 10.1021/acsnano.9b06585.  
  
P. Xie, “Highly efficient decomposition of ammonia using high-entropy alloy catalysts”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Sep. 05, 2019. doi: 10.1038/s41467-019-11848-9.  
  
X. Yan, “Atomic interpretation of high activity on transition metal and nitrogen-doped carbon nanofibers for catalyzing oxygen reduction”, *Journal of Materials Chemistry A*, vol. 5, no. 7. Royal Society of Chemistry (RSC), pp. 3336–3345, 2017. doi: 10.1039/c6ta09462g.  
  
L. Zou, J. Li, Z. Liu, G. Wang, A. Manthiramand C. Wang, “Lattice doping regulated interfacial reactions in cathode for enhanced cycling stability”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Aug. 01, 2019. doi: 10.1038/s41467-019-11299-2.  
  
L. Zou, “Solid–Liquid Interfacial Reaction Trigged Propagation of Phase Transition from Surface into Bulk Lattice of Ni-Rich Layered Cathode”, *Chemistry of Materials*, vol. 30, no. 20. American Chemical Society (ACS), pp. 7016–7026, Sep. 21, 2018. doi: 10.1021/acs.chemmater.8b01958.  
  
L. Zou, “Revealing Cycling Rate-Dependent Structure Evolution in Ni-Rich Layered Cathode Materials”, *ACS Energy Letters*, vol. 3, no. 10. American Chemical Society (ACS), pp. 2433–2440, Sep. 14, 2018. doi: 10.1021/acsenergylett.8b01490.  
  
A. Bajaj, J. P. Janetand H. J. Kulik, “Communication: Recovering the flat-plane condition in electronic structure theory at semi-local DFT cost”, *The Journal of Chemical Physics*, vol. 147, no. 19. AIP Publishing, p. 191101, Nov. 21, 2017. doi: 10.1063/1.5008981.  
  
A. Bajaj, F. Liuand H. J. Kulik, “Non-empirical, low-cost recovery of exact conditions with model-Hamiltonian inspired expressions in jmDFT”, *The Journal of Chemical Physics*, vol. 150, no. 15. AIP Publishing, p. 154115, Apr. 21, 2019. doi: 10.1063/1.5091563.  
  
C. Duan, J. P. Janet, F. Liu, A. Nandyand H. J. Kulik, “Learning from Failure: Predicting Electronic Structure Calculation Outcomes with Machine Learning Models”, *Journal of Chemical Theory and Computation*, vol. 15, no. 4. American Chemical Society (ACS), pp. 2331–2345, Mar. 12, 2019. doi: 10.1021/acs.jctc.9b00057.  
  
T. Z. H. Gani and H. J. Kulik, “Where Does the Density Localize? Convergent Behavior for Global Hybrids, Range Separation, and DFT+U”, *Journal of Chemical Theory and Computation*, vol. 12, no. 12. American Chemical Society (ACS), pp. 5931–5945, Nov. 16, 2016. doi: 10.1021/acs.jctc.6b00937.  
  
T. Z. H. Gani and H. J. Kulik, “Unifying Exchange Sensitivity in Transition-Metal Spin-State Ordering and Catalysis through Bond Valence Metrics”, *Journal of Chemical Theory and Computation*, vol. 13, no. 11. American Chemical Society (ACS), pp. 5443–5457, Nov. 03, 2017. doi: 10.1021/acs.jctc.7b00848.  
  
T. Z. H. Gani and H. J. Kulik, “Understanding and Breaking Scaling Relations in Single-Site Catalysis: Methane to Methanol Conversion by FeIV═O”, *ACS Catalysis*, vol. 8, no. 2. American Chemical Society (ACS), pp. 975–986, Jan. 05, 2018. doi: 10.1021/acscatal.7b03597.  
  
S. Gugler, J. P. Janetand H. J. Kulik, “Enumeration of *de novo* inorganic complexes for chemical discovery and machine learning”, *Molecular Systems Design & Engineering*, vol. 5, no. 1. Royal Society of Chemistry (RSC), pp. 139–152, 2020. doi: 10.1039/c9me00069k.  
  
E. I. Ioannidis and H. J. Kulik, “Towards quantifying the role of exact exchange in predictions of transition metal complex properties”, *The Journal of Chemical Physics*, vol. 143, no. 3. AIP Publishing, p. 034104, Jul. 21, 2015. doi: 10.1063/1.4926836.  
  
E. I. Ioannidis and H. J. Kulik, “Ligand-Field-Dependent Behavior of Meta-GGA Exchange in Transition-Metal Complex Spin-State Ordering”, *The Journal of Physical Chemistry A*, vol. 121, no. 4. American Chemical Society (ACS), pp. 874–884, Jan. 23, 2017. doi: 10.1021/acs.jpca.6b11930.  
  
J. P. Janet, L. Chanand H. J. Kulik, “Accelerating Chemical Discovery with Machine Learning: Simulated Evolution of Spin Crossover Complexes with an Artificial Neural Network”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 5. American Chemical Society (ACS), pp. 1064–1071, Feb. 15, 2018. doi: 10.1021/acs.jpclett.8b00170.  
  
J. P. Janet, C. Duan, T. Yang, A. Nandyand H. J. Kulik, “A quantitative uncertainty metric controls error in neural network-driven chemical discovery”, *Chemical Science*, vol. 10, no. 34. Royal Society of Chemistry (RSC), pp. 7913–7922, 2019. doi: 10.1039/c9sc02298h.  
  
J. P. Janet, T. Z. H. Gani, A. H. Steeves, E. I. Ioannidisand H. J. Kulik, “Leveraging Cheminformatics Strategies for Inorganic Discovery: Application to Redox Potential Design”, *Industrial & Engineering Chemistry Research*, vol. 56, no. 17. American Chemical Society (ACS), pp. 4898–4910, Apr. 19, 2017. doi: 10.1021/acs.iecr.7b00808.  
  
J. P. Janet and H. J. Kulik, “Predicting electronic structure properties of transition metal complexes with neural networks”, *Chemical Science*, vol. 8, no. 7. Royal Society of Chemistry (RSC), pp. 5137–5152, 2017. doi: 10.1039/c7sc01247k.  
  
J. P. Janet and H. J. Kulik, “Resolving Transition Metal Chemical Space: Feature Selection for Machine Learning and Structure–Property Relationships”, *The Journal of Physical Chemistry A*, vol. 121, no. 46. American Chemical Society (ACS), pp. 8939–8954, Nov. 15, 2017. doi: 10.1021/acs.jpca.7b08750.  
  
J. P. Janet, “Designing in the Face of Uncertainty: Exploiting Electronic Structure and Machine Learning Models for Discovery in Inorganic Chemistry”, *Inorganic Chemistry*, vol. 58, no. 16. American Chemical Society (ACS), pp. 10592–10606, Mar. 05, 2019. doi: 10.1021/acs.inorgchem.9b00109.  
  
J. P. Janet, S. Ramesh, C. Duanand H. J. Kulik, “Accurate Multiobjective Design in a Space of Millions of Transition Metal Complexes with Neural-Network-Driven Efficient Global Optimization”, *ACS Central Science*, vol. 6, no. 4. American Chemical Society (ACS), pp. 513–524, Mar. 11, 2020. doi: 10.1021/acscentsci.0c00026.  
  
J. P. Janet, Q. Zhao, E. I. Ioannidisand H. J. Kulik, “Density functional theory for modelling large molecular adsorbate–surface interactions: a mini-review and worked example”, *Molecular Simulation*, vol. 43, no. 5–6. Informa UK Limited, pp. 327–345, Nov. 29, 2016. doi: 10.1080/08927022.2016.1258465.  
  
M. Karelina and H. J. Kulik, “Systematic Quantum Mechanical Region Determination in QM/MM Simulation”, *Journal of Chemical Theory and Computation*, vol. 13, no. 2. American Chemical Society (ACS), pp. 563–576, Jan. 23, 2017. doi: 10.1021/acs.jctc.6b01049.  
  
J. Y. Kim and H. J. Kulik, “When Is Ligand p*K*a a Good Descriptor for Catalyst Energetics? In Search of Optimal CO2 Hydration Catalysts”, *The Journal of Physical Chemistry A*, vol. 122, no. 18. American Chemical Society (ACS), pp. 4579–4590, Apr. 17, 2018. doi: 10.1021/acs.jpca.8b03301.  
  
J. Y. Kim, A. H. Steevesand H. J. Kulik, “Harnessing Organic Ligand Libraries for First-Principles Inorganic Discovery: Indium Phosphide Quantum Dot Precursor Design Strategies”, *Chemistry of Materials*, vol. 29, no. 8. American Chemical Society (ACS), pp. 3632–3643, Apr. 13, 2017. doi: 10.1021/acs.chemmater.7b00472.  
  
H. Kulik, “Large-scale QM/MM free energy simulations of enzyme catalysis reveal the influence of charge transfer”, *[]*. American Chemical Society (ACS), May 07, 2018. doi: 10.26434/chemrxiv.5985187.v2.  
  
F. Liu and H. J. Kulik, “Impact of Approximate DFT Density Delocalization Error on Potential Energy Surfaces in Transition Metal Chemistry”, *Journal of Chemical Theory and Computation*, vol. 16, no. 1. American Chemical Society (ACS), pp. 264–277, Nov. 18, 2019. doi: 10.1021/acs.jctc.9b00842.  
  
F. Liu, T. Yang, J. Yang, E. Xu, A. Bajajand H. J. Kulik, “Bridging the Homogeneous-Heterogeneous Divide: Modeling Spin for Reactivity in Single Atom Catalysis”, *Frontiers in Chemistry*, vol. 7. Frontiers Media SA, Apr. 16, 2019. doi: 10.3389/fchem.2019.00219.  
  
B. D. Mar and H. J. Kulik, “Depolymerization Pathways for Branching Lignin Spirodienone Units Revealed with *ab Initio* Steered Molecular Dynamics”, *The Journal of Physical Chemistry A*, vol. 121, no. 2. American Chemical Society (ACS), pp. 532–543, Jan. 05, 2017. doi: 10.1021/acs.jpca.6b11414.  
  
R. Mehmood and H. J. Kulik, “Both Configuration and QM Region Size Matter: Zinc Stability in QM/MM Models of DNA Methyltransferase”, *Journal of Chemical Theory and Computation*, vol. 16, no. 5. American Chemical Society (ACS), pp. 3121–3134, Apr. 03, 2020. doi: 10.1021/acs.jctc.0c00153.  
  
A. Nandy, C. Duan, J. P. Janet, S. Guglerand H. J. Kulik, “Strategies and Software for Machine Learning Accelerated Discovery in Transition Metal Chemistry”, *Industrial & Engineering Chemistry Research*, vol. 57, no. 42. American Chemical Society (ACS), pp. 13973–13986, Sep. 24, 2018. doi: 10.1021/acs.iecr.8b04015.  
  
A. Nandy, J. Zhu, J. P. Janet, C. Duan, R. B. Getmanand H. J. Kulik, “Machine Learning Accelerates the Discovery of Design Rules and Exceptions in Stable Metal–Oxo Intermediate Formation”, *ACS Catalysis*, vol. 9, no. 9. American Chemical Society (ACS), pp. 8243–8255, Jul. 23, 2019. doi: 10.1021/acscatal.9b02165.  
  
Y.-G. Park, “Protection of tissue physicochemical properties using polyfunctional crosslinkers”, *Nature Biotechnology*, vol. 37, no. 1. Springer Science and Business Media LLC, pp. 73–83, Dec. 17, 2018. doi: 10.1038/nbt.4281.  
  
H. W. Qi and H. J. Kulik, “Evaluating Unexpectedly Short Non-covalent Distances in X-ray Crystal Structures of Proteins with Electronic Structure Analysis”, *Journal of Chemical Information and Modeling*, vol. 59, no. 5. American Chemical Society (ACS), pp. 2199–2211, Mar. 15, 2019. doi: 10.1021/acs.jcim.9b00144.  
  
M. G. Taylor, “Seeing Is Believing: Experimental Spin States from Machine Learning Model Structure Predictions”, *The Journal of Physical Chemistry A*, vol. 124, no. 16. American Chemical Society (ACS), pp. 3286–3299, Mar. 28, 2020. doi: 10.1021/acs.jpca.0c01458.  
  
W. J. Transue, “Anthracene as a Launchpad for a Phosphinidene Sulfide and for Generation of a Phosphorus–Sulfur Material Having the Composition P2S, a Vulcanized Red Phosphorus That Is Yellow”, *Journal of the American Chemical Society*, vol. 141, no. 1. American Chemical Society (ACS), pp. 431–440, Dec. 04, 2018. doi: 10.1021/jacs.8b10775.  
  
L. Xie, Q. Zhao, K. F. Jensenand H. J. Kulik, “Direct Observation of Early-Stage Quantum Dot Growth Mechanisms with High-Temperature Ab Initio Molecular Dynamics”, *The Journal of Physical Chemistry C*, vol. 120, no. 4. American Chemical Society (ACS), pp. 2472–2483, Jan. 25, 2016. doi: 10.1021/acs.jpcc.5b12091.  
  
Z. Yang, F. Liu, A. H. Steevesand H. J. Kulik, “Quantum Mechanical Description of Electrostatics Provides a Unified Picture of Catalytic Action Across Methyltransferases”, *The Journal of Physical Chemistry Letters*, vol. 10, no. 13. American Chemical Society (ACS), pp. 3779–3787, Jun. 18, 2019. doi: 10.1021/acs.jpclett.9b01555.  
  
Z. Yang, R. Mehmood, M. Wang, H. W. Qi, A. H. Steevesand H. J. Kulik, “Revealing quantum mechanical effects in enzyme catalysis with large-scale electronic structure simulation”, *Reaction Chemistry & Engineering*, vol. 4, no. 2. Royal Society of Chemistry (RSC), pp. 298–315, 2019. doi: 10.1039/c8re00213d.  
  
Q. Zhao and H. J. Kulik, “Electronic Structure Origins of Surface-Dependent Growth in III–V Quantum Dots”, *Chemistry of Materials*, vol. 30, no. 20. American Chemical Society (ACS), pp. 7154–7165, Sep. 17, 2018. doi: 10.1021/acs.chemmater.8b03125.  
  
Q. Zhao and H. J. Kulik, “Where Does the Density Localize in the Solid State? Divergent Behavior for Hybrids and DFT+U”, *Journal of Chemical Theory and Computation*, vol. 14, no. 2. American Chemical Society (ACS), pp. 670–683, Jan. 26, 2018. doi: 10.1021/acs.jctc.7b01061.  
  
Q. Zhao and H. J. Kulik, “Stable Surfaces That Bind Too Tightly: Can Range-Separated Hybrids or DFT+U Improve Paradoxical Descriptions of Surface Chemistry?”, *The Journal of Physical Chemistry Letters*, vol. 10, no. 17. American Chemical Society (ACS), pp. 5090–5098, Aug. 14, 2019. doi: 10.1021/acs.jpclett.9b01650.  
  
Q. Zhao, L. Xieand H. J. Kulik, “Discovering Amorphous Indium Phosphide Nanostructures with High-Temperature ab Initio Molecular Dynamics”, *The Journal of Physical Chemistry C*, vol. 119, no. 40. American Chemical Society (ACS), pp. 23238–23249, Sep. 25, 2015. doi: 10.1021/acs.jpcc.5b07264.  
  
S. Wang, K. Goulasand E. Iglesia, “Condensation and esterification reactions of alkanals, alkanones, and alkanols on TiO2: Elementary steps, site requirements, and synergistic effects of bifunctional strategies”, *Journal of Catalysis*, vol. 340. Elsevier BV, pp. 302–320, Aug. 2016. doi: 10.1016/j.jcat.2016.05.026.  
  
S. Wang and E. Iglesia, “Substituent Effects and Molecular Descriptors of Reactivity in Condensation and Esterification Reactions of Oxygenates on Acid–Base Pairs at TiO2 and ZrO2 Surfaces”, *The Journal of Physical Chemistry C*, vol. 120, no. 38. American Chemical Society (ACS), pp. 21589–21616, Sep. 08, 2016. doi: 10.1021/acs.jpcc.6b07304.  
  
S. Wang and E. Iglesia, “Mechanism of Isobutanal–Isobutene Prins Condensation Reactions on Solid Brønsted Acids”, *ACS Catalysis*, vol. 6, no. 11. American Chemical Society (ACS), pp. 7664–7684, Oct. 12, 2016. doi: 10.1021/acscatal.6b02171.  
  
S. Wang and E. Iglesia, “Catalytic diversity conferred by confinement of protons within porous aluminosilicates in Prins condensation reactions”, *Journal of Catalysis*, vol. 352. Elsevier BV, pp. 415–435, Aug. 2017. doi: 10.1016/j.jcat.2017.06.012.  
  
S. Wang and E. Iglesia, “Experimental and Theoretical Evidence for the Reactivity of Bound Intermediates in Ketonization of Carboxylic Acids and Consequences of Acid–Base Properties of Oxide Catalysts”, *The Journal of Physical Chemistry C*, vol. 121, no. 33. American Chemical Society (ACS), pp. 18030–18046, Aug. 10, 2017. doi: 10.1021/acs.jpcc.7b05987.  
  
S. Wang and E. Iglesia, “Experimental and theoretical assessment of the mechanism and site requirements for ketonization of carboxylic acids on oxides”, *Journal of Catalysis*, vol. 345. Elsevier BV, pp. 183–206, Jan. 2017. doi: 10.1016/j.jcat.2016.11.006.  
  
C.-H. Lim, A. M. Holder, J. T. Hynesand C. B. Musgrave, “Catalytic Reduction of CO2 by Renewable Organohydrides”, *The Journal of Physical Chemistry Letters*, vol. 6, no. 24. American Chemical Society (ACS), pp. 5078–5092, Dec. 10, 2015. doi: 10.1021/acs.jpclett.5b01827.  
  
J. C. Theriot, C.-H. Lim, H. Yang, M. D. Ryan, C. B. Musgraveand G. M. Miyake, “Organocatalyzed atom transfer radical polymerization driven by visible light”, *Science*, vol. 352, no. 6289. American Association for the Advancement of Science (AAAS), pp. 1082–1086, May 27, 2016. doi: 10.1126/science.aaf3935.  
  
C.-H. Lim, A. M. Holder, J. T. Hynesand C. B. Musgrave, “Dihydropteridine/Pteridine as a 2H+/2e– Redox Mediator for the Reduction of CO2 to Methanol: A Computational Study”, *The Journal of Physical Chemistry B*, vol. 121, no. 16. American Chemical Society (ACS), pp. 4158–4167, Apr. 18, 2017. doi: 10.1021/acs.jpcb.7b01224.  
  
R. M. Pearson, C.-H. Lim, B. G. McCarthy, C. B. Musgraveand G. M. Miyake, “Organocatalyzed Atom Transfer Radical Polymerization Using *N*-Aryl Phenoxazines as Photoredox Catalysts”, *Journal of the American Chemical Society*, vol. 138, no. 35. American Chemical Society (ACS), pp. 11399–11407, Aug. 24, 2016. doi: 10.1021/jacs.6b08068.  
  
M. Flister and Q. K. Timerghazin, “Structure, Stability, and Substituent Effects in Aromatic *S*-Nitrosothiols: The Crucial Effect of a Cascading Negative Hyperconjugation/Conjugation Interaction”, *The Journal of Physical Chemistry A*, vol. 118, no. 42. American Chemical Society (ACS), pp. 9914–9924, Oct. 09, 2014. doi: 10.1021/jp5079136.  
  
L. V. Ivanova, B. J. Antonand Q. K. Timerghazin, “On the possible biological relevance of HSNO isomers: a computational investigation”, *Phys. Chem. Chem. Phys.*, vol. 16, no. 18. Royal Society of Chemistry (RSC), pp. 8476–8486, 2014. doi: 10.1039/c4cp00469h.  
  
L. V. Ivanova, D. Cibich, G. Deye, M. R. Talipovand Q. K. Timerghazin, “Modeling of *S* ‐Nitrosothiol–Thiol Reactions of Biological Significance: HNO Production by S‐Thiolation Requires a Proton Shuttle and Stabilization of Polar Intermediates”, *ChemBioChem*, vol. 18, no. 8. Wiley, pp. 726–738, Apr. 03, 2017. doi: 10.1002/cbic.201600556.  
  
M. V. Ivanov, M. R. Talipovand Q. K. Timerghazin, “Genetic Algorithm Optimization of Point Charges in Force Field Development: Challenges and Insights”, *The Journal of Physical Chemistry A*, vol. 119, no. 8. American Chemical Society (ACS), pp. 1422–1434, Feb. 16, 2015. doi: 10.1021/acs.jpca.5b00218.  
  
D. G. Khomyakov and Q. K. Timerghazin, “Toward reliable modeling of S-nitrosothiol chemistry: Structure and properties of methyl thionitrite (CH3SNO), an S-nitrosocysteine model”, *The Journal of Chemical Physics*, vol. 147, no. 4. AIP Publishing, p. 044305, Jul. 25, 2017. doi: 10.1063/1.4995300.  
  
M. V. Ivanov, M. R. Talipovand Q. K. Timerghazin, “Electrostatic point charge fitting as an inverse problem: Revealing the underlying ill-conditioning”, *The Journal of Chemical Physics*, vol. 143, no. 13. AIP Publishing, p. 134102, Oct. 07, 2015. doi: 10.1063/1.4932105.  
  
D. Wang, “An Electron‐Rich Calix[4]arene‐Based Receptor with Unprecedented Binding Affinity for Nitric Oxide”, *Chemistry – A European Journal*, vol. 24, no. 66. Wiley, pp. 17439–17443, Oct. 30, 2018. doi: 10.1002/chem.201804245.  
  
N. Z. Rao, J. D. Larkinand C. W. Bock, “A computational investigation of monosubstituted boroxines(RH2B3O3): structure and formation”, *Structural Chemistry*, vol. 26, no. 4. Springer Science and Business Media LLC, pp. 1151–1162, Feb. 25, 2015. doi: 10.1007/s11224-015-0577-9.  
  
Q. Ma, “Postgrowth Tuning of the Bandgap of Single-Layer Molybdenum Disulfide Films by Sulfur/Selenium Exchange”, *ACS Nano*, vol. 8, no. 5. American Chemical Society (ACS), pp. 4672–4677, Apr. 22, 2014. doi: 10.1021/nn5004327.  
  
C. S. Wang, H. Wang, R. Wuand R. Ragan, “Evaluating the Stability of Single-Atom Catalysts with High Chemical Activity”, *The Journal of Physical Chemistry C*, vol. 122, no. 38. American Chemical Society (ACS), pp. 21919–21926, Aug. 31, 2018. doi: 10.1021/acs.jpcc.8b06621.  
  
A. K. Omar and Z.-G. Wang, “Shear-Induced Heterogeneity in Associating Polymer Gels: Role of Network Structure and Dilatancy”, *Physical Review Letters*, vol. 119, no. 11. American Physical Society (APS), Sep. 12, 2017. doi: 10.1103/physrevlett.119.117801.  
  
M. B. Oviedo and B. M. Wong, “Real-Time Quantum Dynamics Reveals Complex, Many-Body Interactions in Solvated Nanodroplets”, *Journal of Chemical Theory and Computation*, vol. 12, no. 4. American Chemical Society (ACS), pp. 1862–1871, Mar. 10, 2016. doi: 10.1021/acs.jctc.5b01019.  
  
P. D. Siders, “Conformational free energy of alkylsilanes by nonequilibrium-pulling Monte Carlo simulation”, *Molecular Simulation*, vol. 42, no. 9. Informa UK Limited, pp. 693–701, Sep. 07, 2015. doi: 10.1080/08927022.2015.1083101.  
  
P. D. Siders, “Simulated molecular-scale interaction of supercritical fluid mobile and stationary phases”, *Journal of Chromatography A*, vol. 1527. Elsevier BV, pp. 97–104, Dec. 2017. doi: 10.1016/j.chroma.2017.10.056.  
  
N. Ekanayake, “H2 roaming chemistry and the formation of H3+ from organic molecules in strong laser fields”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Dec. 05, 2018. doi: 10.1038/s41467-018-07577-0.  
  
M. P. Esch, Y. Shuand B. G. Levine, “A Conical Intersection Perspective on the Low Nonradiative Recombination Rate in Lead Halide Perovskites”, *The Journal of Physical Chemistry A*, vol. 123, no. 13. American Chemical Society (ACS), pp. 2661–2673, Mar. 07, 2019. doi: 10.1021/acs.jpca.9b00952.  
  
B. S. Fales and B. G. Levine, “Nanoscale Multireference Quantum Chemistry: Full Configuration Interaction on Graphical Processing Units”, *Journal of Chemical Theory and Computation*, vol. 11, no. 10. American Chemical Society (ACS), pp. 4708–4716, Oct. 05, 2015. doi: 10.1021/acs.jctc.5b00634.  
  
B. S. Fales, S. Seritan, N. F. Settje, B. G. Levine, H. Kochand T. J. Martínez, “Large-Scale Electron Correlation Calculations: Rank-Reduced Full Configuration Interaction”, *Journal of Chemical Theory and Computation*, vol. 14, no. 8. American Chemical Society (ACS), pp. 4139–4150, Jun. 11, 2018. doi: 10.1021/acs.jctc.8b00382.  
  
B. G. Levine, M. P. Esch, B. S. Fales, D. T. Hardwick, W.-T. Pengand Y. Shu, “Conical Intersections at the Nanoscale: Molecular Ideas for Materials”, *Annual Review of Physical Chemistry*, vol. 70, no. 1. Annual Reviews, pp. 21–43, Jun. 14, 2019. doi: 10.1146/annurev-physchem-042018-052425.  
  
B. G. Levine, W.-T. Pengand M. P. Esch, “Locality of conical intersections in semiconductor nanomaterials”, *Physical Chemistry Chemical Physics*, vol. 21, no. 21. Royal Society of Chemistry (RSC), pp. 10870–10878, 2019. doi: 10.1039/c9cp01584a.  
  
W.-T. Peng and B. G. Levine, “Ab Initio Molecular Dynamics Study of the Interaction between Defects during Nonradiative Recombination”, *The Journal of Physical Chemistry C*, vol. 123, no. 27. American Chemical Society (ACS), pp. 16588–16595, Jun. 20, 2019. doi: 10.1021/acs.jpcc.9b04673.  
  
Y. Shu, B. S. Falesand B. G. Levine, “Defect-Induced Conical Intersections Promote Nonradiative Recombination”, *Nano Letters*, vol. 15, no. 9. American Chemical Society (ACS), pp. 6247–6253, Aug. 24, 2015. doi: 10.1021/acs.nanolett.5b02848.  
  
Y. Shu, B. S. Fales, W.-T. Pengand B. G. Levine, “Understanding Nonradiative Recombination through Defect-Induced Conical Intersections”, *The Journal of Physical Chemistry Letters*, vol. 8, no. 17. American Chemical Society (ACS), pp. 4091–4099, Aug. 16, 2017. doi: 10.1021/acs.jpclett.7b01707.  
  
C. Yang, “Impact of Stokes Shift on the Performance of Near-Infrared Harvesting Transparent Luminescent Solar Concentrators”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, Nov. 05, 2018. doi: 10.1038/s41598-018-34442-3.  
  
J. Zhang, H. J. Kulik, T. J. Martinezand J. P. Klinman, “Mediation of donor–acceptor distance in an enzymatic methyl transfer reaction”, *Proceedings of the National Academy of Sciences*, vol. 112, no. 26. Proceedings of the National Academy of Sciences, pp. 7954–7959, Jun. 15, 2015. doi: 10.1073/pnas.1506792112.  
  
J.-M. Arce-Ramos, L. C. Grabow, B. E. Handyand M.-G. Cárdenas-Galindo, “Nature of Acid Sites in Silica-Supported Zirconium Oxide: A Combined Experimental and Periodic DFT Study”, *The Journal of Physical Chemistry C*, vol. 119, no. 27. American Chemical Society (ACS), pp. 15150–15159, Jun. 26, 2015. doi: 10.1021/acs.jpcc.5b02394.  
  
B. Baek, A. Aboiralor, S. Wang, P. Kharidehal, L. C. Grabowand J. D. Massa, “Strategy to improve catalytic trend predictions for methane oxidation and reforming”, *AIChE Journal*, vol. 63, no. 1. Wiley, pp. 66–77, Jul. 25, 2016. doi: 10.1002/aic.15404.  
  
J. E. Bruno, “On the Limited Role of Electronic Support Effects in Selective Alkyne Hydrogenation: A Kinetic Study of Au/MO x Catalysts Prepared from Oleylamine‐Capped Colloidal Nanoparticles”, *ChemCatChem*, vol. 11, no. 6. Wiley, pp. 1650–1664, Feb. 28, 2019. doi: 10.1002/cctc.201801882.  
  
H. A. Doan, M. K. Sharma, W. S. Eplingand L. C. Grabow, “From Active‐Site Models to Real Catalysts: Importance of the Material Gap in the Design of Pd Catalysts for Methane Oxidation”, *ChemCatChem*, vol. 9, no. 9. Wiley, pp. 1594–1600, Feb. 14, 2017. doi: 10.1002/cctc.201601333.  
  
Q. K. Do, H.-V. Tran, S. Wangand L. C. Grabow, “The Synergy of Dilute Pd and Surface Oxygen Species for Methane Upgrading on Au 3 Pd(111)”, *Energy Technology*, vol. 8, no. 8. Wiley, p. 1900732, Sep. 18, 2019. doi: 10.1002/ente.201900732.  
  
A. Ghorbanpour, J. D. Rimerand L. C. Grabow, “Periodic, vdW-corrected density functional theory investigation of the effect of Al siting in H-ZSM-5 on chemisorption properties and site-specific acidity”, *Catalysis Communications*, vol. 52. Elsevier BV, pp. 98–102, Jul. 2014. doi: 10.1016/j.catcom.2014.04.005.  
  
A. Ghorbanpour, J. D. Rimerand L. C. Grabow, “Computational Assessment of the Dominant Factors Governing the Mechanism of Methanol Dehydration over H-ZSM-5 with Heterogeneous Aluminum Distribution”, *ACS Catalysis*, vol. 6, no. 4. American Chemical Society (ACS), pp. 2287–2298, Mar. 03, 2016. doi: 10.1021/acscatal.5b02367.  
  
K. A. Goulas, “Selectivity tuning over monometallic and bimetallic dehydrogenation catalysts: effects of support and particle size”, *Catalysis Science & Technology*, vol. 8, no. 1. Royal Society of Chemistry (RSC), pp. 314–327, 2018. doi: 10.1039/c7cy01306j.  
  
K. A. Goulas, “Synergistic Effects in Bimetallic Palladium–Copper Catalysts Improve Selectivity in Oxygenate Coupling Reactions”, *Journal of the American Chemical Society*, vol. 138, no. 21. American Chemical Society (ACS), pp. 6805–6812, May 19, 2016. doi: 10.1021/jacs.6b02247.  
  
S. Guo, “Insights into Nitrate Reduction over Indium-Decorated Palladium Nanoparticle Catalysts”, *ACS Catalysis*, vol. 8, no. 1. American Chemical Society (ACS), pp. 503–515, Dec. 13, 2017. doi: 10.1021/acscatal.7b01371.  
  
M. Hsieh, Y. Zhou, H. Thirumalai, L. C. Grabowand J. D. Rimer, “Silver‐Promoted Dehydroaromatization of Ethylene over ZSM‐5 Catalysts”, *ChemCatChem*, vol. 9, no. 9. Wiley, pp. 1675–1682, Apr. 04, 2017. doi: 10.1002/cctc.201700192.  
  
Y. Jangjou, “Nature of Cu Active Centers in Cu-SSZ-13 and Their Responses to SO2 Exposure”, *ACS Catalysis*, vol. 8, no. 2. American Chemical Society (ACS), pp. 1325–1337, Jan. 19, 2018. doi: 10.1021/acscatal.7b03095.  
  
S. Kasiraju and L. C. Grabow, “Learning from the past: Are catalyst design principles transferrable between hydrodesulfurization and deoxygenation?”, *AIChE Journal*, vol. 64, no. 8. Wiley, pp. 3121–3133, Mar. 25, 2018. doi: 10.1002/aic.16151.  
  
Y. Liang, “Interlayer-Expanded Molybdenum Disulfide Nanocomposites for Electrochemical Magnesium Storage”, *Nano Letters*, vol. 15, no. 3. American Chemical Society (ACS), pp. 2194–2202, Mar. 02, 2015. doi: 10.1021/acs.nanolett.5b00388.  
  
A. Mahdavi-Shakib, J. M. Arce-Ramos, R. N. Austin, T. J. Schwartz, L. C. Grabowand B. G. Frederick, “Frequencies and Thermal Stability of Isolated Surface Hydroxyls on Pyrogenic TiO2 Nanoparticles”, *The Journal of Physical Chemistry C*, vol. 123, no. 40. American Chemical Society (ACS), pp. 24533–24548, Sep. 13, 2019. doi: 10.1021/acs.jpcc.9b05699.  
  
M. D. Oleksiak, “Synthesis Strategies for Ultrastable Zeolite GIS Polymorphs as Sorbents for Selective Separations”, *Chemistry – A European Journal*, vol. 22, no. 45. Wiley, pp. 16078–16088, Sep. 02, 2016. doi: 10.1002/chem.201602653.  
  
J. Saavedra, H. A. Doan, C. J. Pursell, L. C. Grabowand B. D. Chandler, “The critical role of water at the gold-titania interface in catalytic CO oxidation”, *Science*, vol. 345, no. 6204. American Association for the Advancement of Science (AAAS), pp. 1599–1602, Sep. 26, 2014. doi: 10.1126/science.1256018.  
  
D. E. Schipper, “Effects of Catalyst Phase on the Hydrogen Evolution Reaction of Water Splitting: Preparation of Phase-Pure Films of FeP, Fe2P, and Fe3P and Their Relative Catalytic Activities”, *Chemistry of Materials*, vol. 30, no. 10. American Chemical Society (ACS), pp. 3588–3598, Apr. 26, 2018. doi: 10.1021/acs.chemmater.8b01624.  
  
J. Shuai, H. D. Yoo, Y. Liang, Y. Li, Y. Yaoand L. C. Grabow, “Density functional theory study of Li, Na, and Mg intercalation and diffusion in MoS2with controlled interlayer spacing”, *Materials Research Express*, vol. 3, no. 6. IOP Publishing, p. 064001, Jun. 08, 2016. doi: 10.1088/2053-1591/3/6/064001.  
  
Y. Song and L. C. Grabow, “Activity Trends for Catalytic CO and NO Co-Oxidation at Low Temperature Diesel Emission Conditions”, *Industrial & Engineering Chemistry Research*, vol. 57, no. 38. American Chemical Society (ACS), pp. 12715–12725, Aug. 28, 2018. doi: 10.1021/acs.iecr.8b01905.  
  
H. Thirumalai and J. R. Kitchin, “The role of vdW interactions in coverage dependent adsorption energies of atomic adsorbates on Pt(111) and Pd(111)”, *Surface Science*, vol. 650. Elsevier BV, pp. 196–202, Aug. 2016. doi: 10.1016/j.susc.2015.10.001.  
  
H. Thirumalai, J. D. Rimerand L. C. Grabow, “Quantification and Statistical Analysis of Errors Related to the Approximate Description of Active Site Models in Metal‐Exchanged Zeolites”, *ChemCatChem*, vol. 11, no. 20. Wiley, pp. 5055–5067, Sep. 26, 2019. doi: 10.1002/cctc.201901229.  
  
T. Whittaker, K. B. S. Kumar, C. Peterson, M. N. Pollock, L. C. Grabowand B. D. Chandler, “H2 Oxidation over Supported Au Nanoparticle Catalysts: Evidence for Heterolytic H2 Activation at the Metal–Support Interface”, *Journal of the American Chemical Society*, vol. 140, no. 48. American Chemical Society (ACS), pp. 16469–16487, Sep. 19, 2018. doi: 10.1021/jacs.8b04991.  
  
Q. Yuan, H. A. Doan, L. C. Grabowand S. R. Brankovic, “Finite Size Effects in Submonolayer Catalysts Investigated by CO Electrosorption on PtsML/Pd(100)”, *Journal of the American Chemical Society*, vol. 139, no. 39. American Chemical Society (ACS), pp. 13676–13679, Sep. 21, 2017. doi: 10.1021/jacs.7b08740.  
  
Z. Zhao, “Vertically Aligned MoS2/Mo2C hybrid Nanosheets Grown on Carbon Paper for Efficient Electrocatalytic Hydrogen Evolution”, *ACS Catalysis*, vol. 7, no. 10. American Chemical Society (ACS), pp. 7312–7318, Sep. 26, 2017. doi: 10.1021/acscatal.7b02885.  
  
Z. Zhao, “Bifunctional metal phosphide FeMnP films from single source metal organic chemical vapor deposition for efficient overall water splitting”, *Nano Energy*, vol. 39. Elsevier BV, pp. 444–453, Sep. 2017. doi: 10.1016/j.nanoen.2017.07.027.  
  
R. C. Nelson, “Experimental and Theoretical Insights into the Hydrogen-Efficient Direct Hydrodeoxygenation Mechanism of Phenol over Ru/TiO2”, *ACS Catalysis*, vol. 5, no. 11. American Chemical Society (ACS), pp. 6509–6523, Oct. 05, 2015. doi: 10.1021/acscatal.5b01554.  
  
T. O. Omotoso, B. Baek, L. C. Grabowand S. P. Crossley, “Experimental and First‐Principles Evidence for Interfacial Activity of Ru/TiO 2 for the Direct Conversion of *m* ‐Cresol to Toluene”, *ChemCatChem*, vol. 9, no. 14. Wiley, pp. 2642–2651, Jul. 03, 2017. doi: 10.1002/cctc.201700157.  
  
C. J. Cooper and J. M. Stubbs, “The effect of unequal strand length on short DNA duplex hybridization in a model microarray system: A Monte Carlo simulation study”, *Chemical Physics Letters*, vol. 634. Elsevier BV, pp. 230–235, Aug. 2015. doi: 10.1016/j.cplett.2015.06.024.  
  
M. Narayanan, V. R. Singh, G. Kodali, K. Moravcevicand R. J. Stanley, “An Ethenoadenine FAD Analog Accelerates UV Dimer Repair by DNA Photolyase”, *Photochemistry and Photobiology*, vol. 93, no. 1. Wiley, pp. 343–354, Jan. 2017. doi: 10.1111/php.12684.  
  
J. E. Barker, “Serendipitous Rediscovery of the Facile Cyclization of *Z* , *Z* ‐3,5‐Octadiene‐1,7‐diyne Derivatives to Afford Stable, Substituted Naphthocyclobutadienes”, *ChemPlusChem*, vol. 84, no. 6. Wiley, pp. 665–672, Jan. 23, 2019. doi: 10.1002/cplu.201800605.  
  
C. J. Holt, K. J. Wentworthand R. P. Johnson, “A Short and Efficient Synthesis of the [3]Triangulene Ring System”, *Angewandte Chemie International Edition*, vol. 58, no. 44. Wiley, pp. 15793–15796, Sep. 24, 2019. doi: 10.1002/anie.201907226.  
  
T. Qin, S. L. Skraba-Joiner, Z. G. Khalil, R. P. Johnson, R. J. Caponand J. A. Porco Jr, “Atropselective syntheses of (−) and (+) rugulotrosin A utilizing point-to-axial chirality transfer”, *Nature Chemistry*, vol. 7, no. 3. Springer Science and Business Media LLC, pp. 234–240, Feb. 02, 2015. doi: 10.1038/nchem.2173.  
  
K. D. Reichl, M. J. Smith, M. K. Song, R. P. Johnsonand J. A. Porco Jr., “Biomimetic Total Synthesis of (±)-Griffipavixanthone via a Cationic Cycloaddition–Cyclization Cascade”, *Journal of the American Chemical Society*, vol. 139, no. 40. American Chemical Society (ACS), pp. 14053–14056, Oct. 02, 2017. doi: 10.1021/jacs.7b09265.  
  
S. L. Skraba-Joiner, C. J. Holtand R. P. Johnson, “Acid-catalyzed rearrangements in arenes: interconversions in the quaterphenyl series”, *Beilstein Journal of Organic Chemistry*, vol. 15. Beilstein Institut, pp. 2655–2663, Nov. 06, 2019. doi: 10.3762/bjoc.15.258.  
  
S. L. Skraba-Joiner, R. P. Johnsonand J. Agarwal, “Dehydropericyclic Reactions: Symmetry-Controlled Routes to Strained Reactive Intermediates”, *The Journal of Organic Chemistry*, vol. 80, no. 23. American Chemical Society (ACS), pp. 11779–11787, Oct. 07, 2015. doi: 10.1021/acs.joc.5b01488.  
  
S. L. Skraba-Joiner, E. C. McLaughlin, A. Ajaz, R. Thamatamand R. P. Johnson, “Scholl Cyclizations of Aryl Naphthalenes: Rearrangement Precedes Cyclization”, *The Journal of Organic Chemistry*, vol. 80, no. 19. American Chemical Society (ACS), pp. 9578–9583, Sep. 14, 2015. doi: 10.1021/acs.joc.5b01559.  
  
M. Assmann, T. Weinachtand S. Matsika, “Surface hopping investigation of the relaxation dynamics in radical cations”, *The Journal of Chemical Physics*, vol. 144, no. 3. AIP Publishing, p. 034301, Jan. 19, 2016. doi: 10.1063/1.4939842.  
  
P. Chakraborty, Y. Liu, T. Weinachtand S. Matsika, “Excited state dynamics of *cis*,*cis*-1,3-cyclooctadiene: Non-adiabatic trajectory surface hopping”, *The Journal of Chemical Physics*, vol. 152, no. 17. AIP Publishing, p. 174302, May 07, 2020. doi: 10.1063/5.0005558.  
  
S. L. Horton, “Strong-field- versus weak-field-ionization pump-probe spectroscopy”, *Physical Review A*, vol. 98, no. 5. American Physical Society (APS), Nov. 14, 2018. doi: 10.1103/physreva.98.053416.  
  
W. Lee, G. Kodali, R. J. Stanleyand S. Matsika, “Coexistence of Different Electron‐Transfer Mechanisms in the DNA Repair Process by Photolyase”, *Chemistry – A European Journal*, vol. 22, no. 32. Wiley, pp. 11371–11381, Jun. 30, 2016. doi: 10.1002/chem.201600656.  
  
W. Lee and S. Matsika, “Conformational and electronic effects on the formation of anti cyclobutane pyrimidine dimers in G-quadruplex structures”, *Physical Chemistry Chemical Physics*, vol. 19, no. 4. Royal Society of Chemistry (RSC), pp. 3325–3336, 2017. doi: 10.1039/c6cp05604k.  
  
W. Lee and S. Matsika, “Photochemical Formation of Cyclobutane Pyrimidine Dimers in DNA through Electron Transfer from a Flanking Base”, *ChemPhysChem*, vol. 19, no. 13. Wiley, pp. 1568–1571, Apr. 25, 2018. doi: 10.1002/cphc.201800151.  
  
Y. Liu, P. Chakraborty, S. Matsikaand T. Weinacht, “Excited state dynamics of *cis*,*cis*-1,3-cyclooctadiene: UV pump VUV probe time-resolved photoelectron spectroscopy”, *The Journal of Chemical Physics*, vol. 153, no. 7. AIP Publishing, p. 074301, Aug. 21, 2020. doi: 10.1063/5.0006920.  
  
Q. L. Nguyen, V. A. Spataand S. Matsika, “Photophysical properties of pyrrolocytosine, a cytosine fluorescent base analogue”, *Physical Chemistry Chemical Physics*, vol. 18, no. 30. Royal Society of Chemistry (RSC), pp. 20189–20198, 2016. doi: 10.1039/c6cp01559j.  
  
V. A. Spata, W. Leeand S. Matsika, “Excimers and Exciplexes in Photoinitiated Processes of Oligonucleotides”, *The Journal of Physical Chemistry Letters*, vol. 7, no. 6. American Chemical Society (ACS), pp. 976–984, Mar. 02, 2016. doi: 10.1021/acs.jpclett.5b02756.  
  
V. A. Spata and S. Matsika, “Role of Excitonic Coupling and Charge-Transfer States in the Absorption and CD Spectra of Adenine-Based Oligonucleotides Investigated through QM/MM Simulations”, *The Journal of Physical Chemistry A*, vol. 118, no. 51. American Chemical Society (ACS), pp. 12021–12030, Sep. 16, 2014. doi: 10.1021/jp507520c.  
  
V. A. Spata and S. Matsika, “Photophysical deactivation pathways in adenine oligonucleotides”, *Physical Chemistry Chemical Physics*, vol. 17, no. 46. Royal Society of Chemistry (RSC), pp. 31073–31083, 2015. doi: 10.1039/c5cp04254b.  
  
M. Thodika, M. Fennimore, T. N. V. Karsiliand S. Matsika, “Comparative study of methodologies for calculating metastable states of small to medium-sized molecules”, *The Journal of Chemical Physics*, vol. 151, no. 24. AIP Publishing, p. 244104, Dec. 28, 2019. doi: 10.1063/1.5134700.  
  
C. Zuluaga, V. A. Spataand S. Matsika, “Benchmarking Quantum Mechanical Methods for the Description of Charge-Transfer States in π-Stacked Nucleobases”, *Journal of Chemical Theory and Computation*, vol. 17, no. 1. American Chemical Society (ACS), pp. 376–387, Dec. 21, 2020. doi: 10.1021/acs.jctc.0c00973.  
  
S. E. Brown, A. W. Götz, X. Cheng, R. P. Steele, V. A. Mandelshtamand F. Paesani, “Monitoring Water Clusters “Melt” Through Vibrational Spectroscopy”, *Journal of the American Chemical Society*, vol. 139, no. 20. American Chemical Society (ACS), pp. 7082–7088, May 12, 2017. doi: 10.1021/jacs.7b03143.  
  
X. Cheng, J. D. Herrand R. P. Steele, “Accelerating *Ab Initio* Path Integral Simulations via Imaginary Multiple-Timestepping”, *Journal of Chemical Theory and Computation*, vol. 12, no. 4. American Chemical Society (ACS), pp. 1627–1638, Mar. 25, 2016. doi: 10.1021/acs.jctc.6b00021.  
  
X. Cheng, J. D. Herrand R. P. Steele, “Accelerating *Ab Initio* Path Integral Simulations via Imaginary Multiple-Timestepping”, *Journal of Chemical Theory and Computation*, vol. 12, no. 4. American Chemical Society (ACS), pp. 1627–1638, Mar. 25, 2016. doi: 10.1021/acs.jctc.6b00021.  
  
X. Cheng, J. J. Talbotand R. P. Steele, “Tuning vibrational mode localization with frequency windowing”, *The Journal of Chemical Physics*, vol. 145, no. 12. AIP Publishing, p. 124112, Sep. 28, 2016. doi: 10.1063/1.4963109.  
  
J. D. Herr and R. P. Steele, “Signatures of Size-Dependent Structural Patterns in Hydrated Copper(I) Clusters, Cu+(H2O)*n*=1–10”, *The Journal of Physical Chemistry A*, vol. 120, no. 51. American Chemical Society (ACS), pp. 10252–10263, Dec. 16, 2016. doi: 10.1021/acs.jpca.6b10346.  
  
J. D. Herr and R. P. Steele, “Ion–Radical Pair Separation in Larger Oxidized Water Clusters, (H2O)+*n*=6–21”, *The Journal of Physical Chemistry A*, vol. 120, no. 36. American Chemical Society (ACS), pp. 7225–7239, Sep. 01, 2016. doi: 10.1021/acs.jpca.6b07465.  
  
J. D. Herr and R. P. Steele, “Accelerating ab initio molecular dynamics simulations by linear prediction methods”, *Chemical Physics Letters*, vol. 661. Elsevier BV, pp. 42–47, Sep. 2016. doi: 10.1016/j.cplett.2016.08.050.  
  
J. D. Herr, J. Talbotand R. P. Steele, “Structural Progression in Clusters of Ionized Water, (H2O)*n*=1–5+”, *The Journal of Physical Chemistry A*, vol. 119, no. 4. American Chemical Society (ACS), pp. 752–766, Jan. 21, 2015. doi: 10.1021/jp509698y.  
  
B. K. Mitchell and R. P. Steele, “Nuclear Motion in the σ-Bound Regime of Metal–H2 Complexes: [Mg(H2)*n*=1–6]2+”, *The Journal of Physical Chemistry A*, vol. 118, no. 43. American Chemical Society (ACS), pp. 10057–10066, Oct. 21, 2014. doi: 10.1021/jp5048979.  
  
A. Y. Pereverzev, X. Cheng, N. S. Nagornova, D. L. Reese, R. P. Steeleand O. V. Boyarkin, “Vibrational Signatures of Conformer-Specific Intramolecular Interactions in Protonated Tryptophan”, *The Journal of Physical Chemistry A*, vol. 120, no. 28. American Chemical Society (ACS), pp. 5598–5608, Jul. 08, 2016. doi: 10.1021/acs.jpca.6b05605.  
  
Y. Shao, “Advances in molecular quantum chemistry contained in the Q-Chem 4 program package”, *Molecular Physics*, vol. 113, no. 2. Informa UK Limited, pp. 184–215, Sep. 03, 2014. doi: 10.1080/00268976.2014.952696.  
  
R. P. Steele, “Multiple-Timestep *ab Initio* Molecular Dynamics Using an Atomic Basis Set Partitioning”, *The Journal of Physical Chemistry A*, vol. 119, no. 50. American Chemical Society (ACS), pp. 12119–12130, Sep. 09, 2015. doi: 10.1021/acs.jpca.5b05850.  
  
J. J. Talbot, X. Cheng, J. D. Herrand R. P. Steele, “Vibrational Signatures of Electronic Properties in Oxidized Water: Unraveling the Anomalous Spectrum of the Water Dimer Cation”, *Journal of the American Chemical Society*, vol. 138, no. 36. American Chemical Society (ACS), pp. 11936–11945, Aug. 30, 2016. doi: 10.1021/jacs.6b07182.  
  
B. D. Stewart, “Computational modeling of amylin-induced calcium dysregulation in rat ventricular cardiomyocytes”, *Cell Calcium*, vol. 71. Elsevier BV, pp. 65–74, May 2018. doi: 10.1016/j.ceca.2017.11.006.  
  
B. Sun, D. Vaughan, S. Tikunova, T. Creamer, J. Davisand P. Kekenes-Huskey, “Molecular basis of calmodulin-dependent calcineurin activation”, *[]*. Cold Spring Harbor Laboratory, Jun. 08, 2019. doi: 10.1101/665158.  
  
Y. A. Jeilani, K. A. Duncan, D. S. Newallo, A. N. Thompson Jr.and N. K. Bose, “Tandem mass spectrometry and density functional theory of RDX fragmentation pathways: Role of ion-molecule complexes in loss of NO3and lack of molecular ion peak”, *Rapid Communications in Mass Spectrometry*, vol. 29, no. 9. Wiley, pp. 802–810, Mar. 25, 2015. doi: 10.1002/rcm.7167.  
  
Y. A. Jeilani, H. Li, I. I. Harruna, K. R. Alhooshaniand A. A. Al-Saadi, “Collision induced dissociations of non-derivatized and trimethylsilyl-derivatized estradiols: similarities in fragmentation patterns”, *Journal of Mass Spectrometry*, vol. 50, no. 2. Wiley, pp. 308–315, Feb. 2015. doi: 10.1002/jms.3529.  
  
T. A. Hamlin, C. S. Hamannand D. J. Tantillo, “Delocalization of Charge and Electron Density in the Humulyl Cation—Implications for Terpene Biosynthesis”, *The Journal of Organic Chemistry*, vol. 80, no. 8. American Chemical Society (ACS), pp. 4046–4053, Apr. 08, 2015. doi: 10.1021/acs.joc.5b00381.  
  
N. Singh, J. Niklas, O. Poluektov, K. M. Van Heuvelenand A. Mukherjee, “Mononuclear nickel (II) and copper (II) coordination complexes supported by bispicen ligand derivatives: Experimental and computational studies”, *Inorganica Chimica Acta*, vol. 455. Elsevier BV, pp. 221–230, Jan. 2017. doi: 10.1016/j.ica.2016.09.001.  
  
K. M. Van Heuvelen, I. Lee, K. Arriola, R. Griffin, C. Yeand M. K. Takase, “Crystal structure and spectroscopic characterization of a cobalt(II) tetraazamacrocycle: completing a series of first-row transition-metal complexes”, *Acta Crystallographica Section C Structural Chemistry*, vol. 73, no. 8. International Union of Crystallography (IUCr), pp. 620–624, Jul. 20, 2017. doi: 10.1107/s2053229617010397.  
  
P. An, T. M. Lewandowski, T. G. Erbay, P. Liuand Q. Lin, “Sterically Shielded, Stabilized Nitrile Imine for Rapid Bioorthogonal Protein Labeling in Live Cells”, *Journal of the American Chemical Society*, vol. 140, no. 14. American Chemical Society (ACS), pp. 4860–4868, Mar. 22, 2018. doi: 10.1021/jacs.8b00126.  
  
B. A. Boon, A. G. Green, P. Liu, K. N. Houkand C. A. Merlic, “Using Ring Strain to Control 4π-Electrocyclization Reactions: Torquoselectivity in Ring Closing of Medium-Ring Dienes and Ring Opening of Bicyclic Cyclobutenes”, *The Journal of Organic Chemistry*, vol. 82, no. 9. American Chemical Society (ACS), pp. 4613–4624, Apr. 21, 2017. doi: 10.1021/acs.joc.7b00203.  
  
C. Boucher-Jacobs, P. Liuand K. M. Nicholas, “Mechanistic Insights into the ReIO2(PPh3)2-Promoted Reductive Coupling of Alcohols”, *Organometallics*, vol. 37, no. 15. American Chemical Society (ACS), pp. 2468–2480, Jul. 19, 2018. doi: 10.1021/acs.organomet.8b00285.  
  
L. C. Burrows, L. T. Jesikiewicz, G. Lu, S. J. Geib, P. Liuand K. M. Brummond, “Computationally Guided Catalyst Design in the Type I Dynamic Kinetic Asymmetric Pauson–Khand Reaction of Allenyl Acetates”, *Journal of the American Chemical Society*, vol. 139, no. 42. American Chemical Society (ACS), pp. 15022–15032, Oct. 12, 2017. doi: 10.1021/jacs.7b07121.  
  
B. Chen, C. Fang, P. Liuand J. M. Ready, “Rhodium-Catalyzed Enantioselective Radical Addition of CX4 Reagents to Olefins”, *Angewandte Chemie International Edition*, vol. 56, no. 30. Wiley, pp. 8780–8784, Jun. 14, 2017. doi: 10.1002/anie.201704074.  
  
C. K. Chu, T.-P. Lin, H. Shao, A. L. Liberman-Martin, P. Liuand R. H. Grubbs, “Disentangling Ligand Effects on Metathesis Catalyst Activity: Experimental and Computational Studies of Ruthenium–Aminophosphine Complexes”, *Journal of the American Chemical Society*, vol. 140, no. 16. American Chemical Society (ACS), pp. 5634–5643, Apr. 05, 2018. doi: 10.1021/jacs.8b02324.  
  
Z. Dong, G. Lu, J. Wang, P. Liuand G. Dong, “Modular *ipso*/*ortho* Difunctionalization of Aryl Bromides via Palladium/Norbornene Cooperative Catalysis”, *Journal of the American Chemical Society*, vol. 140, no. 27. American Chemical Society (ACS), pp. 8551–8562, Jun. 15, 2018. doi: 10.1021/jacs.8b04153.  
  
K. M. Engle, “Origins of Initiation Rate Differences in Ruthenium Olefin Metathesis Catalysts Containing Chelating Benzylidenes”, *Journal of the American Chemical Society*, vol. 137, no. 17. American Chemical Society (ACS), pp. 5782–5792, Apr. 21, 2015. doi: 10.1021/jacs.5b01144.  
  
G. He, G. Lu, Z. Guo, P. Liuand G. Chen, “Benzazetidine synthesis via palladium-catalysed intramolecular C−H amination”, *Nature Chemistry*, vol. 8, no. 12. Springer Science and Business Media LLC, pp. 1131–1136, Aug. 01, 2016. doi: 10.1038/nchem.2585.  
  
K. N. Houk and P. Liu, “Using Computational Chemistry to Understand & Discover Chemical Reactions”, *Daedalus*, vol. 143, no. 4. MIT Press - Journals, pp. 49–66, Oct. 2014. doi: 10.1162/daed\_a\_00305.  
  
G. Huang and P. Liu, “Mechanism and Origins of Ligand-Controlled Linear Versus Branched Selectivity of Iridium-Catalyzed Hydroarylation of Alkenes”, *ACS Catalysis*, vol. 6, no. 2. American Chemical Society (ACS), pp. 809–820, Jan. 05, 2016. doi: 10.1021/acscatal.5b02201.  
  
N. Kennedy, P. Liuand T. Cohen, “Fundamental Difference in Reductive Lithiations with Preformed Radical Anions versus Catalytic Aromatic Electron-Transfer Agents:*N*,*N-*Dimethylaniline as an Advantageous Catalyst”, *Angewandte Chemie International Edition*, vol. 55, no. 1. Wiley, pp. 383–386, Nov. 18, 2015. doi: 10.1002/anie.201508971.  
  
N. Kennedy, G. Lu, P. Liuand T. Cohen, “Reductive Lithiation in the Absence of Aromatic Electron Carriers. A Steric Effect Manifested on the Surface of Lithium Metal Leads to a Difference in Relative Reactivity Depending on Whether the Aromatic Electron Carrier Is Present or Absent”, *The Journal of Organic Chemistry*, vol. 80, no. 17. American Chemical Society (ACS), pp. 8571–8582, Aug. 14, 2015. doi: 10.1021/acs.joc.5b01136.  
  
D. N. Lastovickova, H. Shao, G. Lu, P. Liuand C. W. Bielawski, “A Ring‐Opening Metathesis Polymerization Catalyst That Exhibits Redox‐Switchable Monomer Selectivities”, *Chemistry – A European Journal*, vol. 23, no. 25. Wiley, pp. 5994–6000, Feb. 03, 2017. doi: 10.1002/chem.201605738.  
  
D. N. Lastovickova, A. J. Teator, H. Shao, P. Liuand C. W. Bielawski, “A redox-switchable ring-closing metathesis catalyst”, *Inorganic Chemistry Frontiers*, vol. 4, no. 9. Royal Society of Chemistry (RSC), pp. 1525–1532, 2017. doi: 10.1039/c7qi00018a.  
  
J. W. Lee, W. Zheng, C. A. Morales-Rivera, P. Liuand M.-Y. Ngai, “Catalytic radical difluoromethoxylation of arenes and heteroarenes”, *Chemical Science*, vol. 10, no. 11. Royal Society of Chemistry (RSC), pp. 3217–3222, 2019. doi: 10.1039/c8sc05390a.  
  
K. N. Lee, Z. Lei, C. A. Morales-Rivera, P. Liuand M.-Y. Ngai, “Mechanistic studies on intramolecular C–H trifluoromethoxylation of (hetero)arenes via OCF3-migration”, *Organic & Biomolecular Chemistry*, vol. 14, no. 24. Royal Society of Chemistry (RSC), pp. 5599–5605, 2016. doi: 10.1039/c6ob00132g.  
  
C. Li, R. Y. Liu, L. T. Jesikiewicz, Y. Yang, P. Liuand S. L. Buchwald, “CuH-Catalyzed Enantioselective Ketone Allylation with 1,3-Dienes: Scope, Mechanism, and Applications”, *Journal of the American Chemical Society*, vol. 141, no. 12. American Chemical Society (ACS), pp. 5062–5070, Feb. 28, 2019. doi: 10.1021/jacs.9b01784.  
  
G.-X. Li, “A unified photoredox-catalysis strategy for C(sp3)–H hydroxylation and amidation using hypervalent iodine”, *Chemical Science*, vol. 8, no. 10. Royal Society of Chemistry (RSC), pp. 7180–7185, 2017. doi: 10.1039/c7sc02773g.  
  
G.-X. Li, “Photoredox-mediated Minisci C–H alkylation of N-heteroarenes using boronic acids and hypervalent iodine”, *Chemical Science*, vol. 7, no. 10. Royal Society of Chemistry (RSC), pp. 6407–6412, 2016. doi: 10.1039/c6sc02653b.  
  
M. Liu, P. Yang, M. K. Karunananda, Y. Wang, P. Liuand K. M. Engle, “C(alkenyl)–H Activation via Six-Membered Palladacycles: Catalytic 1,3-Diene Synthesis”, *Journal of the American Chemical Society*, vol. 140, no. 17. American Chemical Society (ACS), pp. 5805–5813, Apr. 09, 2018. doi: 10.1021/jacs.8b02124.  
  
P. Liu, T. Wang, K. Wu, C. Fangand S. Kaur, “Methylene Blue-Catalyzed Oxidative Cleavage of N-Carbonylated Indoles”, *Synthesis*, vol. 50, no. 15. Georg Thieme Verlag KG, pp. 2897–2907, May 08, 2018. doi: 10.1055/s-0036-1592006.  
  
Z. Liu, Y. Wang, Z. Wang, T. Zeng, P. Liuand K. M. Engle, “Catalytic Intermolecular Carboamination of Unactivated Alkenes via Directed Aminopalladation”, *Journal of the American Chemical Society*, vol. 139, no. 32. American Chemical Society (ACS), pp. 11261–11270, Aug. 04, 2017. doi: 10.1021/jacs.7b06520.  
  
X. Li, “Rhodium‐Catalyzed Intramolecular [5+2] Cycloaddition of Inverted 3‐Acyloxy‐1,4‐enyne and Alkyne: Experimental and Theoretical Studies”, *Chemistry – A European Journal*, vol. 22, no. 21. Wiley, pp. 7079–7083, Apr. 20, 2016. doi: 10.1002/chem.201601195.  
  
X. Li, “Rhodium(I)‐Catalyzed Benzannulation of Heteroaryl Propargylic Esters: Synthesis of Indoles and Related Heterocycles”, *Chemistry – A European Journal*, vol. 22, no. 30. Wiley, pp. 10410–10414, Jun. 20, 2016. doi: 10.1002/chem.201602088.  
  
G. Lu, C. Fang, T. Xu, G. Dongand P. Liu, “Computational Study of Rh-Catalyzed Carboacylation of Olefins: Ligand-Promoted Rhodacycle Isomerization Enables Regioselective C–C Bond Functionalization of Benzocyclobutenones”, *Journal of the American Chemical Society*, vol. 137, no. 25. American Chemical Society (ACS), pp. 8274–8283, Jun. 19, 2015. doi: 10.1021/jacs.5b04691.  
  
G. Lu, “Ligand–Substrate Dispersion Facilitates the Copper-Catalyzed Hydroamination of Unactivated Olefins”, *Journal of the American Chemical Society*, vol. 139, no. 46. American Chemical Society (ACS), pp. 16548–16555, Nov. 09, 2017. doi: 10.1021/jacs.7b07373.  
  
G. Lu, H. Shao, H. Omerand P. Liu, “Issues Particular to Organometallic Reactions”, *Applied Theoretical Organic Chemistry*. WORLD SCIENTIFIC (EUROPE), pp. 519–539, Mar. 05, 2018. doi: 10.1142/9781786344090\_0017.  
  
A. Maji, “H-bonded reusable template assisted para-selective ketonisation using soft electrophilic vinyl ethers”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Sep. 04, 2018. doi: 10.1038/s41467-018-06018-2.  
  
A. Maji, “Experimental and Computational Exploration of *para* ‐Selective Silylation with a Hydrogen‐Bonded Template”, *Angewandte Chemie International Edition*, vol. 56, no. 47. Wiley, pp. 14903–14907, Oct. 25, 2017. doi: 10.1002/anie.201708449.  
  
T. R. McFadden, C. Fang, S. J. Geib, E. Merling, P. Liuand D. P. Curran, “Synthesis of Boriranes by Double Hydroboration Reactions of N-Heterocyclic Carbene Boranes and Dimethyl Acetylenedicarboxylate”, *Journal of the American Chemical Society*, vol. 139, no. 5. American Chemical Society (ACS), pp. 1726–1729, Jan. 24, 2017. doi: 10.1021/jacs.6b09873.  
  
C. A. Morales-Rivera, P. E. Floreancigand P. Liu, “Predictive Model for Oxidative C–H Bond Functionalization Reactivity with 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone”, *Journal of the American Chemical Society*, vol. 139, no. 49. American Chemical Society (ACS), pp. 17935–17944, Nov. 30, 2017. doi: 10.1021/jacs.7b08902.  
  
J. A. Nowalk, “Sequence-Controlled Polymers Through Entropy-Driven Ring-Opening Metathesis Polymerization: Theory, Molecular Weight Control, and Monomer Design”, *Journal of the American Chemical Society*, vol. 141, no. 14. American Chemical Society (ACS), pp. 5741–5752, Feb. 04, 2019. doi: 10.1021/jacs.8b13120.  
  
M. L. O’Duill, “Tridentate Directing Groups Stabilize 6-Membered Palladacycles in Catalytic Alkene Hydrofunctionalization”, *Journal of the American Chemical Society*, vol. 139, no. 44. American Chemical Society (ACS), pp. 15576–15579, Oct. 26, 2017. doi: 10.1021/jacs.7b08383.  
  
H. M. Omer and P. Liu, “Computational Study of Ni-Catalyzed C–H Functionalization: Factors That Control the Competition of Oxidative Addition and Radical Pathways”, *Journal of the American Chemical Society*, vol. 139, no. 29. American Chemical Society (ACS), pp. 9909–9920, Jul. 12, 2017. doi: 10.1021/jacs.7b03548.  
  
H. M. Omer and P. Liu, “Computational Study of the Ni-Catalyzed C–H Oxidative Cycloaddition of Aromatic Amides with Alkynes”, *ACS Omega*, vol. 4, no. 3. American Chemical Society (ACS), pp. 5209–5220, Mar. 13, 2019. doi: 10.1021/acsomega.9b00030.  
  
V. Palani, C. L. Hugelshofer, I. Kevlishvili, P. Liuand R. Sarpong, “A Short Synthesis of Delavatine A Unveils New Insights into Site-Selective Cross-Coupling of 3,5-Dibromo-2-pyrone”, *Journal of the American Chemical Society*, vol. 141, no. 6. American Chemical Society (ACS), pp. 2652–2660, Jan. 15, 2019. doi: 10.1021/jacs.8b13012.  
  
X. Pan, “Mechanism of Photoinduced Metal-Free Atom Transfer Radical Polymerization: Experimental and Computational Studies”, *Journal of the American Chemical Society*, vol. 138, no. 7. American Chemical Society (ACS), pp. 2411–2425, Feb. 12, 2016. doi: 10.1021/jacs.5b13455.  
  
K. J. Schwarz, C. M. Pearson, G. A. Cintron‐Rosado, P. Liuand T. N. Snaddon, “Traversing Steric Limitations by Cooperative Lewis Base/Palladium Catalysis: An Enantioselective Synthesis of α‐Branched Esters Using 2‐Substituted Allyl Electrophiles”, *Angewandte Chemie International Edition*, vol. 57, no. 26. Wiley, pp. 7800–7803, May 18, 2018. doi: 10.1002/anie.201803277.  
  
A. L. Short, C. Fang, J. A. Nowalk, R. M. Weiss, P. Liuand T. Y. Meyer, “*Cis*-Selective Metathesis to Enhance the Living Character of Ring-Opening Polymerization: An Approach to Sequenced Copolymers”, *ACS Macro Letters*, vol. 7, no. 7. American Chemical Society (ACS), pp. 858–862, Jun. 29, 2018. doi: 10.1021/acsmacrolett.8b00460.  
  
A. J. Teator, H. Shao, G. Lu, P. Liuand C. W. Bielawski, “A Photoswitchable Olefin Metathesis Catalyst”, *Organometallics*, vol. 36, no. 2. American Chemical Society (ACS), pp. 490–497, Jan. 03, 2017. doi: 10.1021/acs.organomet.6b00913.  
  
A. A. Thomas, K. Speck, I. Kevlishvili, Z. Lu, P. Liuand S. L. Buchwald, “Mechanistically Guided Design of Ligands That Significantly Improve the Efficiency of CuH-Catalyzed Hydroamination Reactions”, *Journal of the American Chemical Society*, vol. 140, no. 42. American Chemical Society (ACS), pp. 13976–13984, Sep. 23, 2018. doi: 10.1021/jacs.8b09565.  
  
H. Wang, G. Lu, G. J. Sormunen, H. A. Malik, P. Liuand J. Montgomery, “NHC Ligands Tailored for Simultaneous Regio- and Enantiocontrol in Nickel-Catalyzed Reductive Couplings”, *Journal of the American Chemical Society*, vol. 139, no. 27. American Chemical Society (ACS), pp. 9317–9324, Jul. 03, 2017. doi: 10.1021/jacs.7b04583.  
  
J. Wang, R. Li, Z. Dong, P. Liuand G. Dong, “Complementary site-selectivity in arene functionalization enabled by overcoming the ortho constraint in palladium/norbornene catalysis”, *Nature Chemistry*, vol. 10, no. 8. Springer Science and Business Media LLC, pp. 866–872, Jun. 25, 2018. doi: 10.1038/s41557-018-0074-z.  
  
Y. Wang, “Epimerization of Tertiary Carbon Centers via Reversible Radical Cleavage of Unactivated C(sp3)–H Bonds”, *Journal of the American Chemical Society*, vol. 140, no. 30. American Chemical Society (ACS), pp. 9678–9684, Jul. 08, 2018. doi: 10.1021/jacs.8b05753.  
  
K. M. Wenz, P. Liuand K. N. Houk, “Intramolecular C–H Activation Reactions of Ru(NHC) Complexes Combined with H2 Transfer to Alkenes: A Theoretical Elucidation of Mechanisms and Effects of Ligands on Reactivities”, *Organometallics*, vol. 36, no. 18. American Chemical Society (ACS), pp. 3613–3623, Sep. 07, 2017. doi: 10.1021/acs.organomet.7b00531.  
  
G. Xiao, “Catalytic Site-Selective Acylation of Carbohydrates Directed by Cation–*n* Interaction”, *Journal of the American Chemical Society*, vol. 139, no. 12. American Chemical Society (ACS), pp. 4346–4349, Mar. 17, 2017. doi: 10.1021/jacs.7b01412.  
  
Y. Xia, G. Lu, P. Liuand G. Dong, “Catalytic activation of carbon–carbon bonds in cyclopentanones”, *Nature*, vol. 539, no. 7630. Springer Science and Business Media LLC, pp. 546–550, Nov. 2016. doi: 10.1038/nature19849.  
  
D. Xing, X. Qi, D. Marchant, P. Liuand G. Dong, “Branched‐Selective Direct α‐Alkylation of Cyclic Ketones with Simple Alkenes”, *Angewandte Chemie International Edition*, vol. 58, no. 13. Wiley, pp. 4366–4370, Feb. 21, 2019. doi: 10.1002/anie.201900301.  
  
Y. Xu, X. Qi, P. Zheng, C. C. Berti, P. Liuand G. Dong, “Deacylative transformations of ketones via aromatization-promoted C–C bond activation”, *Nature*, vol. 567, no. 7748. Springer Science and Business Media LLC, pp. 373–378, Jan. 30, 2019. doi: 10.1038/s41586-019-0926-8.  
  
Y. Yang and P. Liu, “Mechanism and Origins of Selectivities in the Copper-Catalyzed Dearomatization-Induced *ortho* C–H Cyanation of Vinylarenes”, *ACS Catalysis*, vol. 5, no. 5. American Chemical Society (ACS), pp. 2944–2951, Apr. 13, 2015. doi: 10.1021/acscatal.5b00443.  
  
Y. Yang, I. B. Perry, G. Lu, P. Liuand S. L. Buchwald, “Copper-catalyzed asymmetric addition of olefin-derived nucleophiles to ketones”, *Science*, vol. 353, no. 6295. American Association for the Advancement of Science (AAAS), pp. 144–150, Jul. 08, 2016. doi: 10.1126/science.aaf7720.  
  
Y. Yang, S.-L. Shi, D. Niu, P. Liuand S. L. Buchwald, “Catalytic asymmetric hydroamination of unactivated internal olefins to aliphatic amines”, *Science*, vol. 349, no. 6243. American Association for the Advancement of Science (AAAS), pp. 62–66, Jul. 03, 2015. doi: 10.1126/science.aab3753.  
  
X. Zhang, “A general strategy for synthesis of cyclophane-braced peptide macrocycles via palladium-catalysed intramolecular sp3 C−H arylation”, *Nature Chemistry*, vol. 10, no. 5. Springer Science and Business Media LLC, pp. 540–548, Apr. 02, 2018. doi: 10.1038/s41557-018-0006-y.  
  
C. Zhao, “Intermolecular Regio‐ and Stereoselective Hetero‐[5+2] Cycloaddition of Oxidopyrylium Ylides and Cyclic Imines”, *Angewandte Chemie International Edition*, vol. 58, no. 3. Wiley, pp. 887–891, Dec. 13, 2018. doi: 10.1002/anie.201811896.  
  
W. Zheng, J. W. Lee, C. A. Morales‐Rivera, P. Liuand M. Ngai, “Redox‐Active Reagents for Photocatalytic Generation of the OCF 3 Radical and (Hetero)Aryl C−H Trifluoromethoxylation”, *Angewandte Chemie International Edition*, vol. 57, no. 42. Wiley, pp. 13795–13799, Sep. 20, 2018. doi: 10.1002/anie.201808495.  
  
W. Zheng, C. A. Morales‐Rivera, J. W. Lee, P. Liuand M. Ngai, “Catalytic C−H Trifluoromethoxylation of Arenes and Heteroarenes”, *Angewandte Chemie International Edition*, vol. 57, no. 31. Wiley, pp. 9645–9649, Mar. 13, 2018. doi: 10.1002/anie.201800598.  
  
F. Zhu, “Glycosyl Cross-Coupling of Anomeric Nucleophiles: Scope, Mechanism, and Applications in the Synthesis of Aryl *C*-Glycosides”, *Journal of the American Chemical Society*, vol. 139, no. 49. American Chemical Society (ACS), pp. 17908–17922, Nov. 30, 2017. doi: 10.1021/jacs.7b08707.  
  
H. Goel, C. L. Butler, Z. W. Windomand N. Rai, “Vapor Liquid Equilibria of Hydrofluorocarbons Using Dispersion-Corrected and Nonlocal Density Functionals”, *Journal of Chemical Theory and Computation*, vol. 12, no. 7. American Chemical Society (ACS), pp. 3295–3304, Jun. 28, 2016. doi: 10.1021/acs.jctc.6b00305.  
  
P. B. Armentrout, R. M. Cox, B. C. Sweeny, S. G. Ard, N. S. Shumanand A. A. Viggiano, “Lanthanides as Catalysts: Guided Ion Beam and Theoretical Studies of Sm+ + COS”, *The Journal of Physical Chemistry A*, vol. 122, no. 3. American Chemical Society (ACS), pp. 737–749, Jan. 12, 2018. doi: 10.1021/acs.jpca.7b09905.  
  
P. B. Armentrout, M. Demirevaand K. A. Peterson, “Guided ion beam and theoretical studies of the bond energy of SmS+”, *The Journal of Chemical Physics*, vol. 147, no. 21. AIP Publishing, p. 214307, Dec. 07, 2017. doi: 10.1063/1.5009916.  
  
M. Demireva and P. B. Armentrout, “Activation of CO2 by Gadolinium Cation (Gd+): Energetics and Mechanism from Experiment and Theory”, *Topics in Catalysis*, vol. 61, no. 1–2. Springer Science and Business Media LLC, pp. 3–19, Nov. 29, 2017. doi: 10.1007/s11244-017-0858-1.  
  
M. Demireva and P. B. Armentrout, “Activation of H2 by Gadolinium Cation (Gd+): Bond Energy of GdH+ and Mechanistic Insights from Guided Ion Beam and Theoretical Studies”, *The Journal of Physical Chemistry A*, vol. 122, no. 3. American Chemical Society (ACS), pp. 750–761, Jan. 12, 2018. doi: 10.1021/acs.jpca.7b11471.  
  
C. P. McNary and P. B. Armentrout, “Non-adiabatic behavior in the homolytic and heterolytic bond dissociation of protonated hydrazine: A guided ion beam and theoretical investigation”, *The Journal of Chemical Physics*, vol. 147, no. 12. AIP Publishing, p. 124306, Sep. 28, 2017. doi: 10.1063/1.4997415.  
  
C. Liao, “Melittin Aggregation in Aqueous Solutions: Insight from Molecular Dynamics Simulations”, *The Journal of Physical Chemistry B*, vol. 119, no. 33. American Chemical Society (ACS), pp. 10390–10398, Aug. 11, 2015. doi: 10.1021/acs.jpcb.5b03254.  
  
M. Y. Shelley, “A New Mixed All-Atom/Coarse-Grained Model: Application to Melittin Aggregation in Aqueous Solution”, *Journal of Chemical Theory and Computation*, vol. 13, no. 8. American Chemical Society (ACS), pp. 3881–3897, Jun. 21, 2017. doi: 10.1021/acs.jctc.7b00071.  
  
J. Macharia, “A Designed Approach to Enantiodivergent Enamine Catalysis”, *Angewandte Chemie International Edition*, vol. 56, no. 30. Wiley, pp. 8756–8760, Jun. 20, 2017. doi: 10.1002/anie.201703919.  
  
J. E. Stevens, K. D. Utterbeck, A. Piatkowskiand M. N. Spicer, “Density functional theory investigation of mechanisms of degradation reactions of sulfonated PEEK membranes with H radicals in fuel cells: addition–elimination bond-breaking reactions in a model molecule”, *Theoretical Chemistry Accounts*, vol. 137, no. 7. Springer Science and Business Media LLC, Jul. 2018. doi: 10.1007/s00214-018-2281-5.  
  
E. R. Hantz, M. D. Sonntagand C. S. Hamann, “Connecting Organic and Physical Chemistry Students with Raman Spectroscopy”, *Raman Spectroscopy in the Undergraduate Curriculum*. American Chemical Society, pp. 35–51, Jan. 2018. doi: 10.1021/bk-2018-1305.ch003.  
  
C. K. Brozek, A. Ozarowski, S. A. Stoianand M. Dincă, “Dynamic structural flexibility of Fe-MOF-5 evidenced by 57Fe Mössbauer spectroscopy”, *Inorganic Chemistry Frontiers*, vol. 4, no. 5. Royal Society of Chemistry (RSC), pp. 782–788, 2017. doi: 10.1039/c6qi00584e.  
  
M. E. Pascualini, S. A. Stoian, A. Ozarowski, K. A. Abboudand A. S. Veige, “Solid State Collapse of a High-Spin Square-Planar Fe(II) Complex, Solution Phase Dynamics, and Electronic Structure Characterization of an Fe(II)2 Dimer”, *Inorganic Chemistry*, vol. 55, no. 11. American Chemical Society (ACS), pp. 5191–5200, May 16, 2016. doi: 10.1021/acs.inorgchem.6b00075.  
  
M. E. Pascualini, “Synthesis and characterization of a family of M2+ complexes supported by a trianionic ONO3− pincer-type ligand: towards the stabilization of high-spin square-planar complexes”, *Dalton Transactions*, vol. 44, no. 46. Royal Society of Chemistry (RSC), pp. 20207–20215, 2015. doi: 10.1039/c5dt03960f.  
  
K. T. Kuwata, E. J. Guinn, M. R. Hermes, J. A. Fernandez, J. M. Mathisonand K. Huang, “A Computational Re-examination of the Criegee Intermediate–Sulfur Dioxide Reaction”, *The Journal of Physical Chemistry A*, vol. 119, no. 41. American Chemical Society (ACS), pp. 10316–10335, Oct. 06, 2015. doi: 10.1021/acs.jpca.5b06565.  
  
S. Kyasa, R. N. Meier, R. A. Pardini, T. K. Truttmann, K. T. Kuwataand P. H. Dussault, “Synthesis of Ethers via Reaction of Carbanions and Monoperoxyacetals”, *The Journal of Organic Chemistry*, vol. 80, no. 24. American Chemical Society (ACS), pp. 12100–12114, Dec. 07, 2015. doi: 10.1021/acs.joc.5b02043.  
  
D. J. Marell, “Mechanism of the Intramolecular Hexadehydro-Diels–Alder Reaction”, *The Journal of Organic Chemistry*, vol. 80, no. 23. American Chemical Society (ACS), pp. 11744–11754, Aug. 25, 2015. doi: 10.1021/acs.joc.5b01356.  
  
B. J. Cook, G. N. Di Francesco, M. T. Kieber-Emmonsand L. J. Murray, “A Tricopper(I) Complex Competent for O Atom Transfer, C–H Bond Activation, and Multiple O2 Activation Steps”, *Inorganic Chemistry*, vol. 57, no. 18. American Chemical Society (ACS), pp. 11361–11368, May 23, 2018. doi: 10.1021/acs.inorgchem.8b00921.  
  
D. E. Heppner, “Direct cysteine sulfenylation drives activation of the Src kinase”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Oct. 30, 2018. doi: 10.1038/s41467-018-06790-1.  
  
C. Liao, Z. Zhang, J. Kale, D. W. Andrews, J. Linand J. Li, “Conformational Heterogeneity of Bax Helix 9 Dimer for Apoptotic Pore Formation”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Jul. 06, 2016. doi: 10.1038/srep29502.  
  
C. Liao, X. Zhao, M. Brewer, V. Mayand J. Li, “Conformational Transitions of the Pituitary Adenylate Cyclase-Activating Polypeptide Receptor, a Human Class B GPCR”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Jul. 14, 2017. doi: 10.1038/s41598-017-05815-x.  
  
C. Liao, X. Zhao, J. Liu, S. T. Schneebeli, J. C. Shelleyand J. Li, “Capturing the multiscale dynamics of membrane protein complexes with all-atom, mixed-resolution, and coarse-grained models”, *Physical Chemistry Chemical Physics*, vol. 19, no. 13. Royal Society of Chemistry (RSC), pp. 9181–9188, 2017. doi: 10.1039/c7cp00200a.  
  
J. Li, “Controlled Self-Assembly inside C-Shaped Polyaromatic Strips”, *Synlett*, vol. 27, no. 14. Georg Thieme Verlag KG, pp. 2145–2149, Jun. 28, 2016. doi: 10.1055/s-0035-1561479.  
  
J. Liu, “Targeting the apoptotic Mcl-1-PUMA interface with a dual-acting compound”, *Oncotarget*, vol. 8, no. 33. Impact Journals, LLC, pp. 54236–54242, Apr. 20, 2017. doi: 10.18632/oncotarget.17294.  
  
X. Liu, Z. J. Weinert, M. Sharafi, C. Liao, J. Liand S. T. Schneebeli, “Regulating Molecular Recognition with C-Shaped Strips Attained by Chirality-Assisted Synthesis”, *Angewandte Chemie*, vol. 127, no. 43. Wiley, pp. 12963–12967, Sep. 09, 2015. doi: 10.1002/ange.201506793.  
  
J. J. Madsen, A. V. Sinitskiy, J. Liand G. A. Voth, “Highly Coarse-Grained Representations of Transmembrane Proteins”, *Journal of Chemical Theory and Computation*, vol. 13, no. 2. American Chemical Society (ACS), pp. 935–944, Jan. 18, 2017. doi: 10.1021/acs.jctc.6b01076.  
  
K. E. Murphy, “Precise through-space control of an abiotic electrophilic aromatic substitution reaction”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Apr. 05, 2017. doi: 10.1038/ncomms14840.  
  
M. Sharafi, “Crystal‐Packing‐Driven Enrichment of Atropoisomers”, *Angewandte Chemie International Edition*, vol. 56, no. 25. Wiley, pp. 7097–7101, May 16, 2017. doi: 10.1002/anie.201701876.  
  
Z. Zhang, “BH 3‐in‐groove dimerization initiates and helix 9 dimerization expands Bax pore assembly in membranes”, *The EMBO Journal*, vol. 35, no. 2. EMBO, pp. 208–236, Dec. 23, 2015. doi: 10.15252/embj.201591552.  
  
X. Zhao, C. Liao, Y.-T. Ma, J. B. Ferrell, S. T. Schneebeliand J. Li, “Top-down Multiscale Approach To Simulate Peptide Self-Assembly from Monomers”, *Journal of Chemical Theory and Computation*, vol. 15, no. 3. American Chemical Society (ACS), pp. 1514–1522, Jan. 24, 2019. doi: 10.1021/acs.jctc.8b01025.  
  
U. F. Shahul Hameed, “H-NS uses an autoinhibitory conformational switch for environment-controlled gene silencing”, *Nucleic Acids Research*, vol. 47, no. 5. Oxford University Press (OUP), pp. 2666–2680, Dec. 28, 2018. doi: 10.1093/nar/gky1299.  
  
D. L. Cruickshank, C. H. Hendon, M. J. R. Verbeek, A. Walshand C. C. Wilson, “Polymorphism of the azobenzene dye compound methyl yellow”, *CrystEngComm*, vol. 18, no. 19. Royal Society of Chemistry (RSC), pp. 3456–3461, 2016. doi: 10.1039/c6ce00387g.  
  
C. H. Hendon, “A Simple and Non-Destructive Method for Assessing the Incorporation of Bipyridine Dicarboxylates as Linkers within Metal-Organic Frameworks”, *Chemistry - A European Journal*, vol. 22, no. 11. Wiley, pp. 3713–3718, Feb. 02, 2016. doi: 10.1002/chem.201600143.  
  
C. H. Hendon, “One-dimensional Magnus-type platinum double salts”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Jun. 20, 2016. doi: 10.1038/ncomms11950.  
  
I. G. Powers, J. M. Andjaba, X. Luo, J. Meiand C. Uyeda, “Catalytic Azoarene Synthesis from Aryl Azides Enabled by a Dinuclear Ni Complex”, *Journal of the American Chemical Society*, vol. 140, no. 11. American Chemical Society (ACS), pp. 4110–4118, Feb. 28, 2018. doi: 10.1021/jacs.8b00503.  
  
I. G. Powers, C. Kiattisewee, K. C. Mullane, E. J. Schelterand C. Uyeda, “A 1,2‐Addition Pathway for C(sp 2 )−H Activation at a Dinickel Imide”, *Chemistry – A European Journal*, vol. 23, no. 32. Wiley, pp. 7694–7697, May 22, 2017. doi: 10.1002/chem.201701855.  
  
I. G. Powers and C. Uyeda, “Metal–Metal Bonds in Catalysis”, *ACS Catalysis*, vol. 7, no. 2. American Chemical Society (ACS), pp. 936–958, Dec. 29, 2016. doi: 10.1021/acscatal.6b02692.  
  
K. Trerayapiwat, N. Ricke, P. Cohen, A. Poblete, H. Rudeland S. N. Eustis, “Sticking to (first) principles: quantum molecular dynamics and Bayesian probabilistic methods to simulate aquatic pollutant absorption spectra”, *Environmental Science: Processes & Impacts*, vol. 18, no. 8. Royal Society of Chemistry (RSC), pp. 1068–1077, 2016. doi: 10.1039/c6em00233a.  
  
R. L. Kenion and N. Ananth, “Direct simulation of electron transfer in the cobalt hexammine(ii/iii) self-exchange reaction”, *Physical Chemistry Chemical Physics*, vol. 18, no. 37. Royal Society of Chemistry (RSC), pp. 26117–26124, 2016. doi: 10.1039/c6cp04882j.  
  
Y.-G. Wang and E. C. Barnes, “O-Regioselective Synthesis with the Silver Salt Method”, *ACS Omega*, vol. 3, no. 4. American Chemical Society (ACS), pp. 4557–4572, Apr. 26, 2018. doi: 10.1021/acsomega.8b00361.  
  
E. I. Alarcon, H. Poblete, H. Roh, J.-F. Couture, J. Comerand I. E. Kochevar, “Rose Bengal Binding to Collagen and Tissue Photobonding”, *ACS Omega*, vol. 2, no. 10. American Chemical Society (ACS), pp. 6646–6657, Oct. 11, 2017. doi: 10.1021/acsomega.7b00675.  
  
H. Poblete, I. Miranda-Carvajaland J. Comer, “Determinants of Alanine Dipeptide Conformational Equilibria on Graphene and Hydroxylated Derivatives”, *The Journal of Physical Chemistry B*, vol. 121, no. 15. American Chemical Society (ACS), pp. 3895–3907, Mar. 24, 2017. doi: 10.1021/acs.jpcb.7b01130.  
  
J. Shen, S. Magesh, L. Chen, L. Huand Y. He, “Enantiomeric characterization and structure elucidation of LH601A using vibrational circular dichroism spectroscopy”, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 192. Elsevier BV, pp. 312–317, Mar. 2018. doi: 10.1016/j.saa.2017.11.033.  
  
A. Ge, “Interfacial Structure and Electric Field Probed by *in Situ* Electrochemical Vibrational Stark Effect Spectroscopy and Computational Modeling”, *The Journal of Physical Chemistry C*, vol. 121, no. 34. American Chemical Society (ACS), pp. 18674–18682, Aug. 22, 2017. doi: 10.1021/acs.jpcc.7b05563.  
  
S. Hedström, “Thousandfold Enhancement of Photoreduction Lifetime in Re(bpy)(CO)3 via Spin-Dependent Electron Transfer from a Perylenediimide Radical Anion Donor”, *Journal of the American Chemical Society*, vol. 139, no. 46. American Chemical Society (ACS), pp. 16466–16469, Nov. 08, 2017. doi: 10.1021/jacs.7b09438.  
  
N. T. La Porte, “Photoinduced electron transfer from rylenediimide radical anions and dianions to Re(bpy)(CO)3 using red and near-infrared light”, *Chemical Science*, vol. 8, no. 5. Royal Society of Chemistry (RSC), pp. 3821–3831, 2017. doi: 10.1039/c6sc05103k.  
  
B. Rudshteyn, “Water-Nucleophilic Attack Mechanism for the CuII(pyalk)2 Water-Oxidation Catalyst”, *ACS Catalysis*, vol. 8, no. 9. American Chemical Society (ACS), pp. 7952–7960, Jul. 18, 2018. doi: 10.1021/acscatal.8b02466.  
  
Y. Wu, “Electrode-Ligand Interactions Dramatically Enhance CO2 Conversion to CO by the [Ni(cyclam)](PF%3Csub%3E6%3C/sub%3E)2 Catalyst”, *ACS Catalysis*, vol. 7, no. 8. American Chemical Society (ACS), pp. 5282–5288, Jul. 13, 2017. doi: 10.1021/acscatal.7b01109.  
  
K. T. Butler, C. H. Hendonand A. Walsh, “Designing porous electronic thin-film devices: band offsets and heteroepitaxy”, *Faraday Discussions*, vol. 201. Royal Society of Chemistry (RSC), pp. 207–219, 2017. doi: 10.1039/c7fd00019g.  
  
A. Cadiau, “Toward New 2D Zirconium-Based Metal–Organic Frameworks: Synthesis, Structures, and Electronic Properties”, *Chemistry of Materials*, vol. 32, no. 1. American Chemical Society (ACS), pp. 97–104, Dec. 18, 2019. doi: 10.1021/acs.chemmater.9b02462.  
  
M. I. Cameron, “Systematically Improving Espresso: Insights from Mathematical Modeling and Experiment”, *Matter*, vol. 2, no. 3. Elsevier BV, pp. 631–648, Mar. 2020. doi: 10.1016/j.matt.2019.12.019.  
  
M. M. Cerda, J. L. Mancuso, E. J. Mullen, C. H. Hendonand M. D. Pluth, “Use of Dithiasuccinoyl‐Caged Amines Enables COS/H 2 S Release Lacking Electrophilic Byproducts”, *Chemistry – A European Journal*, vol. 26, no. 24. Wiley, pp. 5374–5380, Mar. 04, 2020. doi: 10.1002/chem.201905577.  
  
M. M. Cerda, T. D. Newton, Y. Zhao, B. K. Collins, C. H. Hendonand M. D. Pluth, “Dithioesters: simple, tunable, cysteine-selective H2S donors”, *Chemical Science*, vol. 10, no. 6. Royal Society of Chemistry (RSC), pp. 1773–1779, 2019. doi: 10.1039/c8sc04683b.  
  
R. J. Comito, “Selective Dimerization of Propylene with Ni-MFU-4*l*”, *Organometallics*, vol. 36, no. 9. American Chemical Society (ACS), pp. 1681–1683, Apr. 25, 2017. doi: 10.1021/acs.organomet.7b00178.  
  
R. W. Day, “Single Crystals of Electrically Conductive Two-Dimensional Metal–Organic Frameworks: Structural and Electrical Transport Properties”, *ACS Central Science*, vol. 5, no. 12. American Chemical Society (ACS), pp. 1959–1964, Dec. 10, 2019. doi: 10.1021/acscentsci.9b01006.  
  
J.-H. Dou, “Signature of Metallic Behavior in the Metal–Organic Frameworks M3(hexaiminobenzene)2 (M = Ni, Cu)”, *Journal of the American Chemical Society*, vol. 139, no. 39. American Chemical Society (ACS), pp. 13608–13611, Sep. 21, 2017. doi: 10.1021/jacs.7b07234.  
  
R. J.-C. Dubey, “Highly Stereoselective Heterogeneous Diene Polymerization by Co-MFU-4*l*: A Single-Site Catalyst Prepared by Cation Exchange”, *Journal of the American Chemical Society*, vol. 139, no. 36. American Chemical Society (ACS), pp. 12664–12669, Aug. 29, 2017. doi: 10.1021/jacs.7b06841.  
  
D. M. Hamann, “Influence of Nanoarchitecture on Charge Donation and the Electrical-Transport Properties in [(SnSe)1+δ][TiSe2]*q* Heterostructures”, *Chemistry of Materials*, vol. 32, no. 13. American Chemical Society (ACS), pp. 5802–5813, Jun. 02, 2020. doi: 10.1021/acs.chemmater.0c01691.  
  
C. H. Hendon, “Electroactive Nanoporous Metal Oxides and Chalcogenides by Chemical Design”, *Chemistry of Materials*, vol. 29, no. 8. American Chemical Society (ACS), pp. 3663–3670, Apr. 03, 2017. doi: 10.1021/acs.chemmater.7b00464.  
  
C. H. Hendon, S. T. Hunt, M. Milina, K. T. Butler, A. Walshand Y. Román-Leshkov, “Realistic Surface Descriptions of Heterometallic Interfaces: The Case of TiWC Coated in Noble Metals”, *The Journal of Physical Chemistry Letters*, vol. 7, no. 22. American Chemical Society (ACS), pp. 4475–4482, Oct. 28, 2016. doi: 10.1021/acs.jpclett.6b02293.  
  
C. H. Hendon, “Magnetic coupling in a hybrid Mn(ii) acetylene dicarboxylate”, *Physical Chemistry Chemical Physics*, vol. 18, no. 48. Royal Society of Chemistry (RSC), pp. 33329–33334, 2016. doi: 10.1039/c6cp06886c.  
  
C. H. Hendon, A. J. Rieth, M. D. Korzyńskiand M. Dincă, “Grand Challenges and Future Opportunities for Metal–Organic Frameworks”, *ACS Central Science*, vol. 3, no. 6. American Chemical Society (ACS), pp. 554–563, Jun. 06, 2017. doi: 10.1021/acscentsci.7b00197.  
  
C. H. Hendon, A. Walshand M. Dincă, “Frontier Orbital Engineering of Metal–Organic Frameworks with Extended Inorganic Connectivity: Porous Alkaline-Earth Oxides”, *Inorganic Chemistry*, vol. 55, no. 15. American Chemical Society (ACS), pp. 7265–7269, Jun. 07, 2016. doi: 10.1021/acs.inorgchem.6b00979.  
  
S. T. Hunt, M. Milina, A. C. Alba-Rubio, C. H. Hendon, J. A. Dumesicand Y. Roman-Leshkov, “Self-assembly of noble metal monolayers on transition metal carbide nanoparticle catalysts”, *Science*, vol. 352, no. 6288. American Association for the Advancement of Science (AAAS), pp. 974–978, May 19, 2016. doi: 10.1126/science.aad8471.  
  
D. Jung, “A molecular cross-linking approach for hybrid metal oxides”, *Nature Materials*, vol. 17, no. 4. Springer Science and Business Media LLC, pp. 341–348, Mar. 05, 2018. doi: 10.1038/s41563-018-0021-9.  
  
T. W. Kasel, Z. Deng, A. M. Mroz, C. H. Hendon, K. T. Butlerand P. Canepa, “Metal-free perovskites for non linear optical materials”, *Chemical Science*, vol. 10, no. 35. Royal Society of Chemistry (RSC), pp. 8187–8194, 2019. doi: 10.1039/c9sc03378e.  
  
T. W. Kasel and C. H. Hendon, “Electronic implications of organic nitrogen lone pairs in lead iodide perovskites”, *Journal of Materials Chemistry C*, vol. 6, no. 17. Royal Society of Chemistry (RSC), pp. 4765–4768, 2018. doi: 10.1039/c8tc00376a.  
  
T. W. Kasel, A. T. Murrayand C. H. Hendon, “Cyclopropenium (C3H3)+ as an Aromatic Alternative A-Site Cation for Hybrid Halide Perovskite Architectures”, *The Journal of Physical Chemistry C*, vol. 122, no. 4. American Chemical Society (ACS), pp. 2041–2045, Jan. 17, 2018. doi: 10.1021/acs.jpcc.7b11867.  
  
M. D. Korzyński, “*Quo vadis niobium*? Divergent coordination behavior of early-transition metals towards MOF-5”, *Chemical Science*, vol. 10, no. 23. Royal Society of Chemistry (RSC), pp. 5906–5910, 2019. doi: 10.1039/c9sc01553a.  
  
S.-J. Lee, “Time-Resolved *in Situ* Polymorphic Transformation from One 12-Connected Zr-MOF to Another”, *ACS Materials Letters*, vol. 2, no. 5. American Chemical Society (ACS), pp. 499–504, Apr. 09, 2020. doi: 10.1021/acsmaterialslett.0c00012.  
  
K. N. Le and C. H. Hendon, “Pressure-induced metallicity and piezoreductive transition of metal-centres in conductive 2-dimensional metal–organic frameworks”, *Physical Chemistry Chemical Physics*, vol. 21, no. 46. Royal Society of Chemistry (RSC), pp. 25773–25778, 2019. doi: 10.1039/c9cp04797b.  
  
J. L. Mancuso and C. H. Hendon, “Titanium(IV) Inclusion as a Versatile Route to Photoactivity in Metal–Organic Frameworks”, *Advanced Theory and Simulations*, vol. 2, no. 11. Wiley, p. 1900126, Aug. 26, 2019. doi: 10.1002/adts.201900126.  
  
C. E. McDevitt, “Monofunctional platinum(II) compounds and nucleolar stress: is phenanthriplatin unique?”, *JBIC Journal of Biological Inorganic Chemistry*, vol. 24, no. 6. Springer Science and Business Media LLC, pp. 899–908, Sep. 2019. doi: 10.1007/s00775-019-01707-9.  
  
E. D. Metzger, R. J. Comito, C. H. Hendonand M. Dincă, “Mechanism of Single-Site Molecule-Like Catalytic Ethylene Dimerization in Ni-MFU-4*l*”, *Journal of the American Chemical Society*, vol. 139, no. 2. American Chemical Society (ACS), pp. 757–762, Jan. 04, 2017. doi: 10.1021/jacs.6b10300.  
  
G. Paille, “An unprecedented {Ni14SiW9} hybrid polyoxometalate with high photocatalytic hydrogen evolution activity”, *Chemical Communications*, vol. 55, no. 29. Royal Society of Chemistry (RSC), pp. 4166–4169, 2019. doi: 10.1039/c9cc01269a.  
  
S. S. Park, C. H. Hendon, A. J. Fielding, A. Walsh, M. O’Keeffeand M. Dincă, “The Organic Secondary Building Unit: Strong Intermolecular π Interactions Define Topology in MIT-25, a Mesoporous MOF with Proton-Replete Channels”, *Journal of the American Chemical Society*, vol. 139, no. 10. American Chemical Society (ACS), pp. 3619–3622, Mar. 06, 2017. doi: 10.1021/jacs.6b13176.  
  
S. S. Park, A. J. Rieth, C. H. Hendonand M. Dincă, “Selective Vapor Pressure Dependent Proton Transport in a Metal–Organic Framework with Two Distinct Hydrophilic Pores”, *Journal of the American Chemical Society*, vol. 140, no. 6. American Chemical Society (ACS), pp. 2016–2019, Feb. 06, 2018. doi: 10.1021/jacs.7b12784.  
  
A. J. Rieth, A. M. Wright, G. Skorupskii, J. L. Mancuso, C. H. Hendonand M. Dincă, “Record-Setting Sorbents for Reversible Water Uptake by Systematic Anion Exchanges in Metal–Organic Frameworks”, *Journal of the American Chemical Society*, vol. 141, no. 35. American Chemical Society (ACS), pp. 13858–13866, Aug. 09, 2019. doi: 10.1021/jacs.9b06246.  
  
J. G. Santaclara, “Revisiting the Incorporation of Ti(IV) in UiO-type Metal–Organic Frameworks: Metal Exchange versus Grafting and Their Implications on Photocatalysis”, *Chemistry of Materials*, vol. 29, no. 21. American Chemical Society (ACS), pp. 8963–8967, Oct. 19, 2017. doi: 10.1021/acs.chemmater.7b03320.  
  
G. Skorupskii, B. A. Trump, T. W. Kasel, C. M. Brown, C. H. Hendonand M. Dincă, “Efficient and tunable one-dimensional charge transport in layered lanthanide metal–organic frameworks”, *Nature Chemistry*, vol. 12, no. 2. Springer Science and Business Media LLC, pp. 131–136, Nov. 25, 2019. doi: 10.1038/s41557-019-0372-0.  
  
I. Stassen, J.-H. Dou, C. Hendonand M. Dincă, “Chemiresistive Sensing of Ambient CO2 by an Autogenously Hydrated Cu3(hexaiminobenzene)2 Framework”, *ACS Central Science*, vol. 5, no. 8. American Chemical Society (ACS), pp. 1425–1431, Jun. 27, 2019. doi: 10.1021/acscentsci.9b00482.  
  
L. Sun, “Is iron unique in promoting electrical conductivity in MOFs?”, *Chemical Science*, vol. 8, no. 6. Royal Society of Chemistry (RSC), pp. 4450–4457, 2017. doi: 10.1039/c7sc00647k.  
  
E. C. Sutton, “Nucleolar Stress Induction by Oxaliplatin and Derivatives”, *Journal of the American Chemical Society*, vol. 141, no. 46. American Chemical Society (ACS), pp. 18411–18415, Oct. 31, 2019. doi: 10.1021/jacs.9b10319.  
  
Y. Tulchinsky, “Reversible Capture and Release of Cl2 and Br2 with a Redox-Active Metal–Organic Framework”, *Journal of the American Chemical Society*, vol. 139, no. 16. American Chemical Society (ACS), pp. 5992–5997, Apr. 14, 2017. doi: 10.1021/jacs.7b02161.  
  
A. Walsh, K. T. Butlerand C. H. Hendon, “Chemical principles for electroactive metal–organic frameworks”, *MRS Bulletin*, vol. 41, no. 11. Springer Science and Business Media LLC, pp. 870–876, Nov. 2016. doi: 10.1557/mrs.2016.243.  
  
H. C. Wentz, “Switchable electrical conductivity in a three-dimensional metal–organic framework *via* reversible ligand n-doping”, *Chemical Science*, vol. 11, no. 5. Royal Society of Chemistry (RSC), pp. 1342–1346, 2020. doi: 10.1039/c9sc06150a.  
  
A. M. Wright, “A Structural Mimic of Carbonic Anhydrase in a Metal-Organic Framework”, *Chem*, vol. 4, no. 12. Elsevier BV, pp. 2894–2901, Dec. 2018. doi: 10.1016/j.chempr.2018.09.011.  
  
A. Wuttig, “Tracking a Common Surface-Bound Intermediate during CO2-to-Fuels Catalysis”, *ACS Central Science*, vol. 2, no. 8. American Chemical Society (ACS), pp. 522–528, Aug. 08, 2016. doi: 10.1021/acscentsci.6b00155.  
  
L. S. Xie, “Tunable Mixed-Valence Doping toward Record Electrical Conductivity in a Three-Dimensional Metal–Organic Framework”, *Journal of the American Chemical Society*, vol. 140, no. 24. American Chemical Society (ACS), pp. 7411–7414, May 28, 2018. doi: 10.1021/jacs.8b03604.  
  
E. Berry, G. dos P. Gomes, A. MacLean, J. R. Martinand P. A. Wiget, “Discovery of a Long-Range Perlin Effect in a Conformationally Constrained Oxocane”, *The Journal of Organic Chemistry*, vol. 81, no. 13. American Chemical Society (ACS), pp. 5740–5744, Jun. 22, 2016. doi: 10.1021/acs.joc.6b00819.  
  
G. dos Passos Gomes and I. V. Alabugin, “Drawing Catalytic Power from Charge Separation: Stereoelectronic and Zwitterionic Assistance in the Au(I)-Catalyzed Bergman Cyclization”, *Journal of the American Chemical Society*, vol. 139, no. 9. American Chemical Society (ACS), pp. 3406–3416, Feb. 22, 2017. doi: 10.1021/jacs.6b11054.  
  
G. dos Passos Gomes, “Stereoelectronic Control in the Ozone‐Free Synthesis of Ozonides”, *Angewandte Chemie International Edition*, vol. 56, no. 18. Wiley, pp. 4955–4959, Apr. 05, 2017. doi: 10.1002/anie.201610699.  
  
C. J. Evoniuk, G. dos P. Gomes, S. P. Hill, S. Fujita, K. Hansonand I. V. Alabugin, “Coupling N–H Deprotonation, C–H Activation, and Oxidation: Metal-Free C(sp3)–H Aminations with Unprotected Anilines”, *Journal of the American Chemical Society*, vol. 139, no. 45. American Chemical Society (ACS), pp. 16210–16221, Oct. 31, 2017. doi: 10.1021/jacs.7b07519.  
  
C. J. Evoniuk, G. dos P. Gomes, M. Ly, F. D. Whiteand I. V. Alabugin, “Coupling Radical Homoallylic Expansions with C–C Fragmentations for the Synthesis of Heteroaromatics: Quinolines from Reactions of *o*-Alkenylarylisonitriles with Aryl, Alkyl, and Perfluoroalkyl Radicals”, *The Journal of Organic Chemistry*, vol. 82, no. 8. American Chemical Society (ACS), pp. 4265–4278, Apr. 03, 2017. doi: 10.1021/acs.joc.7b00262.  
  
G. dos P. Gomes, C. J. Evoniuk, M. Lyand I. V. Alabugin, “Changing the path of least resistance, or access to endo-dig products via a sequence of three exo-trig transition states: electronic effects in homoallyic ring expansion cascades of alkenyl isonitriles”, *Organic & Biomolecular Chemistry*, vol. 15, no. 19. Royal Society of Chemistry (RSC), pp. 4135–4143, 2017. doi: 10.1039/c7ob00527j.  
  
T. Harris, G. dos P. Gomes, R. J. Clarkand I. V. Alabugin, “Domino Fragmentations in Traceless Directing Groups of Radical Cascades: Evidence for the Formation of Alkoxy Radicals via C–O Scission”, *The Journal of Organic Chemistry*, vol. 81, no. 14. American Chemical Society (ACS), pp. 6007–6017, Jun. 27, 2016. doi: 10.1021/acs.joc.6b01052.  
  
E. Juaristi, G. dos Passos Gomes, A. O. Terent’ev, R. Notarioand I. V. Alabugin, “Stereoelectronic Interactions as a Probe for the Existence of the Intramolecular α-Effect”, *Journal of the American Chemical Society*, vol. 139, no. 31. American Chemical Society (ACS), pp. 10799–10813, Jul. 25, 2017. doi: 10.1021/jacs.7b05367.  
  
N. H. Park, G. dos P. Gomes, M. Fevre, G. O. Jones, I. V. Alabuginand J. L. Hedrick, “Organocatalyzed synthesis of fluorinated poly(aryl thioethers)”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Aug. 01, 2017. doi: 10.1038/s41467-017-00186-3.  
  
K. Pati, G. dos Passos Gomesand I. V. Alabugin, “Combining Traceless Directing Groups with Hybridization Control of Radical Reactivity: From Skipped Enynes to Defect‐Free Hexagonal Frameworks”, *Angewandte Chemie International Edition*, vol. 55, no. 38. Wiley, pp. 11633–11637, Aug. 18, 2016. doi: 10.1002/anie.201605799.  
  
K. Pati, G. dos P. Gomes, T. Harrisand I. V. Alabugin, “Fused Catechol Ethers from Gold(I)-Catalyzed Intramolecular Reaction of Propargyl Ethers with Acetals”, *Organic Letters*, vol. 18, no. 5. American Chemical Society (ACS), pp. 928–931, Feb. 17, 2016. doi: 10.1021/acs.orglett.5b03522.  
  
P. Poonpatana, “Formaldehyde-Extruding Homolytic Aromatic Substitution via C→O Transposition: Selective ‘Traceless-Linker’ access to Congested Biaryl Bonds”, *Chemistry - A European Journal*, vol. 23, no. 38. Wiley, pp. 9091–9097, Jun. 19, 2017. doi: 10.1002/chem.201700085.  
  
K. N. Sedenkova, “Substituent effects on stereoselectivity of dihalocarbene reactions with cyclohexadiene and on the reactivity of bis-dihalocyclopropanes in electrophilic nitrations en route to pyrimidine *N*-oxides”, *Organic & Biomolecular Chemistry*, vol. 15, no. 44. Royal Society of Chemistry (RSC), pp. 9433–9441, 2017. doi: 10.1039/c7ob02463k.  
  
N. P. Tsvetkov, “Radical Alkyne *peri* ‐Annulation Reactions for the Synthesis of Functionalized Phenalenes, Benzanthrenes, and Olympicene”, *Angewandte Chemie International Edition*, vol. 57, no. 14. Wiley, pp. 3651–3655, Mar. 2018. doi: 10.1002/anie.201712783.  
  
S. Umezu, “Regioselective One‐Pot Synthesis of Triptycenes via Triple‐Cycloadditions of Arynes to Ynolates”, *Angewandte Chemie International Edition*, vol. 56, no. 5. Wiley, pp. 1298–1302, Dec. 28, 2016. doi: 10.1002/anie.201609111.  
  
S. Z. Vatsadze, Y. D. Loginova, G. dos Passos Gomesand I. V. Alabugin, “Stereoelectronic Chameleons: The Donor–Acceptor Dichotomy of Functional Groups”, *Chemistry – A European Journal*, vol. 23, no. 14. Wiley, pp. 3225–3245, Nov. 11, 2016. doi: 10.1002/chem.201603491.  
  
V. A. Vil’, “Interrupted Baeyer–Villiger Rearrangement: Building A Stereoelectronic Trap for the Criegee Intermediate”, *Angewandte Chemie International Edition*, vol. 57, no. 13. Wiley, pp. 3372–3376, Feb. 23, 2018. doi: 10.1002/anie.201712651.  
  
I. A. Yaremenko, “Ozone-Free Synthesis of Ozonides: Assembling Bicyclic Structures from 1,5-Diketones and Hydrogen Peroxide”, *The Journal of Organic Chemistry*, vol. 83, no. 8. American Chemical Society (ACS), pp. 4402–4426, Mar. 13, 2018. doi: 10.1021/acs.joc.8b00130.  
  
J. Anderson, P. T. Lakeand M. McCullagh, “Initial Aggregation and Ordering Mechanism of Diphenylalanine from Microsecond All-Atom Molecular Dynamics Simulations”, *The Journal of Physical Chemistry B*, vol. 122, no. 51. American Chemical Society (ACS), pp. 12331–12341, Dec. 04, 2018. doi: 10.1021/acs.jpcb.8b10335.  
  
R. B. Davidson, J. Hendrix, B. J. Geissand M. McCullagh, “Allostery in the dengue virus NS3 helicase: Insights into the NTPase cycle from molecular simulations”, *PLOS Computational Biology*, vol. 14, no. 4. Public Library of Science (PLoS), p. e1006103, Apr. 16, 2018. doi: 10.1371/journal.pcbi.1006103.  
  
M. A. Mattson, T. D. Green, P. T. Lake, M. McCullaghand A. T. Krummel, “Elucidating Structural Evolution of Perylene Diimide Aggregates Using Vibrational Spectroscopy and Molecular Dynamics Simulations”, *The Journal of Physical Chemistry B*, vol. 122, no. 18. American Chemical Society (ACS), pp. 4891–4900, Apr. 23, 2018. doi: 10.1021/acs.jpcb.8b02355.  
  
A. K. Mishra, “Self‐Assembly of Perylenediimide–Single‐Strand‐DNA Conjugates: Employing Hydrophobic Interactions and DNA Base‐Pairing To Create a Diverse Structural Space”, *Chemistry – A European Journal*, vol. 23, no. 43. Wiley, pp. 10328–10337, Jul. 07, 2017. doi: 10.1002/chem.201700752.  
  
G. Hu, “*Pyro*-Borates, *Spiro*-Borates, and Boroxinates of BINOL—Assembly, Structures, and Reactivity”, *Journal of the American Chemical Society*, vol. 139, no. 30. American Chemical Society (ACS), pp. 10267–10285, Jul. 19, 2017. doi: 10.1021/jacs.7b02317.  
  
J. A. Izzo, Y. Myshchuk, J. S. Hirschiand M. J. Vetticatt, “Transition state analysis of an enantioselective Michael addition by a bifunctional thiourea organocatalyst”, *Organic & Biomolecular Chemistry*, vol. 17, no. 16. Royal Society of Chemistry (RSC), pp. 3934–3939, 2019. doi: 10.1039/c9ob00072k.  
  
J. A. Izzo, P. H. Poulsen, J. A. Intrator, K. A. Jørgensenand M. J. Vetticatt, “Isotope Effects Reveal an Alternative Mechanism for “Iminium-Ion” Catalysis”, *Journal of the American Chemical Society*, vol. 140, no. 27. American Chemical Society (ACS), pp. 8396–8400, Jun. 25, 2018. doi: 10.1021/jacs.8b04856.  
  
C. L. Jarvis, J. S. Hirschi, M. J. Vetticattand D. Seidel, “Catalytic Enantioselective Synthesis of Lactams through Formal [4+2] Cycloaddition of Imines with Homophthalic Anhydride”, *Angewandte Chemie International Edition*, vol. 56, no. 10. Wiley, pp. 2670–2674, Jan. 27, 2017. doi: 10.1002/anie.201612148.  
  
Y. Lin, “A Selenourea-Thiourea Brønsted Acid Catalyst Facilitates Asymmetric Conjugate Additions of Amines to α,β-Unsaturated Esters”, *Journal of the American Chemical Society*, vol. 142, no. 12. American Chemical Society (ACS), pp. 5627–5635, Mar. 02, 2020. doi: 10.1021/jacs.9b12457.  
  
J. Novacek, J. A. Izzo, M. J. Vetticattand M. Waser, “Bifunctional Ammonium Salt Catalyzed Asymmetric α-Hydroxylation of β-Ketoesters by Simultaneous Resolution of Oxaziridines”, *Chemistry - A European Journal*, vol. 22, no. 48. Wiley, pp. 17339–17344, Oct. 20, 2016. doi: 10.1002/chem.201604153.  
  
S. P. Lockwood, T. G. Fullerand J. J. Newby, “Structure and Spectroscopy of Furan:H2O Complexes”, *The Journal of Physical Chemistry A*, vol. 122, no. 36. American Chemical Society (ACS), pp. 7160–7170, Aug. 24, 2018. doi: 10.1021/acs.jpca.8b06308.  
  
D. Dumett Torres, P. Banerjee, S. Pamidighantamand P. K. Jain, “A Non-Natural Wurtzite Polymorph of HgSe: A Potential 3D Topological Insulator”, *Chemistry of Materials*, vol. 29, no. 15. American Chemical Society (ACS), pp. 6356–6366, Jul. 21, 2017. doi: 10.1021/acs.chemmater.7b01674.  
  
C. Van Dyck, T. J. Marksand M. A. Ratner, “Chain Length Dependence of the Dielectric Constant and Polarizability in Conjugated Organic Thin Films”, *ACS Nano*, vol. 11, no. 6. American Chemical Society (ACS), pp. 5970–5981, Jun. 14, 2017. doi: 10.1021/acsnano.7b01807.  
  
L. Zeng, “Measuring Dipole Inversion in Self-Assembled Nano-Dielectric Molecular Layers”, *ACS Applied Materials & Interfaces*, vol. 10, no. 7. American Chemical Society (ACS), pp. 6484–6490, Feb. 12, 2018. doi: 10.1021/acsami.7b16160.  
  
E. P. Hoy, D. A. Mazziottiand T. Seideman, “Development and application of a 2-electron reduced density matrix approach to electron transport via molecular junctions”, *The Journal of Chemical Physics*, vol. 147, no. 18. AIP Publishing, p. 184110, Nov. 14, 2017. doi: 10.1063/1.4986804.  
  
J. M. Lipchock, “Characterization of Protein Tyrosine Phosphatase 1B Inhibition by Chlorogenic Acid and Cichoric Acid”, *Biochemistry*, vol. 56, no. 1. American Chemical Society (ACS), pp. 96–106, Dec. 27, 2016. doi: 10.1021/acs.biochem.6b01025.  
  
E. D. Hummel and S. C. E. Stieber, “Student-led Computational Inorganic Chemistry Research in a Classroom Setting”, *The Journal of Computational Science Education*, vol. 10, no. 1. The Shodor Education Foundation, Inc., pp. 12–15, Jan. 2019. doi: 10.22369/issn.2153-4136/10/1/2.  
  
B. J. Hale, “Evaluating the influence of heteroatoms on the electronic properties of aryl[3,4-c]pyrroledione based copolymers”, *Polymer*, vol. 109. Elsevier BV, pp. 85–92, Jan. 2017. doi: 10.1016/j.polymer.2016.12.013.  
  
M. Abubekerov, “Exploring Oxidation State-Dependent Selectivity in Polymerization of Cyclic Esters and Carbonates with Zinc(II) Complexes”, *iScience*, vol. 7. Elsevier BV, pp. 120–131, Sep. 2018. doi: 10.1016/j.isci.2018.08.020.  
  
M. Abubekerov, J. Wei, K. R. Swartz, Z. Xie, Q. Peiand P. L. Diaconescu, “Preparation of multiblock copolymers *via* step-wise addition of l-lactide and trimethylene carbonate”, *Chemical Science*, vol. 9, no. 8. Royal Society of Chemistry (RSC), pp. 2168–2178, 2018. doi: 10.1039/c7sc04507g.  
  
S. M. Quan, J. Weiand P. L. Diaconescu, “Mechanistic Studies of Redox-Switchable Copolymerization of Lactide and Cyclohexene Oxide by a Zirconium Complex”, *Organometallics*, vol. 36, no. 22. American Chemical Society (ACS), pp. 4451–4457, Nov. 07, 2017. doi: 10.1021/acs.organomet.7b00672.  
  
J. Wei and P. L. Diaconescu, “Redox-Switchable Ring-Opening Polymerization with Ferrocene Derivatives”, *Accounts of Chemical Research*, vol. 52, no. 2. American Chemical Society (ACS), pp. 415–424, Feb. 01, 2019. doi: 10.1021/acs.accounts.8b00523.  
  
J. Wei, M. N. Riffeland P. L. Diaconescu, “Redox Control of Aluminum Ring-Opening Polymerization: A Combined Experimental and DFT Investigation”, *Macromolecules*, vol. 50, no. 5. American Chemical Society (ACS), pp. 1847–1861, Mar. 02, 2017. doi: 10.1021/acs.macromol.6b02402.  
  
N. A. Eschmann, “Signature of an aggregation-prone conformation of tau”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Mar. 17, 2017. doi: 10.1038/srep44739.  
  
P. Ganguly, P. Boserman, N. F. A. van der Vegtand J.-E. Shea, “Trimethylamine *N*-oxide Counteracts Urea Denaturation by Inhibiting Protein–Urea Preferential Interaction”, *Journal of the American Chemical Society*, vol. 140, no. 1. American Chemical Society (ACS), pp. 483–492, Dec. 22, 2017. doi: 10.1021/jacs.7b11695.  
  
P. Ganguly, N. F. A. van der Vegtand J.-E. Shea, “Hydrophobic Association in Mixed Urea–TMAO Solutions”, *The Journal of Physical Chemistry Letters*, vol. 7, no. 15. American Chemical Society (ACS), pp. 3052–3059, Jul. 27, 2016. doi: 10.1021/acs.jpclett.6b01344.  
  
A. Alherz, C.-H. Lim, J. T. Hynesand C. B. Musgrave, “Predicting Hydride Donor Strength via Quantum Chemical Calculations of Hydride Transfer Activation Free Energy”, *The Journal of Physical Chemistry B*, vol. 122, no. 3. American Chemical Society (ACS), pp. 1278–1288, Jan. 05, 2018. doi: 10.1021/acs.jpcb.7b12093.  
  
A. Alherz, “Renewable Hydride Donors for the Catalytic Reduction of CO2: A Thermodynamic and Kinetic Study”, *The Journal of Physical Chemistry B*, vol. 122, no. 44. American Chemical Society (ACS), pp. 10179–10189, Oct. 05, 2018. doi: 10.1021/acs.jpcb.8b08536.  
  
J. P. Cole, D.-F. Chen, M. Kudisch, R. M. Pearson, C.-H. Limand G. M. Miyake, “Organocatalyzed Birch Reduction Driven by Visible Light”, *Journal of the American Chemical Society*, vol. 142, no. 31. American Chemical Society (ACS), pp. 13573–13581, Jul. 14, 2020. doi: 10.1021/jacs.0c05899.  
  
Y. Du, “Strongly Reducing, Visible‐Light Organic Photoredox Catalysts as Sustainable Alternatives to Precious Metals”, *Chemistry – A European Journal*, vol. 23, no. 46. Wiley, pp. 10962–10968, Aug. 2017. doi: 10.1002/chem.201702926.  
  
C.-H. Lim, “Benzimidazoles as Metal-Free and Recyclable Hydrides for CO2 Reduction to Formate”, *Journal of the American Chemical Society*, vol. 141, no. 1. American Chemical Society (ACS), pp. 272–280, Nov. 27, 2018. doi: 10.1021/jacs.8b09653.  
  
C.-H. Lim, M. Kudisch, B. Liuand G. M. Miyake, “C–N Cross-Coupling via Photoexcitation of Nickel–Amine Complexes”, *Journal of the American Chemical Society*, vol. 140, no. 24. American Chemical Society (ACS), pp. 7667–7673, May 22, 2018. doi: 10.1021/jacs.8b03744.  
  
C.-H. Lim, “Intramolecular Charge Transfer and Ion Pairing in *N,N*-Diaryl Dihydrophenazine Photoredox Catalysts for Efficient Organocatalyzed Atom Transfer Radical Polymerization”, *Journal of the American Chemical Society*, vol. 139, no. 1. American Chemical Society (ACS), pp. 348–355, Dec. 27, 2016. doi: 10.1021/jacs.6b11022.  
  
B. Liu, C.-H. Limand G. M. Miyake, “Visible-Light-Promoted C–S Cross-Coupling via Intermolecular Charge Transfer”, *Journal of the American Chemical Society*, vol. 139, no. 39. American Chemical Society (ACS), pp. 13616–13619, Sep. 19, 2017. doi: 10.1021/jacs.7b07390.  
  
B. Liu, C.-H. Limand G. M. Miyake, “Light-Driven Intermolecular Charge Transfer Induced Reactivity of Ethynylbenziodoxol(on)e and Phenols”, *Journal of the American Chemical Society*, vol. 140, no. 40. American Chemical Society (ACS), pp. 12829–12835, Sep. 14, 2018. doi: 10.1021/jacs.8b05870.  
  
S. Mavila, “Dynamic and Responsive DNA-like Polymers”, *Journal of the American Chemical Society*, vol. 140, no. 42. American Chemical Society (ACS), pp. 13594–13598, Oct. 10, 2018. doi: 10.1021/jacs.8b09105.  
  
B. G. McCarthy, R. M. Pearson, C.-H. Lim, S. M. Sartor, N. H. Damrauerand G. M. Miyake, “Structure–Property Relationships for Tailoring Phenoxazines as Reducing Photoredox Catalysts”, *Journal of the American Chemical Society*, vol. 140, no. 15. American Chemical Society (ACS), pp. 5088–5101, Mar. 07, 2018. doi: 10.1021/jacs.7b12074.  
  
H. Rao, C.-H. Lim, J. Bonin, G. M. Miyakeand M. Robert, “Visible-Light-Driven Conversion of CO2 to CH4 with an Organic Sensitizer and an Iron Porphyrin Catalyst”, *Journal of the American Chemical Society*, vol. 140, no. 51. American Chemical Society (ACS), pp. 17830–17834, Dec. 07, 2018. doi: 10.1021/jacs.8b09740.  
  
M. D. Ryan, “Solvent effects on the intramolecular charge transfer character of *N* ,*N* -diaryl dihydrophenazine catalysts for organocatalyzed atom transfer radical polymerization”, *Journal of Polymer Science Part A: Polymer Chemistry*, vol. 55, no. 18. Wiley, pp. 3017–3027, Mar. 16, 2017. doi: 10.1002/pola.28574.  
  
J. C. Theriot, B. G. McCarthy, C. Limand G. M. Miyake, “Organocatalyzed Atom Transfer Radical Polymerization: Perspectives on Catalyst Design and Performance”, *Macromolecular Rapid Communications*, vol. 38, no. 13. Wiley, p. 1700040, Apr. 03, 2017. doi: 10.1002/marc.201700040.  
  
B. T. Worrell, “A user’s guide to the thiol-thioester exchange in organic media: scope, limitations, and applications in material science”, *Polymer Chemistry*, vol. 9, no. 36. Royal Society of Chemistry (RSC), pp. 4523–4534, 2018. doi: 10.1039/c8py01031e.  
  
B. T. Worrell, “Bistable and photoswitchable states of matter”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Jul. 18, 2018. doi: 10.1038/s41467-018-05300-7.  
  
C. Wu, “Guiding the Design of Organic Photocatalyst for PET-RAFT Polymerization: Halogenated Xanthene Dyes”, *Macromolecules*, vol. 52, no. 1. American Chemical Society (ACS), pp. 236–248, Dec. 20, 2018. doi: 10.1021/acs.macromol.8b02517.  
  
N. M. Antczak, “Characterization of Nine Cancer-Associated Variants in Human DNA Polymerase κ”, *Chemical Research in Toxicology*, vol. 31, no. 8. American Chemical Society (ACS), pp. 697–711, Jul. 13, 2018. doi: 10.1021/acs.chemrestox.8b00055.  
  
E. G. Blanco-Díaz, E. A. Vázquez-Montelongo, G. A. Cisnerosand E. O. Castrejón-González, “Computational investigation of non-covalent interactions in 1-butyl 3-methylimidazolium/bis(trifluoromethylsulfonyl)imide [bmim][Tf2N] in EMD and NEMD”, *The Journal of Chemical Physics*, vol. 148, no. 5. AIP Publishing, p. 054303, Feb. 07, 2018. doi: 10.1063/1.5017987.  
  
J. E. DeNizio, M. Y. Liu, E. M. Leddin, G. A. Cisnerosand R. M. Kohli, “Selectivity and Promiscuity in TET-Mediated Oxidation of 5-Methylcytosine in DNA and RNA”, *Biochemistry*, vol. 58, no. 5. American Chemical Society (ACS), pp. 411–421, Nov. 02, 2018. doi: 10.1021/acs.biochem.8b00912.  
  
H. L. Gahlon, A. R. Walker, G. A. Cisneros, M. H. Lamersand D. S. Rueda, “Reduced structural flexibility for an exonuclease deficient DNA polymerase III mutant”, *Physical Chemistry Chemical Physics*, vol. 20, no. 42. Royal Society of Chemistry (RSC), pp. 26892–26902, 2018. doi: 10.1039/c8cp04112a.  
  
H. Gökcan, E. Kratz, T. A. Darden, J.-P. Piquemaland G. A. Cisneros, “QM/MM Simulations with the Gaussian Electrostatic Model: A Density-based Polarizable Potential”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 11. American Chemical Society (ACS), pp. 3062–3067, May 18, 2018. doi: 10.1021/acs.jpclett.8b01412.  
  
L. Lagardère, “Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields”, *Chemical Science*, vol. 9, no. 4. Royal Society of Chemistry (RSC), pp. 956–972, 2018. doi: 10.1039/c7sc04531j.  
  
P. S. Liyanage, A. R. Walker, A. Brenlla, G. A. Cisneros, L. J. Romanoand D. Rueda, “Bulky Lesion Bypass Requires Dpo4 Binding in Distinct Conformations”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Dec. 12, 2017. doi: 10.1038/s41598-017-17643-0.  
  
P. Silvestrov, S. J. Maier, M. Fangand G. A. Cisneros, “DNArCdb: A database of cancer biomarkers in DNA repair genes that includes variants related to multiple cancer phenotypes”, *DNA Repair*, vol. 70. Elsevier BV, pp. 10–17, Oct. 2018. doi: 10.1016/j.dnarep.2018.07.010.  
  
H. Torabifard and G. A. Cisneros, “Computational investigation of O2diffusion through an intra-molecular tunnel in AlkB; influence of polarization on O2transport”, *Chemical Science*, vol. 8, no. 9. Royal Society of Chemistry (RSC), pp. 6230–6238, 2017. doi: 10.1039/c7sc00997f.  
  
H. Torabifard and G. A. Cisneros, “Insight into wild-type and T1372E TET2-mediated 5hmC oxidation using *ab initio* QM/MM calculations”, *Chemical Science*, vol. 9, no. 44. Royal Society of Chemistry (RSC), pp. 8433–8445, 2018. doi: 10.1039/c8sc02961j.  
  
Y.-J. Tu, Z. Lin, M. J. Allenand G. A. Cisneros, “Molecular dynamics investigation of water-exchange reactions on lanthanide ions in water/1-ethyl-3-methylimidazolium trifluoromethylsufate ([EMIm][OTf])”, *The Journal of Chemical Physics*, vol. 148, no. 2. AIP Publishing, p. 024503, Jan. 14, 2018. doi: 10.1063/1.4997008.  
  
A. R. Walker and G. A. Cisneros, “Computational Simulations of DNA Polymerases: Detailed Insights on Structure/Function/Mechanism from Native Proteins to Cancer Variants”, *Chemical Research in Toxicology*, vol. 30, no. 11. American Chemical Society (ACS), pp. 1922–1935, Sep. 06, 2017. doi: 10.1021/acs.chemrestox.7b00161.  
  
R. E. Black and R. F. Jordan, “Synthesis and Reactivity of Palladium(II) Alkyl Complexes that Contain Phosphine-cyclopentanesulfonate Ligands”, *Organometallics*, vol. 36, no. 17. American Chemical Society (ACS), pp. 3415–3428, Aug. 23, 2017. doi: 10.1021/acs.organomet.7b00572.  
  
M. R. Hennefarth and A. N. Alexandrova, “Direct Look at the Electric Field in Ketosteroid Isomerase and Its Variants”, *ACS Catalysis*, vol. 10, no. 17. American Chemical Society (ACS), pp. 9915–9924, Aug. 07, 2020. doi: 10.1021/acscatal.0c02795.  
  
E. T. Baxter, M.-A. Ha, A. C. Cass, A. N. Alexandrovaand S. L. Anderson, “Ethylene Dehydrogenation on Pt4,7,8 Clusters on Al2O3: Strong Cluster Size Dependence Linked to Preferred Catalyst Morphologies”, *ACS Catalysis*, vol. 7, no. 5. American Chemical Society (ACS), pp. 3322–3335, Apr. 10, 2017. doi: 10.1021/acscatal.7b00409.  
  
D. Dumett Torres and P. K. Jain, “Strain Stabilization of Superionicity in Copper and Lithium Selenides”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 6. American Chemical Society (ACS), pp. 1200–1205, Feb. 20, 2018. doi: 10.1021/acs.jpclett.8b00236.  
  
J. Heo, D. Dumett Torres, P. Banerjeeand P. K. Jain, “In-situ electron microscopy mapping of an order-disorder transition in a superionic conductor”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Apr. 03, 2019. doi: 10.1038/s41467-019-09502-5.  
  
J. Heo, D. Dumett Torresand P. K. Jain, “Unconventional Long-Range Cation Ordering in Copper Selenide Nanocrystals”, *Chemistry of Materials*, vol. 31, no. 1. American Chemical Society (ACS), pp. 68–72, Dec. 20, 2018. doi: 10.1021/acs.chemmater.8b04053.  
  
H. Hou, “A novel calcium-binding peptide from Antarctic krill protein hydrolysates and identification of binding sites of calcium-peptide complex”, *Food Chemistry*, vol. 243. Elsevier BV, pp. 389–395, Mar. 2018. doi: 10.1016/j.foodchem.2017.09.152.  
  
A. Ray, N. Ahalawatand J. Mondal, “Atomistic Insights into Structural Differences between E3 and E4 Isoforms of Apolipoprotein E”, *Biophysical Journal*, vol. 113, no. 12. Elsevier BV, pp. 2682–2694, Dec. 2017. doi: 10.1016/j.bpj.2017.10.006.  
  
S. Ray, A. Maitra, A. Biswas, S. Panjikar, J. Mondaland R. Anand, “Functional insights into the mode of DNA and ligand binding of the TetR family regulator TylP from Streptomyces fradiae”, *Journal of Biological Chemistry*, vol. 292, no. 37. Elsevier BV, pp. 15301–15311, Sep. 2017. doi: 10.1074/jbc.m117.788000.  
  
S. Ray, A. Maitra, A. Biswas, S. Panjikar, J. Mondaland R. Anand, “Functional insights into the mode of DNA and ligand binding of the TetR family regulator TylP from Streptomyces fradiae”, *Journal of Biological Chemistry*, vol. 292, no. 37. Elsevier BV, pp. 15301–15311, Sep. 2017. doi: 10.1074/jbc.m117.788000.  
  
S. Kundu, “Nitrosyl Linkage Isomers: NO Coupling to N2O at a Mononuclear Site”, *Journal of the American Chemical Society*, vol. 141, no. 4. American Chemical Society (ACS), pp. 1415–1419, Jan. 02, 2019. doi: 10.1021/jacs.8b09769.  
  
S. G. Minasian, “Quantitative Evidence for Lanthanide-Oxygen Orbital Mixing in CeO2, PrO2, and TbO2”, *Journal of the American Chemical Society*, vol. 139, no. 49. American Chemical Society (ACS), pp. 18052–18064, Nov. 28, 2017. doi: 10.1021/jacs.7b10361.  
  
M. H. Fung, M. DeVault, K. T. Kuwataand R. Suryanarayanan, “Drug-Excipient Interactions: Effect on Molecular Mobility and Physical Stability of Ketoconazole–Organic Acid Coamorphous Systems”, *Molecular Pharmaceutics*, vol. 15, no. 3. American Chemical Society (ACS), pp. 1052–1061, Jan. 08, 2018. doi: 10.1021/acs.molpharmaceut.7b00932.  
  
K. T. Kuwata, “Quantum Chemical and Statistical Rate Theory Studies of the Vinyl Hydroperoxides Formed in *trans*-2-Butene and 2,3-Dimethyl-2-butene Ozonolysis”, *The Journal of Physical Chemistry A*, vol. 122, no. 9. American Chemical Society (ACS), pp. 2485–2502, Feb. 12, 2018. doi: 10.1021/acs.jpca.8b00287.  
  
M. J. Chalkley, T. J. Del Castillo, B. D. Matson, J. P. Roddyand J. C. Peters, “Catalytic N2-to-NH3 Conversion by Fe at Lower Driving Force: A Proposed Role for Metallocene-Mediated PCET”, *ACS Central Science*, vol. 3, no. 3. American Chemical Society (ACS), pp. 217–223, Feb. 14, 2017. doi: 10.1021/acscentsci.7b00014.  
  
T. Phongpreecha, J. Liu, D. B. Hodgeand Y. Qi, “Adsorption of Lignin β-O-4 Dimers on Metal Surfaces in Vacuum and Solvated Environments”, *ACS Sustainable Chemistry & Engineering*, vol. 7, no. 2. American Chemical Society (ACS), pp. 2667–2678, Dec. 14, 2018. doi: 10.1021/acssuschemeng.8b05736.  
  
S.-M. Hyun, M. Yuan, A. Maity, O. Gutierrezand D. C. Powers, “The Role of Iodanyl Radicals as Critical Chain Carriers in Aerobic Hypervalent Iodine Chemistry”, *Chem*, vol. 5, no. 9. Elsevier BV, pp. 2388–2404, Sep. 2019. doi: 10.1016/j.chempr.2019.06.006.  
  
Y. Luo, “Oxa- and Azabenzonorbornadienes as Electrophilic Partners under Photoredox/Nickel Dual Catalysis”, *ACS Catalysis*, vol. 9, no. 9. American Chemical Society (ACS), pp. 8835–8842, Aug. 28, 2019. doi: 10.1021/acscatal.9b02458.  
  
J. P. Phelan, “Redox-Neutral Photocatalytic Cyclopropanation via Radical/Polar Crossover”, *Journal of the American Chemical Society*, vol. 140, no. 25. American Chemical Society (ACS), pp. 8037–8047, Jun. 19, 2018. doi: 10.1021/jacs.8b05243.  
  
M. E. Rotella, R. M. B. Dyer, M. K. Hilinskiand O. Gutierrez, “Mechanism of Iminium Salt-Catalyzed C(sp3)–H Amination: Factors Controlling Hydride Transfer versus H-Atom Abstraction”, *ACS Catalysis*, vol. 10, no. 1. American Chemical Society (ACS), pp. 897–906, Dec. 09, 2019. doi: 10.1021/acscatal.9b03588.  
  
A. M. Sorlin, J. C. Mixdorf, M. E. Rotella, R. T. Martin, O. Gutierrezand H. M. Nguyen, “The Role of Trichloroacetimidate To Enable Iridium-Catalyzed Regio- and Enantioselective Allylic Fluorination: A Combined Experimental and Computational Study”, *Journal of the American Chemical Society*, vol. 141, no. 37. American Chemical Society (ACS), pp. 14843–14852, Aug. 22, 2019. doi: 10.1021/jacs.9b07575.  
  
R. R. Thompson, “Siloxide Podand Ligand as a Scaffold for Molybdenum-Catalyzed Alkyne Metathesis and Isolation of a Dynamic Metallatetrahedrane Intermediate”, *Organometallics*, vol. 38, no. 21. American Chemical Society (ACS), pp. 4054–4059, Oct. 28, 2019. doi: 10.1021/acs.organomet.9b00430.  
  
H. Wang, “Engaging α-Fluorocarboxylic Acids Directly in Decarboxylative C–C Bond Formation”, *ACS Catalysis*, vol. 10, no. 7. American Chemical Society (ACS), pp. 4451–4459, Mar. 24, 2020. doi: 10.1021/acscatal.0c00789.  
  
B. Xu, L. Troian-Gautier, R. Dykstra, R. T. Martin, O. Gutierrezand U. K. Tambar, “Photocatalyzed Diastereoselective Isomerization of Cinnamyl Chlorides to Cyclopropanes”, *Journal of the American Chemical Society*, vol. 142, no. 13. American Chemical Society (ACS), pp. 6206–6215, Mar. 04, 2020. doi: 10.1021/jacs.0c00147.  
  
M. Yuan, Z. Song, S. O. Badir, G. A. Molanderand O. Gutierrez, “On the Nature of C(sp3)–C(sp2) Bond Formation in Nickel-Catalyzed Tertiary Radical Cross-Couplings: A Case Study of Ni/Photoredox Catalytic Cross-Coupling of Alkyl Radicals and Aryl Halides”, *Journal of the American Chemical Society*, vol. 142, no. 15. American Chemical Society (ACS), pp. 7225–7234, Mar. 20, 2020. doi: 10.1021/jacs.0c02355.  
  
M. J. Cabrera-Afonso, “Engaging sulfinate salts *via* Ni/photoredox dual catalysis enables facile Csp2–SO2R coupling”, *Chemical Science*, vol. 9, no. 12. Royal Society of Chemistry (RSC), pp. 3186–3191, 2018. doi: 10.1039/c7sc05402e.  
  
W. Lee, M. Yuan, C. Acha, A. Onwuand O. Gutierrez, “Mechanism of nitrones and allenoates cascade reactions for the synthesis of dihydro[1,2-*a*]indoles”, *Organic & Biomolecular Chemistry*, vol. 17, no. 7. Royal Society of Chemistry (RSC), pp. 1767–1772, 2019. doi: 10.1039/c8ob02346h.  
  
L. Liu, W. Lee, M. Yuanand O. Gutierrez, “Mechanisms of Bisphosphine Iron-Catalyzed C(SP2)-C(SP3) Cross-Coupling Reactions: Inner-Sphere or Outer-Sphere Arylation?”, *Comments on Inorganic Chemistry*, vol. 38, no. 6. Informa UK Limited, pp. 210–237, Nov. 02, 2018. doi: 10.1080/02603594.2018.1539392.  
  
L. Liu, W. Lee, J. Zhou, S. Bandyopadhyayand O. Gutierrez, “Radical-clock α-halo-esters as mechanistic probes for bisphosphine iron-catalyzed cross-coupling reactions”, *Tetrahedron*, vol. 75, no. 2. Elsevier BV, pp. 129–136, Jan. 2019. doi: 10.1016/j.tet.2018.11.043.  
  
J. K. Matsui, Á. Gutiérrez-Bonet, M. Rotella, R. Alam, O. Gutierrezand G. A. Molander, “Photoredox/Nickel-Catalyzed Single-Electron Tsuji-Trost Reaction: Development and Mechanistic Insights”, *Angewandte Chemie International Edition*, vol. 57, no. 48. Wiley, pp. 15847–15851, Nov. 07, 2018. doi: 10.1002/anie.201809919.  
  
K. B. Sutyak, W. Lee, P. V. Zavalij, O. Gutierrezand J. T. Davis, “Templating and Catalyzing [2+2] Photocycloaddition in Solution Using a Dynamic G‐Quadruplex”, *Angewandte Chemie International Edition*, vol. 57, no. 52. Wiley, pp. 17146–17150, Nov. 26, 2018. doi: 10.1002/anie.201811202.  
  
A. R. Akbashev, “Activation of ultrathin SrTiO3 with subsurface SrRuO3 for the oxygen evolution reaction”, *Energy & Environmental Science*, vol. 11, no. 7. Royal Society of Chemistry (RSC), pp. 1762–1769, 2018. doi: 10.1039/c8ee00210j.  
  
V. Vlček, E. Rabaniand D. Neuhauser, “Quasiparticle spectra from molecules to bulk”, *Physical Review Materials*, vol. 2, no. 3. American Physical Society (APS), Mar. 16, 2018. doi: 10.1103/physrevmaterials.2.030801.  
  
V. Vlček, E. Rabani, D. Neuhauserand R. Baer, “Stochastic GW Calculations for Molecules”, *Journal of Chemical Theory and Computation*, vol. 13, no. 10. American Chemical Society (ACS), pp. 4997–5003, Oct. 02, 2017. doi: 10.1021/acs.jctc.7b00770.  
  
P. R. Jothi, Y. Zhang, J. P. Scheifers, H. Parkand B. P. T. Fokwa, “Molybdenum diboride nanoparticles as a highly efficient electrocatalyst for the hydrogen evolution reaction”, *Sustainable Energy & Fuels*, vol. 1, no. 9. Royal Society of Chemistry (RSC), pp. 1928–1934, 2017. doi: 10.1039/c7se00397h.  
  
H. Park, Y. Zhang, J. P. Scheifers, P. R. Jothi, A. Encinasand B. P. T. Fokwa, “Graphene- and Phosphorene-like Boron Layers with Contrasting Activities in Highly Active Mo2B4 for Hydrogen Evolution”, *Journal of the American Chemical Society*, vol. 139, no. 37. American Chemical Society (ACS), pp. 12915–12918, Sep. 08, 2017. doi: 10.1021/jacs.7b07247.  
  
M. Radzieowski, T. Block, T. Fickenscher, Y. Zhang, B. P. T. Fokwaand O. Janka, “Synthesis, crystal and electronic structures, physical properties and121Sb and151Eu Mössbauer spectroscopy of the alumo-antimonide Zintl-phase Eu5Al2Sb6”, *Materials Chemistry Frontiers*, vol. 1, no. 8. Royal Society of Chemistry (RSC), pp. 1563–1572, 2017. doi: 10.1039/c7qm00057j.  
  
P. Shankhari, Y. Zhang, D. Stekovic, M. E. Itkisand B. P. T. Fokwa, “Unexpected Competition between Antiferromagnetic and Ferromagnetic States in Hf2MnRu5B2: Predicted and Realized”, *Inorganic Chemistry*, vol. 56, no. 21. American Chemical Society (ACS), pp. 12674–12677, Oct. 11, 2017. doi: 10.1021/acs.inorgchem.7b01758.  
  
S. J. Bailey, “Lewis-Acid-Mediated Union of Epoxy-Carvone Diastereomers with Anisole Derivatives: Mechanistic Insight and Application to the Synthesis of Non-natural CBD Analogues”, *Organic Letters*, vol. 20, no. 15. American Chemical Society (ACS), pp. 4618–4621, Jul. 23, 2018. doi: 10.1021/acs.orglett.8b01909.  
  
R. D. Bongard, “Discovery and characterization of halogenated xanthene inhibitors of DUSP5 as potential photodynamic therapeutics”, *Journal of Photochemistry and Photobiology A: Chemistry*, vol. 375. Elsevier BV, pp. 114–131, Apr. 2019. doi: 10.1016/j.jphotochem.2019.01.005.  
  
A. Gupta, “Role of Conserved Histidine and Serine in the HCXXXXXRS Motif of Human Dual-Specificity Phosphatase 5”, *Journal of Chemical Information and Modeling*, vol. 59, no. 4. American Chemical Society (ACS), pp. 1563–1574, Mar. 05, 2019. doi: 10.1021/acs.jcim.8b00919.  
  
F. Li, M. R. Talipov, C. Dong, S. Baliand K. Ding, “Acid-facilitated product release from a Mo(IV) center: relevance to oxygen atom transfer reactivity of molybdenum oxotransferases”, *JBIC Journal of Biological Inorganic Chemistry*, vol. 23, no. 2. Springer Science and Business Media LLC, pp. 193–207, Nov. 25, 2017. doi: 10.1007/s00775-017-1518-4.  
  
R. R. Sapkota, J. M. Jarvis, T. M. Schaub, M. R. Talipovand J. B. Arterburn, “Bimolecular Cross‐Metathesis of a Tetrasubstituted Alkene with Allylic Sulfones”, *ChemistryOpen*, vol. 8, no. 2. Wiley, pp. 201–205, Feb. 2019. doi: 10.1002/open.201800296.  
  
R. R. Syrlybaeva and M. R. Talipov, “Ab Initio Study Predicts That Enigmatic Isonitrosyl Fluoride Should Be Stable at Low Temperatures yet Unnoticeable Due to Its Photoreactivity”, *The Journal of Physical Chemistry A*, vol. 122, no. 4. American Chemical Society (ACS), pp. 1027–1033, Jan. 22, 2018. doi: 10.1021/acs.jpca.7b12130.  
  
A. Barrozo, M. Y. El‐Naggarand A. I. Krylov, “Distinct Electron Conductance Regimes in Bacterial Decaheme Cytochromes”, *Angewandte Chemie International Edition*, vol. 57, no. 23. Wiley, pp. 6805–6809, May 02, 2018. doi: 10.1002/anie.201800294.  
  
A. Watson, S. Hackbuschand A. H. Franz, “NMR solution geometry of saccharides containing the 6-O-(α-D-glucopyranosyl)-α/β-D-glucopyranose (isomaltose) or 6-O-(α-D-galactopyranosyl)-α/β-D-glucopyranose (melibiose) core”, *Carbohydrate Research*, vol. 473. Elsevier BV, pp. 18–35, Feb. 2019. doi: 10.1016/j.carres.2018.12.012.  
  
P. Tarakeshwar, P. R. Buseckand F. X. Timmes, “On the Structure, Magnetic Properties, and Infrared Spectra of Iron Pseudocarbynes in the Interstellar Medium”, *The Astrophysical Journal*, vol. 879, no. 1. American Astronomical Society, p. 2, Jun. 26, 2019. doi: 10.3847/1538-4357/ab22b7.  
  
M. D. Ellison, “Transport of Amino Acid Cations through a 2.25-nm-Diameter Carbon Nanotube Nanopore: Electrokinetic Motion and Trapping/Desorption”, *The Journal of Physical Chemistry C*, vol. 121, no. 49. American Chemical Society (ACS), pp. 27709–27720, Dec. 06, 2017. doi: 10.1021/acs.jpcc.7b08727.  
  
D. M. Love, “Amine Induced Retardation of the Radical-Mediated Thiol–Ene Reaction via the Formation of Metastable Disulfide Radical Anions”, *The Journal of Organic Chemistry*, vol. 83, no. 5. American Chemical Society (ACS), pp. 2912–2919, Feb. 09, 2018. doi: 10.1021/acs.joc.8b00143.  
  
A. Acharya, S. Chaudhuriand V. S. Batista, “Can TDDFT Describe Excited Electronic States of Naphthol Photoacids? A Closer Look with EOM-CCSD”, *Journal of Chemical Theory and Computation*, vol. 14, no. 2. American Chemical Society (ACS), pp. 867–876, Jan. 26, 2018. doi: 10.1021/acs.jctc.7b01101.  
  
J. A. Christensen, B. T. Phelan, S. Chaudhuri, A. Acharya, V. S. Batistaand M. R. Wasielewski, “Phenothiazine Radical Cation Excited States as Super-oxidants for Energy-Demanding Reactions”, *Journal of the American Chemical Society*, vol. 140, no. 15. American Chemical Society (ACS), pp. 5290–5299, Mar. 28, 2018. doi: 10.1021/jacs.8b01778.  
  
B. Rudshteyn, A. Acharyaand V. S. Batista, “Is the Supporting Information the Venue for Reproducibility and Transparency?”, *The Journal of Physical Chemistry A*, vol. 121, no. 51. American Chemical Society (ACS), pp. 9680–9681, Dec. 28, 2017. doi: 10.1021/acs.jpca.7b11663.  
  
D. A. Penchoff, “Structural Analysis of the Complexation of Uranyl, Neptunyl, Plutonyl, and Americyl with Cyclic Imide Dioximes”, *ACS Omega*, vol. 3, no. 10. American Chemical Society (ACS), pp. 13984–13993, Oct. 24, 2018. doi: 10.1021/acsomega.8b02068.  
  
D. A. Penchoff, “Structural Characteristics, Population Analysis, and Binding Energies of [An(NO3)]2+(with An = Ac to Lr)”, *ACS Omega*, vol. 3, no. 10. American Chemical Society (ACS), pp. 14127–14143, Oct. 25, 2018. doi: 10.1021/acsomega.8b01800.  
  
N. N. Intan, K. Klyukin, T. J. Zimudzi, M. A. Hicknerand V. Alexandrov, “A combined theoretical-experimental study of interactions between vanadium ions and Nafion membrane in all-vanadium redox flow batteries”, *Journal of Power Sources*, vol. 373. Elsevier BV, pp. 150–160, Jan. 2018. doi: 10.1016/j.jpowsour.2017.10.050.  
  
K. Klyukin and V. Alexandrov, “CO2 Adsorption and Reactivity on Rutile TiO2(110) in Water: An *Ab Initio* Molecular Dynamics Study”, *The Journal of Physical Chemistry C*, vol. 121, no. 19. American Chemical Society (ACS), pp. 10476–10483, May 08, 2017. doi: 10.1021/acs.jpcc.7b02777.  
  
Z. Jiang, K. Klyukin, K. Millerand V. Alexandrov, “Mechanistic Theoretical Investigation of Self-Discharge Reactions in a Vanadium Redox Flow Battery”, *The Journal of Physical Chemistry B*, vol. 123, no. 18. American Chemical Society (ACS), pp. 3976–3983, Apr. 17, 2019. doi: 10.1021/acs.jpcb.8b10980.  
  
D. C. Ashley and E. Jakubikova, “Ray-Dutt and Bailar Twists in Fe(II)-Tris(2,2′-bipyridine): Spin States, Sterics, and Fe–N Bond Strengths”, *Inorganic Chemistry*, vol. 57, no. 9. American Chemical Society (ACS), pp. 5585–5596, Apr. 23, 2018. doi: 10.1021/acs.inorgchem.8b00560.  
  
S. Xu, “A flexible, redox-active macrocycle enables the electrocatalytic reduction of nitrate to ammonia by a cobalt complex”, *Chemical Science*, vol. 9, no. 22. Royal Society of Chemistry (RSC), pp. 4950–4958, 2018. doi: 10.1039/c8sc00721g.  
  
G. Dey, L. Yang, K.-B. Leeand L. Wang, “Characterizing Molecular Adsorption on Biodegradable MnO2 Nanoscaffolds”, *The Journal of Physical Chemistry C*, vol. 122, no. 50. American Chemical Society (ACS), pp. 29017–29027, Nov. 27, 2018. doi: 10.1021/acs.jpcc.8b09562.  
  
L. Yang, “A biodegradable hybrid inorganic nanoscaffold for advanced stem cell therapy”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Aug. 08, 2018. doi: 10.1038/s41467-018-05599-2.  
  
T. J. Summers, Q. Chengand N. J. DeYonker, “A transition state “trapped”? QM-cluster models of engineered threonyl-tRNA synthetase”, *Organic & Biomolecular Chemistry*, vol. 16, no. 22. Royal Society of Chemistry (RSC), pp. 4090–4100, 2018. doi: 10.1039/c8ob00540k.  
  
C.-C. Zho, V. Vlček, D. Neuhauserand B. J. Schwartz, “Thermal Equilibration Controls H-Bonding and the Vertical Detachment Energy of Water Cluster Anions”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 17. American Chemical Society (ACS), pp. 5173–5178, Aug. 21, 2018. doi: 10.1021/acs.jpclett.8b02152.  
  
H. Jiang, P. G. Debenedettiand A. Z. Panagiotopoulos, “Communication: Nucleation rates of supersaturated aqueous NaCl using a polarizable force field”, *The Journal of Chemical Physics*, vol. 149, no. 14. AIP Publishing, p. 141102, Oct. 14, 2018. doi: 10.1063/1.5053652.  
  
H. Jiang, A. Haji-Akbari, P. G. Debenedettiand A. Z. Panagiotopoulos, “Forward flux sampling calculation of homogeneous nucleation rates from aqueous NaCl solutions”, *The Journal of Chemical Physics*, vol. 148, no. 4. AIP Publishing, p. 044505, Jan. 28, 2018. doi: 10.1063/1.5016554.  
  
G. Sun and P. Sautet, “Metastable Structures in Cluster Catalysis from First-Principles: Structural Ensemble in Reaction Conditions and Metastability Triggered Reactivity”, *Journal of the American Chemical Society*, vol. 140, no. 8. American Chemical Society (ACS), pp. 2812–2820, Feb. 20, 2018. doi: 10.1021/jacs.7b11239.  
  
G. Sun and P. Sautet, “Toward Fast and Reliable Potential Energy Surfaces for Metallic Pt Clusters by Hierarchical Delta Neural Networks”, *Journal of Chemical Theory and Computation*, vol. 15, no. 10. American Chemical Society (ACS), pp. 5614–5627, Aug. 29, 2019. doi: 10.1021/acs.jctc.9b00465.  
  
M. A. van Spronsen, “Dynamics of Surface Alloys: Rearrangement of Pd/Ag(111) Induced by CO and O2”, *The Journal of Physical Chemistry C*, vol. 123, no. 13. American Chemical Society (ACS), pp. 8312–8323, Nov. 19, 2018. doi: 10.1021/acs.jpcc.8b08849.  
  
G. Yan and P. Sautet, “Surface Structure of Co3O4 (111) under Reactive Gas-Phase Environments”, *ACS Catalysis*, vol. 9, no. 7. American Chemical Society (ACS), pp. 6380–6392, Jun. 04, 2019. doi: 10.1021/acscatal.9b01485.  
  
G. Yan, “Water on Oxide Surfaces: A Triaqua Surface Coordination Complex on Co3O4(111)”, *Journal of the American Chemical Society*, vol. 141, no. 14. American Chemical Society (ACS), pp. 5623–5627, Mar. 21, 2019. doi: 10.1021/jacs.9b00898.  
  
B. Zhang, “Atomically Dispersed Pt1–Polyoxometalate Catalysts: How Does Metal–Support Interaction Affect Stability and Hydrogenation Activity?”, *Journal of the American Chemical Society*, vol. 141, no. 20. American Chemical Society (ACS), pp. 8185–8197, Apr. 29, 2019. doi: 10.1021/jacs.9b00486.  
  
K. M. Lebold and W. G. Noid, “Dual approach for effective potentials that accurately model structure and energetics”, *The Journal of Chemical Physics*, vol. 150, no. 23. AIP Publishing, p. 234107, Jun. 21, 2019. doi: 10.1063/1.5094330.  
  
N. V. Karimova, L. M. McCaslinand R. B. Gerber, “Ion reactions in atmospherically-relevant clusters: mechanisms, dynamics and spectroscopic signatures”, *Faraday Discussions*, vol. 217. Royal Society of Chemistry (RSC), pp. 342–360, 2019. doi: 10.1039/c8fd00230d.  
  
N. V. Karimova, “SN2 Reactions of N2O5 with Ions in Water: Microscopic Mechanisms, Intermediates, and Products”, *The Journal of Physical Chemistry A*, vol. 124, no. 4. American Chemical Society (ACS), pp. 711–720, Dec. 27, 2019. doi: 10.1021/acs.jpca.9b09095.  
  
L. M. McCaslin, M. A. Johnsonand R. B. Gerber, “Mechanisms and competition of halide substitution and hydrolysis in reactions of N 2 O 5 with seawater”, *Science Advances*, vol. 5, no. 6. American Association for the Advancement of Science (AAAS), Jun. 07, 2019. doi: 10.1126/sciadv.aav6503.  
  
E. Rossich Molina and R. B. Gerber, “Microscopic Mechanisms of N2O5 Hydrolysis on the Surface of Water Droplets”, *The Journal of Physical Chemistry A*, vol. 124, no. 1. American Chemical Society (ACS), pp. 224–228, Dec. 12, 2019. doi: 10.1021/acs.jpca.9b08900.  
  
S. Staudt, “Sulfate and Carboxylate Suppress the Formation of ClNO2 at Atmospheric Interfaces”, *ACS Earth and Space Chemistry*, vol. 3, no. 9. American Chemical Society (ACS), pp. 1987–1997, Jul. 22, 2019. doi: 10.1021/acsearthspacechem.9b00177.  
  
S. Bhattacharya, M. P. Yothers, L. Huangand L. A. Bumm, “Interaction of the (2√3 × 3)rect. Adsorption-Site Basis and Alkyl-Chain Close Packing in Alkanethiol Self-Assembled Monolayers on Au(111): A Molecular Dynamics Study of Alkyl-Chain Conformation”, *ACS Omega*, vol. 5, no. 23. American Chemical Society (ACS), pp. 13802–13812, Jun. 02, 2020. doi: 10.1021/acsomega.0c01111.  
  
V. M. Breslin, N. A. Barbour, D.-K. Dang, S. A. Lopezand M. A. Garcia-Garibay, “Nanosecond laser flash photolysis of a 6-nitroindolinospiropyran in solution and in nanocrystalline suspension under single excitation conditions”, *Photochemical & Photobiological Sciences*, vol. 17, no. 6. Springer Science and Business Media LLC, pp. 741–749, Jun. 2018. doi: 10.1039/c8pp00095f.  
  
D. P. Donnelly, “Cyclic Thiosulfinates and Cyclic Disulfides Selectively Cross-Link Thiols While Avoiding Modification of Lone Thiols”, *Journal of the American Chemical Society*, vol. 140, no. 24. American Chemical Society (ACS), pp. 7377–7380, May 31, 2018. doi: 10.1021/jacs.8b01136.  
  
R. J. Xu, B. Blasiak, M. Cho, J. P. Layfieldand C. H. Londergan, “A Direct, Quantitative Connection between Molecular Dynamics Simulations and Vibrational Probe Line Shapes”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 10. American Chemical Society (ACS), pp. 2560–2567, Apr. 26, 2018. doi: 10.1021/acs.jpclett.8b00969.  
  
E. D. Entz, J. E. A. Russell, L. V. Hookerand S. R. Neufeldt, “Small Phosphine Ligands Enable Selective Oxidative Addition of Ar–O over Ar–Cl Bonds at Nickel(0)”, *Journal of the American Chemical Society*, vol. 142, no. 36. American Chemical Society (ACS), pp. 15454–15463, Aug. 17, 2020. doi: 10.1021/jacs.0c06995.  
  
L. V. Hooker and S. R. Neufeldt, “Ligation state of nickel during C O bond activation with monodentate phosphines”, *Tetrahedron*, vol. 74, no. 47. Elsevier BV, pp. 6717–6725, Nov. 2018. doi: 10.1016/j.tet.2018.10.025.  
  
E. K. Reeves, O. R. Bauman, G. B. Mitchemand S. R. Neufeldt, “Solvent Effects on the Selectivity of Palladium‐Catalyzed Suzuki‐Miyaura Couplings”, *Israel Journal of Chemistry*, vol. 60, no. 3–4. Wiley, pp. 406–409, Aug. 30, 2019. doi: 10.1002/ijch.201900082.  
  
E. K. Reeves, J. N. Humkeand S. R. Neufeldt, “N-Heterocyclic Carbene Ligand-Controlled Chemodivergent Suzuki–Miyaura Cross Coupling”, *The Journal of Organic Chemistry*, vol. 84, no. 18. American Chemical Society (ACS), pp. 11799–11812, Sep. 02, 2019. doi: 10.1021/acs.joc.9b01692.  
  
J. E. A. Russell, E. D. Entz, I. M. Joyceand S. R. Neufeldt, “Nickel-Catalyzed Stille Cross Coupling of C–O Electrophiles”, *ACS Catalysis*, vol. 9, no. 4. American Chemical Society (ACS), pp. 3304–3310, Mar. 04, 2019. doi: 10.1021/acscatal.9b00744.  
  
R. Forsythe, J. P. Scheifers, Y. Zhangand B. P. T. Fokwa, “HT‐NbOsB: Experimental and Theoretical Investigations of a Boride Structure Type Containing Boron Chains and Isolated Boron Atoms”, *European Journal of Inorganic Chemistry*, vol. 2018, no. 28. Wiley, pp. 3297–3303, Jun. 19, 2018. doi: 10.1002/ejic.201800235.  
  
Z. R. Kehoe, G. R. Woller, E. D. Speetzen, J. B. Lawrence, E. Boschand N. P. Bowling, “Effects of Halogen and Hydrogen Bonding on the Electronics of a Conjugated Rotor”, *The Journal of Organic Chemistry*, vol. 83, no. 11. American Chemical Society (ACS), pp. 6142–6150, May 04, 2018. doi: 10.1021/acs.joc.8b01064.  
  
C. I. Nwachukwu, Z. R. Kehoe, N. P. Bowling, E. D. Speetzenand E. Bosch, “Cooperative halogen bonding and polarized π-stacking in the formation of coloured charge-transfer co-crystals”, *New Journal of Chemistry*, vol. 42, no. 13. Royal Society of Chemistry (RSC), pp. 10615–10622, 2018. doi: 10.1039/c8nj00693h.  
  
H. Albright, “Catalytic Carbonyl-Olefin Metathesis of Aliphatic Ketones: Iron(III) Homo-Dimers as Lewis Acidic Superelectrophiles”, *Journal of the American Chemical Society*, vol. 141, no. 4. American Chemical Society (ACS), pp. 1690–1700, Dec. 31, 2018. doi: 10.1021/jacs.8b11840.  
  
N. Hananya, J. P. Reid, O. Green, M. S. Sigmanand D. Shabat, “Rapid chemiexcitation of phenoxy-dioxetane luminophores yields ultrasensitive chemiluminescence assays”, *Chemical Science*, vol. 10, no. 5. Royal Society of Chemistry (RSC), pp. 1380–1385, 2019. doi: 10.1039/c8sc04280b.  
  
S. Zhao, T. Gensch, B. Murray, Z. L. Niemeyer, M. S. Sigmanand M. R. Biscoe, “Enantiodivergent Pd-catalyzed C–C bond formation enabled through ligand parameterization”, *Science*, vol. 362, no. 6415. American Association for the Advancement of Science (AAAS), pp. 670–674, Nov. 09, 2018. doi: 10.1126/science.aat2299.  
  
D. Ascough, F. Duarteand R. Paton, “Stereospecific 1,3-H Transfer of Indenols Proceeds via Persistent Ion-Pairs Anchored By NH···Pi Interactions”, *[]*. American Chemical Society (ACS), Sep. 07, 2018. doi: 10.26434/chemrxiv.7057892.v1.  
  
M. Formica, G. Sorin, A. J. M. Farley, J. Díaz, R. S. Patonand D. J. Dixon, “Bifunctional iminophosphorane catalysed enantioselective sulfa-Michael addition of alkyl thiols to alkenyl benzimidazoles”, *Chemical Science*, vol. 9, no. 34. Royal Society of Chemistry (RSC), pp. 6969–6974, 2018. doi: 10.1039/c8sc01804a.  
  
G. Pupo, “Asymmetric nucleophilic fluorination under hydrogen bonding phase-transfer catalysis”, *Science*, vol. 360, no. 6389. American Association for the Advancement of Science (AAAS), pp. 638–642, May 11, 2018. doi: 10.1126/science.aar7941.  
  
L. Simón and R. S. Paton, “The True Catalyst Revealed: The Intervention of Chiral Ca and Mg Phosphates in Brønsted Acid Promoted Asymmetric Mannich Reactions”, *Journal of the American Chemical Society*, vol. 140, no. 16. American Chemical Society (ACS), pp. 5412–5420, Mar. 30, 2018. doi: 10.1021/jacs.7b13678.  
  
A. Brethomé, S. P. Fletcherand R. Paton, “Conformational Effects on Physical-Organic Descriptors – the Case of Sterimol Steric Parameters”, *[]*. American Chemical Society (ACS), Sep. 26, 2018. doi: 10.26434/chemrxiv.7125656.v1.  
  
S. Sung, “Synergistic Effects of Imidazolium-Functionalization on *fac*-Mn(CO)3 Bipyridine Catalyst Platforms for Electrocatalytic Carbon Dioxide Reduction”, *Journal of the American Chemical Society*, vol. 141, no. 16. American Chemical Society (ACS), pp. 6569–6582, Mar. 29, 2019. doi: 10.1021/jacs.8b13657.  
  
J. M. L. Ribeiro, P. Bravo, Y. Wangand P. Tiwary, “Reweighted autoencoded variational Bayes for enhanced sampling (RAVE)”, *The Journal of Chemical Physics*, vol. 149, no. 7. AIP Publishing, p. 072301, Aug. 21, 2018. doi: 10.1063/1.5025487.  
  
J. M. Lamim Ribeiro and P. Tiwary, “Toward Achieving Efficient and Accurate Ligand-Protein Unbinding with Deep Learning and Molecular Dynamics through RAVE”, *Journal of Chemical Theory and Computation*, vol. 15, no. 1. American Chemical Society (ACS), pp. 708–719, Dec. 07, 2018. doi: 10.1021/acs.jctc.8b00869.  
  
J. M. L. Ribeiro, S.-T. Tsai, D. Pramanik, Y. Wangand P. Tiwary, “Kinetics of Ligand–Protein Dissociation from All-Atom Simulations: Are We There Yet?”, *Biochemistry*, vol. 58, no. 3. American Chemical Society (ACS), pp. 156–165, Dec. 14, 2018. doi: 10.1021/acs.biochem.8b00977.  
  
Z. Smith, D. Pramanik, S.-T. Tsaiand P. Tiwary, “Multi-dimensional spectral gap optimization of order parameters (SGOOP) through conditional probability factorization”, *The Journal of Chemical Physics*, vol. 149, no. 23. AIP Publishing, p. 234105, Dec. 21, 2018. doi: 10.1063/1.5064856.  
  
C. I. Drexler, “Counter Cations Affect Transport in Aqueous Hydroxide Solutions with Ion Specificity”, *Journal of the American Chemical Society*, vol. 141, no. 17. American Chemical Society (ACS), pp. 6930–6936, Apr. 22, 2019. doi: 10.1021/jacs.8b13458.  
  
J. N. Dahanayake and K. R. Mitchell-Koch, “How Does Solvation Layer Mobility Affect Protein Structural Dynamics?”, *Frontiers in Molecular Biosciences*, vol. 5. Frontiers Media SA, Jul. 13, 2018. doi: 10.3389/fmolb.2018.00065.  
  
J. N. Dahanayake and K. R. Mitchell-Koch, “Entropy connects water structure and dynamics in protein hydration layer”, *Physical Chemistry Chemical Physics*, vol. 20, no. 21. Royal Society of Chemistry (RSC), pp. 14765–14777, 2018. doi: 10.1039/c8cp01674g.  
  
J. N. Dahanayake, E. Shahryari, K. M. Roberts, M. E. Heikes, C. Kasireddyand K. R. Mitchell-Koch, “Protein Solvent Shell Structure Provides Rapid Analysis of Hydration Dynamics”, *Journal of Chemical Information and Modeling*, vol. 59, no. 5. American Chemical Society (ACS), pp. 2407–2422, Mar. 13, 2019. doi: 10.1021/acs.jcim.9b00009.  
  
D. Su, M. P. Kabir, Y. Orozco‐Gonzalez, S. Gozemand G. Gadda, “Fluorescence Properties of Flavin Semiquinone Radicals in Nitronate Monooxygenase”, *ChemBioChem*, vol. 20, no. 13. Wiley, pp. 1646–1652, May 20, 2019. doi: 10.1002/cbic.201900016.  
  
S. Gozem, “Excited-State Vibronic Dynamics of Bacteriorhodopsin from Two-Dimensional Electronic Photon Echo Spectroscopy and Multiconfigurational Quantum Chemistry”, *The Journal of Physical Chemistry Letters*, vol. 11, no. 10. American Chemical Society (ACS), pp. 3889–3896, Apr. 24, 2020. doi: 10.1021/acs.jpclett.0c01063.  
  
S. Gozem, “Probing the Electronic Structure of Bulk Water at the Molecular Length Scale with Angle-Resolved Photoelectron Spectroscopy”, *The Journal of Physical Chemistry Letters*, vol. 11, no. 13. American Chemical Society (ACS), pp. 5162–5170, Jun. 01, 2020. doi: 10.1021/acs.jpclett.0c00968.  
  
M. P. Kabir, Y. Orozco-Gonzalezand S. Gozem, “Electronic spectra of flavin in different redox and protonation states: a computational perspective on the effect of the electrostatic environment”, *Physical Chemistry Chemical Physics*, vol. 21, no. 30. Royal Society of Chemistry (RSC), pp. 16526–16537, 2019. doi: 10.1039/c9cp02230a.  
  
Y. Orozco-Gonzalez, M. P. Kabirand S. Gozem, “Electrostatic Spectral Tuning Maps for Biological Chromophores”, *The Journal of Physical Chemistry B*, vol. 123, no. 23. American Chemical Society (ACS), pp. 4813–4824, Mar. 14, 2019. doi: 10.1021/acs.jpcb.9b00489.  
  
C. P. Constantinides, “Ferromagnetic interactions in a 1D Heisenberg linear chain of 1-phenyl-3,7-bis(trifluoromethyl)-1,4-dihydro-1,2,4-benzotriazin-4-yls”, *CrystEngComm*, vol. 21, no. 31. Royal Society of Chemistry (RSC), pp. 4599–4606, 2019. doi: 10.1039/c9ce00739c.  
  
J. R. Rogers and P. L. Geissler, “Breakage of Hydrophobic Contacts Limits the Rate of Passive Lipid Exchange between Membranes”, *The Journal of Physical Chemistry B*, vol. 124, no. 28. American Chemical Society (ACS), pp. 5884–5898, Jul. 07, 2020. doi: 10.1021/acs.jpcb.0c04139.  
  
C. O’Hara, C.-H. Yang, A. J. Francis, B. S. Newell, H. Wangand M. J. E. Resendiz, “Photocycloaddition of *S*,*S*-Dioxo-benzothiophene-2-methanol, Reactivity in the Solid State and in Solution: Mechanistic Studies and Diastereoselective Formation of Cyclobutyl Rings”, *The Journal of Organic Chemistry*, vol. 84, no. 15. American Chemical Society (ACS), pp. 9714–9725, Jul. 12, 2019. doi: 10.1021/acs.joc.9b01354.  
  
D. Rodriquez, “Measurement of Cohesion and Adhesion of Semiconducting Polymers by Scratch Testing: Effect of Side-Chain Length and Degree of Polymerization”, *ACS Macro Letters*, vol. 7, no. 8. American Chemical Society (ACS), pp. 1003–1009, Aug. 01, 2018. doi: 10.1021/acsmacrolett.8b00412.  
  
J. Li, “Epoxidation Catalyzed by the Nonheme Iron(II)- and 2-Oxoglutarate-Dependent Oxygenase, AsqJ: Mechanistic Elucidation of Oxygen Atom Transfer by a Ferryl Intermediate”, *Journal of the American Chemical Society*, vol. 142, no. 13. American Chemical Society (ACS), pp. 6268–6284, Mar. 04, 2020. doi: 10.1021/jacs.0c00484.  
  
H. Hao, J. Shee, S. Upadhyay, C. Ataca, K. D. Jordanand B. M. Rubenstein, “Accurate Predictions of Electron Binding Energies of Dipole-Bound Anions via Quantum Monte Carlo Methods”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 21. American Chemical Society (ACS), pp. 6185–6190, Oct. 09, 2018. doi: 10.1021/acs.jpclett.8b02733.  
  
J. P. Cole, C. R. Federico, C.-H. Limand G. M. Miyake, “Photoinduced Organocatalyzed Atom Transfer Radical Polymerization Using Low ppm Catalyst Loading”, *Macromolecules*, vol. 52, no. 2. American Chemical Society (ACS), pp. 747–754, Jan. 10, 2019. doi: 10.1021/acs.macromol.8b02688.  
  
Z. J. Schiffer, N. Lazouski, N. Corbinand K. Manthiram, “Nature of the First Electron Transfer in Electrochemical Ammonia Activation in a Nonaqueous Medium”, *The Journal of Physical Chemistry C*, vol. 123, no. 15. American Chemical Society (ACS), pp. 9713–9720, Mar. 21, 2019. doi: 10.1021/acs.jpcc.9b00669.  
  
V. Vlček, “Stochastic Vertex Corrections: Linear Scaling Methods for Accurate Quasiparticle Energies”, *Journal of Chemical Theory and Computation*, vol. 15, no. 11. American Chemical Society (ACS), pp. 6254–6266, Sep. 26, 2019. doi: 10.1021/acs.jctc.9b00317.  
  
V. Vlček, R. Baerand D. Neuhauser, “Stochastic time-dependent DFT with optimally tuned range-separated hybrids: Application to excitonic effects in large phosphorene sheets”, *The Journal of Chemical Physics*, vol. 150, no. 18. AIP Publishing, p. 184118, May 14, 2019. doi: 10.1063/1.5093707.  
  
V. Vlček, E. Rabani, R. Baerand D. Neuhauser, “Nonmonotonic band gap evolution in bent phosphorene nanosheets”, *Physical Review Materials*, vol. 3, no. 6. American Physical Society (APS), Jun. 07, 2019. doi: 10.1103/physrevmaterials.3.064601.  
  
D. Pramanik, Z. Smith, A. Kellsand P. Tiwary, “Can One Trust Kinetic and Thermodynamic Observables from Biased Metadynamics Simulations?: Detailed Quantitative Benchmarks on Millimolar Drug Fragment Dissociation”, *The Journal of Physical Chemistry B*, vol. 123, no. 17. American Chemical Society (ACS), pp. 3672–3678, Apr. 11, 2019. doi: 10.1021/acs.jpcb.9b01813.  
  
P. Ravindra, Z. Smithand P. Tiwary, “Automatic mutual information noise omission (AMINO): generating order parameters for molecular systems”, *Molecular Systems Design & Engineering*, vol. 5, no. 1. Royal Society of Chemistry (RSC), pp. 339–348, 2020. doi: 10.1039/c9me00115h.  
  
S.-T. Tsai, Z. Smithand P. Tiwary, “Reaction coordinates and rate constants for liquid droplet nucleation: Quantifying the interplay between driving force and memory”, *The Journal of Chemical Physics*, vol. 151, no. 15. AIP Publishing, p. 154106, Oct. 21, 2019. doi: 10.1063/1.5124385.  
  
Y. Wang, J. M. L. Ribeiroand P. Tiwary, “Past–future information bottleneck for sampling molecular reaction coordinate simultaneously with thermodynamics and kinetics”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Aug. 08, 2019. doi: 10.1038/s41467-019-11405-4.  
  
T. K. Achar, “Palladium‐Catalyzed Directed *meta* ‐Selective C−H Allylation of Arenes: Unactivated Internal Olefins as Allyl Surrogates”, *Angewandte Chemie International Edition*, vol. 58, no. 30. Wiley, pp. 10353–10360, Jul. 22, 2019. doi: 10.1002/anie.201904608.  
  
D. M. H. Ascough, F. Duarteand R. S. Paton, “Stereospecific 1,3-H Transfer of Indenols Proceeds via Persistent Ion-Pairs Anchored by NH···π Interactions”, *Journal of the American Chemical Society*, vol. 140, no. 48. American Chemical Society (ACS), pp. 16740–16748, Oct. 19, 2018. doi: 10.1021/jacs.8b09874.  
  
A. V. Brethomé, S. P. Fletcherand R. S. Paton, “Conformational Effects on Physical-Organic Descriptors: The Case of Sterimol Steric Parameters”, *ACS Catalysis*, vol. 9, no. 3. American Chemical Society (ACS), pp. 2313–2323, Jan. 25, 2019. doi: 10.1021/acscatal.8b04043.  
  
A. V. Brethomé, R. S. Patonand S. P. Fletcher, “Retooling Asymmetric Conjugate Additions for Sterically Demanding Substrates with an Iterative Data-Driven Approach”, *ACS Catalysis*, vol. 9, no. 8. American Chemical Society (ACS), pp. 7179–7187, Jul. 02, 2019. doi: 10.1021/acscatal.9b01814.  
  
Q. Dan, “Fungal indole alkaloid biogenesis through evolution of a bifunctional reductase/Diels–Alderase”, *Nature Chemistry*, vol. 11, no. 11. Springer Science and Business Media LLC, pp. 972–980, Sep. 23, 2019. doi: 10.1038/s41557-019-0326-6.  
  
B. D. Etz, “Elucidating the chemical pathways responsible for the sooting tendency of 1 and 2-phenylethanol”, *Proceedings of the Combustion Institute*, vol. 38, no. 1. Elsevier BV, pp. 1327–1334, 2021. doi: 10.1016/j.proci.2020.06.072.  
  
A. Franchino, J. Chapman, I. Funes-Ardoiz, R. S. Patonand D. J. Dixon, “Catalytic Enantio- and Diastereoselective Mannich Addition of TosMIC to Ketimines”, *Chemistry - A European Journal*, vol. 24, no. 67. Wiley, pp. 17660–17664, Oct. 31, 2018. doi: 10.1002/chem.201804099.  
  
A. J. Fugard, A. S. K. Lahdenperä, J. S. J. Tan, A. Mekareeya, R. S. Patonand M. D. Smith, “Hydrogen‐Bond‐Enabled Dynamic Kinetic Resolution of Axially Chiral Amides Mediated by a Chiral Counterion”, *Angewandte Chemie*, vol. 131, no. 9. Wiley, pp. 2821–2824, Feb. 25, 2019. doi: 10.1002/ange.201814362.  
  
A. J. Fugard, A. S. K. Lahdenperä, J. S. J. Tan, A. Mekareeya, R. S. Patonand M. D. Smith, “Hydrogen‐Bond‐Enabled Dynamic Kinetic Resolution of Axially Chiral Amides Mediated by a Chiral Counterion”, *Angewandte Chemie International Edition*, vol. 58, no. 9. Wiley, pp. 2795–2798, Feb. 25, 2019. doi: 10.1002/anie.201814362.  
  
J. C. Golec, “BIMP‐Catalyzed 1,3‐Prototropic Shift for the Highly Enantioselective Synthesis of Conjugated Cyclohexenones”, *Angewandte Chemie International Edition*, vol. 59, no. 40. Wiley, pp. 17417–17422, Aug. 07, 2020. doi: 10.1002/anie.202006202.  
  
S. Guin, “Iterative Arylation of Amino Acids and Aliphatic Amines via δ‐C(sp 3 )−H Activation: Experimental and Computational Exploration”, *Angewandte Chemie International Edition*, vol. 58, no. 17. Wiley, pp. 5633–5638, Mar. 21, 2019. doi: 10.1002/anie.201900479.  
  
S. Guin, “Iterative Arylation of Amino Acids and Aliphatic Amines via δ‐C(sp 3 )−H Activation: Experimental and Computational Exploration”, *Angewandte Chemie*, vol. 131, no. 17. Wiley, pp. 5689–5694, Mar. 21, 2019. doi: 10.1002/ange.201900479.  
  
M. C. Hilton, X. Zhang, B. T. Boyle, J. V. Alegre-Requena, R. S. Patonand A. McNally, “Heterobiaryl synthesis by contractive C–C coupling via P(V) intermediates”, *Science*, vol. 362, no. 6416. American Association for the Advancement of Science (AAAS), pp. 799–804, Nov. 16, 2018. doi: 10.1126/science.aas8961.  
  
J. C. J. Hintzen, “Comparison of Molecular Recognition of Trimethyllysine and Trimethylthialysine by Epigenetic Reader Proteins”, *Molecules*, vol. 25, no. 8. MDPI AG, p. 1918, Apr. 21, 2020. doi: 10.3390/molecules25081918.  
  
S. Hyde, J. Veliks, D. M. H. Ascough, R. Szpera, R. S. Patonand V. Gouverneur, “Enantioselective rhodium-catalysed insertion of trifluorodiazoethanes into tin hydrides”, *Tetrahedron*, vol. 75, no. 1. Elsevier BV, pp. 17–25, Jan. 2019. doi: 10.1016/j.tet.2018.11.022.  
  
S. Karabiyikoglu, A. V. Brethomé, T. Palacin, R. S. Patonand S. P. Fletcher, “Enantiomerically enriched tetrahydropyridine allyl chlorides”, *Chemical Science*, vol. 11, no. 16. Royal Society of Chemistry (RSC), pp. 4125–4130, 2020. doi: 10.1039/d0sc00377h.  
  
J. L. Koniarczyk, J. W. Greenwood, J. V. Alegre‐Requena, R. S. Patonand A. McNally, “A Pyridine–Pyridine Cross‐Coupling Reaction via Dearomatized Radical Intermediates”, *Angewandte Chemie International Edition*, vol. 58, no. 42. Wiley, pp. 14882–14886, Sep. 09, 2019. doi: 10.1002/anie.201906267.  
  
J. N. Levy, J. V. Alegre-Requena, R. Liu, R. S. Patonand A. McNally, “Selective Halogenation of Pyridines Using Designed Phosphine Reagents”, *Journal of the American Chemical Society*, vol. 142, no. 25. American Chemical Society (ACS), pp. 11295–11305, May 29, 2020. doi: 10.1021/jacs.0c04674.  
  
C. T. Lohans, “Non-Hydrolytic β-Lactam Antibiotic Fragmentation byl,d-Transpeptidases and Serine β-Lactamase Cysteine Variants”, *Angewandte Chemie International Edition*, vol. 58, no. 7. Wiley, pp. 1990–1994, Jan. 21, 2019. doi: 10.1002/anie.201809424.  
  
J. Luccarelli and R. S. Paton, “Hydrogen-Bond-Dependent Conformational Switching: A Computational Challenge from Experimental Thermochemistry”, *The Journal of Organic Chemistry*, vol. 84, no. 2. American Chemical Society (ACS), pp. 613–621, Dec. 26, 2018. doi: 10.1021/acs.joc.8b02436.  
  
G. Luchini, J. V. Alegre-Requena, I. Funes-Ardoizand R. S. Paton, “GoodVibes: automated thermochemistry for heterogeneous computational chemistry data”, *F1000Research*, vol. 9. F1000 Research Ltd, p. 291, Apr. 24, 2020. doi: 10.12688/f1000research.22758.1.  
  
G. Luchini, D. M. H. Ascough, J. V. Alegre-Requena, V. Gouverneurand R. S. Paton, “Data-mining the diaryl(thio)urea conformational landscape: Understanding the contrasting behavior of ureas and thioureas with quantum chemistry”, *Tetrahedron*, vol. 75, no. 6. Elsevier BV, pp. 697–702, Feb. 2019. doi: 10.1016/j.tet.2018.12.033.  
  
B. J. G. E. Pieters, “Mechanism of biomolecular recognition of trimethyllysine by the fluorinated aromatic cage of KDM5A PHD3 finger”, *Communications Chemistry*, vol. 3, no. 1. Springer Science and Business Media LLC, Jun. 01, 2020. doi: 10.1038/s42004-020-0313-2.  
  
M. V. Popescu, A. Mekereeya, J. V. Alegre‐Requena, R. S. Patonand M. D. Smith, “Visible‐Light‐Mediated Heterocycle Functionalization via Geometrically Interrupted [2+2] Cycloaddition”, *Angewandte Chemie International Edition*, vol. 59, no. 51. Wiley, pp. 23020–23024, Oct. 08, 2020. doi: 10.1002/anie.202009704.  
  
S. Porey, “Alkyne Linchpin Strategy for Drug:Pharmacophore Conjugation: Experimental and Computational Realization of a *Meta*-Selective Inverse Sonogashira Coupling”, *Journal of the American Chemical Society*, vol. 142, no. 8. American Chemical Society (ACS), pp. 3762–3774, Jan. 07, 2020. doi: 10.1021/jacs.9b10646.  
  
G. Pupo, “Hydrogen Bonding Phase-Transfer Catalysis with Potassium Fluoride: Enantioselective Synthesis of β-Fluoroamines”, *Journal of the American Chemical Society*, vol. 141, no. 7. American Chemical Society (ACS), pp. 2878–2883, Jan. 28, 2019. doi: 10.1021/jacs.8b12568.  
  
G. Roagna, “Hydrogen Bonding Phase-Transfer Catalysis with Ionic Reactants: Enantioselective Synthesis of γ-Fluoroamines”, *Journal of the American Chemical Society*, vol. 142, no. 33. American Chemical Society (ACS), pp. 14045–14051, Jul. 01, 2020. doi: 10.1021/jacs.0c05131.  
  
H. S. Sam Chan, Q. N. N. Nguyen, R. S. Patonand J. W. Burton, “Synthesis, Characterization, and Reactivity of Complex Tricyclic Oxonium Ions, Proposed Intermediates in Natural Product Biosynthesis”, *Journal of the American Chemical Society*, vol. 141, no. 40. American Chemical Society (ACS), pp. 15951–15962, Sep. 27, 2019. doi: 10.1021/jacs.9b07438.  
  
E. D. Shepherd, “Structure Determination of a Chloroenyne from *Laurencia majuscula* Using Computational Methods and Total Synthesis”, *The Journal of Organic Chemistry*, vol. 84, no. 9. American Chemical Society (ACS), pp. 4971–4991, Apr. 12, 2019. doi: 10.1021/acs.joc.8b02975.  
  
P. C. St. John, Y. Guan, Y. Kim, B. D. Etz, S. Kimand R. S. Paton, “Quantum chemical calculations for over 200,000 organic radical species and 40,000 associated closed-shell molecules”, *Scientific Data*, vol. 7, no. 1. Springer Science and Business Media LLC, Jul. 21, 2020. doi: 10.1038/s41597-020-00588-x.  
  
P. C. St. John, Y. Guan, Y. Kim, S. Kimand R. S. Paton, “Prediction of organic homolytic bond dissociation enthalpies at near chemical accuracy with sub-second computational cost”, *Nature Communications*, vol. 11, no. 1. Springer Science and Business Media LLC, May 11, 2020. doi: 10.1038/s41467-020-16201-z.  
  
B. Tang and R. S. Paton, “Biosynthesis of Providencin: Understanding Photochemical Cyclobutane Formation with Density Functional Theory”, *Organic Letters*, vol. 21, no. 5. American Chemical Society (ACS), pp. 1243–1247, Feb. 15, 2019. doi: 10.1021/acs.orglett.8b03838.  
  
J. S. J. Tan and R. S. Paton, “Frontier molecular orbital effects control the hole-catalyzed racemization of atropisomeric biaryls”, *Chemical Science*, vol. 10, no. 8. Royal Society of Chemistry (RSC), pp. 2285–2289, 2019. doi: 10.1039/c8sc05066j.  
  
Y. Ye, “Fungal-derived brevianamide assembly by a stereoselective semipinacolase”, *Nature Catalysis*, vol. 3, no. 6. Springer Science and Business Media LLC, pp. 497–506, May 18, 2020. doi: 10.1038/s41929-020-0454-9.  
  
H. Yuan, “Effects of substituents X and Y on the NMR chemical shifts of 2-(4-X phenyl)-5-Y pyrimidines”, *Journal of Molecular Structure*, vol. 1204. Elsevier BV, p. 127489, Mar. 2020. doi: 10.1016/j.molstruc.2019.127489.  
  
X. Zhang and R. S. Paton, “Stereoretention in styrene heterodimerisation promoted by one-electron oxidants”, *Chemical Science*, vol. 11, no. 34. Royal Society of Chemistry (RSC), pp. 9309–9324, 2020. doi: 10.1039/d0sc03059g.  
  
S. F. Alamudun, “Structure–Photochemical Function Relationships in Nitrogen-Containing Heterocyclic Aromatic Photobases Derived from Quinoline”, *The Journal of Physical Chemistry A*, vol. 124, no. 13. American Chemical Society (ACS), pp. 2537–2546, Mar. 20, 2020. doi: 10.1021/acs.jpca.9b11375.  
  
L. K. Ulloa, S. Kong, A. M. Vigiland A. S. Petit, “Computational Investigation of Substituent Effects on the Formation and Intramolecular Cyclization of 2′-Arylbenzaldehyde and 2′-Arylacetophenone Oxime Ether Radical Cations”, *The Journal of Organic Chemistry*, vol. 84, no. 22. American Chemical Society (ACS), pp. 14659–14669, Nov. 05, 2019. doi: 10.1021/acs.joc.9b02240.  
  
A. Adeagbo, T. Weiand A. Z. Clayborne, “Computational Comparative Analysis of Small Atomically Precise Copper Clusters”, *The Journal of Physical Chemistry A*, vol. 124, no. 32. American Chemical Society (ACS), pp. 6504–6510, Jul. 21, 2020. doi: 10.1021/acs.jpca.0c03992.  
  
S. Kenzler, “Synthesis and Characterization of Three Multi‐Shell Metalloid Gold Clusters Au 32 (R 3 P) 12 Cl 8”, *Angewandte Chemie International Edition*, vol. 58, no. 18. Wiley, pp. 5902–5905, Mar. 26, 2019. doi: 10.1002/anie.201900644.  
  
J.-C. Lemay, “Relative Abundances of Surface Diastereomeric Complexes Formed by Two Chiral Modifiers That Differ by a Methyl Group”, *ACS Catalysis*, vol. 10, no. 5. American Chemical Society (ACS), pp. 3034–3041, Jan. 30, 2020. doi: 10.1021/acscatal.9b04682.  
  
M. T. Whited, M. J. Trenerry, K. E. DeMeulenaereand B. L. H. Taylor, “Computational and Experimental Investigation of Alkene Hydrogenation by a Pincer-Type [P2Si]Rh Complex: Alkane Release via Competitive σ-Bond Metathesis and Reductive Elimination”, *Organometallics*, vol. 38, no. 7. American Chemical Society (ACS), pp. 1493–1501, Mar. 07, 2019. doi: 10.1021/acs.organomet.8b00922.  
  
N. P. Burlow, S. Y. Howard, C. M. Saunders, J. C. Fettinger, D. J. Tantilloand J. T. Shaw, “Formal [4 + 2] Cycloadditions of Anhydrides and α,β-Unsaturated *N*-Tosyl Ketimines”, *Organic Letters*, vol. 21, no. 4. American Chemical Society (ACS), pp. 1046–1049, Feb. 05, 2019. doi: 10.1021/acs.orglett.8b04091.  
  
R. Chen, G. T. Cravenand A. Nitzan, “Electron-transfer-induced and phononic heat transport in molecular environments”, *The Journal of Chemical Physics*, vol. 147, no. 12. AIP Publishing, p. 124101, Sep. 28, 2017. doi: 10.1063/1.4990410.  
  
G. T. Craven, R. Chenand A. Nitzan, “Upside/Downside statistical mechanics of nonequilibrium Brownian motion. II. Heat transfer and energy partitioning of a free particle”, *The Journal of Chemical Physics*, vol. 149, no. 10. AIP Publishing, p. 104103, Sep. 14, 2018. doi: 10.1063/1.5045361.  
  
G. T. Craven, D. Heand A. Nitzan, “Electron-Transfer-Induced Thermal and Thermoelectric Rectification”, *Physical Review Letters*, vol. 121, no. 24. American Physical Society (APS), Dec. 14, 2018. doi: 10.1103/physrevlett.121.247704.  
  
W. Dou, M. A. Ochoa, A. Nitzanand J. E. Subotnik, “Universal approach to quantum thermodynamics in the strong coupling regime”, *Physical Review B*, vol. 98, no. 13. American Physical Society (APS), Oct. 15, 2018. doi: 10.1103/physrevb.98.134306.  
  
O. S. Lumbroso, L. Simine, A. Nitzan, D. Segaland O. Tal, “Electronic noise due to temperature differences in atomic-scale junctions”, *Nature*, vol. 562, no. 7726. Springer Science and Business Media LLC, pp. 240–244, Oct. 2018. doi: 10.1038/s41586-018-0592-2.  
  
M. A. Ochoa, N. Zimbovskayaand A. Nitzan, “Quantum thermodynamics for driven dissipative bosonic systems”, *Physical Review B*, vol. 97, no. 8. American Physical Society (APS), Feb. 23, 2018. doi: 10.1103/physrevb.97.085434.  
  
B. Rudshteyn, “Predicting Ligand-Dissociation Energies of 3d Coordination Complexes with Auxiliary-Field Quantum Monte Carlo”, *Journal of Chemical Theory and Computation*, vol. 16, no. 5. American Chemical Society (ACS), pp. 3041–3054, Apr. 15, 2020. doi: 10.1021/acs.jctc.0c00070.  
  
S. Agrawal, W. Lin, O. V. Prezhdoand D. J. Trivedi, “*Ab initio* quantum dynamics of charge carriers in graphitic carbon nitride nanosheets”, *The Journal of Chemical Physics*, vol. 153, no. 5. AIP Publishing, p. 054701, Aug. 07, 2020. doi: 10.1063/5.0010628.  
  
A. He, “Structural Complexity and High Thermoelectric Performance of the Zintl Phase: Yb21Mn4Sb18”, *Chemistry of Materials*, vol. 31, no. 19. American Chemical Society (ACS), pp. 8076–8086, Sep. 09, 2019. doi: 10.1021/acs.chemmater.9b02671.  
  
C. M. Wehrmann, M. Imran, C. Pointer, L. A. Fredin, E. R. Youngand M. S. Chen, “Spin multiplicity effects in doublet *versus* singlet emission: the photophysical consequences of a single electron”, *Chemical Science*, vol. 11, no. 37. Royal Society of Chemistry (RSC), pp. 10212–10219, 2020. doi: 10.1039/d0sc04211k.  
  
Y. Luo, “Colloidal Assembly of Au–Quantum Dot–Au Sandwiched Nanostructures with Strong Plasmon–Exciton Coupling”, *The Journal of Physical Chemistry Letters*, vol. 11, no. 7. American Chemical Society (ACS), pp. 2449–2456, Mar. 10, 2020. doi: 10.1021/acs.jpclett.0c00110.  
  
Q. Wang, L. Ma, W. Cui, M. Chenand S. Zou, “Ultra-narrow electromagnetically induced transparency in the visible and near-infrared regions”, *Applied Physics Letters*, vol. 114, no. 21. AIP Publishing, p. 213103, May 27, 2019. doi: 10.1063/1.5093648.  
  
J. X. Xu, Y. Yuan, M. Liu, S. Zou, O. Chenand D. Zhang, “Quantification of the Photon Absorption, Scattering, and On-Resonance Emission Properties of CdSe/CdS Core/Shell Quantum Dots: Effect of Shell Geometry and Volumes”, *Analytical Chemistry*, vol. 92, no. 7. American Chemical Society (ACS), pp. 5346–5353, Mar. 03, 2020. doi: 10.1021/acs.analchem.0c00016.  
  
J. X. Xu, Y. Yuan, S. Zou, O. Chenand D. Zhang, “A Divide-and-Conquer Strategy for Quantification of Light Absorption, Scattering, and Emission Properties of Fluorescent Nanomaterials in Solutions”, *Analytical Chemistry*, vol. 91, no. 13. American Chemical Society (ACS), pp. 8540–8548, May 28, 2019. doi: 10.1021/acs.analchem.9b01803.  
  
Q. Zhang, “Photothermal Effect, Local Field Dependence, and Charge Carrier Relaying Species in Plasmon-Driven Photocatalysis: A Case Study of Aerobic Nitrothiophenol Coupling Reaction”, *The Journal of Physical Chemistry C*, vol. 123, no. 43. American Chemical Society (ACS), pp. 26695–26704, Oct. 04, 2019. doi: 10.1021/acs.jpcc.9b08181.  
  
N. C. Iovanac and B. M. Savoie, “Simpler is Better: How Linear Prediction Tasks Improve Transfer Learning in Chemical Autoencoders”, *The Journal of Physical Chemistry A*, vol. 124, no. 18. American Chemical Society (ACS), pp. 3679–3685, Apr. 08, 2020. doi: 10.1021/acs.jpca.0c00042.  
  
A. Khot, S. B. Shiringand B. M. Savoie, “Evidence of information limitations in coarse-grained models”, *The Journal of Chemical Physics*, vol. 151, no. 24. AIP Publishing, p. 244105, Dec. 28, 2019. doi: 10.1063/1.5129398.  
  
Q. Zhao and B. M. Savoie, “Self-Consistent Component Increment Theory for Predicting Enthalpy of Formation”, *Journal of Chemical Information and Modeling*, vol. 60, no. 4. American Chemical Society (ACS), pp. 2199–2207, Mar. 11, 2020. doi: 10.1021/acs.jcim.0c00092.  
  
A. V. Balueva, I. N. Dashevskiy, P. Todebushand C. Campbell, “Modeling Bonding Energy in Novel Bio-active Nano Coatings on Dental Implants”, *Procedia Structural Integrity*, vol. 23. Elsevier BV, pp. 173–178, 2019. doi: 10.1016/j.prostr.2020.01.082.  
  
A. V. Balueva, I. N. Dashevskiy, P. Todebush, C. Campbelland E. Valdez, “First-Principle Calculations of the Binding Energy of the Coating Components of New Generation Dental Implants”, *Volume 10: Micro- and Nano-Systems Engineering and Packaging*. American Society of Mechanical Engineers, Nov. 11, 2019. doi: 10.1115/imece2019-10059.  
  
I. Dashevskiy, A. Balueva, P. Todebush, C. Campbell, J. Maganaand N. Clement, “On Estimation of Adhesive Strength of Implants Bioactive Coating with Titanium by Density Functional Theory and Molecular Dynamics Simulations”, *Materials Research*, vol. 22, no. 3. FapUNIFESP (SciELO), 2019. doi: 10.1590/1980-5373-mr-2019-0030.  
  
S. P. Ross, A. A. Rahmanand M. S. Sigman, “Development and Mechanistic Interrogation of Interrupted Chain-Walking in the Enantioselective Relay Heck Reaction”, *Journal of the American Chemical Society*, vol. 142, no. 23. American Chemical Society (ACS), pp. 10516–10525, May 15, 2020. doi: 10.1021/jacs.0c03589.  
  
B. B. Dangi and S. Kattel, “Growth of carbonaceous material on silicon surface: Case study of 1,3-butadiene molecule”, *Chemical Physics Letters*, vol. 745. Elsevier BV, p. 137248, Apr. 2020. doi: 10.1016/j.cplett.2020.137248.  
  
Q. He, “Electrochemical Conversion of CO 2 to Syngas with Controllable CO/H 2 Ratios over Co and Ni Single‐Atom Catalysts”, *Angewandte Chemie International Edition*, vol. 59, no. 8. Wiley, pp. 3033–3037, Jan. 09, 2020. doi: 10.1002/anie.201912719.  
  
N. Humphrey, S. Bacand S. Mallikarjun Sharada, “Ab Initio Molecular Dynamics Reveals New Metal-Binding Sites in Atomically Dispersed Pt1/TiO2 Catalysts”, *The Journal of Physical Chemistry C*, vol. 124, no. 44. American Chemical Society (ACS), pp. 24187–24195, Oct. 23, 2020. doi: 10.1021/acs.jpcc.0c06771.  
  
J. T. Perryman, F. P. Hyler, J. C. Ortiz-Rodríguez, A. Mehta, A. R. Kulkarniand J. M. Velázquez, “X-ray absorption spectroscopy study of the electronic structure and local coordination of 1st row transition metal-promoted Chevrel-phase sulfides”, *Journal of Coordination Chemistry*, vol. 72, no. 8. Informa UK Limited, pp. 1322–1335, Apr. 18, 2019. doi: 10.1080/00958972.2019.1613532.  
  
J. T. Perryman, A. R. Kulkarniand J. M. Velázquez, “Direct solid-state nucleation and charge-transport dynamics of alkali metal-intercalated M2Mo6S6 (M = K, Rb, Cs) nanorods”, *Journal of Materials Chemistry C*, vol. 8, no. 31. Royal Society of Chemistry (RSC), pp. 10742–10748, 2020. doi: 10.1039/d0tc01674h.  
  
J. T. Perryman, “Metal-promoted Mo6S8 clusters: a platform for probing ensemble effects on the electrochemical conversion of CO2 and CO to methanol”, *Materials Horizons*, vol. 7, no. 1. Royal Society of Chemistry (RSC), pp. 193–202, 2020. doi: 10.1039/c9mh00745h.  
  
A. S. Hansen, Z. Liu, S. Chen, M. G. Schumer, P. J. Walshand M. I. Lester, “Unraveling Conformer-Specific Sources of Hydroxyl Radical Production from an Isoprene-Derived Criegee Intermediate by Deuteration”, *The Journal of Physical Chemistry A*, vol. 124, no. 24. American Chemical Society (ACS), pp. 4929–4938, May 25, 2020. doi: 10.1021/acs.jpca.0c02867.  
  
C. R. Reinhardt, P. Li, G. Kang, J. Stubbe, C. L. Drennanand S. Hammes-Schiffer, “Conformational Motions and Water Networks at the α/β Interface in *E. coli* Ribonucleotide Reductase”, *Journal of the American Chemical Society*, vol. 142, no. 32. American Chemical Society (ACS), pp. 13768–13778, Jul. 07, 2020. doi: 10.1021/jacs.0c04325.  
  
R. A. Daley, A. S. Morrenzin, S. R. Neufeldtand J. J. Topczewski, “Gold Catalyzed Decarboxylative Cross-Coupling of Iodoarenes”, *Journal of the American Chemical Society*, vol. 142, no. 30. American Chemical Society (ACS), pp. 13210–13218, Jul. 07, 2020. doi: 10.1021/jacs.0c06244.  
  
Y. Zhang, J. Furness, R. Zhang, Z. Wang, A. Zungerand J. Sun, “Symmetry-breaking polymorphous descriptions for correlated materials without interelectronic *U*”, *Physical Review B*, vol. 102, no. 4. American Physical Society (APS), Jul. 08, 2020. doi: 10.1103/physrevb.102.045112.  
  
C. Sandford, L. R. Fries, T. E. Ball, S. D. Minteerand M. S. Sigman, “Mechanistic Studies into the Oxidative Addition of Co(I) Complexes: Combining Electroanalytical Techniques with Parameterization”, *Journal of the American Chemical Society*, vol. 141, no. 47. American Chemical Society (ACS), pp. 18877–18889, Nov. 08, 2019. doi: 10.1021/jacs.9b10771.  
  
C. Tsai, C. Sandford, T. Wu, B. Chen, M. S. Sigmanand F. D. Toste, “Enantioselective Intramolecular Allylic Substitution via Synergistic Palladium/Chiral Phosphoric Acid Catalysis: Insight into Stereoinduction through Statistical Modeling”, *Angewandte Chemie International Edition*, vol. 59, no. 34. Wiley, pp. 14647–14655, Jun. 30, 2020. doi: 10.1002/anie.202006237.  
  
M. Singh, N. Garza, Z. Pearson, J. Douglasand Z. Boskovic, “Broad assessment of bioactivity of a collection of spiroindane pyrrolidines through “cell painting””, *Bioorganic & Medicinal Chemistry*, vol. 28, no. 13. Elsevier BV, p. 115547, Jul. 2020. doi: 10.1016/j.bmc.2020.115547.  
  
L. Cheng, C. Zhangand Y. Liu, “Why Two-Dimensional Semiconductors Generally Have Low Electron Mobility”, *Physical Review Letters*, vol. 125, no. 17. American Physical Society (APS), Oct. 19, 2020. doi: 10.1103/physrevlett.125.177701.  
  
G. Li, “Engineering Substrate Interaction To Improve Hydrogen Evolution Catalysis of Monolayer MoS2 Films beyond Pt”, *ACS Nano*, vol. 14, no. 2. American Chemical Society (ACS), pp. 1707–1714, Jan. 16, 2020. doi: 10.1021/acsnano.9b07324.  
  
J. Shi, X. Zhao, Z. Wangand Y. Liu, “Eliminating Trap‐States and Functionalizing Vacancies in 2D Semiconductors by Electrochemistry”, *Small*, vol. 15, no. 47. Wiley, p. 1901899, Oct. 22, 2019. doi: 10.1002/smll.201901899.  
  
C. Tang, “CO2 Reduction on Copper’s Twin Boundary”, *ACS Catalysis*, vol. 10, no. 3. American Chemical Society (ACS), pp. 2026–2032, Jan. 08, 2020. doi: 10.1021/acscatal.9b03814.  
  
X. Zhao and Y. Liu, “Unveiling the Active Structure of Single Nickel Atom Catalysis: Critical Roles of Charge Capacity and Hydrogen Bonding”, *Journal of the American Chemical Society*, vol. 142, no. 12. American Chemical Society (ACS), pp. 5773–5777, Mar. 03, 2020. doi: 10.1021/jacs.9b13872.  
  
N. S. Abularrage, B. J. Levandowskiand R. T. Raines, “Synthesis and Diels–Alder Reactivity of 4-Fluoro-4-Methyl-4H-Pyrazoles”, *International Journal of Molecular Sciences*, vol. 21, no. 11. MDPI AG, p. 3964, May 31, 2020. doi: 10.3390/ijms21113964.  
  
B. J. Levandowski, N. S. Abularrage, K. N. Houkand R. T. Raines, “Hyperconjugative Antiaromaticity Activates 4*H*-Pyrazoles as Inverse-Electron-Demand Diels–Alder Dienes”, *Organic Letters*, vol. 21, no. 20. American Chemical Society (ACS), pp. 8492–8495, Oct. 07, 2019. doi: 10.1021/acs.orglett.9b03351.  
  
B. J. Levandowski, N. S. Abularrageand R. T. Raines, “Differential Effects of Nitrogen Substitution in 5‐ and 6‐Membered Aromatic Motifs”, *Chemistry – A European Journal*, vol. 26, no. 41. Wiley, pp. 8862–8866, Jun. 12, 2020. doi: 10.1002/chem.202000825.  
  
P. C. Bevilacqua, “An Ontology for Facilitating Discussion of Catalytic Strategies of RNA-Cleaving Enzymes”, *ACS Chemical Biology*, vol. 14, no. 6. American Chemical Society (ACS), pp. 1068–1076, May 16, 2019. doi: 10.1021/acschembio.9b00202.  
  
Ş. Ekesan and D. M. York, “Dynamical ensemble of the active state and transition state mimic for the RNA-cleaving 8–17 DNAzyme in solution”, *Nucleic Acids Research*, vol. 47, no. 19. Oxford University Press (OUP), pp. 10282–10295, Sep. 12, 2019. doi: 10.1093/nar/gkz773.  
  
C. S. Gaines, J. A. Piccirilliand D. M. York, “The L-platform/L-scaffold framework: a blueprint for RNA-cleaving nucleic acid enzyme design”, *RNA*, vol. 26, no. 2. Cold Spring Harbor Laboratory, pp. 111–125, Nov. 27, 2019. doi: 10.1261/rna.071894.119.  
  
A. Ganguly, “Confluence of theory and experiment reveals the catalytic mechanism of the Varkud satellite ribozyme”, *Nature Chemistry*, vol. 12, no. 2. Springer Science and Business Media LLC, pp. 193–201, Jan. 20, 2020. doi: 10.1038/s41557-019-0391-x.  
  
A. Ganguly, B. P. Weissman, J. A. Piccirilliand D. M. York, “Evidence for a Catalytic Strategy to Promote Nucleophile Activation in Metal-Dependent RNA-Cleaving Ribozymes and 8-17 DNAzyme”, *ACS Catalysis*, vol. 9, no. 12. American Chemical Society (ACS), pp. 10612–10617, Oct. 27, 2019. doi: 10.1021/acscatal.9b02035.  
  
T. J. Giese and D. M. York, “Development of a Robust Indirect Approach for MM → QM Free Energy Calculations That Combines Force-Matched Reference Potential and Bennett’s Acceptance Ratio Methods”, *Journal of Chemical Theory and Computation*, vol. 15, no. 10. American Chemical Society (ACS), pp. 5543–5562, Sep. 11, 2019. doi: 10.1021/acs.jctc.9b00401.  
  
K. Kostenbader and D. M. York, “Molecular simulations of the pistol ribozyme: unifying the interpretation of experimental data and establishing functional links with the hammerhead ribozyme”, *RNA*, vol. 25, no. 11. Cold Spring Harbor Laboratory, pp. 1439–1456, Jul. 30, 2019. doi: 10.1261/rna.071944.119.  
  
L. F. Song, T.-S. Lee, C. Zhu, D. M. Yorkand K. M. Merz Jr., “Using AMBER18 for Relative Free Energy Calculations”, *Journal of Chemical Information and Modeling*, vol. 59, no. 7. American Chemical Society (ACS), pp. 3128–3135, Jun. 06, 2019. doi: 10.1021/acs.jcim.9b00105.  
  
J. W. Bennett, “Exploring the A2BX3 Family for New Functional Materials Using Crystallographic Database Mining and First-Principles Calculations”, *The Journal of Physical Chemistry C*, vol. 124, no. 36. American Chemical Society (ACS), pp. 19413–19425, Aug. 12, 2020. doi: 10.1021/acs.jpcc.0c03093.  
  
V. P. Barber, A. S. Hansen, Y. Georgievskii, S. J. Klippensteinand M. I. Lester, “Experimental and theoretical studies of the doubly substituted methyl-ethyl Criegee intermediate: Infrared action spectroscopy and unimolecular decay to OH radical products”, *The Journal of Chemical Physics*, vol. 152, no. 9. AIP Publishing, p. 094301, Mar. 07, 2020. doi: 10.1063/5.0002422.  
  
C.-W. Tai, S. Wangand V. Narsimhan, “Cross-stream migration of non-spherical particles in a second-order fluid – theories of particle dynamics in arbitrary quadratic flows”, *Journal of Fluid Mechanics*, vol. 895. Cambridge University Press (CUP), May 15, 2020. doi: 10.1017/jfm.2020.300.  
  
S. Wang, D. Ramkrishnaand V. Narsimhan, “Exact sampling of polymer conformations using Brownian bridges”, *The Journal of Chemical Physics*, vol. 153, no. 3. AIP Publishing, p. 034901, Jul. 21, 2020. doi: 10.1063/5.0010368.  
  
E. J. Peterson, W. Qi, I. N. Stanton, P. Zhangand M. J. Therien, “Driving high quantum yield NIR emission through proquinoidal linkage motifs in conjugated supermolecular arrays”, *Chemical Science*, vol. 11, no. 31. Royal Society of Chemistry (RSC), pp. 8095–8104, 2020. doi: 10.1039/d0sc03446k.  
  
J. V. Alegre‐Requena, R. P. Herreraand D. Díaz Díaz, “Self‐Assembly of Hollow Organic Nanotubes Driven by Arene Regioisomerism”, *ChemPlusChem*, vol. 85, no. 11. Wiley, pp. 2372–2375, Aug. 18, 2020. doi: 10.1002/cplu.202000473.  
  
J. V. Alegre-Requena, A. Valero-Tena, I. G. Sonsona, S. Urieland R. P. Herrera, “Simple iodoalkyne-based organocatalysts for the activation of carbonyl compounds”, *Organic & Biomolecular Chemistry*, vol. 18, no. 8. Royal Society of Chemistry (RSC), pp. 1594–1601, 2020. doi: 10.1039/c9ob02688f.  
  
I. G. Sonsona, J. V. Alegre‐Requena, E. Marqués‐López, M. C. Gimenoand R. P. Herrera, “Asymmetric Organocatalyzed Aza‐Henry Reaction of Hydrazones: Experimental and Computational Studies”, *Chemistry – A European Journal*, vol. 26, no. 24. Wiley, pp. 5469–5478, Apr. 15, 2020. doi: 10.1002/chem.202000232.  
  
C.-H. Yang and H. Wang, “Heat Transport in a Spin-Boson Model at Low Temperatures: A Multilayer Multiconfiguration Time-Dependent Hartree Study”, *Entropy*, vol. 22, no. 10. MDPI AG, p. 1099, Sep. 29, 2020. doi: 10.3390/e22101099.  
  
C. Desgranges and J. Delhommelle, “Unraveling liquid polymorphism in silicon driven out-of-equilibrium”, *The Journal of Chemical Physics*, vol. 153, no. 5. AIP Publishing, p. 054502, Aug. 07, 2020. doi: 10.1063/5.0015417.  
  
C. Desgranges and J. Delhommelle, “The central role of entropy in adiabatic ensembles and its application to phase transitions in the grand-isobaric adiabatic ensemble”, *The Journal of Chemical Physics*, vol. 153, no. 9. AIP Publishing, p. 094114, Sep. 07, 2020. doi: 10.1063/5.0021488.  
  
S. Gusarov and S. R. Stoyanov, “COSMO-RS-Based Descriptors for the Machine Learning-Enabled Screening of Nucleotide Analogue Drugs against SARS-CoV-2”, *The Journal of Physical Chemistry Letters*, vol. 11, no. 21. American Chemical Society (ACS), pp. 9408–9414, Oct. 26, 2020. doi: 10.1021/acs.jpclett.0c02836.  
  
J. Diaz, G. von Laszewski, F. Wang, A. J. Youngeand G. Fox, “FutureGrid Image Repository: A Generic Catalog and Storage System for Heterogeneous Virtual Machine Images”, *2011 IEEE Third International Conference on Cloud Computing Technology and Science*. IEEE, Nov. 2011. doi: 10.1109/cloudcom.2011.85.  
  
J. Cao, G. Kerr, K. Aryaand G. Cooperman, “Transparent checkpoint-restart over infiniband”, *Proceedings of the 23rd international symposium on High-performance parallel and distributed computing*. ACM, Jun. 23, 2014. doi: 10.1145/2600212.2600219.  
  
A. Hassani, A. Skjellum, P. V. Bangaloreand R. Brightwell, “Practical resilient cases for FA-MPI, a transactional fault-tolerant MPI”, *Proceedings of the 3rd Workshop on Exascale MPI*. ACM, Nov. 15, 2015. doi: 10.1145/2831129.2831130.  
  
S. De, S. Chowdhary, A. Shirke, Y. L. Lo, R. Kravetsand H. Sundaram, “Finding by Counting”, *Proceedings of the 11th Workshop on Wireless Network Testbeds, Experimental evaluation & CHaracterization*. ACM, Oct. 20, 2017. doi: 10.1145/3131473.3131482.  
  
A. Krishnan, A. Sharma, A. Sankarand H. Sundaram, “An Adversarial Approach to Improve Long-Tail Performance in Neural Collaborative Filtering”, *Proceedings of the 27th ACM International Conference on Information and Knowledge Management*. ACM, Oct. 17, 2018. doi: 10.1145/3269206.3269264.  
  
A. Krishnan, A. Sharmaand H. Sundaram, “Insights from the Long-Tail”, *Proceedings of the 27th ACM International Conference on Information and Knowledge Management*. ACM, Oct. 17, 2018. doi: 10.1145/3269206.3271706.  
  
H. Cao, Q. Ma, X. Chenand Y. Xu, “DOOR: a prokaryotic operon database for genome analyses and functional inference”, *Briefings in Bioinformatics*, vol. 20, no. 4. Oxford University Press (OUP), pp. 1568–1577, Jul. 28, 2017. doi: 10.1093/bib/bbx088.  
  
S. Cao, T. Sheng, X. Chen, Q. Maand C. Zhang, “A probabilistic model-based bi-clustering method for single-cell transcriptomic data analysis”, *[]*. Cold Spring Harbor Laboratory, Aug. 27, 2017. doi: 10.1101/181362.  
  
X. Chen, “RECTA: Regulon Identification Based on Comparative Genomics and Transcriptomics Analysis”, *[]*. Cold Spring Harbor Laboratory, Feb. 08, 2018. doi: 10.1101/261453.  
  
S. Liang, A. Ma, S. Yang, Y. Wangand Q. Ma, “A Review of Matched-pairs Feature Selection Methods for Gene Expression Data Analysis”, *Computational and Structural Biotechnology Journal*, vol. 16. Elsevier BV, pp. 88–97, 2018. doi: 10.1016/j.csbj.2018.02.005.  
  
B. Liu, L. Han, X. Liu, J. Wuand Q. Ma, “Computational Prediction of Sigma-54 Promoters in Bacterial Genomes by Integrating Motif Finding and Machine Learning Strategies”, *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, vol. 16, no. 4. Institute of Electrical and Electronics Engineers (IEEE), pp. 1211–1218, Jul. 01, 2019. doi: 10.1109/tcbb.2018.2816032.  
  
A. McDermaid, X. Chen, Y. Zhang, J. Xie, C. Wangand Q. Ma, “GeneQC: A quality control tool for gene expression estimation based on RNA-sequencing reads mapping”, *[]*. Cold Spring Harbor Laboratory, Feb. 15, 2018. doi: 10.1101/266445.  
  
A. McDermaid, B. Monier, J. Zhaoand Q. Ma, “ViDGER: An R package for integrative interpretation of differential gene expression results of RNA-seq data”, *[]*. Cold Spring Harbor Laboratory, Feb. 21, 2018. doi: 10.1101/268896.  
  
B. Monier, A. McDermaid, J. Zhao, A. Fennelland Q. Ma, “IRIS-DGE: An integrated RNA-seq data analysis and interpretation system for differential gene expression”, *[]*. Cold Spring Harbor Laboratory, Mar. 16, 2018. doi: 10.1101/283341.  
  
S.-Y. Niu, J. Yang, A. McDermaid, J. Zhao, Y. Kangand Q. Ma, “Bioinformatics tools for quantitative and functional metagenome and metatranscriptome data analysis in microbes”, *Briefings in Bioinformatics*. Oxford University Press (OUP), May 08, 2017. doi: 10.1093/bib/bbx051.  
  
J. Xie, A. Ma, A. Fennell, Q. Maand J. Zhao, “It is time to apply biclustering: a comprehensive review of biclustering applications in biological and biomedical data”, *Briefings in Bioinformatics*, vol. 20, no. 4. Oxford University Press (OUP), pp. 1450–1465, Feb. 27, 2018. doi: 10.1093/bib/bby014.  
  
J. Yang, X. Chen, A. McDermaidand Q. Ma, “DMINDA 2.0: integrated and systematic views of regulatory DNA motif identification and analyses”, *Bioinformatics*, vol. 33, no. 16. Oxford University Press (OUP), pp. 2586–2588, Apr. 13, 2017. doi: 10.1093/bioinformatics/btx223.  
  
Y. Zhang, S. Cao, J. Zhao, B. Alsaihati, Q. Maand C. Zhang, “MRHCA: a nonparametric statistics based method for hub and co-expression module identification in large gene co-expression network”, *Quantitative Biology*, vol. 6, no. 1. Engineering Sciences Press, pp. 40–55, Feb. 13, 2018. doi: 10.1007/s40484-018-0131-z.  
  
X. Chen, R. Dathathri, G. Gilland K. Pingali, “Pangolin”, *Proceedings of the VLDB Endowment*, vol. 13, no. 8. Association for Computing Machinery (ACM), pp. 1190–1205, Apr. 2020. doi: 10.14778/3389133.3389137.  
  
H.-V. Dang, “A Lightweight Communication Runtime for Distributed Graph Analytics”, *2018 IEEE International Parallel and Distributed Processing Symposium (IPDPS)*. IEEE, May 2018. doi: 10.1109/ipdps.2018.00107.  
  
R. Dathathri, “Gluon: a communication-optimizing substrate for distributed heterogeneous graph analytics”, *Proceedings of the 39th ACM SIGPLAN Conference on Programming Language Design and Implementation*. ACM, Jun. 11, 2018. doi: 10.1145/3192366.3192404.  
  
R. Dathathri, “Gluon-Async: A Bulk-Asynchronous System for Distributed and Heterogeneous Graph Analytics”, *2019 28th International Conference on Parallel Architectures and Compilation Techniques (PACT)*. IEEE, Sep. 2019. doi: 10.1109/pact.2019.00010.  
  
R. Dathathri, G. Gill, L. Hoangand K. Pingali, “Phoenix”, *Proceedings of the Twenty-Fourth International Conference on Architectural Support for Programming Languages and Operating Systems*. ACM, Apr. 04, 2019. doi: 10.1145/3297858.3304056.  
  
L. Hoang, R. Dathathri, G. Gilland K. Pingali, “CuSP: A Customizable Streaming Edge Partitioner for Distributed Graph Analytics”, *2019 IEEE International Parallel and Distributed Processing Symposium (IPDPS)*. IEEE, May 2019. doi: 10.1109/ipdps.2019.00054.  
  
L. Hoang, “DistTC: High Performance Distributed Triangle Counting”, *2019 IEEE High Performance Extreme Computing Conference (HPEC)*. IEEE, Sep. 2019. doi: 10.1109/hpec.2019.8916438.  
  
L. Hoang, “A round-efficient distributed betweenness centrality algorithm”, *Proceedings of the 24th Symposium on Principles and Practice of Parallel Programming*. ACM, Feb. 16, 2019. doi: 10.1145/3293883.3295729.  
  
E. Arslan and T. Kosar, “High-Speed Transfer Optimization Based on Historical Analysis and Real-Time Tuning”, *IEEE Transactions on Parallel and Distributed Systems*, vol. 29, no. 6. Institute of Electrical and Electronics Engineers (IEEE), pp. 1303–1316, Jun. 01, 2018. doi: 10.1109/tpds.2018.2790948.  
  
B. Langmead, C. Wilks, V. Antonescuand R. Charles, “Scaling read aligners to hundreds of threads on general-purpose processors”, *Bioinformatics*, vol. 35, no. 3. Oxford University Press (OUP), pp. 421–432, Jul. 18, 2018. doi: 10.1093/bioinformatics/bty648.  
  
J. Finocchiaro and H. D. Mathias, “Evolving cooperation for the iterated prisoner’s dilemma”, *Proceedings of the Genetic and Evolutionary Computation Conference Companion*. ACM, Jul. 13, 2019. doi: 10.1145/3319619.3322021.  
  
V. R. Ragusa, H. D. Mathias, V. A. Kazakovaand A. S. Wu, “Enhanced genetic path planning for autonomous flight”, *Proceedings of the Genetic and Evolutionary Computation Conference*. ACM, Jul. 2017. doi: 10.1145/3071178.3071293.  
  
A.-V. Vo, N. Konda, N. Chauhan, H. Aljumailyand D. F. Laefer, “Lessons Learned with Laser Scanning Point Cloud Management in Hadoop HBase”, *Advanced Computing Strategies for Engineering*. Springer International Publishing, pp. 231–253, 2018. doi: 10.1007/978-3-319-91635-4\_13.  
  
M. H. Choudhury, J. Wu, W. A. Ingramand E. A. Fox, “A Heuristic Baseline Method for Metadata Extraction from Scanned Electronic Theses and Dissertations”, *Proceedings of the ACM/IEEE Joint Conference on Digital Libraries in 2020*. ACM, Aug. 2020. doi: 10.1145/3383583.3398590.  
  
P. S. Bernard, “The hairpin vortex illusion”, *Journal of Physics: Conference Series*, vol. 318, no. 6. IOP Publishing, p. 062004, Dec. 22, 2011. doi: 10.1088/1742-6596/318/6/062004.  
  
P. Balogh and P. Bagchi, “Analysis of red blood cell partitioning at bifurcations in simulated microvascular networks”, *Physics of Fluids*, vol. 30, no. 5. AIP Publishing, p. 051902, May 2018. doi: 10.1063/1.5024783.  
  
P. Balogh and P. Bagchi, “Three‐dimensional distribution of wall shear stress and its gradient in red cell‐resolved computational modeling of blood flow in in vivo‐like microvascular networks”, *Physiological Reports*, vol. 7, no. 9. Wiley, p. e14067, May 2019. doi: 10.14814/phy2.14067.  
  
P. Balogh and P. Bagchi, “The cell-free layer in simulated microvascular networks”, *Journal of Fluid Mechanics*, vol. 864. Cambridge University Press (CUP), pp. 768–806, Feb. 11, 2019. doi: 10.1017/jfm.2019.45.  
  
E. J. Campbell and P. Bagchi, “A computational model of amoeboid cell motility in the presence of obstacles”, *Soft Matter*, vol. 14, no. 28. Royal Society of Chemistry (RSC), pp. 5741–5763, 2018. doi: 10.1039/c8sm00457a.  
  
D. Cordasco and P. Bagchi, “Orbital drift of capsules and red blood cells in shear flow”, *Physics of Fluids*, vol. 25, no. 9. AIP Publishing, p. 091902, Sep. 2013. doi: 10.1063/1.4820472.  
  
D. Cordasco and P. Bagchi, “Intermittency and synchronized motion of red blood cell dynamics in shear flow”, *Journal of Fluid Mechanics*, vol. 759. Cambridge University Press (CUP), pp. 472–488, Oct. 24, 2014. doi: 10.1017/jfm.2014.587.  
  
D. Cordasco, A. Yazdaniand P. Bagchi, “Comparison of erythrocyte dynamics in shear flow under different stress-free configurations”, *Physics of Fluids*, vol. 26, no. 4. AIP Publishing, p. 041902, Apr. 2014. doi: 10.1063/1.4871300.  
  
K. Vahidkhah and P. Bagchi, “Microparticle shape effects on margination, near-wall dynamics and adhesion in a three-dimensional simulation of red blood cell suspension”, *Soft Matter*, vol. 11, no. 11. Royal Society of Chemistry (RSC), pp. 2097–2109, 2015. doi: 10.1039/c4sm02686a.  
  
K. Vahidkhah, P. Baloghand P. Bagchi, “Flow of Red Blood Cells in Stenosed Microvessels”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Jun. 20, 2016. doi: 10.1038/srep28194.  
  
K. Vahidkhah, S. L. Diamondand P. Bagchi, “Platelet Dynamics in Three-Dimensional Simulation of Whole Blood”, *Biophysical Journal*, vol. 106, no. 11. Elsevier BV, pp. 2529–2540, Jun. 2014. doi: 10.1016/j.bpj.2014.04.028.  
  
A. Yazdani and P. Bagchi, “Influence of membrane viscosity on capsule dynamics in shear flow”, *Journal of Fluid Mechanics*, vol. 718. Cambridge University Press (CUP), pp. 569–595, Feb. 08, 2013. doi: 10.1017/jfm.2012.637.  
  
K. Vahidkhah, “Flow-Induced Damage to Blood Cells in Aortic Valve Stenosis”, *Annals of Biomedical Engineering*, vol. 44, no. 9. Springer Science and Business Media LLC, pp. 2724–2736, Apr. 05, 2016. doi: 10.1007/s10439-016-1577-7.  
  
S. Menon, K. G. Mooney, K. G. Stapfand D. P. Schmidt, “Parallel adaptive simplical re-meshing for deforming domain CFD computations”, *Journal of Computational Physics*, vol. 298. Elsevier BV, pp. 62–78, Oct. 2015. doi: 10.1016/j.jcp.2015.05.044.  
  
J. R. Finn, M. Liand S. V. Apte, “Particle based modelling and simulation of natural sand dynamics in the wave bottom boundary layer”, *Journal of Fluid Mechanics*, vol. 796. Cambridge University Press (CUP), pp. 340–385, May 04, 2016. doi: 10.1017/jfm.2016.246.  
  
C. D. Ghodke and S. V. Apte, “Roughness effects on the second-order turbulence statistics in oscillatory flows”, *Computers & Fluids*, vol. 162. Elsevier BV, pp. 160–170, Jan. 2018. doi: 10.1016/j.compfluid.2017.09.021.  
  
X. He, S. Apte, K. Schneiderand B. Kadoch, “Angular multiscale statistics of turbulence in a porous bed”, *Physical Review Fluids*, vol. 3, no. 8. American Physical Society (APS), Aug. 02, 2018. doi: 10.1103/physrevfluids.3.084501.  
  
X. He, S. Karra, P. Pakseresht, S. V. Apteand S. Elghobashi, “Effect of heated-air blanket on the dispersion of squames in an operating room”, *International Journal for Numerical Methods in Biomedical Engineering*, vol. 34, no. 5. Wiley, p. e2960, Feb. 20, 2018. doi: 10.1002/cnm.2960.  
  
P. Pakseresht and S. V. Apte, “Volumetric displacement effects in Euler-Lagrange LES of particle-laden jet flows”, *International Journal of Multiphase Flow*, vol. 113. Elsevier BV, pp. 16–32, Apr. 2019. doi: 10.1016/j.ijmultiphaseflow.2018.12.013.  
  
S. V. Apte and J. R. Finn, “A variable-density fictitious domain method for particulate flows with broad range of particle–fluid density ratios”, *Journal of Computational Physics*, vol. 243. Elsevier BV, pp. 109–129, Jun. 2013. doi: 10.1016/j.jcp.2012.12.021.  
  
A. J. Cihonski, J. R. Finnand S. V. Apte, “Modeling and Simulation of Multiple Bubble Entrainment and Interactions With a Traveling Vortex Ring”, *Volume 2: Fora*. American Society of Mechanical Engineers, Jul. 08, 2012. doi: 10.1115/fedsm2012-72378.  
  
K. Drost, T. Jackson, S. V. Apteand R. Haggerty, “RANS Predictions of Turbulent Scalar Transport in Dead Zones of Natural Streams”, *Volume 1: Symposia, Parts A and B*. American Society of Mechanical Engineers, Jul. 08, 2012. doi: 10.1115/fedsm2012-72380.  
  
J. Finn and S. V. Apte, “Relative performance of body fitted and fictitious domain simulations of flow through fixed packed beds of spheres”, *International Journal of Multiphase Flow*, vol. 56. Elsevier BV, pp. 54–71, Oct. 2013. doi: 10.1016/j.ijmultiphaseflow.2013.05.001.  
  
J. R. Finn, S. V. Apteand M. Li, “Numerical Simulation of Sand Ripple Evolution in Oscillatory Boundary Layers”, *Volume 1B, Symposia: Fluid Machinery; Fluid-Structure Interaction and Flow-Induced Noise in Industrial Applications; Flow Applications in Aerospace; Flow Manipulation and Active Control: Theory, Experiments and Implementation; Multiscale Methods for Multiphase Flow; Noninvasive Measurements in Single and Multiphase Flows*. American Society of Mechanical Engineers, Aug. 03, 2014. doi: 10.1115/fedsm2014-22065.  
  
J. Finn, E. Shamsand S. V. Apte, “Modeling and simulation of multiple bubble entrainment and interactions with two dimensional vortical flows”, *Physics of Fluids*, vol. 23, no. 2. AIP Publishing, p. 023301, Feb. 2011. doi: 10.1063/1.3541813.  
  
C. D. Ghodke and S. V. Apte, “DNS of Oscillatory Boundary Layer Over a Closely Packed Layer of Sediment Particles”, *Volume 1A, Symposia: Advances in Fluids Engineering Education; Turbomachinery Flow Predictions and Optimization; Applications in CFD; Bio-Inspired Fluid Mechanics; Droplet-Surface Interactions; CFD Verification and Validation; Development and Applications of Immersed Boundary Methods; DNS, LES, and Hybrid RANS/LES Methods*. American Society of Mechanical Engineers, Aug. 03, 2014. doi: 10.1115/fedsm2014-21719.  
  
C. D. Ghodke, J. Skitkaand S. V. Apte, “Characterization of Oscillatory Boundary Layer over a Closely Packed Bed of Sediment Particles”, *The Journal of Computational Multiphase Flows*, vol. 6, no. 4. SAGE Publications, pp. 447–456, Dec. 2014. doi: 10.1260/1757-482x.6.4.447.  
  
X. He, S. V. Apte, J. R. Finnand B. D. Wood, “Characteristics of turbulence in a face-centred cubic porous unit cell”, *Journal of Fluid Mechanics*, vol. 873. Cambridge University Press (CUP), pp. 608–645, Jun. 25, 2019. doi: 10.1017/jfm.2019.403.  
  
T. R. Jackson, R. Haggerty, S. V. Apte, A. Colemanand K. J. Drost, “Defining and measuring the mean residence time of lateral surface transient storage zones in small streams”, *Water Resources Research*, vol. 48, no. 10. American Geophysical Union (AGU), Oct. 2012. doi: 10.1029/2012wr012096.  
  
T. R. Jackson, R. Haggerty, S. V. Apteand B. L. O’Connor, “A mean residence time relationship for lateral cavities in gravel-bed rivers and streams: Incorporating streambed roughness and cavity shape”, *Water Resources Research*, vol. 49, no. 6. American Geophysical Union (AGU), pp. 3642–3650, Jun. 2013. doi: 10.1002/wrcr.20272.  
  
V. Patil, “Experimental Versus Computational Methods in the Study of Flow in Porous Media”, *Volume 1D, Symposia: Transport Phenomena in Mixing; Turbulent Flows; Urban Fluid Mechanics; Fluid Dynamic Behavior of Complex Particles; Analysis of Elementary Processes in Dispersed Multiphase Flows; Multiphase Flow With Heat/Mass Transfer in Process Technology; Fluid Mechanics of Aircraft and Rocket Emissions and Their Environmental Impacts; High Performance CFD Computation; Performance of Multiphase Flow Systems; Wind Energy; Uncertainty Quantification in Flow Measurements and Simulations*. American Society of Mechanical Engineers, Aug. 03, 2014. doi: 10.1115/fedsm2014-21886.  
  
B. D. Wood, X. Heand S. V. Apte, “Modeling Turbulent Flows in Porous Media”, *Annual Review of Fluid Mechanics*, vol. 52, no. 1. Annual Reviews, pp. 171–203, Jan. 05, 2020. doi: 10.1146/annurev-fluid-010719-060317.  
  
C. D. Ghodke and S. V. Apte, “DNS study of particle-bed–turbulence interactions in an oscillatory wall-bounded flow”, *Journal of Fluid Mechanics*, vol. 792. Cambridge University Press (CUP), pp. 232–251, Mar. 01, 2016. doi: 10.1017/jfm.2016.85.  
  
B. D. Wood, “A comparison of measured and modeled velocity fields for a laminar flow in a porous medium”, *Advances in Water Resources*, vol. 85. Elsevier BV, pp. 45–63, Nov. 2015. doi: 10.1016/j.advwatres.2015.08.013.  
  
P. H. Pisciuneri, S. L. Yilmaz, P. A. Strakeyand P. Givi, “An Irregularly Portioned FDF Simulator”, *SIAM Journal on Scientific Computing*, vol. 35, no. 4. Society for Industrial & Applied Mathematics (SIAM), pp. C438–C452, Jan. 2013. doi: 10.1137/130911512.  
  
P. H. Pisciuneri, S. L. Yilmaz, P. A. Strakeyand P. Givi, “Massively Parallel FDF Simulation of Turbulent Reacting Flows”, *Mathematical Engineering*. Springer International Publishing, pp. 175–192, 2015. doi: 10.1007/978-3-319-18206-3\_8.  
  
A. Rastegari and R. Akhavan, “On the mechanism of turbulent drag reduction with super-hydrophobic surfaces”, *Journal of Fluid Mechanics*, vol. 773. Cambridge University Press (CUP), May 22, 2015. doi: 10.1017/jfm.2015.266.  
  
Y. Tang and R. Akhavan, “Computations of equilibrium and non-equilibrium turbulent channel flows using a nested-LES approach”, *Journal of Fluid Mechanics*, vol. 793. Cambridge University Press (CUP), pp. 709–748, Mar. 22, 2016. doi: 10.1017/jfm.2016.137.  
  
Z. K. Issa, C. W. Manke, B. P. Jenaand J. J. Potoff, “Ca2+ Bridging of Apposed Phospholipid Bilayers”, *The Journal of Physical Chemistry B*, vol. 114, no. 41. American Chemical Society (ACS), pp. 13249–13254, Sep. 13, 2010. doi: 10.1021/jp105781z.  
  
S. V. Kathuria, “Advances in turbulent mixing techniques to study microsecond protein folding reactions”, *Biopolymers*, vol. 99, no. 11. Wiley, pp. 888–896, Aug. 28, 2013. doi: 10.1002/bip.22355.  
  
Y. Song and J. B. Perot, “CFD Simulation of the NREL Phase VI Rotor”, *Wind Engineering*, vol. 39, no. 3. SAGE Publications, pp. 299–309, Jun. 2015. doi: 10.1260/0309-524x.39.3.299.  
  
T. P. Eiting, J. B. Perotand E. R. Dumont, “How much does nasal cavity morphology matter? Patterns and rates of olfactory airflow in phyllostomid bats”, *Proceedings of the Royal Society B: Biological Sciences*, vol. 282, no. 1800. The Royal Society, p. 20142161, Feb. 07, 2015. doi: 10.1098/rspb.2014.2161.  
  
A. Khajeh-Saeed and J. Blair Perot, “Direct numerical simulation of turbulence using GPU accelerated supercomputers”, *Journal of Computational Physics*, vol. 235. Elsevier BV, pp. 241–257, Feb. 2013. doi: 10.1016/j.jcp.2012.10.050.  
  
A. Khajeh-Saeed and J. B. Perot, “Computational Fluid Dynamics Simulations Using Many Graphics Processors”, *Computing in Science & Engineering*, vol. 14, no. 3. Institute of Electrical and Electronics Engineers (IEEE), pp. 10–19, May 2012. doi: 10.1109/mcse.2011.117.  
  
B. Koren, R. Abgrall, P. Bochev, J. Frankand B. Perot, “Physics-compatible numerical methods”, *Journal of Computational Physics*, vol. 257. Elsevier BV, p. 1039, Jan. 2014. doi: 10.1016/j.jcp.2013.10.015.  
  
M. B. Martell and J. B. Perot, “The Oriented-Eddy Collision Turbulence Model”, *Flow, Turbulence and Combustion*, vol. 89, no. 3. Springer Science and Business Media LLC, pp. 335–359, May 04, 2012. doi: 10.1007/s10494-012-9395-y.  
  
N. Athreyas, “Memristor-CMOS Analog Coprocessor for Acceleration of High-Performance Computing Applications”, *ACM Journal on Emerging Technologies in Computing Systems*, vol. 14, no. 3. Association for Computing Machinery (ACM), pp. 1–30, Jul. 31, 2018. doi: 10.1145/3269985.  
  
S. H. Bader, V. Inguvaand J. B. Perot, “Improving the efficiency of wind farms via wake manipulation”, *Wind Energy*, vol. 21, no. 12. Wiley, pp. 1239–1253, Jul. 30, 2018. doi: 10.1002/we.2226.  
  
J. Blair Perot and C. J. Zusi, “Differential forms for scientists and engineers”, *Journal of Computational Physics*, vol. 257. Elsevier BV, pp. 1373–1393, Jan. 2014. doi: 10.1016/j.jcp.2013.08.007.  
  
T. P. Eiting, T. D. Smith, J. B. Perotand E. R. Dumont, “The role of the olfactory recess in olfactory airflow”, *Journal of Experimental Biology*. The Company of Biologists, Jan. 01, 2014. doi: 10.1242/jeb.097402.  
  
V. Inguva, S. V. Kathuria, O. Bilseland B. J. Perot, “Computer design of microfluidic mixers for protein/RNA folding studies”, *PLOS ONE*, vol. 13, no. 6. Public Library of Science (PLoS), p. e0198534, Jun. 20, 2018. doi: 10.1371/journal.pone.0198534.  
  
V. Inguva, J. P. Rothstein, O. Bilseland B. J. Perot, “High-speed velocimetry in microfluidic protein mixers using confocal fluorescence decay microscopy”, *Experiments in Fluids*, vol. 59, no. 12. Springer Science and Business Media LLC, Nov. 09, 2018. doi: 10.1007/s00348-018-2630-0.  
  
K. Rao, P. Malanand J. B. Perot, “A stopping criterion for the iterative solution of partial differential equations”, *Journal of Computational Physics*, vol. 352. Elsevier BV, pp. 265–284, Jan. 2018. doi: 10.1016/j.jcp.2017.09.033.  
  
C. J. Zusi and J. B. Perot, “Simulation and modeling of turbulence subjected to a period of uniform plane strain”, *Physics of Fluids*, vol. 25, no. 11. AIP Publishing, p. 110819, Nov. 2013. doi: 10.1063/1.4821450.  
  
C. J. Zusi and J. B. Perot, “Simulation and modeling of turbulence subjected to a period of axisymmetric contraction or expansion”, *Physics of Fluids*, vol. 26, no. 11. AIP Publishing, p. 115103, Nov. 2014. doi: 10.1063/1.4901188.  
  
R. Xiong, S. I. Sandlerand D. G. Vlachos, “Alcohol Adsorption onto Silicalite from Aqueous Solution”, *The Journal of Physical Chemistry C*, vol. 115, no. 38. American Chemical Society (ACS), pp. 18659–18669, Sep. 08, 2011. doi: 10.1021/jp205312k.  
  
R. Xiong, S. I. Sandlerand D. G. Vlachos, “Molecular Screening of Alcohol and Polyol Adsorption onto MFI-Type Zeolites”, *Langmuir*, vol. 28, no. 9. American Chemical Society (ACS), pp. 4491–4499, Feb. 22, 2012. doi: 10.1021/la204710j.  
  
J. Capecelatro, D. J. Bodonyand J. B. Freund, “Adjoint-based sensitivity and ignition threshold mapping in a turbulent mixing layer”, *Combustion Theory and Modelling*, vol. 23, no. 1. Informa UK Limited, pp. 147–179, Jul. 11, 2018. doi: 10.1080/13647830.2018.1495342.  
  
J. Kim, D. J. Bodonyand J. B. Freund, “Adjoint-based control of loud events in a turbulent jet”, *Journal of Fluid Mechanics*, vol. 741. Cambridge University Press (CUP), pp. 28–59, Feb. 07, 2014. doi: 10.1017/jfm.2013.654.  
  
A. Mishra and D. J. Bodony, “Evaluation of actuator disk theory for predicting indirect combustion noise”, *Journal of Sound and Vibration*, vol. 332, no. 4. Elsevier BV, pp. 821–838, Feb. 2013. doi: 10.1016/j.jsv.2012.09.025.  
  
M. Natarajan, J. B. Freundand D. J. Bodony, “Actuator selection and placement for localized feedback flow control”, *Journal of Fluid Mechanics*, vol. 809. Cambridge University Press (CUP), pp. 775–792, Nov. 18, 2016. doi: 10.1017/jfm.2016.700.  
  
C. M. Ostoich, D. J. Bodonyand P. H. Geubelle, “Interaction of a Mach 2.25 turbulent boundary layer with a fluttering panel using direct numerical simulation”, *Physics of Fluids*, vol. 25, no. 11. AIP Publishing, p. 110806, Nov. 2013. doi: 10.1063/1.4819350.  
  
N. Shahriari, D. J. Bodony, A. Hanifiand D. S. Henningson, “Acoustic receptivity simulations of flow past a flat plate with elliptic leading edge”, *Journal of Fluid Mechanics*, vol. 800. Cambridge University Press (CUP), Jul. 13, 2016. doi: 10.1017/jfm.2016.433.  
  
N. Sharan, C. Pantanoand D. J. Bodony, “Time-stable overset grid method for hyperbolic problems using summation-by-parts operators”, *Journal of Computational Physics*, vol. 361. Elsevier BV, pp. 199–230, May 2018. doi: 10.1016/j.jcp.2018.01.049.  
  
M. M. Sucheendran, D. J. Bodonyand P. H. Geubelle, “Coupled Structural-Acoustic Response of a Duct-Mounted Elastic Plate with Grazing Flow”, *AIAA Journal*, vol. 52, no. 1. American Institute of Aeronautics and Astronautics (AIAA), pp. 178–194, Jan. 2014. doi: 10.2514/1.j052168.  
  
R. Vishnampet, D. J. Bodonyand J. B. Freund, “A practical discrete-adjoint method for high-fidelity compressible turbulence simulations”, *Journal of Computational Physics*, vol. 285. Elsevier BV, pp. 173–192, Mar. 2015. doi: 10.1016/j.jcp.2015.01.009.  
  
Q. Zhang and D. J. Bodony, “Numerical investigation and modelling of acoustically excited flow through a circular orifice backed by a hexagonal cavity”, *Journal of Fluid Mechanics*, vol. 693. Cambridge University Press (CUP), pp. 367–401, Jan. 18, 2012. doi: 10.1017/jfm.2011.537.  
  
Q. Zhang and D. J. Bodony, “Numerical investigation of a honeycomb liner grazed by laminar and turbulent boundary layers”, *Journal of Fluid Mechanics*, vol. 792. Cambridge University Press (CUP), pp. 936–980, Mar. 08, 2016. doi: 10.1017/jfm.2016.79.  
  
N. Nangia, R. Bale, N. Chen, Y. Hannaand N. A. Patankar, “Optimal specific wavelength for maximum thrust production in undulatory propulsion”, *PLOS ONE*, vol. 12, no. 6. Public Library of Science (PLoS), p. e0179727, Jun. 27, 2017. doi: 10.1371/journal.pone.0179727.  
  
N. K. Patel, A. P. Singh Bhallaand N. A. Patankar, “A new constraint-based formulation for hydrodynamically resolved computational neuromechanics of swimming animals”, *Journal of Computational Physics*, vol. 375. Elsevier BV, pp. 684–716, Dec. 2018. doi: 10.1016/j.jcp.2018.08.035.  
  
J. Kim and S. B. Pope, “Effects of combined dimension reduction and tabulation on the simulations of a turbulent premixed flame using a large-eddy simulation/probability density function method”, *Combustion Theory and Modelling*, vol. 18, no. 3. Informa UK Limited, pp. 388–413, May 04, 2014. doi: 10.1080/13647830.2014.919411.  
  
P. P. Popov and S. B. Pope, “Implicit and explicit schemes for mass consistency preservation in hybrid particle/finite-volume algorithms for turbulent reactive flows”, *Journal of Computational Physics*, vol. 257. Elsevier BV, pp. 352–373, Jan. 2014. doi: 10.1016/j.jcp.2013.09.005.  
  
T. A. Alam, Q. L. Pham, V. I. Sikavitsas, D. V. Papavassiliou, R. L. Shambaughand R. S. Voronov, “Image-based modeling: A novel tool for realistic simulations of artificial bone cultures”, *TECHNOLOGY*, vol. 4, no. 4. World Scientific Pub Co Pte Ltd, pp. 229–233, Dec. 2016. doi: 10.1142/s233954781620003x.  
  
K. Bui, B. P. Grady, M. C. Sahaand D. V. Papavassiliou, “Effect of carbon nanotube persistence length on heat transfer in nanocomposites: A simulation approach”, *Applied Physics Letters*, vol. 102, no. 20. AIP Publishing, p. 203116, May 20, 2013. doi: 10.1063/1.4807769.  
  
K. Bui and D. V. Papavassiliou, “Numerical Calculation of the Effective Thermal Conductivity of Nanocomposites”, *Numerical Heat Transfer, Part A: Applications*, vol. 63, no. 8. Informa UK Limited, pp. 590–603, Apr. 15, 2013. doi: 10.1080/10407782.2013.742813.  
  
F. Gong, K. Bui, D. V. Papavassiliouand H. M. Duong, “Thermal transport phenomena and limitations in heterogeneous polymer composites containing carbon nanotubes and inorganic nanoparticles”, *Carbon*, vol. 78. Elsevier BV, pp. 305–316, Nov. 2014. doi: 10.1016/j.carbon.2014.07.007.  
  
F. Gong, H. M. Duongand D. V. Papavassiliou, “Inter-Carbon Nanotube Contact and Thermal Resistances in Heat Transport of Three-Phase Composites”, *The Journal of Physical Chemistry C*, vol. 119, no. 14. American Chemical Society (ACS), pp. 7614–7620, Mar. 25, 2015. doi: 10.1021/acs.jpcc.5b00651.  
  
F. Gong, Z. Hongyan, D. V. Papavassiliou, K. Bui, C. Limand H. M. Duong, “Mesoscopic modeling of cancer photothermal therapy using single-walled carbon nanotubes and near infrared radiation: insights through an off-lattice Monte Carlo approach”, *Nanotechnology*, vol. 25, no. 20. IOP Publishing, p. 205101, Apr. 30, 2014. doi: 10.1088/0957-4484/25/20/205101.  
  
F. Gong, D. V. Papavassiliouand H. M. Duong, “Off-Lattice Monte Carlo Simulation of Heat Transfer through Carbon Nanotube Multiphase Systems Taking into Account Thermal Boundary Resistances”, *Numerical Heat Transfer, Part A: Applications*, vol. 65, no. 11. Informa UK Limited, pp. 1023–1043, Mar. 17, 2014. doi: 10.1080/10407782.2013.850972.  
  
A. K. Karna and D. V. Papavassiliou, “Near-wall velocity structures that drive turbulent transport from a line source at the wall”, *Physics of Fluids*, vol. 24, no. 3. AIP Publishing, p. 035102, Mar. 2012. doi: 10.1063/1.3689194.  
  
Q. Nguyen and D. Papavassiliou, “Quality Measures of Mixing in Turbulent Flow and Effects of Molecular Diffusivity”, *Fluids*, vol. 3, no. 3. MDPI AG, p. 53, Jul. 30, 2018. doi: 10.3390/fluids3030053.  
  
Q. Nguyen, C. Srinivasanand D. V. Papavassiliou, “Flow-induced separation in wall turbulence”, *Physical Review E*, vol. 91, no. 3. American Physical Society (APS), Mar. 27, 2015. doi: 10.1103/physreve.91.033019.  
  
V. Nguyen and D. V. Papavassiliou, “Hydrodynamic Dispersion in Porous Media and the Significance of Lagrangian Time and Space Scales”, *Fluids*, vol. 5, no. 2. MDPI AG, p. 79, May 21, 2020. doi: 10.3390/fluids5020079.  
  
N. H. Pham, J. H. Harwell, D. E. Resasco, D. V. Papavassiliou, C. Chenand B. Shiau, “Transport and deposition kinetics of polymer-coated multiwalled carbon nanotubes in packed beds”, *AIChE Journal*, vol. 62, no. 10. Wiley, pp. 3774–3783, Apr. 28, 2016. doi: 10.1002/aic.15273.  
  
N. H. Pham and D. V. Papavassiliou, “Flow Recovery Downstream from Nanoposts Grown at the Wall of a Microchannel”, *Nanoscale and Microscale Thermophysical Engineering*, vol. 18, no. 1. Informa UK Limited, pp. 1–17, Jan. 02, 2014. doi: 10.1080/15567265.2013.787568.  
  
N. H. Pham, D. P. Swatske, J. H. Harwell, B.-J. Shiauand D. V. Papavassiliou, “Transport of nanoparticles and kinetics in packed beds: A numerical approach with lattice Boltzmann simulations and particle tracking”, *International Journal of Heat and Mass Transfer*, vol. 72. Elsevier BV, pp. 319–328, May 2014. doi: 10.1016/j.ijheatmasstransfer.2013.12.075.  
  
C. Srinivasan and D. V. Papavassiliou, “Direction of scalar transport in turbulent channel flow”, *Physics of Fluids*, vol. 23, no. 11. AIP Publishing, p. 115105, Nov. 2011. doi: 10.1063/1.3657825.  
  
C. Srinivasan and D. V. Papavassiliou, “Heat Transfer Scaling Close to the Wall for Turbulent Channel Flows”, *Applied Mechanics Reviews*, vol. 65, no. 3. ASME International, May 01, 2013. doi: 10.1115/1.4024428.  
  
S. B. VanGordon, R. S. Voronov, T. B. Blue, R. L. Shambaugh, D. V. Papavassiliouand V. I. Sikavitsas, “Effects of Scaffold Architecture on Preosteoblastic Cultures under Continuous Fluid Shear”, *Industrial & Engineering Chemistry Research*, vol. 50, no. 2. American Chemical Society (ACS), pp. 620–629, Jan. 19, 2011. doi: 10.1021/ie902041v.  
  
M. D. Vo and D. V. Papavassiliou, “Physical adsorption of polyvinyl pyrrolidone on carbon nanotubes under shear studied with dissipative particle dynamics simulations”, *Carbon*, vol. 100. Elsevier BV, pp. 291–301, Apr. 2016. doi: 10.1016/j.carbon.2015.12.105.  
  
M. Vo and D. Papavassiliou, “Effect of Sodium Dodecyl Sulfate Adsorption on the Behavior of Water inside Single Walled Carbon Nanotubes with Dissipative Particle Dynamics Simulation”, *Molecules*, vol. 21, no. 4. MDPI AG, p. 500, Apr. 15, 2016. doi: 10.3390/molecules21040500.  
  
M. D. Vo and D. V. Papavassiliou, “Interaction between polymer-coated carbon nanotubes with coarse-grained computations”, *Chemical Physics Letters*, vol. 685. Elsevier BV, pp. 77–83, Oct. 2017. doi: 10.1016/j.cplett.2017.07.037.  
  
M. D. Vo and D. V. Papavassiliou, “Effects of Temperature and Shear on the Adsorption of Surfactants on Carbon Nanotubes”, *The Journal of Physical Chemistry C*, vol. 121, no. 26. American Chemical Society (ACS), pp. 14339–14348, Jun. 26, 2017. doi: 10.1021/acs.jpcc.7b03904.  
  
M. D. Vo, B. Shiau, J. H. Harwelland D. V. Papavassiliou, “Adsorption of anionic and non-ionic surfactants on carbon nanotubes in water with dissipative particle dynamics simulation”, *The Journal of Chemical Physics*, vol. 144, no. 20. AIP Publishing, p. 204701, May 28, 2016. doi: 10.1063/1.4949364.  
  
R. S. Voronov, S. B. VanGordon, R. L. Shambaugh, D. V. Papavassiliouand V. I. Sikavitsas, “3D Tissue-Engineered Construct Analysis via Conventional High-Resolution Microcomputed Tomography Without X-Ray Contrast”, *Tissue Engineering Part C: Methods*, vol. 19, no. 5. Mary Ann Liebert Inc, pp. 327–335, May 2013. doi: 10.1089/ten.tec.2011.0612.  
  
R. Voronov, S. VanGordon, V. I. Sikavitsasand D. V. Papavassiliou, “Computational modeling of flow-induced shear stresses within 3D salt-leached porous scaffolds imaged via micro-CT”, *Journal of Biomechanics*, vol. 43, no. 7. Elsevier BV, pp. 1279–1286, May 2010. doi: 10.1016/j.jbiomech.2010.01.007.  
  
T. V. Vu and D. V. Papavassiliou, “Modification of Oil–Water Interfaces by Surfactant-Stabilized Carbon Nanotubes”, *The Journal of Physical Chemistry C*, vol. 122, no. 48. American Chemical Society (ACS), pp. 27734–27744, Nov. 06, 2018. doi: 10.1021/acs.jpcc.8b08735.  
  
T. V. Vu and D. V. Papavassiliou, “Synergistic effects of surfactants and heterogeneous nanoparticles at oil-water interface: Insights from computations”, *Journal of Colloid and Interface Science*, vol. 553. Elsevier BV, pp. 50–58, Oct. 2019. doi: 10.1016/j.jcis.2019.05.102.  
  
F. Gong, “Effective thermal transport properties in multiphase biological systems containing carbon nanomaterials”, *RSC Advances*, vol. 7, no. 22. Royal Society of Chemistry (RSC), pp. 13615–13622, 2017. doi: 10.1039/c6ra27768c.  
  
Q. Nguyen and D. V. Papavassiliou, “A statistical model to predict streamwise turbulent dispersion from the wall at small times”, *Physics of Fluids*, vol. 28, no. 12. AIP Publishing, p. 125103, Dec. 2016. doi: 10.1063/1.4968182.  
  
Q. Nguyen and D. V. Papavassiliou, “Scalar mixing in anisotropic turbulent flow”, *AIChE Journal*, vol. 64, no. 7. Wiley, pp. 2803–2815, Feb. 08, 2018. doi: 10.1002/aic.16104.  
  
M. Ozturk, E. A. O’Rearand D. V. Papavassiliou, “Hemolysis Related to Turbulent Eddy Size Distributions Using Comparisons of Experiments to Computations”, *Artificial Organs*, vol. 39, no. 12. Wiley, pp. E227–E239, Sep. 28, 2015. doi: 10.1111/aor.12572.  
  
Q. Nguyen, S. Feherand D. Papavassiliou, “Lagrangian Modeling of Turbulent Dispersion from Instantaneous Point Sources at the Center of a Turbulent Flow Channel”, *Fluids*, vol. 2, no. 3. MDPI AG, p. 46, Sep. 08, 2017. doi: 10.3390/fluids2030046.  
  
N. H. Pham and D. V. Papavassiliou, “Nanoparticle transport in heterogeneous porous media with particle tracking numerical methods”, *Computational Particle Mechanics*, vol. 4, no. 1. Springer Science and Business Media LLC, pp. 87–100, Aug. 27, 2016. doi: 10.1007/s40571-016-0130-7.  
  
N. H. Pham and D. V. Papavassiliou, “Effect of spatial distribution of porous matrix surface charge heterogeneity on nanoparticle attachment in a packed bed”, *Physics of Fluids*, vol. 29, no. 8. AIP Publishing, p. 082007, Aug. 2017. doi: 10.1063/1.4999344.  
  
N. H. Pham and D. V. Papavassiliou, “Hydrodynamic effects on the aggregation of nanoparticles in porous media”, *International Journal of Heat and Mass Transfer*, vol. 121. Elsevier BV, pp. 477–487, Jun. 2018. doi: 10.1016/j.ijheatmasstransfer.2017.12.150.  
  
M. Vo and D. V. Papavassiliou, “Interaction parameters between carbon nanotubes and water in Dissipative Particle Dynamics”, *Molecular Simulation*, vol. 42, no. 9. Informa UK Limited, pp. 737–744, Oct. 2015. doi: 10.1080/08927022.2015.1089989.  
  
T. V. Vu and D. V. Papavassiliou, “Oil-water interfaces with surfactants: A systematic approach to determine coarse-grained model parameters”, *The Journal of Chemical Physics*, vol. 148, no. 20. AIP Publishing, p. 204704, May 28, 2018. doi: 10.1063/1.5022798.  
  
J. Capecelatro and O. Desjardins, “Eulerian–Lagrangian modeling of turbulent liquid–solid slurries in horizontal pipes”, *International Journal of Multiphase Flow*, vol. 55. Elsevier BV, pp. 64–79, Oct. 2013. doi: 10.1016/j.ijmultiphaseflow.2013.04.006.  
  
J. Capecelatro and O. Desjardins, “An Euler–Lagrange strategy for simulating particle-laden flows”, *Journal of Computational Physics*, vol. 238. Elsevier BV, pp. 1–31, Apr. 2013. doi: 10.1016/j.jcp.2012.12.015.  
  
J. Capecelatro, O. Desjardinsand R. O. Fox, “Numerical study of collisional particle dynamics in cluster-induced turbulence”, *Journal of Fluid Mechanics*, vol. 747. Cambridge University Press (CUP), Apr. 23, 2014. doi: 10.1017/jfm.2014.194.  
  
J. Capecelatro, P. Pepiotand O. Desjardins, “Numerical characterization and modeling of particle clustering in wall-bounded vertical risers”, *Chemical Engineering Journal*, vol. 245. Elsevier BV, pp. 295–310, Jun. 2014. doi: 10.1016/j.cej.2014.02.040.  
  
O. Desjardins, J. McCaslin, M. Owkesand P. Brady, “DIRECT NUMERICAL AND LARGE-EDDY SIMULATION OF PRIMARY ATOMIZATION IN COMPLEX GEOMETRIES”, *Atomization and Sprays*, vol. 23, no. 11. Begell House, pp. 1001–1048, 2013. doi: 10.1615/atomizspr.2013007679.  
  
K. Luo, H. Pitsch, M. G. Paiand O. Desjardins, “Direct numerical simulations and analysis of three-dimensional n-heptane spray flames in a model swirl combustor”, *Proceedings of the Combustion Institute*, vol. 33, no. 2. Elsevier BV, pp. 2143–2152, Jan. 2011. doi: 10.1016/j.proci.2010.06.077.  
  
J. O. McCaslin and O. Desjardins, “Numerical investigation of gravitational effects in horizontal annular liquid–gas flow”, *International Journal of Multiphase Flow*, vol. 67. Elsevier BV, pp. 88–105, Dec. 2014. doi: 10.1016/j.ijmultiphaseflow.2014.08.006.  
  
P. Pepiot and O. Desjardins, “Numerical analysis of the dynamics of two- and three-dimensional fluidized bed reactors using an Euler–Lagrange approach”, *Powder Technology*, vol. 220. Elsevier BV, pp. 104–121, Apr. 2012. doi: 10.1016/j.powtec.2011.09.021.  
  
B. P. Van Poppel, O. Desjardinsand J. W. Daily, “A ghost fluid, level set methodology for simulating multiphase electrohydrodynamic flows with application to liquid fuel injection”, *Journal of Computational Physics*, vol. 229, no. 20. Elsevier BV, pp. 7977–7996, Oct. 2010. doi: 10.1016/j.jcp.2010.07.003.  
  
J. T. Buchman, “Research highlights: examining the effect of shape on nanoparticle interactions with organisms”, *Environmental Science: Nano*, vol. 3, no. 4. Royal Society of Chemistry (RSC), pp. 696–700, 2016. doi: 10.1039/c6en90015a.  
  
J. T. Buchman, “Using an environmentally-relevant panel of Gram-negative bacteria to assess the toxicity of polyallylamine hydrochloride-wrapped gold nanoparticles”, *Environmental Science: Nano*, vol. 5, no. 2. Royal Society of Chemistry (RSC), pp. 279–288, 2018. doi: 10.1039/c7en00832e.  
  
H. R. Bureau, D. R. Merz, E. Hershkovits, S. Quirkand R. Hernandez, “Constrained Unfolding of a Helical Peptide: Implicit versus Explicit Solvents”, *PLOS ONE*, vol. 10, no. 5. Public Library of Science (PLoS), p. e0127034, May 13, 2015. doi: 10.1371/journal.pone.0127034.  
  
G. Chong, “Defects in Self-Assembled Monolayers on Nanoparticles Prompt Phospholipid Extraction and Bilayer-Curvature-Dependent Deformations”, *The Journal of Physical Chemistry C*, vol. 123, no. 45. American Chemical Society (ACS), pp. 27951–27958, Oct. 23, 2019. doi: 10.1021/acs.jpcc.9b08583.  
  
G. Chong and R. Hernandez, “Adsorption Dynamics and Structure of Polycations on Citrate-Coated Gold Nanoparticles”, *The Journal of Physical Chemistry C*, vol. 122, no. 34. American Chemical Society (ACS), pp. 19962–19969, Aug. 01, 2018. doi: 10.1021/acs.jpcc.8b05202.  
  
G. Chong, E. D. Laudadio, M. Wu, C. J. Murphy, R. J. Hamersand R. Hernandez, “Density, Structure, and Stability of Citrate3– and H2citrate– on Bare and Coated Gold Nanoparticles”, *The Journal of Physical Chemistry C*, vol. 122, no. 49. American Chemical Society (ACS), pp. 28393–28404, Nov. 19, 2018. doi: 10.1021/acs.jpcc.8b09666.  
  
Q. Cui, R. Hernandez, S. E. Mason, T. Frauenheim, J. A. Pedersenand F. Geiger, “Sustainable Nanotechnology: Opportunities and Challenges for Theoretical/Computational Studies”, *The Journal of Physical Chemistry B*, vol. 120, no. 30. American Chemical Society (ACS), pp. 7297–7306, Jul. 13, 2016. doi: 10.1021/acs.jpcb.6b03976.  
  
M. C. Hagy and R. Hernandez, “Dynamical simulation of dipolar Janus colloids: Equilibrium structure and thermodynamics”, *The Journal of Chemical Physics*, vol. 137, no. 4. AIP Publishing, p. 044505, Jul. 28, 2012. doi: 10.1063/1.4737432.  
  
M. C. Hagy and R. Hernandez, “Dynamical simulation of dipolar Janus colloids: Dynamical properties”, *The Journal of Chemical Physics*, vol. 138, no. 18. AIP Publishing, p. 184903, May 14, 2013. doi: 10.1063/1.4803864.  
  
M. C. Hagy and R. Hernandez, “Dynamical simulation of electrostatic striped colloidal particles”, *The Journal of Chemical Physics*, vol. 140, no. 3. AIP Publishing, p. 034701, Jan. 21, 2014. doi: 10.1063/1.4859855.  
  
B. D. Mahala and R. Hernandez, “Order parameters in the diffusion of rods through two- and three-dimensional fixed scatterers”, *Physical Review E*, vol. 98, no. 4. American Physical Society (APS), Oct. 29, 2018. doi: 10.1103/physreve.98.042607.  
  
E. S. Melby, “Peripheral Membrane Proteins Facilitate Nanoparticle Binding at Lipid Bilayer Interfaces”, *Langmuir*, vol. 34, no. 36. American Chemical Society (ACS), pp. 10793–10805, Aug. 13, 2018. doi: 10.1021/acs.langmuir.8b02060.  
  
L. L. Olenick, “Lipid Corona Formation from Nanoparticle Interactions with Bilayers”, *Chem*, vol. 4, no. 11. Elsevier BV, pp. 2709–2723, Nov. 2018. doi: 10.1016/j.chempr.2018.09.018.  
  
G. Ozer, S. Quirkand R. Hernandez, “Thermodynamics of Decaalanine Stretching in Water Obtained by Adaptive Steered Molecular Dynamics Simulations”, *Journal of Chemical Theory and Computation*, vol. 8, no. 11. American Chemical Society (ACS), pp. 4837–4844, Oct. 24, 2012. doi: 10.1021/ct300709u.  
  
S. Quirk, “Mutational Analysis of Neuropeptide Y Reveals Unusual Thermal Stability Linked to Higher-Order Self-Association”, *ACS Omega*, vol. 3, no. 2. American Chemical Society (ACS), pp. 2141–2154, Feb. 21, 2018. doi: 10.1021/acsomega.7b01949.  
  
R. S. Singh and R. Hernandez, “Modeling soft core-shell colloids using stochastic hard collision dynamics”, *Chemical Physics Letters*, vol. 708. Elsevier BV, pp. 233–240, Sep. 2018. doi: 10.1016/j.cplett.2018.08.032.  
  
E. J. Tollefson, “Preferential Binding of Cytochrome *c* to Anionic Ligand-Coated Gold Nanoparticles: A Complementary Computational and Experimental Approach”, *ACS Nano*, vol. 13, no. 6. American Chemical Society (ACS), pp. 6856–6866, May 13, 2019. doi: 10.1021/acsnano.9b01622.  
  
I. S. Ulusoy, D. A. Andrienko, I. D. Boydand R. Hernandez, “Erratum: “Quantum and quasi-classical collisional dynamics of O2–Ar at high temperatures” [J. Chem. Phys. 144, 234311 (2016)]”, *The Journal of Chemical Physics*, vol. 145, no. 23. AIP Publishing, p. 239902, Dec. 21, 2016. doi: 10.1063/1.4972054.  
  
I. S. Ulusoy, D. Andrienko, I. D. Boydand R. Hernandez, “Quantal treatment of O2–Ar vibrational relaxation at hypersonic temperatures”, *55th AIAA Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 05, 2017. doi: 10.2514/6.2017-0661.  
  
I. S. Ulusoy and R. Hernandez, “Revisiting roaming trajectories in ketene isomerization at higher dimensionality”, *Theoretical Chemistry Accounts*, vol. 133, no. 9. Springer Science and Business Media LLC, Jul. 15, 2014. doi: 10.1007/s00214-014-1528-z.  
  
I. S. Ulusoy, J. F. Stantonand R. Hernandez, “Correction to “Effects of Roaming Trajectories on the Transition State Theory Rates of a Reduced-Dimensional Model of Ketene Isomerization””, *The Journal of Physical Chemistry A*, vol. 117, no. 40. American Chemical Society (ACS), pp. 10567–10568, Oct. 01, 2013. doi: 10.1021/jp408997z.  
  
I. S. Ulusoy, J. F. Stantonand R. Hernandez, “Effects of Roaming Trajectories on the Transition State Theory Rates of a Reduced-Dimensional Model of Ketene Isomerization”, *The Journal of Physical Chemistry A*, vol. 117, no. 32. American Chemical Society (ACS), pp. 7553–7560, Jul. 02, 2013. doi: 10.1021/jp402322h.  
  
M. Wu, “Solution NMR Analysis of Ligand Environment in Quaternary Ammonium-Terminated Self-Assembled Monolayers on Gold Nanoparticles: The Effect of Surface Curvature and Ligand Structure”, *Journal of the American Chemical Society*, vol. 141, no. 10. American Chemical Society (ACS), pp. 4316–4327, Feb. 14, 2019. doi: 10.1021/jacs.8b11445.  
  
G. Ozer, S. Quirkand R. Hernandez, “Adaptive steered molecular dynamics: Validation of the selection criterion and benchmarking energetics in vacuum”, *The Journal of Chemical Physics*, vol. 136, no. 21. AIP Publishing, p. 215104, Jun. 07, 2012. doi: 10.1063/1.4725183.  
  
G. Ozer, E. F. Valeev, S. Quirkand R. Hernandez, “Adaptive Steered Molecular Dynamics of the Long-Distance Unfolding of Neuropeptide Y”, *Journal of Chemical Theory and Computation*, vol. 6, no. 10. American Chemical Society (ACS), pp. 3026–3038, Sep. 14, 2010. doi: 10.1021/ct100320g.  
  
H. R. Bureau, E. Hershkovits, S. Quirkand R. Hernandez, “Determining the Energetics of Small β-Sheet Peptides using Adaptive Steered Molecular Dynamics”, *Journal of Chemical Theory and Computation*, vol. 12, no. 4. American Chemical Society (ACS), pp. 2028–2037, Mar. 10, 2016. doi: 10.1021/acs.jctc.5b01110.  
  
I. S. Ulusoy, D. A. Andrienko, I. D. Boydand R. Hernandez, “Quantum and quasi-classical collisional dynamics of O2–Ar at high temperatures”, *The Journal of Chemical Physics*, vol. 144, no. 23. AIP Publishing, p. 234311, Jun. 21, 2016. doi: 10.1063/1.4954041.  
  
S. C. Ammal and A. Heyden, “Reaction kinetics of the electrochemical oxidation of CO and syngas fuels on a Sr2Fe1.5Mo0.5O6−δ perovskite anode”, *Journal of Materials Chemistry A*, vol. 3, no. 43. Royal Society of Chemistry (RSC), pp. 21618–21629, 2015. doi: 10.1039/c5ta05056a.  
  
S. C. Ammal and A. Heyden, “Water-Gas Shift Activity of Atomically Dispersed Cationic Platinum versus Metallic Platinum Clusters on Titania Supports”, *ACS Catalysis*, vol. 7, no. 1. American Chemical Society (ACS), pp. 301–309, Dec. 08, 2016. doi: 10.1021/acscatal.6b02764.  
  
S. C. Ammal and A. Heyden, “Titania‐Supported Single‐Atom Platinum Catalyst for Water‐Gas Shift Reaction”, *Chemie Ingenieur Technik*, vol. 89, no. 10. Wiley, pp. 1343–1349, Sep. 05, 2017. doi: 10.1002/cite.201700046.  
  
S. Behtash, J. Lu, O. Mamun, C. T. Williams, J. R. Monnierand A. Heyden, “Solvation Effects in the Hydrodeoxygenation of Propanoic Acid over a Model Pd(211) Catalyst”, *The Journal of Physical Chemistry C*, vol. 120, no. 5. American Chemical Society (ACS), pp. 2724–2736, Feb. 01, 2016. doi: 10.1021/acs.jpcc.5b10419.  
  
S. Behtash, J. Lu, E. Walker, O. Mamunand A. Heyden, “Solvent effects in the liquid phase hydrodeoxygenation of methyl propionate over a Pd(1 1 1) catalyst model”, *Journal of Catalysis*, vol. 333. Elsevier BV, pp. 171–183, Jan. 2016. doi: 10.1016/j.jcat.2015.10.027.  
  
S. Behtash, J. Lu, C. T. Williams, J. R. Monnierand A. Heyden, “Effect of Palladium Surface Structure on the Hydrodeoxygenation of Propanoic Acid: Identification of Active Sites”, *The Journal of Physical Chemistry C*, vol. 119, no. 4. American Chemical Society (ACS), pp. 1928–1942, Jan. 16, 2015. doi: 10.1021/jp511618u.  
  
A. J. Chowdhury, W. Yang, E. Walker, O. Mamun, A. Heydenand G. A. Terejanu, “Prediction of Adsorption Energies for Chemical Species on Metal Catalyst Surfaces Using Machine Learning”, *The Journal of Physical Chemistry C*, vol. 122, no. 49. American Chemical Society (ACS), pp. 28142–28150, Nov. 09, 2018. doi: 10.1021/acs.jpcc.8b09284.  
  
A. S. Duke, “*In Situ* Ambient Pressure X-ray Photoelectron Spectroscopy Studies of Methanol Oxidation on Pt(111) and Pt–Re Alloys”, *The Journal of Physical Chemistry C*, vol. 119, no. 40. American Chemical Society (ACS), pp. 23082–23093, Sep. 23, 2015. doi: 10.1021/acs.jpcc.5b07625.  
  
A. S. Duke, “Understanding Active Sites in the Water–Gas Shift Reaction for Pt–Re Catalysts on Titania”, *ACS Catalysis*, vol. 7, no. 4. American Chemical Society (ACS), pp. 2597–2606, Mar. 15, 2017. doi: 10.1021/acscatal.7b00086.  
  
M. Faheem, M. Saleheen, J. Luand A. Heyden, “Ethylene glycol reforming on Pt(111): first-principles microkinetic modeling in vapor and aqueous phases”, *Catalysis Science & Technology*, vol. 6, no. 23. Royal Society of Chemistry (RSC), pp. 8242–8256, 2016. doi: 10.1039/c6cy02111e.  
  
M. Faheem, S. Suthirakunand A. Heyden, “New Implicit Solvation Scheme for Solid Surfaces”, *The Journal of Physical Chemistry C*, vol. 116, no. 42. American Chemical Society (ACS), pp. 22458–22462, Oct. 16, 2012. doi: 10.1021/jp308212h.  
  
M. Faheem, S. Suthirakunand A. Heyden, “New Implicit Solvation Scheme for Solid Surfaces”, *The Journal of Physical Chemistry C*, vol. 116, no. 42. American Chemical Society (ACS), pp. 22458–22462, Oct. 16, 2012. doi: 10.1021/jp308212h.  
  
M. Faheem, S. Suthirakunand A. Heyden, “New Implicit Solvation Scheme for Solid Surfaces”, *The Journal of Physical Chemistry C*, vol. 116, no. 42. American Chemical Society (ACS), pp. 22458–22462, Oct. 16, 2012. doi: 10.1021/jp308212h.  
  
Y. K. Lugo-José, S. Behtash, M. Nicholson, J. R. Monnier, A. Heydenand C. T. Williams, “Unraveling the mechanism of propanoic acid hydrodeoxygenation on palladium using deuterium kinetic isotope effects”, *Journal of Molecular Catalysis A: Chemical*, vol. 406. Elsevier BV, pp. 85–93, Sep. 2015. doi: 10.1016/j.molcata.2015.05.019.  
  
J. Lu, S. Behtash, O. Mamunand A. Heyden, “Theoretical Investigation of the Reaction Mechanism of the Guaiacol Hydrogenation over a Pt(111) Catalyst”, *ACS Catalysis*, vol. 5, no. 4. American Chemical Society (ACS), pp. 2423–2435, Mar. 16, 2015. doi: 10.1021/cs5016244.  
  
J. Lu, M. Faheem, S. Behtashand A. Heyden, “Theoretical investigation of the decarboxylation and decarbonylation mechanism of propanoic acid over a Ru(0 0 0 1) model surface”, *Journal of Catalysis*, vol. 324. Elsevier BV, pp. 14–24, Apr. 2015. doi: 10.1016/j.jcat.2015.01.005.  
  
J. Lu and A. Heyden, “Theoretical investigation of the reaction mechanism of the hydrodeoxygenation of guaiacol over a Ru(0 0 0 1) model surface”, *Journal of Catalysis*, vol. 321. Elsevier BV, pp. 39–50, Jan. 2015. doi: 10.1016/j.jcat.2014.11.003.  
  
M. Saleheen and A. Heyden, “Liquid-Phase Modeling in Heterogeneous Catalysis”, *ACS Catalysis*, vol. 8, no. 3. American Chemical Society (ACS), pp. 2188–2194, Feb. 07, 2018. doi: 10.1021/acscatal.7b04367.  
  
E. Walker, S. C. Ammal, G. A. Terejanuand A. Heyden, “Uncertainty Quantification Framework Applied to the Water–Gas Shift Reaction over Pt-Based Catalysts”, *The Journal of Physical Chemistry C*, vol. 120, no. 19. American Chemical Society (ACS), pp. 10328–10339, May 11, 2016. doi: 10.1021/acs.jpcc.6b01348.  
  
E. A. Walker, D. Mitchell, G. A. Terejanuand A. Heyden, “Identifying Active Sites of the Water–Gas Shift Reaction over Titania Supported Platinum Catalysts under Uncertainty”, *ACS Catalysis*, vol. 8, no. 5. American Chemical Society (ACS), pp. 3990–3998, Mar. 30, 2018. doi: 10.1021/acscatal.7b03531.  
  
W. Wan, S. C. Ammal, Z. Lin, K.-E. You, A. Heydenand J. G. Chen, “Controlling reaction pathways of selective C–O bond cleavage of glycerol”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Nov. 05, 2018. doi: 10.1038/s41467-018-07047-7.  
  
Y. Xi, W. Yang, S. C. Ammal, J. Lauterbach, Y. Pagan-Torresand A. Heyden, “Mechanistic study of the ceria supported, re-catalyzed deoxydehydration of vicinal OH groups”, *Catalysis Science & Technology*, vol. 8, no. 22. Royal Society of Chemistry (RSC), pp. 5750–5762, 2018. doi: 10.1039/c8cy01782d.  
  
A. Kilimnik, W. Maoand A. Alexeev, “Inertial migration of deformable capsules in channel flow”, *Physics of Fluids*, vol. 23, no. 12. AIP Publishing, p. 123302, Dec. 2011. doi: 10.1063/1.3664402.  
  
H. Masoud and A. Alexeev, “Resonance of flexible flapping wings at low Reynolds number”, *Physical Review E*, vol. 81, no. 5. American Physical Society (APS), May 06, 2010. doi: 10.1103/physreve.81.056304.  
  
H. Masoud and A. Alexeev, “Efficient Flapping Flight Using Flexible Wings Oscillating at Resonance”, *Natural Locomotion in Fluids and on Surfaces*. Springer New York, pp. 235–245, 2012. doi: 10.1007/978-1-4614-3997-4\_19.  
  
S. Bailoor, J.-H. Seoand R. Mittal, “Vortex shedding from a circular cylinder in shear-thinning Carreau fluids”, *Physics of Fluids*, vol. 31, no. 1. AIP Publishing, p. 011703, Jan. 2019. doi: 10.1063/1.5086032.  
  
Y. J. Choi, V. Vedulaand R. Mittal, “Computational Study of the Dynamics of a Bileaflet Mechanical Heart Valve in the Mitral Position”, *Annals of Biomedical Engineering*, vol. 42, no. 8. Springer Science and Business Media LLC, pp. 1668–1680, Apr. 29, 2014. doi: 10.1007/s10439-014-1018-4.  
  
P. Eslami, J.-H. Seo, A. A. Rahsepar, R. George, A. C. Lardoand R. Mittal, “Computational Study of Computed Tomography Contrast Gradients in Models of Stenosed Coronary Arteries”, *Journal of Biomechanical Engineering*, vol. 137, no. 9. ASME International, Sep. 01, 2015. doi: 10.1115/1.4030891.  
  
R. Mittal, B. D. Erathand M. W. Plesniak, “Fluid Dynamics of Human Phonation and Speech”, *Annual Review of Fluid Mechanics*, vol. 45, no. 1. Annual Reviews, pp. 437–467, Jan. 03, 2013. doi: 10.1146/annurev-fluid-011212-140636.  
  
R. Mittal, “Computational modeling of cardiac hemodynamics: Current status and future outlook”, *Journal of Computational Physics*, vol. 305. Elsevier BV, pp. 1065–1082, Jan. 2016. doi: 10.1016/j.jcp.2015.11.022.  
  
J.-H. Seo, T. L. Hedrickand R. Mittal, “Mechanism and scaling of wing tone generation in mosquitoes”, *Bioinspiration & Biomimetics*, vol. 15, no. 1. IOP Publishing, p. 016008, Dec. 04, 2019. doi: 10.1088/1748-3190/ab54fc.  
  
J. H. Seo and R. Mittal, “A coupled flow-acoustic computational study of bruits from a modeled stenosed artery”, *Medical & Biological Engineering & Computing*, vol. 50, no. 10. Springer Science and Business Media LLC, pp. 1025–1035, May 21, 2012. doi: 10.1007/s11517-012-0917-5.  
  
J. H. Seo and R. Mittal, “Effect of diastolic flow patterns on the function of the left ventricle”, *Physics of Fluids*, vol. 25, no. 11. AIP Publishing, p. 110801, Nov. 2013. doi: 10.1063/1.4819067.  
  
J. H. Seo, “Effect of the mitral valve on diastolic flow patterns”, *Physics of Fluids*, vol. 26, no. 12. AIP Publishing, p. 121901, Dec. 2014. doi: 10.1063/1.4904094.  
  
J. H. Seo, V. Vedula, T. Abrahamand R. Mittal, “Multiphysics computational models for cardiac flow and virtual cardiography”, *International Journal for Numerical Methods in Biomedical Engineering*, vol. 29, no. 8. Wiley, pp. 850–869, May 10, 2013. doi: 10.1002/cnm.2556.  
  
V. Vedula, S. Fortini, J.-H. Seo, G. Querzoliand R. Mittal, “Computational modeling and validation of intraventricular flow in a simple model of the left ventricle”, *Theoretical and Computational Fluid Dynamics*, vol. 28, no. 6. Springer Science and Business Media LLC, pp. 589–604, Nov. 09, 2014. doi: 10.1007/s00162-014-0335-4.  
  
V. Vedula, J.-H. Seo, A. C. Lardoand R. Mittal, “Effect of trabeculae and papillary muscles on the hemodynamics of the left ventricle”, *Theoretical and Computational Fluid Dynamics*, vol. 30, no. 1–2. Springer Science and Business Media LLC, pp. 3–21, May 07, 2015. doi: 10.1007/s00162-015-0349-6.  
  
W. Wu, C. Meneveauand R. Mittal, “Spatio-temporal dynamics of turbulent separation bubbles”, *Journal of Fluid Mechanics*, vol. 883. Cambridge University Press (CUP), Nov. 28, 2019. doi: 10.1017/jfm.2019.911.  
  
X. I. A. Yang and R. Mittal, “Acceleration of the Jacobi iterative method by factors exceeding 100 using scheduled relaxation”, *Journal of Computational Physics*, vol. 274. Elsevier BV, pp. 695–708, Oct. 2014. doi: 10.1016/j.jcp.2014.06.010.  
  
X. Yang and R. Mittal, “Efficient relaxed-Jacobi smoothers for multigrid on parallel computers”, *Journal of Computational Physics*, vol. 332. Elsevier BV, pp. 135–142, Mar. 2017. doi: 10.1016/j.jcp.2016.12.010.  
  
C. Zhu, J.-H. Seoand R. Mittal, “Computational Modeling and Analysis of Murmurs Generated by Modeled Aortic Stenoses”, *Journal of Biomechanical Engineering*, vol. 141, no. 4. ASME International, Mar. 05, 2019. doi: 10.1115/1.4042765.  
  
C. Zhu, J.-H. Seoand R. Mittal, “A graph-partitioned sharp-interface immersed boundary solver for efficient solution of internal flows”, *Journal of Computational Physics*, vol. 386. Elsevier BV, pp. 37–46, Jun. 2019. doi: 10.1016/j.jcp.2019.01.038.  
  
F. Ahmed, M. Mehrabadi, Z. Liu, G. A. Barabinoand C. K. Aidun, “Internal Viscosity-Dependent Margination of Red Blood Cells in Microfluidic Channels”, *Journal of Biomechanical Engineering*, vol. 140, no. 6. ASME International, Apr. 30, 2018. doi: 10.1115/1.4039897.  
  
M. T. Griffin, Y. Zhu, Z. Liu, C. K. Aidunand D. N. Ku, “Inhibition of high shear arterial thrombosis by charged nanoparticles”, *Biomicrofluidics*, vol. 12, no. 4. AIP Publishing, p. 042210, Jul. 2018. doi: 10.1063/1.5025349.  
  
I. Khan and C. K. Aidun, “Modeling the macroscopic behavior of saturated deformable porous media using direct numerical simulations”, *International Journal of Multiphase Flow*, vol. 71. Elsevier BV, pp. 74–82, May 2015. doi: 10.1016/j.ijmultiphaseflow.2014.12.003.  
  
Z. Liu, J. R. Clausen, R. R. Raoand C. K. Aidun, “A unified analysis of nano-to-microscale particle dispersion in tubular blood flow”, *Physics of Fluids*, vol. 31, no. 8. AIP Publishing, p. 081903, Aug. 2019. doi: 10.1063/1.5110604.  
  
Z. Liu, J. R. Clausen, R. R. Raoand C. K. Aidun, “Nanoparticle diffusion in sheared cellular blood flow”, *Journal of Fluid Mechanics*, vol. 871. Cambridge University Press (CUP), pp. 636–667, May 24, 2019. doi: 10.1017/jfm.2019.320.  
  
Z. Liu, Y. Zhu, J. R. Clausen, J. B. Lechman, R. R. Raoand C. K. Aidun, “Multiscale method based on coupled lattice‐Boltzmann and Langevin‐dynamics for direct simulation of nanoscale particle/polymer suspensions in complex flows”, *International Journal for Numerical Methods in Fluids*, vol. 91, no. 5. Wiley, pp. 228–246, Jul. 05, 2019. doi: 10.1002/fld.4752.  
  
Z. Liu, Y. Zhu, R. R. Rao, J. R. Clausenand C. K. Aidun, “Nanoparticle transport in cellular blood flow”, *Computers & Fluids*, vol. 172. Elsevier BV, pp. 609–620, Aug. 2018. doi: 10.1016/j.compfluid.2018.03.022.  
  
M. Mehrabadi, D. N. Kuand C. K. Aidun, “A Continuum Model for Platelet Transport in Flowing Blood Based on Direct Numerical Simulations of Cellular Blood Flow”, *Annals of Biomedical Engineering*, vol. 43, no. 6. Springer Science and Business Media LLC, pp. 1410–1421, Oct. 28, 2014. doi: 10.1007/s10439-014-1168-4.  
  
T. Rosén, Y. Kotsubo, C. K. Aidun, M. Do-Quangand F. Lundell, “Orientational dynamics of a triaxial ellipsoid in simple shear flow: Influence of inertia”, *Physical Review E*, vol. 96, no. 1. American Physical Society (APS), Jul. 18, 2017. doi: 10.1103/physreve.96.013109.  
  
T. Rosén, A. Nordmark, C. K. Aidun, M. Do-Quangand F. Lundell, “Quantitative analysis of the angular dynamics of a single spheroid in simple shear flow at moderate Reynolds numbers”, *Physical Review Fluids*, vol. 1, no. 4. American Physical Society (APS), Aug. 01, 2016. doi: 10.1103/physrevfluids.1.044201.  
  
B. Min Yun, C. K. Aidunand A. P. Yoganathan, “Blood Damage Through a Bileaflet Mechanical Heart Valve: A Quantitative Computational Study Using a Multiscale Suspension Flow Solver”, *Journal of Biomechanical Engineering*, vol. 136, no. 10. ASME International, Aug. 12, 2014. doi: 10.1115/1.4028105.  
  
B. M. Yun, L. P. Dasi, C. K. Aidunand A. P. Yoganathan, “Highly resolved pulsatile flows through prosthetic heart valves using the entropic lattice-Boltzmann method”, *Journal of Fluid Mechanics*, vol. 754. Cambridge University Press (CUP), pp. 122–160, Jul. 30, 2014. doi: 10.1017/jfm.2014.393.  
  
B. M. Yun, D. B. McElhinney, S. Arjunon, L. Mirabella, C. K. Aidunand A. P. Yoganathan, “Computational simulations of flow dynamics and blood damage through a bileaflet mechanical heart valve scaled to pediatric size and flow”, *Journal of Biomechanics*, vol. 47, no. 12. Elsevier BV, pp. 3169–3177, Sep. 2014. doi: 10.1016/j.jbiomech.2014.06.018.  
  
M. Mehrabadi, L. D. C. Casa, C. K. Aidunand D. N. Ku, “A Predictive Model of High Shear Thrombus Growth”, *Annals of Biomedical Engineering*, vol. 44, no. 8. Springer Science and Business Media LLC, pp. 2339–2350, Jan. 21, 2016. doi: 10.1007/s10439-016-1550-5.  
  
M. Mehrabadi, D. N. Kuand C. K. Aidun, “Effects of shear rate, confinement, and particle parameters on margination in blood flow”, *Physical Review E*, vol. 93, no. 2. American Physical Society (APS), Feb. 16, 2016. doi: 10.1103/physreve.93.023109.  
  
D. Tyler Landfried, A. Janaand M. Kimber, “Characterization of the Behavior of Confined Laminar Round Jets”, *Journal of Fluids Engineering*, vol. 137, no. 3. ASME International, Nov. 06, 2014. doi: 10.1115/1.4028834.  
  
A. Baraldi, M. S. Doddand A. Ferrante, “A mass-conserving volume-of-fluid method: Volume tracking and droplet surface-tension in incompressible isotropic turbulence”, *Computers & Fluids*, vol. 96. Elsevier BV, pp. 322–337, Jun. 2014. doi: 10.1016/j.compfluid.2013.12.018.  
  
M. S. Dodd and A. Ferrante, “A fast pressure-correction method for incompressible two-fluid flows”, *Journal of Computational Physics*, vol. 273. Elsevier BV, pp. 416–434, Sep. 2014. doi: 10.1016/j.jcp.2014.05.024.  
  
M. S. Dodd and A. Ferrante, “On the interaction of Taylor length scale size droplets and isotropic turbulence”, *Journal of Fluid Mechanics*, vol. 806. Cambridge University Press (CUP), pp. 356–412, Sep. 30, 2016. doi: 10.1017/jfm.2016.550.  
  
A. Freund and A. Ferrante, “Wavelet-spectral analysis of droplet-laden isotropic turbulence”, *Journal of Fluid Mechanics*, vol. 875. Cambridge University Press (CUP), pp. 914–928, Jul. 26, 2019. doi: 10.1017/jfm.2019.515.  
  
T. Chen and T. A. Manz, “Bond orders of the diatomic molecules”, *RSC Advances*, vol. 9, no. 30. Royal Society of Chemistry (RSC), pp. 17072–17092, 2019. doi: 10.1039/c9ra00974d.  
  
T. Chen and T. A. Manz, “Identifying misbonded atoms in the 2019 CoRE metal–organic framework database”, *RSC Advances*, vol. 10, no. 45. Royal Society of Chemistry (RSC), pp. 26944–26951, 2020. doi: 10.1039/d0ra02498h.  
  
C. Dong, D. A. Dickie, W. A. Maioand T. A. Manz, “Synthesis and Characterization of *N*,*N*′-Bismesityl Phenanthrene-9,10-diimine and Imine–Nitrone”, *ACS Omega*, vol. 3, no. 12. American Chemical Society (ACS), pp. 16858–16865, Dec. 07, 2018. doi: 10.1021/acsomega.8b02981.  
  
I. Erucar, T. A. Manzand S. Keskin, “Effects of electrostatic interactions on gas adsorption and permeability of MOF membranes”, *Molecular Simulation*, vol. 40, no. 7–9. Informa UK Limited, pp. 557–570, Feb. 05, 2014. doi: 10.1080/08927022.2013.829219.  
  
L. P. Lee, N. G. Limas, D. J. Cole, M. C. Payne, C.-K. Skylarisand T. A. Manz, “Expanding the Scope of Density Derived Electrostatic and Chemical Charge Partitioning to Thousands of Atoms”, *Journal of Chemical Theory and Computation*, vol. 10, no. 12. American Chemical Society (ACS), pp. 5377–5390, Nov. 20, 2014. doi: 10.1021/ct500766v.  
  
N. G. Limas and T. A. Manz, “Introducing DDEC6 atomic population analysis: part 2. Computed results for a wide range of periodic and nonperiodic materials”, *RSC Advances*, vol. 6, no. 51. Royal Society of Chemistry (RSC), pp. 45727–45747, 2016. doi: 10.1039/c6ra05507a.  
  
N. G. Limas and T. A. Manz, “Introducing DDEC6 atomic population analysis: part 4. Efficient parallel computation of net atomic charges, atomic spin moments, bond orders, and more”, *RSC Advances*, vol. 8, no. 5. Royal Society of Chemistry (RSC), pp. 2678–2707, 2018. doi: 10.1039/c7ra11829e.  
  
T. A. Manz and D. S. Sholl, “Computing Accurate Net Atomic Charges, Atomic Spin Moments, and Effective Bond Orders in Complex Materials”, *Computational Catalysis*. The Royal Society of Chemistry, pp. 192–222, Dec. 02, 2013. doi: 10.1039/9781849734905-00192.  
  
T. A. Manz, “Introducing DDEC6 atomic population analysis: part 3. Comprehensive method to compute bond orders”, *RSC Adv.*, vol. 7, no. 72. Royal Society of Chemistry (RSC), pp. 45552–45581, 2017. doi: 10.1039/c7ra07400j.  
  
T. A. Manz and N. G. Limas, “Introducing DDEC6 atomic population analysis: part 1. Charge partitioning theory and methodology”, *RSC Advances*, vol. 6, no. 53. Royal Society of Chemistry (RSC), pp. 47771–47801, 2016. doi: 10.1039/c6ra04656h.  
  
T. A. Manz and D. S. Sholl, “Chemically Meaningful Atomic Charges That Reproduce the Electrostatic Potential in Periodic and Nonperiodic Materials”, *Journal of Chemical Theory and Computation*, vol. 6, no. 8. American Chemical Society (ACS), pp. 2455–2468, Jul. 15, 2010. doi: 10.1021/ct100125x.  
  
T. A. Manz and D. S. Sholl, “Methods for Computing Accurate Atomic Spin Moments for Collinear and Noncollinear Magnetism in Periodic and Nonperiodic Materials”, *Journal of Chemical Theory and Computation*, vol. 7, no. 12. American Chemical Society (ACS), pp. 4146–4164, Oct. 26, 2011. doi: 10.1021/ct200539n.  
  
T. A. Manz and D. S. Sholl, “Improved Atoms-in-Molecule Charge Partitioning Functional for Simultaneously Reproducing the Electrostatic Potential and Chemical States in Periodic and Nonperiodic Materials”, *Journal of Chemical Theory and Computation*, vol. 8, no. 8. American Chemical Society (ACS), pp. 2844–2867, Jul. 18, 2012. doi: 10.1021/ct3002199.  
  
T. A. Manz and B. Yang, “Selective oxidation passing through η3-ozone intermediates: applications to direct propene epoxidation using molecular oxygen oxidant”, *RSC Adv.*, vol. 4, no. 53. Royal Society of Chemistry (RSC), pp. 27755–27774, 2014. doi: 10.1039/c4ra03729d.  
  
B. Yang and T. A. Manz, “Computationally designed zirconium organometallic catalyst for direct epoxidation of alkenes without allylic H atoms: aromatic linkage eliminates formation of inert octahedral complexes”, *Theoretical Chemistry Accounts*, vol. 135, no. 1. Springer Science and Business Media LLC, Jan. 2016. doi: 10.1007/s00214-015-1789-1.  
  
B. Yang and T. A. Manz, “Computationally designed tandem direct selective oxidation using molecular oxygen as oxidant without coreductant”, *RSC Advances*, vol. 6, no. 91. Royal Society of Chemistry (RSC), pp. 88189–88215, 2016. doi: 10.1039/c6ra17731j.  
  
D. Huang, R. Ma, T. Zhangand T. Luo, “Origin of Hydrophilic Surface Functionalization-Induced Thermal Conductance Enhancement across Solid–Water Interfaces”, *ACS Applied Materials & Interfaces*, vol. 10, no. 33. American Chemical Society (ACS), pp. 28159–28165, Jul. 30, 2018. doi: 10.1021/acsami.8b03709.  
  
X. Mu, Z. Song, Y. Wang, Z. Xu, D. B. Goand T. Luo, “Thermal transport in oxidized polycrystalline graphene”, *Carbon*, vol. 108. Elsevier BV, pp. 318–326, Nov. 2016. doi: 10.1016/j.carbon.2016.07.023.  
  
X. Mu, X. Wu, T. Zhang, D. B. Goand T. Luo, “Thermal Transport in Graphene Oxide – From Ballistic Extreme to Amorphous Limit”, *Scientific Reports*, vol. 4, no. 1. Springer Science and Business Media LLC, Jan. 28, 2014. doi: 10.1038/srep03909.  
  
D. Rish, S. Luo, B. Kurtzand T. Luo, “Exceptional ion rejection ability of directional solvent for non-membrane desalination”, *Applied Physics Letters*, vol. 104, no. 2. AIP Publishing, p. 024102, Jan. 13, 2014. doi: 10.1063/1.4861835.  
  
F. Sun, “Molecular Bridge Enables Anomalous Enhancement in Thermal Transport across Hard-Soft Material Interfaces”, *Advanced Materials*, vol. 26, no. 35. Wiley, pp. 6093–6099, May 20, 2014. doi: 10.1002/adma.201400954.  
  
X. Wei and T. Luo, “The effect of the block ratio on the thermal conductivity of amorphous polyethylene–polypropylene (PE–PP) diblock copolymers”, *Physical Chemistry Chemical Physics*, vol. 20, no. 31. Royal Society of Chemistry (RSC), pp. 20534–20539, 2018. doi: 10.1039/c8cp03433h.  
  
X. Wei, T. Zhangand T. Luo, “Chain conformation-dependent thermal conductivity of amorphous polymer blends: the impact of inter- and intra-chain interactions”, *Physical Chemistry Chemical Physics*, vol. 18, no. 47. Royal Society of Chemistry (RSC), pp. 32146–32154, 2016. doi: 10.1039/c6cp06643g.  
  
X. Wei, T. Zhangand T. Luo, “Thermal Energy Transport across Hard–Soft Interfaces”, *ACS Energy Letters*, vol. 2, no. 10. American Chemical Society (ACS), pp. 2283–2292, Sep. 12, 2017. doi: 10.1021/acsenergylett.7b00570.  
  
X. Wei, T. Zhangand T. Luo, “Molecular Fin Effect from Heterogeneous Self-Assembled Monolayer Enhances Thermal Conductance across Hard–Soft Interfaces”, *ACS Applied Materials & Interfaces*, vol. 9, no. 39. American Chemical Society (ACS), pp. 33740–33748, Sep. 19, 2017. doi: 10.1021/acsami.7b07169.  
  
X. Wu, “Hydrogenation of Penta-Graphene Leads to Unexpected Large Improvement in Thermal Conductivity”, *Nano Letters*, vol. 16, no. 6. American Chemical Society (ACS), pp. 3925–3935, May 10, 2016. doi: 10.1021/acs.nanolett.6b01536.  
  
T. Zhang, “Role of Hydrogen Bonds in Thermal Transport across Hard/Soft Material Interfaces”, *ACS Applied Materials & Interfaces*, vol. 8, no. 48. American Chemical Society (ACS), pp. 33326–33334, Nov. 22, 2016. doi: 10.1021/acsami.6b12073.  
  
T. Zhang and T. Luo, “Giant Thermal Rectification from Polyethylene Nanofiber Thermal Diodes”, *Small*, vol. 11, no. 36. Wiley, pp. 4657–4665, Jul. 14, 2015. doi: 10.1002/smll.201501127.  
  
T. Zhang and T. Luo, “Role of Chain Morphology and Stiffness in Thermal Conductivity of Amorphous Polymers”, *The Journal of Physical Chemistry B*, vol. 120, no. 4. American Chemical Society (ACS), pp. 803–812, Jan. 25, 2016. doi: 10.1021/acs.jpcb.5b09955.  
  
T. Zhang, X. Wuand T. Luo, “Polymer Nanofibers with Outstanding Thermal Conductivity and Thermal Stability: Fundamental Linkage between Molecular Characteristics and Macroscopic Thermal Properties”, *The Journal of Physical Chemistry C*, vol. 118, no. 36. American Chemical Society (ACS), pp. 21148–21159, Aug. 29, 2014. doi: 10.1021/jp5051639.  
  
P. Li, G. Henkelman, J. A. Keithand J. K. Johnson, “Elucidation of Aqueous Solvent-Mediated Hydrogen-Transfer Reactions by ab Initio Molecular Dynamics and Nudged Elastic-Band Studies of NaBH4 Hydrolysis”, *The Journal of Physical Chemistry C*, vol. 118, no. 37. American Chemical Society (ACS), pp. 21385–21399, Sep. 09, 2014. doi: 10.1021/jp507872d.  
  
P. Li, L. Yu, M. A. Matthews, W. A. Saidiand J. K. Johnson, “Deliquescence of NaBH4 from Density Functional Theory and Experiments”, *Industrial & Engineering Chemistry Research*, vol. 52, no. 38. American Chemical Society (ACS), pp. 13849–13861, Sep. 10, 2013. doi: 10.1021/ie401742u.  
  
M. Barisik and A. Beskok, “Boundary treatment effects on molecular dynamics simulations of interface thermal resistance”, *Journal of Computational Physics*, vol. 231, no. 23. Elsevier BV, pp. 7881–7892, Oct. 2012. doi: 10.1016/j.jcp.2012.07.026.  
  
M. Barisik and A. Beskok, “Boundary treatment effects on molecular dynamics simulations of interface thermal resistance”, *Journal of Computational Physics*, vol. 231, no. 23. Elsevier BV, pp. 7881–7892, Oct. 2012. doi: 10.1016/j.jcp.2012.07.026.  
  
Z. Shi, M. Barisikand A. Beskok, “Molecular dynamics modeling of thermal resistance at argon-graphite and argon-silver interfaces”, *International Journal of Thermal Sciences*, vol. 59. Elsevier BV, pp. 29–37, Sep. 2012. doi: 10.1016/j.ijthermalsci.2012.04.009.  
  
A. Aboulhassan, D. Baum, O. Wodo, B. Ganapathysubramanian, A. Amassianand M. Hadwiger, “A Novel Framework for Visual Detection and Exploration of Performance Bottlenecks in Organic Photovoltaic Solar Cell Materials”, *Computer Graphics Forum*, vol. 34, no. 3. Wiley, pp. 401–410, Jun. 2015. doi: 10.1111/cgf.12652.  
  
D. M. Ackerman, K. Delaney, G. H. Fredricksonand B. Ganapathysubramanian, “A finite element approach to self-consistent field theory calculations of multiblock polymers”, *Journal of Computational Physics*, vol. 331. Elsevier BV, pp. 280–296, Feb. 2017. doi: 10.1016/j.jcp.2016.11.020.  
  
T. Fast, O. Wodo, B. Ganapathysubramanianand S. R. Kalidindi, “Microstructure taxonomy based on spatial correlations: Application to microstructure coarsening”, *Acta Materialia*, vol. 108. Elsevier BV, pp. 176–185, Apr. 2016. doi: 10.1016/j.actamat.2016.01.046.  
  
A. D. Fontanini, K. M. Pr’Out, J. Kosnyand B. Ganapathysubramanian, “Exploring future climate trends on the thermal performance of attics: Part 1 – Standard roofs”, *Energy and Buildings*, vol. 129. Elsevier BV, pp. 32–45, Oct. 2016. doi: 10.1016/j.enbuild.2016.07.045.  
  
A. D. Fontanini, U. Vaidyaand B. Ganapathysubramanian, “Constructing Markov matrices for real-time transient contaminant transport analysis for indoor environments”, *Building and Environment*, vol. 94. Elsevier BV, pp. 68–81, Dec. 2015. doi: 10.1016/j.buildenv.2015.07.020.  
  
A. D. Fontanini, U. Vaidyaand B. Ganapathysubramanian, “A methodology for optimal placement of sensors in enclosed environments: A dynamical systems approach”, *Building and Environment*, vol. 100. Elsevier BV, pp. 145–161, May 2016. doi: 10.1016/j.buildenv.2016.02.003.  
  
A. D. Fontanini, U. Vaidya, A. Passalacquaand B. Ganapathysubramanian, “Quantifying mechanical ventilation performance: The connection between transport equations and Markov matrices”, *Building and Environment*, vol. 104. Elsevier BV, pp. 253–262, Aug. 2016. doi: 10.1016/j.buildenv.2016.05.019.  
  
A. D. Fontanini, U. Vaidya, A. Passalacquaand B. Ganapathysubramanian, “Contaminant transport at large Courant numbers using Markov matrices”, *Building and Environment*, vol. 112. Elsevier BV, pp. 1–16, Feb. 2017. doi: 10.1016/j.buildenv.2016.11.007.  
  
R. S. Gebhardt, “Utilizing Wide Band Gap, High Dielectric Constant Nanoparticles as Additives in Organic Solar Cells”, *The Journal of Physical Chemistry C*, vol. 119, no. 42. American Chemical Society (ACS), pp. 23883–23889, Oct. 13, 2015. doi: 10.1021/acs.jpcc.5b08581.  
  
A. J. Herrema, N. M. Wiese, C. N. Darling, B. Ganapathysubramanian, A. Krishnamurthyand M.-C. Hsu, “A framework for parametric design optimization using isogeometric analysis”, *Computer Methods in Applied Mechanics and Engineering*, vol. 316. Elsevier BV, pp. 944–965, Apr. 2017. doi: 10.1016/j.cma.2016.10.048.  
  
M. A. Khanwale, A. D. Lofquist, H. Sundar, J. A. Rossmanithand B. Ganapathysubramanian, “Simulating two-phase flows with thermodynamically consistent energy stable Cahn-Hilliard Navier-Stokes equations on parallel adaptive octree based meshes”, *Journal of Computational Physics*, vol. 419. Elsevier BV, p. 109674, Oct. 2020. doi: 10.1016/j.jcp.2020.109674.  
  
D. Kipp, O. Wodo, B. Ganapathysubramanianand V. Ganesan, “Achieving Bicontinuous Microemulsion Like Morphologies in Organic Photovoltaics”, *ACS Macro Letters*, vol. 4, no. 2. American Chemical Society (ACS), pp. 266–270, Feb. 05, 2015. doi: 10.1021/acsmacrolett.5b00007.  
  
D. Kipp, O. Wodo, B. Ganapathysubramanianand V. Ganesan, “Utilizing morphological correlators for device performance to optimize ternary blend organic solar cells based on block copolymer additives”, *Solar Energy Materials and Solar Cells*, vol. 161. Elsevier BV, pp. 206–218, Mar. 2017. doi: 10.1016/j.solmat.2016.11.025.  
  
J. Pace, C. Gardner, C. Romay, B. Ganapathysubramanianand T. Lübberstedt, “Genome-wide association analysis of seedling root development in maize (Zea mays L.)”, *BMC Genomics*, vol. 16, no. 1. Springer Science and Business Media LLC, Feb. 05, 2015. doi: 10.1186/s12864-015-1226-9.  
  
B. S. S. Pokuri and B. Ganapathysubramanian, “Morphology control in polymer blend fibers—a high throughput computing approach”, *Modelling and Simulation in Materials Science and Engineering*, vol. 24, no. 6. IOP Publishing, p. 065012, Aug. 01, 2016. doi: 10.1088/0965-0393/24/6/065012.  
  
S. K. Samudrala, P. V. Balachandran, J. Zola, K. Rajanand B. Ganapathysubramanian, “A software framework for data dimensionality reduction: application to chemical crystallography”, *Integrating Materials and Manufacturing Innovation*, vol. 3, no. 1. Springer Science and Business Media LLC, pp. 205–224, Jun. 29, 2014. doi: 10.1186/s40192-014-0017-5.  
  
S. Samudrala, O. Wodo, S. K. Suram, S. Broderick, K. Rajanand B. Ganapathysubramanian, “A graph-theoretic approach for characterization of precipitates from atom probe tomography data”, *Computational Materials Science*, vol. 77. Elsevier BV, pp. 335–342, Sep. 2013. doi: 10.1016/j.commatsci.2013.04.038.  
  
A. Singh, B. Ganapathysubramanian, A. K. Singhand S. Sarkar, “Machine Learning for High-Throughput Stress Phenotyping in Plants”, *Trends in Plant Science*, vol. 21, no. 2. Elsevier BV, pp. 110–124, Feb. 2016. doi: 10.1016/j.tplants.2015.10.015.  
  
D. Stoecklein, C.-Y. Wu, D. Kim, D. Di Carloand B. Ganapathysubramanian, “Optimization of micropillar sequences for fluid flow sculpting”, *Physics of Fluids*, vol. 28, no. 1. AIP Publishing, p. 012003, Jan. 2016. doi: 10.1063/1.4939512.  
  
O. Wodo and B. Ganapathysubramanian, “Computationally efficient solution to the Cahn–Hilliard equation: Adaptive implicit time schemes, mesh sensitivity analysis and the 3D isoperimetric problem”, *Journal of Computational Physics*, vol. 230, no. 15. Elsevier BV, pp. 6037–6060, Jul. 2011. doi: 10.1016/j.jcp.2011.04.012.  
  
O. Wodo and B. Ganapathysubramanian, “Modeling morphology evolution during solvent-based fabrication of organic solar cells”, *Computational Materials Science*, vol. 55. Elsevier BV, pp. 113–126, Apr. 2012. doi: 10.1016/j.commatsci.2011.12.012.  
  
Y. Xie, O. Wodoand B. Ganapathysubramanian, “A Diffuse Interface Model for Incompressible Two-Phase Flow with Large Density Ratios”, *Advances in Computational Fluid-Structure Interaction and Flow Simulation*. Springer International Publishing, pp. 203–215, 2016. doi: 10.1007/978-3-319-40827-9\_16.  
  
Y. Xie, O. Wodoand B. Ganapathysubramanian, “Incompressible two-phase flow: Diffuse interface approach for large density ratios, grid resolution study, and 3D patterned substrate wetting problem”, *Computers & Fluids*, vol. 141. Elsevier BV, pp. 223–234, Dec. 2016. doi: 10.1016/j.compfluid.2016.04.011.  
  
K. Zhao, “Vertical Phase Separation in Small Molecule:Polymer Blend Organic Thin Film Transistors Can Be Dynamically Controlled”, *Advanced Functional Materials*, vol. 26, no. 11. Wiley, pp. 1737–1746, Feb. 03, 2016. doi: 10.1002/adfm.201503943.  
  
Z. Cheng, N. A. Fineand C. S. Lo, “Platinum Nanoclusters Exhibit Enhanced Catalytic Activity for Methane Dehydrogenation”, *Topics in Catalysis*, vol. 55, no. 5–6. Springer Science and Business Media LLC, pp. 345–352, Apr. 24, 2012. doi: 10.1007/s11244-012-9803-5.  
  
Z. Cheng and C. S. Lo, “Formation of Active Sites on WO3 Catalysts: A Density Functional Theory Study of Olefin Metathesis”, *ACS Catalysis*, vol. 2, no. 3. American Chemical Society (ACS), pp. 341–349, Feb. 01, 2012. doi: 10.1021/cs2005778.  
  
Z. Cheng and C. S. Lo, “Effect of Support Structure and Composition on the Catalytic Activity of Pt Nanoclusters for Methane Dehydrogenation”, *Industrial & Engineering Chemistry Research*, vol. 52, no. 44. American Chemical Society (ACS), pp. 15447–15454, Jun. 12, 2013. doi: 10.1021/ie400776n.  
  
Z. Cheng and C. S. Lo, “Propagation of Olefin Metathesis to Propene on WO3Catalysts: A Mechanistic and Kinetic Study”, *ACS Catalysis*, vol. 5, no. 1. American Chemical Society (ACS), pp. 59–72, Nov. 25, 2014. doi: 10.1021/cs500531b.  
  
Z. Cheng, B. J. Shermanand C. S. Lo, “Carbon dioxide activation and dissociation on ceria (110): A density functional theory study”, *The Journal of Chemical Physics*, vol. 138, no. 1. AIP Publishing, p. 014702, Jan. 07, 2013. doi: 10.1063/1.4773248.  
  
A. Faghaninia, J. W. Agerand C. S. Lo, “*Ab initio*electronic transport model with explicit solution to the linearized Boltzmann transport equation”, *Physical Review B*, vol. 91, no. 23. American Physical Society (APS), Jun. 12, 2015. doi: 10.1103/physrevb.91.235123.  
  
A. Faghaninia and C. S. Lo, “First principles study of defect formation in thermoelectric zinc antimonide, *β*-Zn4Sb3”, *Journal of Physics: Condensed Matter*, vol. 27, no. 12. IOP Publishing, p. 125502, Mar. 10, 2015. doi: 10.1088/0953-8984/27/12/125502.  
  
S. Á. Kovács, W. P. Bricker, D. M. Niedzwiedzki, P. F. Collettiand C. S. Lo, “Computational determination of the pigment binding motif in the chlorosome protein a of green sulfur bacteria”, *Photosynthesis Research*, vol. 118, no. 3. Springer Science and Business Media LLC, pp. 231–247, Sep. 27, 2013. doi: 10.1007/s11120-013-9920-4.  
  
M. Stoica and C. S Lo, “P-type zinc oxide spinels: application to transparent conductors and spintronics”, *New Journal of Physics*, vol. 16, no. 5. IOP Publishing, p. 055011, May 14, 2014. doi: 10.1088/1367-2630/16/5/055011.  
  
V. Coralic and T. Colonius, “Shock-induced collapse of a bubble inside a deformable vessel”, *European Journal of Mechanics - B/Fluids*, vol. 40. Elsevier BV, pp. 64–74, Jul. 2013. doi: 10.1016/j.euromechflu.2013.01.003.  
  
N. R. Stuckert, L. Wangand R. T. Yang, “Characteristics of Hydrogen Storage by Spillover on Pt-Doped Carbon and Catalyst-Bridged Metal Organic Framework”, *Langmuir*, vol. 26, no. 14. American Chemical Society (ACS), pp. 11963–11971, Jun. 09, 2010. doi: 10.1021/la101377u.  
  
C. Carson, H. Luoand B. Yin, “CFD Based Optimization of A Flexible Flapping Wing”, *21st AIAA Computational Fluid Dynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 22, 2013. doi: 10.2514/6.2013-2454.  
  
Y. Chen and H. Luo, “A computational study of the three-dimensional fluid–structure interaction of aortic valve”, *Journal of Fluids and Structures*, vol. 80. Elsevier BV, pp. 332–349, Jul. 2018. doi: 10.1016/j.jfluidstructs.2018.04.009.  
  
Y. Chen and H. Luo, “Pressure distribution over the leaflets and effect of bending stiffness on fluid–structure interaction of the aortic valve”, *Journal of Fluid Mechanics*, vol. 883. Cambridge University Press (CUP), Nov. 28, 2019. doi: 10.1017/jfm.2019.904.  
  
H. Dai, H. Luo, P. J. S. A. F. de Sousaand J. F. Doyle, “Thrust performance of a flexible low-aspect-ratio pitching plate”, *Physics of Fluids*, vol. 24, no. 10. AIP Publishing, p. 101903, Oct. 2012. doi: 10.1063/1.4764047.  
  
H. Dai, H. Luoand J. F. Doyle, “Dynamic pitching of an elastic rectangular wing in hovering motion”, *Journal of Fluid Mechanics*, vol. 693. Cambridge University Press (CUP), pp. 473–499, Jan. 17, 2012. doi: 10.1017/jfm.2011.543.  
  
Z. Li, Y. Chen, S. Changand H. Luo, “A Reduced-Order Flow Model for Fluid–Structure Interaction Simulation of Vocal Fold Vibration”, *Journal of Biomechanical Engineering*, vol. 142, no. 2. ASME International, Oct. 07, 2019. doi: 10.1115/1.4044033.  
  
H. Luo, H. Dai, P. J. S. A. Ferreira de Sousaand B. Yin, “On the numerical oscillation of the direct-forcing immersed-boundary method for moving boundaries”, *Computers & Fluids*, vol. 56. Elsevier BV, pp. 61–76, Mar. 2012. doi: 10.1016/j.compfluid.2011.11.015.  
  
J. Song, H. Luoand T. Hedrick, “Lift characteristics of a hovering rufous hummingbird”, *31st AIAA Applied Aerodynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 22, 2013. doi: 10.2514/6.2013-3050.  
  
F. Tian, X. Luand H. Luo, “Onset of instability of a flag in uniform flow”, *Theoretical and Applied Mechanics Letters*, vol. 2, no. 2. Elsevier BV, p. 022005, 2012. doi: 10.1063/2.1202205.  
  
F.-B. Tian, H. Luo, L. Zhu, J. C. Liaoand X.-Y. Lu, “An efficient immersed boundary-lattice Boltzmann method for the hydrodynamic interaction of elastic filaments”, *Journal of Computational Physics*, vol. 230, no. 19. Elsevier BV, pp. 7266–7283, Aug. 2011. doi: 10.1016/j.jcp.2011.05.028.  
  
F.-B. Tian, H. Luo, L. Zhuand X.-Y. Lu, “Coupling modes of three filaments in side-by-side arrangement”, *Physics of Fluids*, vol. 23, no. 11. AIP Publishing, p. 111903, Nov. 2011. doi: 10.1063/1.3659892.  
  
B. Yin and H. Luo, “Effect of wing inertia on hovering performance of flexible flapping wings”, *Physics of Fluids*, vol. 22, no. 11. AIP Publishing, p. 111902, Nov. 2010. doi: 10.1063/1.3499739.  
  
B. Yin and H. Luo, “Numerical simulation of drops inside an asymmetric microchannel with protrusions”, *Computers & Fluids*, vol. 82. Elsevier BV, pp. 14–28, Aug. 2013. doi: 10.1016/j.compfluid.2013.05.005.  
  
B. Yin and H. Luo, “Hydrodynamic interaction of oblique sheets in tandem arrangement”, *Physics of Fluids*, vol. 25, no. 1. AIP Publishing, p. 011902, Jan. 2013. doi: 10.1063/1.4774345.  
  
A. Baranwal, D. A. Donzisand R. D. Bowersox, “Vibrational turbulent Prandtl number in flows with thermal non-equilibrium”, *AIAA Scitech 2020 Forum*. American Institute of Aeronautics and Astronautics, Jan. 05, 2020. doi: 10.2514/6.2020-2052.  
  
C. H. Chen, D. A. Donzisand R. D. Bowersox, “Characteristic Locations in Shock-Turbulence Interactions”, *AIAA Scitech 2020 Forum*. American Institute of Aeronautics and Astronautics, Jan. 05, 2020. doi: 10.2514/6.2020-1812.  
  
D. A. Donzis and K. Aditya, “Asynchronous finite-difference schemes for partial differential equations”, *Journal of Computational Physics*, vol. 274. Elsevier BV, pp. 370–392, Oct. 2014. doi: 10.1016/j.jcp.2014.06.017.  
  
D. A. Donzis, K. Aditya, K. R. Sreenivasanand P. K. Yeung, “The Turbulent Schmidt Number”, *Journal of Fluids Engineering*, vol. 136, no. 6. ASME International, Apr. 28, 2014. doi: 10.1115/1.4026619.  
  
D. A. Donzis and S. Jagannathan, “Fluctuations of thermodynamic variables in stationary compressible turbulence”, *Journal of Fluid Mechanics*, vol. 733. Cambridge University Press (CUP), pp. 221–244, Sep. 23, 2013. doi: 10.1017/jfm.2013.445.  
  
S. Jagannathan and D. A. Donzis, “Massively parallel direct numerical simulations of forced compressible turbulence”, *Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment: Bridging from the eXtreme to the campus and beyond*. ACM, Jul. 16, 2012. doi: 10.1145/2335755.2335819.  
  
S. Jagannathan and D. A. Donzis, “Reynolds and Mach number scaling in solenoidally-forced compressible turbulence using high-resolution direct numerical simulations”, *Journal of Fluid Mechanics*, vol. 789. Cambridge University Press (CUP), pp. 669–707, Jan. 26, 2016. doi: 10.1017/jfm.2015.754.  
  
D. A. Donzis, J. D. Gibbon, A. Gupta, R. M. Kerr, R. Panditand D. Vincenzi, “Vorticity moments in four numerical simulations of the 3D Navier–Stokes equations”, *Journal of Fluid Mechanics*, vol. 732. Cambridge University Press (CUP), pp. 316–331, Sep. 04, 2013. doi: 10.1017/jfm.2013.409.  
  
J. D. Gibbon, D. A. Donzis, A. Gupta, R. M. Kerr, R. Panditand D. Vincenzi, “Regimes of nonlinear depletion and regularity in the 3D Navier–Stokes equations”, *Nonlinearity*, vol. 27, no. 10. IOP Publishing, pp. 2605–2625, Sep. 22, 2014. doi: 10.1088/0951-7715/27/10/2605.  
  
J. Schumacher, J. D. Scheel, D. Krasnov, D. A. Donzis, V. Yakhotand K. R. Sreenivasan, “Small-scale universality in fluid turbulence”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 30. Proceedings of the National Academy of Sciences, pp. 10961–10965, Jul. 14, 2014. doi: 10.1073/pnas.1410791111.  
  
Y. Lv and M. Ihme, “Computational analysis of re-ignition and re-initiation mechanisms of quenched detonation waves behind a backward facing step”, *Proceedings of the Combustion Institute*, vol. 35, no. 2. Elsevier BV, pp. 1963–1972, 2015. doi: 10.1016/j.proci.2014.07.041.  
  
B. X. Dong, “Structure Control of a π-Conjugated Oligothiophene-Based Liquid Crystal for Enhanced Mixed Ion/Electron Transport Characteristics”, *ACS Nano*, vol. 13, no. 7. American Chemical Society (ACS), pp. 7665–7675, Jun. 13, 2019. doi: 10.1021/acsnano.9b01055.  
  
B. X. Dong, “Influence of Side-Chain Chemistry on Structure and Ionic Conduction Characteristics of Polythiophene Derivatives: A Computational and Experimental Study”, *Chemistry of Materials*, vol. 31, no. 4. American Chemical Society (ACS), pp. 1418–1429, Feb. 15, 2019. doi: 10.1021/acs.chemmater.8b05257.  
  
F. A. Escobedo, “Effect of inter-species selective interactions on the thermodynamics and nucleation free-energy barriers of a tessellating polyhedral compound”, *The Journal of Chemical Physics*, vol. 145, no. 21. AIP Publishing, p. 211903, Dec. 07, 2016. doi: 10.1063/1.4953862.  
  
F. A. Escobedo, “Optimizing the formation of solid solutions with components of different shapes”, *The Journal of Chemical Physics*, vol. 146, no. 13. AIP Publishing, p. 134508, Apr. 07, 2017. doi: 10.1063/1.4979091.  
  
F. A. Escobedo, “Optimizing the formation of colloidal compounds with components of different shapes”, *The Journal of Chemical Physics*, vol. 147, no. 21. AIP Publishing, p. 214501, Dec. 07, 2017. doi: 10.1063/1.5006047.  
  
U. Gupta, T. Hanrathand F. A. Escobedo, “Modeling the orientational and positional behavior of polyhedral nanoparticles at fluid-fluid interfaces”, *Physical Review Materials*, vol. 1, no. 5. American Physical Society (APS), Oct. 27, 2017. doi: 10.1103/physrevmaterials.1.055602.  
  
C. Liu, “Single polymer growth dynamics”, *Science*, vol. 358, no. 6361. American Association for the Advancement of Science (AAAS), pp. 352–355, Oct. 20, 2017. doi: 10.1126/science.aan6837.  
  
Z. Liu, “Self‐Assembly Behavior of an Oligothiophene‐Based Conjugated Liquid Crystal and Its Implication for Ionic Conductivity Characteristics”, *Advanced Functional Materials*, vol. 29, no. 2. Wiley, p. 1805220, Nov. 14, 2018. doi: 10.1002/adfm.201805220.  
  
S. P. Mahajan, “Computational affinity maturation of camelid single-domain intrabodies against the nonamyloid component of alpha-synuclein”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, Dec. 04, 2018. doi: 10.1038/s41598-018-35464-7.  
  
M. Misra, “Thermal Stability of π-Conjugated *n*-Ethylene-Glycol-Terminated Quaterthiophene Oligomers: A Computational and Experimental Study”, *ACS Macro Letters*, vol. 9, no. 3. American Chemical Society (ACS), pp. 295–300, Feb. 11, 2020. doi: 10.1021/acsmacrolett.9b00935.  
  
C. Nowak and F. A. Escobedo, “Optimizing the network topology of block copolymer liquid crystal elastomers for enhanced extensibility and toughness”, *Physical Review Materials*, vol. 1, no. 3. American Physical Society (APS), Aug. 02, 2017. doi: 10.1103/physrevmaterials.1.035601.  
  
C. Nowak and F. A. Escobedo, “Stability of the Gyroid Phase in Rod–Coil Systems via Thermodynamic Integration with Molecular Dynamics”, *Journal of Chemical Theory and Computation*, vol. 14, no. 11. American Chemical Society (ACS), pp. 5984–5991, Sep. 14, 2018. doi: 10.1021/acs.jctc.8b00419.  
  
C. Nowak and F. A. Escobedo, “Effect of Block Immiscibility on Strain-Induced Microphase Segregation and Crystallization of Model Block Copolymer Elastomers”, *Macromolecules*, vol. 51, no. 15. American Chemical Society (ACS), pp. 5685–5693, Jul. 20, 2018. doi: 10.1021/acs.macromol.8b00965.  
  
C. Nowak, M. Misraand F. A. Escobedo, “Framework for Inverse Mapping Chemistry-Agnostic Coarse-Grained Simulation Models into Chemistry-Specific Models”, *Journal of Chemical Information and Modeling*, vol. 59, no. 12. American Chemical Society (ACS), pp. 5045–5056, Nov. 19, 2019. doi: 10.1021/acs.jcim.9b00232.  
  
P. Padmanabhan, F. Martinez-Veracoecheaand F. A. Escobedo, “Computation of Free Energies of Cubic Bicontinuous Phases for Blends of Diblock Copolymer and Selective Homopolymer”, *Macromolecules*, vol. 49, no. 14. American Chemical Society (ACS), pp. 5232–5243, Jul. 05, 2016. doi: 10.1021/acs.macromol.6b00123.  
  
Y. Sun, P. Padmanabhan, M. Misraand F. A. Escobedo, “Molecular dynamics simulation of thermotropic bolaamphiphiles with a swallow-tail lateral chain: formation of cubic network phases”, *Soft Matter*, vol. 13, no. 45. Royal Society of Chemistry (RSC), pp. 8542–8555, 2017. doi: 10.1039/c7sm01819c.  
  
E. Wang and F. Escobedo, “Swelling and Tensile Properties of Tetra‐Polyethylene glycol via Coarse‐Grained Molecular Models”, *Macromolecular Theory and Simulations*, vol. 26, no. 3. Wiley, p. 1600098, May 2017. doi: 10.1002/mats.201600098.  
  
C. Nowak and F. A. Escobedo, “Tuning the Sawtooth Tensile Response and Toughness of Multiblock Copolymer Diamond Networks”, *Macromolecules*, vol. 49, no. 17. American Chemical Society (ACS), pp. 6711–6721, Sep. 01, 2016. doi: 10.1021/acs.macromol.6b00733.  
  
X. Wu, H. Chang, C. Mello, R. Nagarajanand G. Narsimhan, “Effect of interaction with coesite silica on the conformation of Cecropin P1 using explicit solvent molecular dynamics simulation”, *The Journal of Chemical Physics*, vol. 138, no. 4. AIP Publishing, p. 045103, Jan. 28, 2013. doi: 10.1063/1.4788662.  
  
C. P. Andersen, H. Hu, G. Qiu, V. Kalraand Y. Sun, “Pore-Scale Transport Resolved Model Incorporating Cathode Microstructure and Peroxide Growth in Lithium-Air Batteries”, *Journal of The Electrochemical Society*, vol. 162, no. 7. The Electrochemical Society, pp. A1135–A1145, 2015. doi: 10.1149/2.0051507jes.  
  
P. A. Boettcher, H. Hu, S. P. M. Bane, M. McCarthyand Y. Sun, “Dust ignition of pure and encapsulated paraffin phase change materials”, *Journal of Loss Prevention in the Process Industries*, vol. 40. Elsevier BV, pp. 298–303, Mar. 2016. doi: 10.1016/j.jlp.2016.01.008.  
  
H. Hu and Y. Sun, “Effect of nanopatterns on Kapitza resistance at a water-gold interface during boiling: A molecular dynamics study”, *Journal of Applied Physics*, vol. 112, no. 5. AIP Publishing, p. 053508, Sep. 2012. doi: 10.1063/1.4749393.  
  
H. Hu and Y. Sun, “Molecular dynamics simulations of disjoining pressure effect in ultra-thin water film on a metal surface”, *Applied Physics Letters*, vol. 103, no. 26. AIP Publishing, p. 263110, Dec. 23, 2013. doi: 10.1063/1.4858469.  
  
H. Hu and Y. Sun, “Effect of nanostructures on heat transfer coefficient of an evaporating meniscus”, *International Journal of Heat and Mass Transfer*, vol. 101. Elsevier BV, pp. 878–885, Oct. 2016. doi: 10.1016/j.ijheatmasstransfer.2016.05.092.  
  
H. Hu, C. R. Weinbergerand Y. Sun, “Effect of Nanostructures on the Meniscus Shape and Disjoining Pressure of Ultrathin Liquid Film”, *Nano Letters*, vol. 14, no. 12. American Chemical Society (ACS), pp. 7131–7137, Nov. 17, 2014. doi: 10.1021/nl5037066.  
  
H. Hu, C. R. Weinbergerand Y. Sun, “Model of Meniscus Shape and Disjoining Pressure of Thin Liquid Films on Nanostructured Surfaces with Electrostatic Interactions”, *The Journal of Physical Chemistry C*, vol. 119, no. 21. American Chemical Society (ACS), pp. 11777–11785, May 15, 2015. doi: 10.1021/acs.jpcc.5b03250.  
  
D.-O. Kim, M. Pack, H. Hu, H. Kimand Y. Sun, “Deposition of Colloidal Drops Containing Ellipsoidal Particles: Competition between Capillary and Hydrodynamic Forces”, *Langmuir*, vol. 32, no. 45. American Chemical Society (ACS), pp. 11899–11906, Nov. 04, 2016. doi: 10.1021/acs.langmuir.6b03221.  
  
G. Lu, H. Hu, Y. Duanand Y. Sun, “Wetting kinetics of water nano-droplet containing non-surfactant nanoparticles: A molecular dynamics study”, *Applied Physics Letters*, vol. 103, no. 25. AIP Publishing, p. 253104, Dec. 16, 2013. doi: 10.1063/1.4837717.  
  
M. Pack, H. Hu, D.-O. Kim, X. Yangand Y. Sun, “Colloidal Drop Deposition on Porous Substrates: Competition among Particle Motion, Evaporation, and Infiltration”, *Langmuir*, vol. 31, no. 29. American Chemical Society (ACS), pp. 7953–7961, Jul. 14, 2015. doi: 10.1021/acs.langmuir.5b01846.  
  
M. Pack, H. Hu, D. Kim, Z. Zheng, H. A. Stoneand Y. Sun, “Failure mechanisms of air entrainment in drop impact on lubricated surfaces”, *Soft Matter*, vol. 13, no. 12. Royal Society of Chemistry (RSC), pp. 2402–2409, 2017. doi: 10.1039/c7sm00117g.  
  
M. Pack, P. Kaneelil, H. Kimand Y. Sun, “Contact Line Instability Caused by Air Rim Formation under Nonsplashing Droplets”, *Langmuir*, vol. 34, no. 17. American Chemical Society (ACS), pp. 4962–4969, Apr. 05, 2018. doi: 10.1021/acs.langmuir.8b01082.  
  
G. Qiu, C. R. Dennison, K. W. Knehr, E. C. Kumburand Y. Sun, “Pore-scale analysis of effects of electrode morphology and electrolyte flow conditions on performance of vanadium redox flow batteries”, *Journal of Power Sources*, vol. 219. Elsevier BV, pp. 223–234, Dec. 2012. doi: 10.1016/j.jpowsour.2012.07.042.  
  
G. Qiu, A. S. Joshi, C. R. Dennison, K. W. Knehr, E. C. Kumburand Y. Sun, “3-D pore-scale resolved model for coupled species/charge/fluid transport in a vanadium redox flow battery”, *Electrochimica Acta*, vol. 64. Elsevier BV, pp. 46–64, Mar. 2012. doi: 10.1016/j.electacta.2011.12.065.  
  
H. Shabgard, H. Hu, P. A. Boettcher, M. McCarthyand Y. Sun, “Heat transfer analysis of PCM slurry flow between parallel plates”, *International Journal of Heat and Mass Transfer*, vol. 99. Elsevier BV, pp. 895–903, Aug. 2016. doi: 10.1016/j.ijheatmasstransfer.2016.04.020.  
  
L. Sun, H. Hu, A. A. Rokoniand Y. Sun, “Intrinsic instability of thin liquid films on nanostructured surfaces”, *Applied Physics Letters*, vol. 109, no. 11. AIP Publishing, p. 111601, Sep. 12, 2016. doi: 10.1063/1.4962654.  
  
M. Temirel, H. Hu, H. Shabgard, P. Boettcher, M. McCarthyand Y. Sun, “Solidification of additive-enhanced phase change materials in spherical enclosures with convective cooling”, *Applied Thermal Engineering*, vol. 111. Elsevier BV, pp. 134–142, Jan. 2017. doi: 10.1016/j.applthermaleng.2016.09.090.  
  
Z. Tian, H. Huand Y. Sun, “A molecular dynamics study of effective thermal conductivity in nanocomposites”, *International Journal of Heat and Mass Transfer*, vol. 61. Elsevier BV, pp. 577–582, Jun. 2013. doi: 10.1016/j.ijheatmasstransfer.2013.02.023.  
  
D. Zong, H. Hu, Y. Duanand Y. Sun, “Viscosity of Water under Electric Field: Anisotropy Induced by Redistribution of Hydrogen Bonds”, *The Journal of Physical Chemistry B*, vol. 120, no. 21. American Chemical Society (ACS), pp. 4818–4827, May 18, 2016. doi: 10.1021/acs.jpcb.6b01686.  
  
A. Hsieh and S. Biringen, “The minimal flow unit in complex turbulent flows”, *Physics of Fluids*, vol. 28, no. 12. AIP Publishing, p. 125102, Dec. 2016. doi: 10.1063/1.4968827.  
  
A. S. Hsieh, S. Biringenand A. Kucala, “Simulation of Rotating Channel Flow With Heat Transfer: Evaluation of Closure Models”, *Journal of Turbomachinery*, vol. 138, no. 11. ASME International, May 24, 2016. doi: 10.1115/1.4033463.  
  
M. I. Hussein, S. Biringen, O. R. Bilaland A. Kucala, “Flow stabilization by subsurface phonons”, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 471, no. 2177. The Royal Society, p. 20140928, May 2015. doi: 10.1098/rspa.2014.0928.  
  
A. Kucala and S. Biringen, “Spatial simulation of channel flow instability and control”, *Journal of Fluid Mechanics*, vol. 738. Cambridge University Press (CUP), pp. 105–123, Dec. 04, 2013. doi: 10.1017/jfm.2013.532.  
  
S. W. Martlatt, S. B. Waggyand S. Biringen, “Direct Numerical Simulation of the Turbulent Ekman Layer: Turbulent Energy Budgets”, *Journal of Thermophysics and Heat Transfer*, vol. 24, no. 3. American Institute of Aeronautics and Astronautics (AIAA), pp. 544–555, Jul. 2010. doi: 10.2514/1.45200.  
  
S. B. Waggy, S. Biringenand P. P. Sullivan, “Direct numerical simulation of top-down and bottom-up diffusion in the convective boundary layer”, *Journal of Fluid Mechanics*, vol. 724. Cambridge University Press (CUP), pp. 581–606, Apr. 30, 2013. doi: 10.1017/jfm.2013.130.  
  
S. B. Waggy, A. Hsiehand S. Biringen, “Modeling high-order statistics in the turbulent Ekman layer”, *Geophysical & Astrophysical Fluid Dynamics*, vol. 110, no. 5. Informa UK Limited, pp. 391–408, Jun. 13, 2016. doi: 10.1080/03091929.2016.1196202.  
  
S. H. Bryngelson, K. Schmidmayerand T. Colonius, “A quantitative comparison of phase-averaged models for bubbly, cavitating flows”, *International Journal of Multiphase Flow*, vol. 115. Elsevier BV, pp. 137–143, Jun. 2019. doi: 10.1016/j.ijmultiphaseflow.2019.03.028.  
  
V. Coralic and T. Colonius, “Numerical simulation of bubble dynamics in deformable vessels.”, *The Journal of the Acoustical Society of America*, vol. 129, no. 4. Acoustical Society of America (ASA), pp. 2375–2375, Apr. 2011. doi: 10.1121/1.3587690.  
  
V. Coralic and T. Colonius, “Modeling vascular injury due to shock-induced bubble collapse in lithotripsy”, *The Journal of the Acoustical Society of America*, vol. 136, no. 4. Acoustical Society of America (ASA), pp. 2192–2192, Oct. 2014. doi: 10.1121/1.4899946.  
  
V. Coralic and T. Colonius, “Finite-volume WENO scheme for viscous compressible multicomponent flows”, *Journal of Computational Physics*, vol. 274. Elsevier BV, pp. 95–121, Oct. 2014. doi: 10.1016/j.jcp.2014.06.003.  
  
B. Dorschner, K. Yu, G. Mengaldoand T. Colonius, “A fast multi-resolution lattice Green’s function method for elliptic difference equations”, *Journal of Computational Physics*, vol. 407. Elsevier BV, p. 109270, Apr. 2020. doi: 10.1016/j.jcp.2020.109270.  
  
A. Goza and T. Colonius, “A strongly-coupled immersed-boundary formulation for thin elastic structures”, *Journal of Computational Physics*, vol. 336. Elsevier BV, pp. 401–411, May 2017. doi: 10.1016/j.jcp.2017.02.027.  
  
T. Jardin and T. Colonius, “On the lift-optimal aspect ratio of a revolving wing at low Reynolds number”, *Journal of The Royal Society Interface*, vol. 15, no. 143. The Royal Society, p. 20170933, Jun. 2018. doi: 10.1098/rsif.2017.0933.  
  
K. Maeda and T. Colonius, “A source term approach for generation of one-way acoustic waves in the Euler and Navier–Stokes equations”, *Wave Motion*, vol. 75. Elsevier BV, pp. 36–49, Dec. 2017. doi: 10.1016/j.wavemoti.2017.08.004.  
  
K. Maeda and T. Colonius, “A source term approach for generation of one-way acoustic waves in the Euler and Navier–Stokes equations”, *Wave Motion*, vol. 75. Elsevier BV, pp. 36–49, Dec. 2017. doi: 10.1016/j.wavemoti.2017.08.004.  
  
K. Maeda and T. Colonius, “Eulerian–Lagrangian method for simulation of cloud cavitation”, *Journal of Computational Physics*, vol. 371. Elsevier BV, pp. 994–1017, Oct. 2018. doi: 10.1016/j.jcp.2018.05.029.  
  
K. Maeda and T. Colonius, “Eulerian–Lagrangian method for simulation of cloud cavitation”, *Journal of Computational Physics*, vol. 371. Elsevier BV, pp. 994–1017, Oct. 2018. doi: 10.1016/j.jcp.2018.05.029.  
  
K. Maeda and T. Colonius, “Bubble cloud dynamics in an ultrasound field”, *Journal of Fluid Mechanics*, vol. 862. Cambridge University Press (CUP), pp. 1105–1134, Jan. 16, 2019. doi: 10.1017/jfm.2018.968.  
  
K. Maeda, T. Colonius, W. Kreider, A. Maxwelland M. Bailey, “Modeling and experimental analysis of acoustic cavitation bubble clouds for burst-wave lithotripsy”, *The Journal of the Acoustical Society of America*, vol. 140, no. 4. Acoustical Society of America (ASA), pp. 3307–3307, Oct. 2016. doi: 10.1121/1.4970532.  
  
G. Mengaldo, S. Liska, K. Yu, T. Coloniusand T. Jardin, “Immersed Boundary Lattice Green Function methods for External Aerodynamics”, *23rd AIAA Computational Fluid Dynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 02, 2017. doi: 10.2514/6.2017-3621.  
  
J. C. Meng and T. Colonius, “Numerical simulations of the early stages of high-speed droplet breakup”, *Shock Waves*, vol. 25, no. 4. Springer Science and Business Media LLC, pp. 399–414, Dec. 20, 2014. doi: 10.1007/s00193-014-0546-z.  
  
J. C. Meng and T. Colonius, “Numerical simulation of the aerobreakup of a water droplet”, *Journal of Fluid Mechanics*, vol. 835. Cambridge University Press (CUP), pp. 1108–1135, Nov. 29, 2017. doi: 10.1017/jfm.2017.804.  
  
A. Ahmed and S. I. Sandler, “Hydration Free Energies of Multifunctional Nitroaromatic Compounds”, *Journal of Chemical Theory and Computation*, vol. 9, no. 6. American Chemical Society (ACS), pp. 2774–2785, Jun. 03, 2013. doi: 10.1021/ct3011002.  
  
A. Ahmed and S. I. Sandler, “Physicochemical Properties of Hazardous Energetic Compounds from Molecular Simulation”, *Journal of Chemical Theory and Computation*, vol. 9, no. 5. American Chemical Society (ACS), pp. 2389–2397, Apr. 02, 2013. doi: 10.1021/ct301129x.  
  
S. Verma, Y. Xuanand G. Blanquart, “An improved bounded semi-Lagrangian scheme for the turbulent transport of passive scalars”, *Journal of Computational Physics*, vol. 272. Elsevier BV, pp. 1–22, Sep. 2014. doi: 10.1016/j.jcp.2014.03.062.  
  
K. R. Reddy, J. A. Ryonand P. A. Durbin, “A DDES model with a Smagorinsky-type eddy viscosity formulation and log-layer mismatch correction”, *International Journal of Heat and Fluid Flow*, vol. 50. Elsevier BV, pp. 103–113, Dec. 2014. doi: 10.1016/j.ijheatfluidflow.2014.06.002.  
  
C. K. Bennett, “Strong Influence of the Nucleophile on the Rate and Selectivity of 1,2-Epoxyoctane Ring Opening Catalyzed by Tris(pentafluorophenyl)borane, B(C6F5)3”, *ACS Catalysis*, vol. 9, no. 12. American Chemical Society (ACS), pp. 11589–11602, Oct. 30, 2019. doi: 10.1021/acscatal.9b02607.  
  
M. N. Bhagat, “Enhancing the Regioselectivity of B(C6F5)3-Catalyzed Epoxide Alcoholysis Reactions Using Hydrogen-Bond Acceptors”, *ACS Catalysis*, vol. 9, no. 10. American Chemical Society (ACS), pp. 9663–9670, Sep. 13, 2019. doi: 10.1021/acscatal.9b03089.  
  
L. H. Oakley, F. Casadio, K. R. Shulland L. J. Broadbelt, “Theoretical Study of Epoxidation Reactions Relevant to Hydrocarbon Oxidation”, *Industrial & Engineering Chemistry Research*, vol. 56, no. 26. American Chemical Society (ACS), pp. 7454–7461, Jun. 26, 2017. doi: 10.1021/acs.iecr.7b01443.  
  
A. Irannejad, A. Banaeizadehand F. Jaberi, “Large eddy simulation of turbulent spray combustion”, *Combustion and Flame*, vol. 162, no. 2. Elsevier BV, pp. 431–450, Feb. 2015. doi: 10.1016/j.combustflame.2014.07.029.  
  
A. Irannejad and F. Jaberi, “Large Eddy Simulation of Spray Mixing and Combustion with Two-Phase Mass Density Function”, *43rd Fluid Dynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 22, 2013. doi: 10.2514/6.2013-2599.  
  
A. Irannejad and F. Jaberi, “Numerical study of high speed evaporating sprays”, *International Journal of Multiphase Flow*, vol. 70. Elsevier BV, pp. 58–76, Apr. 2015. doi: 10.1016/j.ijmultiphaseflow.2014.11.014.  
  
A. Irannejad, F. A. Jaberi, J. Komperdaand F. Mashayek, “Large Eddy Simulation of Supersonic Turbulent Combustion with FMDF”, *52nd Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 10, 2014. doi: 10.2514/6.2014-1188.  
  
A. Jammalamadaka and F. Jaberi, “Subgrid-scale turbulence in shock–boundary layer flows”, *Theoretical and Computational Fluid Dynamics*, vol. 29, no. 1–2. Springer Science and Business Media LLC, pp. 29–54, Jan. 18, 2015. doi: 10.1007/s00162-015-0339-8.  
  
S. Srivastava and F. Jaberi, “Large eddy simulations of complex multicomponent diesel fuels in high temperature and pressure turbulent flows”, *International Journal of Heat and Mass Transfer*, vol. 104. Elsevier BV, pp. 819–834, Jan. 2017. doi: 10.1016/j.ijheatmasstransfer.2016.07.011.  
  
A. Bodling and A. Sharma, “Numerical Investigation of Low-Noise Airfoils Inspired by the Down Coat of Owls”, *2018 AIAA/CEAS Aeroacoustics Conference*. American Institute of Aeronautics and Astronautics, Jun. 24, 2018. doi: 10.2514/6.2018-3925.  
  
L. Chen, C. Harding, A. Sharmaand E. MacDonald, “Modeling noise and lease soft costs improves wind farm design and cost-of-energy predictions”, *Renewable Energy*, vol. 97. Elsevier BV, pp. 849–859, Nov. 2016. doi: 10.1016/j.renene.2016.05.045.  
  
H. Ju, R. Mani, M. Vysohlidand A. Sharma, “Investigation of Fan-Wake/Outlet-Guide-Vane Interaction Broadband Noise”, *AIAA Journal*, vol. 53, no. 12. American Institute of Aeronautics and Astronautics (AIAA), pp. 3534–3550, Dec. 2015. doi: 10.2514/1.j053167.  
  
B. Moghadassian and A. Sharma, “Inverse Design of Single- and Multi-Rotor Horizontal Axis Wind Turbine Blades Using Computational Fluid Dynamics”, *Journal of Solar Energy Engineering*, vol. 140, no. 2. ASME International, Jan. 22, 2018. doi: 10.1115/1.4038811.  
  
A. Rosenberg, S. Selvarajand A. Sharma, “A Novel Dual-Rotor Turbine for Increased Wind Energy Capture”, *Journal of Physics: Conference Series*, vol. 524. IOP Publishing, p. 012078, Jun. 16, 2014. doi: 10.1088/1742-6596/524/1/012078.  
  
A. Rosenberg and A. Sharma, “A Prescribed-Wake Vortex Lattice Method for Preliminary Design of Co-Axial, Dual-Rotor Wind Turbines”, *Journal of Solar Energy Engineering*, vol. 138, no. 6. ASME International, Sep. 02, 2016. doi: 10.1115/1.4034350.  
  
A. Sharma and M. R. Visbal, “Airfoil Thickness Effects on Dynamic Stall Onset”, *23rd AIAA Computational Fluid Dynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 02, 2017. doi: 10.2514/6.2017-3957.  
  
E. S. Takle, D. A. Rajewski, J. K. Lundquist, W. A. Gallus Jrand A. Sharma, “Measurements in support of wind farm simulations and power forecasts: The Crop/Wind-energy Experiments (CWEX)”, *Journal of Physics: Conference Series*, vol. 524. IOP Publishing, p. 012174, Jun. 16, 2014. doi: 10.1088/1742-6596/524/1/012174.  
  
A. Thelen, L. Leifsson, A. Sharmaand S. Koziel, “RANS-based design optimization of dual-rotor wind turbines”, *Engineering Computations*, vol. 35, no. 1. Emerald, pp. 35–52, Mar. 05, 2018. doi: 10.1108/ec-10-2016-0354.  
  
A. Bodling and A. Sharma, “Numerical investigation of low-noise airfoils inspired by the down coat of owls”, *Bioinspiration & Biomimetics*, vol. 14, no. 1. IOP Publishing, p. 016013, Dec. 07, 2018. doi: 10.1088/1748-3190/aaf19c.  
  
S. Alahyari Beig and E. Johnsen, “Maintaining interface equilibrium conditions in compressible multiphase flows using interface capturing”, *Journal of Computational Physics*, vol. 302. Elsevier BV, pp. 548–566, Dec. 2015. doi: 10.1016/j.jcp.2015.09.018.  
  
S. A. Beig, B. Aboulhasanzadehand E. Johnsen, “Temperatures produced by inertially collapsing bubbles near rigid surfaces”, *Journal of Fluid Mechanics*, vol. 852. Cambridge University Press (CUP), pp. 105–125, Aug. 02, 2018. doi: 10.1017/jfm.2018.525.  
  
P. E. Johnson, L. H. Khieuand E. Johnsen, “Analysis of Recovery-assisted discontinuous Galerkin methods for the compressible Navier-Stokes equations”, *Journal of Computational Physics*, vol. 423. Elsevier BV, p. 109813, Dec. 2020. doi: 10.1016/j.jcp.2020.109813.  
  
P. Movahed and E. Johnsen, “Turbulence diffusion effects at material interfaces, with application to the Rayleigh-Taylor instability”, *43rd Fluid Dynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 22, 2013. doi: 10.2514/6.2013-3121.  
  
P. Movahed and E. Johnsen, “The mixing region in freely decaying variable-density turbulence”, *Journal of Fluid Mechanics*, vol. 772. Cambridge University Press (CUP), pp. 386–426, May 05, 2015. doi: 10.1017/jfm.2015.200.  
  
S. Pan and E. Johnsen, “The role of bulk viscosity on the decay of compressible, homogeneous, isotropic turbulence”, *Journal of Fluid Mechanics*, vol. 833. Cambridge University Press (CUP), pp. 717–744, Nov. 08, 2017. doi: 10.1017/jfm.2017.598.  
  
B. Patterson and E. Johnsen, “Dynamics of an acoustically driven liquid-gas interface”, *The Journal of the Acoustical Society of America*, vol. 140, no. 4. Acoustical Society of America (ASA), pp. 3368–3368, Oct. 2016. doi: 10.1121/1.4970754.  
  
B. Patterson and E. Johnsen, “Dynamics of pulsed-ultrasound driven gas-liquid interfaces”, *The Journal of the Acoustical Society of America*, vol. 141, no. 5. Acoustical Society of America (ASA), pp. 4014–4014, May 2017. doi: 10.1121/1.4989225.  
  
B. Patterson and E. Johnsen, “Growth of liquid-gas interfacial perturbations driven by acoustic waves”, *Physical Review Fluids*, vol. 3, no. 7. American Physical Society (APS), Jul. 13, 2018. doi: 10.1103/physrevfluids.3.074002.  
  
M. J. Wadas and E. Johnsen, “Interactions of two bubbles along a gaseous interface undergoing the Richtmyer–Meshkov instability in two dimensions”, *Physica D: Nonlinear Phenomena*, vol. 409. Elsevier BV, p. 132489, Aug. 2020. doi: 10.1016/j.physd.2020.132489.  
  
B. Bobbitt and G. Blanquart, “Vorticity isotropy in high Karlovitz number premixed flames”, *Physics of Fluids*, vol. 28, no. 10. AIP Publishing, p. 105101, Oct. 2016. doi: 10.1063/1.4962305.  
  
B. Bobbitt, S. Lapointeand G. Blanquart, “Vorticity transformation in high Karlovitz number premixed flames”, *Physics of Fluids*, vol. 28, no. 1. AIP Publishing, p. 015101, Jan. 2016. doi: 10.1063/1.4937947.  
  
P. L. Carroll and G. Blanquart, “The effect of velocity field forcing techniques on the Karman–Howarth equation”, *Journal of Turbulence*, vol. 15, no. 7. Informa UK Limited, pp. 429–448, May 13, 2014. doi: 10.1080/14685248.2014.911876.  
  
P. L. Carroll and G. Blanquart, “A new framework for simulating forced homogeneous buoyant turbulent flows”, *Theoretical and Computational Fluid Dynamics*, vol. 29, no. 3. Springer Science and Business Media LLC, pp. 225–244, May 06, 2015. doi: 10.1007/s00162-015-0350-0.  
  
P. L. Carroll, S. Vermaand G. Blanquart, “A novel forcing technique to simulate turbulent mixing in a decaying scalar field”, *Physics of Fluids*, vol. 25, no. 9. AIP Publishing, p. 095102, Sep. 2013. doi: 10.1063/1.4819782.  
  
S. Lapointe and G. Blanquart, “Fuel and chemistry effects in high Karlovitz premixed turbulent flames”, *Combustion and Flame*, vol. 167. Elsevier BV, pp. 294–307, May 2016. doi: 10.1016/j.combustflame.2016.01.035.  
  
J. Smolke, “Experimental and numerical studies of fuel and hydrodynamic effects on piloted turbulent premixed jet flames”, *Proceedings of the Combustion Institute*, vol. 36, no. 2. Elsevier BV, pp. 1877–1884, 2017. doi: 10.1016/j.proci.2016.07.127.  
  
V. S. Acharya and T. C. Lieuwen, “Sound Generation from Swirling, Premixed Flames Excited by Helical Flow Disturbances”, *Combustion Science and Technology*, vol. 187, no. 1–2. Informa UK Limited, pp. 206–229, Dec. 10, 2014. doi: 10.1080/00102202.2014.973492.  
  
V. Acharya and T. Lieuwen, “Effect of azimuthal flow fluctuations on flow and flame dynamics of axisymmetric swirling flames”, *Physics of Fluids*, vol. 27, no. 10. AIP Publishing, p. 105106, Oct. 2015. doi: 10.1063/1.4933135.  
  
V. Acharya and T. Lieuwen, “Premixed flame response to helical disturbances: Mean flame non-axisymmetry effects”, *Combustion and Flame*, vol. 165. Elsevier BV, pp. 188–197, Mar. 2016. doi: 10.1016/j.combustflame.2015.12.003.  
  
V. Acharya, M. Malanoski, M. Aguilarand T. Lieuwen, “Dynamics of a Transversely Excited Swirling, Lifted Flame: Flame Response Modeling and Comparison With Experiments”, *Journal of Engineering for Gas Turbines and Power*, vol. 136, no. 5. ASME International, Jan. 02, 2014. doi: 10.1115/1.4025790.  
  
V. S. Acharya, D.-H. Shinand T. Lieuwen, “Premixed Flames Excited by Helical Disturbances: Flame Wrinkling and Heat Release Oscillations”, *Journal of Propulsion and Power*, vol. 29, no. 6. American Institute of Aeronautics and Astronautics (AIAA), pp. 1282–1291, Nov. 2013. doi: 10.2514/1.b34883.  
  
M. Aguilar, “Helical Flow Disturbances in a Multinozzle Combustor”, *Journal of Engineering for Gas Turbines and Power*, vol. 137, no. 9. ASME International, Feb. 25, 2015. doi: 10.1115/1.4029696.  
  
N. Magina, V. Acharya, T. Sunand T. Lieuwen, “Propagation, dissipation, and dispersion of disturbances on harmonically forced, non-premixed flames”, *Proceedings of the Combustion Institute*, vol. 35, no. 1. Elsevier BV, pp. 1097–1105, 2015. doi: 10.1016/j.proci.2014.07.050.  
  
J. O’Connor, V. Acharyaand T. Lieuwen, “Transverse combustion instabilities: Acoustic, fluid mechanic, and flame processes”, *Progress in Energy and Combustion Science*, vol. 49. Elsevier BV, pp. 1–39, Aug. 2015. doi: 10.1016/j.pecs.2015.01.001.  
  
M. Esmaily-Moghadam, Y. Bazilevsand A. L. Marsden, “Impact of data distribution on the parallel performance of iterative linear solvers with emphasis on CFD of incompressible flows”, *Computational Mechanics*, vol. 55, no. 1. Springer Science and Business Media LLC, pp. 93–103, Oct. 25, 2014. doi: 10.1007/s00466-014-1084-3.  
  
M. Esmaily-Moghadam, T.-Y. Hsiaand A. L. Marsden, “The assisted bidirectional Glenn: A novel surgical approach for first-stage single-ventricle heart palliation”, *The Journal of Thoracic and Cardiovascular Surgery*, vol. 149, no. 3. Elsevier BV, pp. 699–705, Mar. 2015. doi: 10.1016/j.jtcvs.2014.10.035.  
  
M. Esmaily Moghadam, I. E. Vignon-Clementel, R. Figliolaand A. L. Marsden, “A modular numerical method for implicit 0D/3D coupling in cardiovascular finite element simulations”, *Journal of Computational Physics*, vol. 244. Elsevier BV, pp. 63–79, Jul. 2013. doi: 10.1016/j.jcp.2012.07.035.  
  
J. Lee, “Spatial and temporal variations in hemodynamic forces initiate cardiac trabeculation”, *JCI Insight*, vol. 3, no. 13. American Society for Clinical Investigation, Jul. 12, 2018. doi: 10.1172/jci.insight.96672.  
  
J. Liu and A. L. Marsden, “A unified continuum and variational multiscale formulation for fluids, solids, and fluid–structure interaction”, *Computer Methods in Applied Mechanics and Engineering*, vol. 337. Elsevier BV, pp. 549–597, Aug. 2018. doi: 10.1016/j.cma.2018.03.045.  
  
C. C. Long, M.-C. Hsu, Y. Bazilevs, J. A. Feinsteinand A. L. Marsden, “Fluid-structure interaction simulations of the Fontan procedure using variable wall properties”, *International Journal for Numerical Methods in Biomedical Engineering*, vol. 28, no. 5. Wiley, pp. 513–527, Jan. 17, 2012. doi: 10.1002/cnm.1485.  
  
A. L. Marsden and M. Esmaily-Moghadam, “Multiscale Modeling of Cardiovascular Flows for Clinical Decision Support”, *Applied Mechanics Reviews*, vol. 67, no. 3. ASME International, May 01, 2015. doi: 10.1115/1.4029909.  
  
A. B. Ramachandra, A. M. Kahnand A. L. Marsden, “Patient-Specific Simulations Reveal Significant Differences in Mechanical Stimuli in Venous and Arterial Coronary Grafts”, *Journal of Cardiovascular Translational Research*, vol. 9, no. 4. Springer Science and Business Media LLC, pp. 279–290, Jul. 22, 2016. doi: 10.1007/s12265-016-9706-0.  
  
D. E. Schiavazzi, A. Baretta, G. Pennati, T. Hsiaand A. L. Marsden, “Patient‐specific parameter estimation in single‐ventricle lumped circulation models under uncertainty”, *International Journal for Numerical Methods in Biomedical Engineering*, vol. 33, no. 3. Wiley, Jun. 08, 2016. doi: 10.1002/cnm.2799.  
  
D. E. Schiavazzi, A. Doostan, G. Iaccarinoand A. L. Marsden, “A generalized multi-resolution expansion for uncertainty propagation with application to cardiovascular modeling”, *Computer Methods in Applied Mechanics and Engineering*, vol. 314. Elsevier BV, pp. 196–221, Feb. 2017. doi: 10.1016/j.cma.2016.09.024.  
  
D. E. Schiavazzi, T. Y. Hsiaand A. L. Marsden, “On a sparse pressure-flow rate condensation of rigid circulation models”, *Journal of Biomechanics*, vol. 49, no. 11. Elsevier BV, pp. 2174–2186, Jul. 2016. doi: 10.1016/j.jbiomech.2015.11.028.  
  
D. E. Schiavazzi, “Hemodynamic effects of left pulmonary artery stenosis after superior cavopulmonary connection: A patient-specific multiscale modeling study”, *The Journal of Thoracic and Cardiovascular Surgery*, vol. 149, no. 3. Elsevier BV, pp. 689–696.e3, Mar. 2015. doi: 10.1016/j.jtcvs.2014.12.040.  
  
J. S. Tran, D. E. Schiavazzi, A. B. Ramachandra, A. M. Kahnand A. L. Marsden, “Automated tuning for parameter identification and uncertainty quantification in multi-scale coronary simulations”, *Computers & Fluids*, vol. 142. Elsevier BV, pp. 128–138, Jan. 2017. doi: 10.1016/j.compfluid.2016.05.015.  
  
V. Vedula, J. Lee, H. Xu, C.-C. J. Kuo, T. K. Hsiaiand A. L. Marsden, “A method to quantify mechanobiologic forces during zebrafish cardiac development using 4-D light sheet imaging and computational modeling”, *PLOS Computational Biology*, vol. 13, no. 10. Public Library of Science (PLoS), p. e1005828, Oct. 30, 2017. doi: 10.1371/journal.pcbi.1005828.  
  
A. Verma, “Optimization of the Assisted Bidirectional Glenn Procedure for First Stage Single Ventricle Repair”, *World Journal for Pediatric and Congenital Heart Surgery*, vol. 9, no. 2. SAGE Publications, pp. 157–170, Mar. 2018. doi: 10.1177/2150135117745026.  
  
W. Yang, J. A. Feinstein, S. C. Shadden, I. E. Vignon-Clementeland A. L. Marsden, “Optimization of a Y-Graft Design for Improved Hepatic Flow Distribution in the Fontan Circulation”, *Journal of Biomechanical Engineering*, vol. 135, no. 1. ASME International, Dec. 27, 2012. doi: 10.1115/1.4023089.  
  
A. Updegrove, N. M. Wilson, J. Merkow, H. Lan, A. L. Marsdenand S. C. Shadden, “SimVascular: An Open Source Pipeline for Cardiovascular Simulation”, *Annals of Biomedical Engineering*, vol. 45, no. 3. Springer Science and Business Media LLC, pp. 525–541, Dec. 08, 2016. doi: 10.1007/s10439-016-1762-8.  
  
L. C. Johnson, B. J. Landrumand R. N. Zia, “Yield of reversible colloidal gels during flow start-up: release from kinetic arrest”, *Soft Matter*, vol. 14, no. 24. Royal Society of Chemistry (RSC), pp. 5048–5068, 2018. doi: 10.1039/c8sm00109j.  
  
L. C. Johnson, R. N. Zia, E. Moghimiand G. Petekidis, “Influence of structure on the linear response rheology of colloidal gels”, *Journal of Rheology*, vol. 63, no. 4. Society of Rheology, pp. 583–608, Jul. 2019. doi: 10.1122/1.5082796.  
  
P. Padmanabhan and R. Zia, “Gravitational collapse of colloidal gels: non-equilibrium phase separation driven by osmotic pressure”, *Soft Matter*, vol. 14, no. 17. Royal Society of Chemistry (RSC), pp. 3265–3287, 2018. doi: 10.1039/c8sm00002f.  
  
X. Peng, J. G. Wang, Q. Li, D. Chen, R. N. Ziaand G. B. McKenna, “Exploring the validity of time-concentration superposition in glassy colloids: Experiments and simulations”, *Physical Review E*, vol. 98, no. 6. American Physical Society (APS), Dec. 06, 2018. doi: 10.1103/physreve.98.062602.  
  
R. N. Zia, B. J. Landrumand W. B. Russel, “A micro-mechanical study of coarsening and rheology of colloidal gels: Cage building, cage hopping, and Smoluchowski’s ratchet”, *Journal of Rheology*, vol. 58, no. 5. Society of Rheology, pp. 1121–1157, Sep. 2014. doi: 10.1122/1.4892115.  
  
V. Rashidi and K. P. Pipe, “Contributions of strain relaxation and interface modes to thermal transport in superlattices”, *Computational Materials Science*, vol. 107. Elsevier BV, pp. 151–156, Sep. 2015. doi: 10.1016/j.commatsci.2015.04.056.  
  
E. T. Baldwin, “String flash-boiling in gasoline direct injection simulations with transient needle motion”, *International Journal of Multiphase Flow*, vol. 87. Elsevier BV, pp. 90–101, Dec. 2016. doi: 10.1016/j.ijmultiphaseflow.2016.09.004.  
  
M. A. Benitz, D. W. Carlson, B. Seyed-Aghazadeh, Y. Modarres-Sadeghi, M. A. Lacknerand D. P. Schmidt, “CFD simulations and experimental measurements of flow past free-surface piercing, finite length cylinders with varying aspect ratios”, *Computers & Fluids*, vol. 136. Elsevier BV, pp. 247–259, Sep. 2016. doi: 10.1016/j.compfluid.2016.06.013.  
  
G. L. Jacobsohn, E. T. Baldwin, D. P. Schmidt, B. R. Halls, A. Kastengrenand T. R. Meyer, “Diffuse Interface Eulerian Spray Atomization Modeling of Impinging Jet Sprays”, *2018 AIAA Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 07, 2018. doi: 10.2514/6.2018-2078.  
  
G. L. Jacobsohn, C. K. Mohapatra, R. O. Grover, D. J. Dukeand D. P. Schmidt, “Comparison of Turbulence Modeling Methods for Evaluating GDI Sprays with Transient Needle Motion”, *SAE Technical Paper Series*. SAE International, Apr. 02, 2019. doi: 10.4271/2019-01-0271.  
  
H. M. Johlas, “Modeling Breaking Waves for Fixed-Bottom Support Structures for Offshore Wind Turbines”, *ASME 2018 1st International Offshore Wind Technical Conference*. American Society of Mechanical Engineers, Nov. 04, 2018. doi: 10.1115/iowtc2018-1095.  
  
P. Mitra, “Identification and Characterization of Steady Spray Conditions in Convergent, Single-Hole Diesel Injectors”, *SAE Technical Paper Series*. SAE International, Apr. 02, 2019. doi: 10.4271/2019-01-0281.  
  
M. Moulai, R. Grover, S. Parrishand D. Schmidt, “Internal and Near-Nozzle Flow in a Multi-Hole Gasoline Injector Under Flashing and Non-Flashing Conditions”, *SAE Technical Paper Series*. SAE International, Apr. 14, 2015. doi: 10.4271/2015-01-0944.  
  
A. Pandal, J. M. Pastor, J. M. García-Oliver, E. Baldwinand D. P. Schmidt, “A consistent, scalable model for Eulerian spray modeling”, *International Journal of Multiphase Flow*, vol. 83. Elsevier BV, pp. 162–171, Jul. 2016. doi: 10.1016/j.ijmultiphaseflow.2016.04.003.  
  
S. K. Rachakonda, A. Paydarfarand D. P. Schmidt, “Prediction of spray collapse in multi-hole gasoline direct-injection fuel injectors”, *International Journal of Engine Research*, vol. 20, no. 1. SAGE Publications, pp. 18–33, Dec. 19, 2018. doi: 10.1177/1468087418819527.  
  
S. K. Rachakonda, “A computational approach to predict external spray characteristics for flashing and cavitating nozzles”, *International Journal of Multiphase Flow*, vol. 106. Elsevier BV, pp. 21–33, Sep. 2018. doi: 10.1016/j.ijmultiphaseflow.2018.04.012.  
  
S. K. Rachakonda, Y. Wangand D. P. Schmidt, “FLASH-BOILING INITIALIZATION FOR SPRAY SIMULATIONS BASED ON PARAMETRIC STUDIES”, *Atomization and Sprays*, vol. 28, no. 2. Begell House, pp. 111–140, 2018. doi: 10.1615/atomizspr.2018020769.  
  
D. P. Schmidt and F. Bedford, “An analysis of the convergence of stochastic Lagrangian/Eulerian spray simulations”, *International Journal of Multiphase Flow*, vol. 102. Elsevier BV, pp. 95–101, May 2018. doi: 10.1016/j.ijmultiphaseflow.2018.01.024.  
  
P. Strek, D. Duke, A. Swantek, A. Kastengren, C. F. Powelland D. P. Schmidt, “X-Ray Radiography and CFD Studies of the Spray G Injector”, *SAE Technical Paper Series*. SAE International, Apr. 05, 2016. doi: 10.4271/2016-01-0858.  
  
H. M. Johlas, L. A. Martí­nez-Tossas, D. P. Schmidt, M. A. Lacknerand M. J. Churchfield, “Large eddy simulations of floating offshore wind turbine wakes with coupled platform motion”, *Journal of Physics: Conference Series*, vol. 1256, no. 1. IOP Publishing, p. 012018, Jul. 01, 2019. doi: 10.1088/1742-6596/1256/1/012018.  
  
A. Zandian, W. A. Sirignanoand F. Hussain, “Length-scale cascade and spread rate of atomizing planar liquid jets”, *International Journal of Multiphase Flow*, vol. 113. Elsevier BV, pp. 117–141, Apr. 2019. doi: 10.1016/j.ijmultiphaseflow.2019.01.004.  
  
Y. He and S. Laursen, “Trends in the Surface and Catalytic Chemistry of Transition-Metal Ceramics in the Deoxygenation of a Woody Biomass Pyrolysis Model Compound”, *ACS Catalysis*, vol. 7, no. 5. American Chemical Society (ACS), pp. 3169–3180, Apr. 03, 2017. doi: 10.1021/acscatal.6b02806.  
  
V. Gururajan, F. N. Egolfopoulosand K. Kohse-Höinghaus, “Direct numerical simulations of probe effects in low-pressure flame sampling”, *Proceedings of the Combustion Institute*, vol. 35, no. 1. Elsevier BV, pp. 821–829, 2015. doi: 10.1016/j.proci.2014.06.046.  
  
R. S. Maier, E. Nybo, J. D. Seymourand S. L. Codd, “Electroosmotic Flow and Dispersion in Open and Closed Porous Media”, *Transport in Porous Media*, vol. 113, no. 1. Springer Science and Business Media LLC, pp. 67–89, Mar. 24, 2016. doi: 10.1007/s11242-016-0680-4.  
  
H. Fujioka, “A continuum model of interfacial surfactant transport for particle methods”, *Journal of Computational Physics*, vol. 234. Elsevier BV, pp. 280–294, Feb. 2013. doi: 10.1016/j.jcp.2012.09.041.  
  
C. Wang and J. D. Eldredge, “Strongly coupled dynamics of fluids and rigid-body systems with the immersed boundary projection method”, *Journal of Computational Physics*, vol. 295. Elsevier BV, pp. 87–113, Aug. 2015. doi: 10.1016/j.jcp.2015.04.005.  
  
M. Shen, S. Ketenand R. M. Lueptow, “Dynamics of water and solute transport in polymeric reverse osmosis membranes via molecular dynamics simulations”, *Journal of Membrane Science*, vol. 506. Elsevier BV, pp. 95–108, May 2016. doi: 10.1016/j.memsci.2016.01.051.  
  
N. Ren, Y. Wang, S. Vilfayeauand A. Trouvé, “Large eddy simulation of turbulent vertical wall fires supplied with gaseous fuel through porous burners”, *Combustion and Flame*, vol. 169. Elsevier BV, pp. 194–208, Jul. 2016. doi: 10.1016/j.combustflame.2015.12.008.  
  
S. Vilfayeau, T. Myers, A. W. Marshalland A. Trouvé, “Large eddy simulation of suppression of turbulent line fires by base-injected water mist”, *Proceedings of the Combustion Institute*, vol. 36, no. 2. Elsevier BV, pp. 3287–3295, 2017. doi: 10.1016/j.proci.2016.06.058.  
  
S. Vilfayeau, J. P. White, P. B. Sunderland, A. W. Marshalland A. Trouvé, “Large eddy simulation of flame extinction in a turbulent line fire exposed to air-nitrogen co-flow”, *Fire Safety Journal*, vol. 86. Elsevier BV, pp. 16–31, Nov. 2016. doi: 10.1016/j.firesaf.2016.09.003.  
  
F. Anaya, L. Zhang, Q. Tanand D. E. Resasco, “Tuning the acid–metal balance in Pd/ and Pt/zeolite catalysts for the hydroalkylation of m-cresol”, *Journal of Catalysis*, vol. 328. Elsevier BV, pp. 173–185, Aug. 2015. doi: 10.1016/j.jcat.2015.01.004.  
  
P. S. Deimel, “Direct quantitative identification of the “surface trans-effect””, *Chemical Science*, vol. 7, no. 9. Royal Society of Chemistry (RSC), pp. 5647–5656, 2016. doi: 10.1039/c6sc01677d.  
  
N. Duong, Q. Tanand D. E. Resasco, “Controlling phenolic hydrodeoxygenation by tailoring metal–O bond strength via specific catalyst metal type and particle size selection”, *Comptes Rendus Chimie*, vol. 21, no. 3–4. Elsevier BV, pp. 155–163, Mar. 2018. doi: 10.1016/j.crci.2017.07.008.  
  
N. Pino, S. Sitthisa, Q. Tan, T. Souza, D. Lópezand D. E. Resasco, “Structure, activity, and selectivity of bimetallic Pd-Fe/SiO2 and Pd-Fe/γ-Al2O3 catalysts for the conversion of furfural”, *Journal of Catalysis*, vol. 350. Elsevier BV, pp. 30–40, Jun. 2017. doi: 10.1016/j.jcat.2017.03.016.  
  
A. Rozenblit, A. J. Avoian, Q. Tan, T. Sooknoiand D. E. Resasco, “Reaction mechanism of aqueous-phase conversion of γ-valerolactone (GVL) over a Ru/C catalyst”, *Journal of Energy Chemistry*, vol. 25, no. 6. Elsevier BV, pp. 1008–1014, Nov. 2016. doi: 10.1016/j.jechem.2016.11.010.  
  
Q. Tan, “Mechanistic analysis of the role of metal oxophilicity in the hydrodeoxygenation of anisole”, *Journal of Catalysis*, vol. 347. Elsevier BV, pp. 102–115, Mar. 2017. doi: 10.1016/j.jcat.2017.01.008.  
  
Q. Tan, “Different Product Distributions and Mechanistic Aspects of the Hydrodeoxygenation of m-Cresol over Platinum and Ruthenium Catalysts”, *ACS Catalysis*, vol. 5, no. 11. American Chemical Society (ACS), pp. 6271–6283, Sep. 25, 2015. doi: 10.1021/acscatal.5b00765.  
  
L. Zhang, “Synthesis of C4and C8Chemicals from Ethanol on MgO-Incorporated Faujasite Catalysts with Balanced Confinement Effects and Basicity”, *ChemSusChem*, vol. 9, no. 7. Wiley, pp. 736–748, Mar. 03, 2016. doi: 10.1002/cssc.201501518.  
  
H. Adamji, M. Stevens, K. Grossklaus, T. E. Vanderveldeand P. Deshlahra, “Density functional theory analysis of the effect of structural configurations on the stability of GaAsBi compounds”, *Computational Materials Science*, vol. 173. Elsevier BV, p. 109401, Feb. 2020. doi: 10.1016/j.commatsci.2019.109401.  
  
L. Annamalai, Y. Liuand P. Deshlahra, “Selective C–H Bond Activation via NO*x*-Mediated Generation of Strong H-Abstractors”, *ACS Catalysis*, vol. 9, no. 11. American Chemical Society (ACS), pp. 10324–10338, Oct. 04, 2019. doi: 10.1021/acscatal.9b03862.  
  
A. Asok, P. Deshlahra, A. M. Ramachandranand A. R. Kulkarni, “Multifunctional Photostable Nanocomplex of ZnO Quantum Dots and Avobenzone via the Promotion of Enolate Tautomer”, *Global Challenges*, vol. 2, no. 11. Wiley, p. 1800025, Jul. 04, 2018. doi: 10.1002/gch2.201800025.  
  
L. A. Cramer, Y. Liu, P. Deshlahraand E. C. H. Sykes, “Dynamic Restructuring Induced Oxygen Activation on AgCu Near-Surface Alloys”, *The Journal of Physical Chemistry Letters*, vol. 11, no. 15. American Chemical Society (ACS), pp. 5844–5848, Jun. 30, 2020. doi: 10.1021/acs.jpclett.0c00887.  
  
P. Deshlahra and E. Iglesia, “Reactivity descriptors in acid catalysis: acid strength, proton affinity and host–guest interactions”, *Chemical Communications*, vol. 56, no. 54. Royal Society of Chemistry (RSC), pp. 7371–7398, 2020. doi: 10.1039/d0cc02593c.  
  
S. Kwon, P. Deshlahraand E. Iglesia, “Dioxygen activation routes in Mars-van Krevelen redox cycles catalyzed by metal oxides”, *Journal of Catalysis*, vol. 364. Elsevier BV, pp. 228–247, Aug. 2018. doi: 10.1016/j.jcat.2018.05.016.  
  
S. Kwon, P. Deshlahraand E. Iglesia, “Reactivity and selectivity descriptors of dioxygen activation routes on metal oxides”, *Journal of Catalysis*, vol. 377. Elsevier BV, pp. 692–710, Sep. 2019. doi: 10.1016/j.jcat.2019.07.048.  
  
Y. Liu, L. Annamalaiand P. Deshlahra, “Effects of Lattice O Atom Coordination and Pore Confinement on Selectivity Limitations for Ethane Oxidative Dehydrogenation Catalyzed by Vanadium-Oxo Species”, *The Journal of Physical Chemistry C*, vol. 123, no. 46. American Chemical Society (ACS), pp. 28168–28191, Nov. 08, 2019. doi: 10.1021/acs.jpcc.9b07778.  
  
B. Savard, Y. Xuan, B. Bobbittand G. Blanquart, “A computationally-efficient, semi-implicit, iterative method for the time-integration of reacting flows with stiff chemistry”, *Journal of Computational Physics*, vol. 295. Elsevier BV, pp. 740–769, Aug. 2015. doi: 10.1016/j.jcp.2015.04.018.  
  
R. Chen, H. (Whitney) . Yu, L. Zhu, R. M. Patiland T. Lee, “Spatial and temporal scaling of unequal microbubble coalescence”, *AIChE Journal*, vol. 63, no. 4. Wiley, pp. 1441–1450, Oct. 04, 2016. doi: 10.1002/aic.15504.  
  
R. Chen, W. Yu, Y. Xuand L. Zhu, “Scalings of inverse energy transfer and energy decay in 3-D decaying isotropic turbulence with non-rotating or rotating frame of reference”, *J. Appl. Comput. Mech.*, no. Online First, Oct. 2018, doi: 10.22055/jacm.2018.26826.1361.  
  
J. Baltrusaitis, T. Bučko, W. Michaels, M. Makkeeand G. Mul, “Catalytic methyl mercaptan coupling to ethylene in chabazite: DFT study of the first C C bond formation”, *Applied Catalysis B: Environmental*, vol. 187. Elsevier BV, pp. 195–203, Jun. 2016. doi: 10.1016/j.apcatb.2016.01.021.  
  
D. Kiani, G. Belletti, P. Quaino, F. Tielensand J. Baltrusaitis, “Structure and Vibrational Properties of Potassium-Promoted Tungsten Oxide Catalyst Monomeric Sites Supported on Alumina (K2O/WO3/Al2O3) Characterized Using Periodic Density Functional Theory”, *The Journal of Physical Chemistry C*, vol. 122, no. 42. American Chemical Society (ACS), pp. 24190–24201, Oct. 03, 2018. doi: 10.1021/acs.jpcc.8b08214.  
  
W. E. Taifan, T. Bučkoand J. Baltrusaitis, “Catalytic conversion of ethanol to 1,3-butadiene on MgO: A comprehensive mechanism elucidation using DFT calculations”, *Journal of Catalysis*, vol. 346. Elsevier BV, pp. 78–91, Feb. 2017. doi: 10.1016/j.jcat.2016.11.042.  
  
W. E. Taifan, G. X. Yanand J. Baltrusaitis, “Surface chemistry of MgO/SiO2 catalyst during the ethanol catalytic conversion to 1,3-butadiene: in-situ DRIFTS and DFT study”, *Catalysis Science & Technology*, vol. 7, no. 20. Royal Society of Chemistry (RSC), pp. 4648–4668, 2017. doi: 10.1039/c7cy01556a.  
  
P. J. Sakievich, Y. T. Peetand R. J. Adrian, “Large-scale thermal motions of turbulent Rayleigh–Bénard convection in a wide aspect-ratio cylindrical domain”, *International Journal of Heat and Fluid Flow*, vol. 61. Elsevier BV, pp. 183–196, Oct. 2016. doi: 10.1016/j.ijheatfluidflow.2016.04.011.  
  
M. J. P. Hack and T. A. Zaki, “Data-enabled prediction of streak breakdown in pressure-gradient boundary layers”, *Journal of Fluid Mechanics*, vol. 801. Cambridge University Press (CUP), pp. 43–64, Jul. 19, 2016. doi: 10.1017/jfm.2016.441.  
  
J. Lee, H. J. Sungand T. A. Zaki, “Signature of large-scale motions on turbulent/non-turbulent interface in boundary layers”, *Journal of Fluid Mechanics*, vol. 819. Cambridge University Press (CUP), pp. 165–187, Apr. 18, 2017. doi: 10.1017/jfm.2017.170.  
  
S. J. Lee and T. A. Zaki, “Simulations of natural transition in viscoelastic channel flow”, *Journal of Fluid Mechanics*, vol. 820. Cambridge University Press (CUP), pp. 232–262, May 05, 2017. doi: 10.1017/jfm.2017.198.  
  
A. D. La Croix, “Design of a Hole Trapping Ligand”, *Nano Letters*, vol. 17, no. 2. American Chemical Society (ACS), pp. 909–914, Jan. 19, 2017. doi: 10.1021/acs.nanolett.6b04213.  
  
A. Alsinan, E. Meiburgand P. Garaud, “A settling-driven instability in two-component, stably stratified fluids”, *Journal of Fluid Mechanics*, vol. 816. Cambridge University Press (CUP), pp. 243–267, Mar. 06, 2017. doi: 10.1017/jfm.2017.94.  
  
E. Biegert, B. Vowinckeland E. Meiburg, “A collision model for grain-resolving simulations of flows over dense, mobile, polydisperse granular sediment beds”, *Journal of Computational Physics*, vol. 340. Elsevier BV, pp. 105–127, Jul. 2017. doi: 10.1016/j.jcp.2017.03.035.  
  
R. Ouillon, E. Meiburg, N. T. Ouelletteand J. R. Koseff, “Interaction of a downslope gravity current with an internal wave”, *Journal of Fluid Mechanics*, vol. 873. Cambridge University Press (CUP), pp. 889–913, Jun. 28, 2019. doi: 10.1017/jfm.2019.414.  
  
J. F. Reali, P. Garaud, A. Alsinanand E. Meiburg, “Layer formation in sedimentary fingering convection”, *Journal of Fluid Mechanics*, vol. 816. Cambridge University Press (CUP), pp. 268–305, Mar. 07, 2017. doi: 10.1017/jfm.2017.26.  
  
M. Mohagheghi and B. Khomami, “Molecular Processes Leading to Shear Banding in Well Entangled Polymeric Melts”, *ACS Macro Letters*, vol. 4, no. 7. American Chemical Society (ACS), pp. 684–688, Jun. 15, 2015. doi: 10.1021/acsmacrolett.5b00238.  
  
M. Mohagheghi and B. Khomami, “Elucidating the flow-microstructure coupling in the entangled polymer melts. Part I: Single chain dynamics in shear flow”, *Journal of Rheology*, vol. 60, no. 5. Society of Rheology, pp. 849–859, Sep. 2016. doi: 10.1122/1.4961481.  
  
M. Mohagheghi and B. Khomami, “Molecularly based criteria for shear banding in transient flow of entangled polymeric fluids”, *Physical Review E*, vol. 93, no. 6. American Physical Society (APS), Jun. 13, 2016. doi: 10.1103/physreve.93.062606.  
  
M. Mohagheghi and B. Khomami, “Elucidating the flow-microstructure coupling in entangled polymer melts. Part II: Molecular mechanism of shear banding”, *Journal of Rheology*, vol. 60, no. 5. Society of Rheology, pp. 861–872, Sep. 2016. doi: 10.1122/1.4961525.  
  
M. H. Nafar Sefiddashti, B. J. Edwardsand B. Khomami, “Individual chain dynamics of a polyethylene melt undergoing steady shear flow”, *Journal of Rheology*, vol. 59, no. 1. Society of Rheology, pp. 119–153, Jan. 2015. doi: 10.1122/1.4903498.  
  
M. H. Nafar Sefiddashti, B. J. Edwardsand B. Khomami, “Evaluation of reptation-based modeling of entangled polymeric fluids including chain rotation via nonequilibrium molecular dynamics simulation”, *Physical Review Fluids*, vol. 2, no. 8. American Physical Society (APS), Aug. 09, 2017. doi: 10.1103/physrevfluids.2.083301.  
  
M. H. Nafar Sefiddashti, B. J. Edwardsand B. Khomami, “Configurational Microphase Separation in Elongational Flow of an Entangled Polymer Liquid”, *Physical Review Letters*, vol. 121, no. 24. American Physical Society (APS), Dec. 14, 2018. doi: 10.1103/physrevlett.121.247802.  
  
S. A. Akhade, N. J. Bernstein, M. R. Esopi, M. J. Regulaand M. J. Janik, “A simple method to approximate electrode potential-dependent activation energies using density functional theory”, *Catalysis Today*, vol. 288. Elsevier BV, pp. 63–73, Jun. 2017. doi: 10.1016/j.cattod.2017.01.050.  
  
S. A. Akhade, R. M. Nidzyn, G. Rostamikiaand M. J. Janik, “Using Brønsted-Evans-Polanyi relations to predict electrode potential-dependent activation energies”, *Catalysis Today*, vol. 312. Elsevier BV, pp. 82–91, Aug. 2018. doi: 10.1016/j.cattod.2018.03.048.  
  
X. Chen, I. T. McCrum, K. A. Schwarz, M. J. Janikand M. T. M. Koper, “Co‐adsorption of Cations as the Cause of the Apparent pH Dependence of Hydrogen Adsorption on a Stepped Platinum Single‐Crystal Electrode”, *Angewandte Chemie International Edition*, vol. 56, no. 47. Wiley, pp. 15025–15029, Oct. 23, 2017. doi: 10.1002/anie.201709455.  
  
Y. Cong, “Uniform Pd0.33Ir0.67 nanoparticles supported on nitrogen-doped carbon with remarkable activity toward the alkaline hydrogen oxidation reaction”, *Journal of Materials Chemistry A*, vol. 7, no. 7. Royal Society of Chemistry (RSC), pp. 3161–3169, 2019. doi: 10.1039/c8ta11019k.  
  
S. Deo, W. Medlin, E. Nikollaand M. J. Janik, “Reaction paths for hydrodeoxygenation of furfuryl alcohol at TiO2/Pd interfaces”, *Journal of Catalysis*, vol. 377. Elsevier BV, pp. 28–40, Sep. 2019. doi: 10.1016/j.jcat.2019.07.012.  
  
D. Gao, “Activity and Selectivity Control in CO2 Electroreduction to Multicarbon Products over CuO*x* Catalysts via Electrolyte Design”, *ACS Catalysis*, vol. 8, no. 11. American Chemical Society (ACS), pp. 10012–10020, Sep. 11, 2018. doi: 10.1021/acscatal.8b02587.  
  
L. Gong, N. Agrawal, A. Roman, A. Holewinskiand M. J. Janik, “Density functional theory study of furfural electrochemical oxidation on the Pt (1 1 1) surface”, *Journal of Catalysis*, vol. 373. Elsevier BV, pp. 322–335, May 2019. doi: 10.1016/j.jcat.2019.04.012.  
  
L. Gong, Y. Muand M. J. Janik, “Mechanistic roles of catalyst surface coating in nitrobenzene selective reduction: A first-principles study”, *Applied Catalysis B: Environmental*, vol. 236. Elsevier BV, pp. 509–517, Nov. 2018. doi: 10.1016/j.apcatb.2018.05.015.  
  
C. M. Gunathunge, V. J. Ovalle, Y. Li, M. J. Janikand M. M. Waegele, “Existence of an Electrochemically Inert CO Population on Cu Electrodes in Alkaline pH”, *ACS Catalysis*, vol. 8, no. 8. American Chemical Society (ACS), pp. 7507–7516, Jul. 06, 2018. doi: 10.1021/acscatal.8b01552.  
  
Y. Guo, “Ring-opening and hydrodenitrogenation of indole under hydrothermal conditions over Ni, Pt, Ru, and Ni-Ru bimetallic catalysts”, *Chemical Engineering Journal*, vol. 406. Elsevier BV, p. 126853, Feb. 2021. doi: 10.1016/j.cej.2020.126853.  
  
H. He, A. Dasgupta, R. M. Rioux, R. J. Meyerand M. J. Janik, “Competitive Hydrogenation between Linear Alkenes and Aromatics on Close-Packed Late Transition Metal Surfaces”, *The Journal of Physical Chemistry C*, vol. 123, no. 13. American Chemical Society (ACS), pp. 8370–8378, Dec. 07, 2018. doi: 10.1021/acs.jpcc.8b09564.  
  
C. Jiang, M. R. Akkullu, B. Li, J. C. Davila, M. J. Janikand K. M. Dooley, “Rapid screening of ternary rare-earth – Transition metal catalysts for dry reforming of methane and characterization of final structures”, *Journal of Catalysis*, vol. 377. Elsevier BV, pp. 332–342, Sep. 2019. doi: 10.1016/j.jcat.2019.07.020.  
  
A. S. M. Jonayat, S. Chen, A. C. T. van Duinand M. Janik, “Predicting Monolayer Oxide Stability over Low-Index Surfaces of TiO2 Polymorphs Using ab Initio Thermodynamics”, *Langmuir*, vol. 34, no. 39. American Chemical Society (ACS), pp. 11685–11694, Aug. 31, 2018. doi: 10.1021/acs.langmuir.8b02426.  
  
A. S. M. Jonayat, “A first-principles study of stability of surface confined mixed metal oxides with corundum structure (Fe2O3, Cr2O3, V2O3)”, *Physical Chemistry Chemical Physics*, vol. 20, no. 10. Royal Society of Chemistry (RSC), pp. 7073–7081, 2018. doi: 10.1039/c8cp00154e.  
  
A. S. M. Jonayat, A. C. T. van Duinand M. J. Janik, “*Ab Initio* Thermodynamic Investigation of Monolayer Stability of Multicomponent Metal Oxides: M*x*O*y*/ZnO(0001) and M*x*O*y*/TiO2(110) (M = Pd, Ru, Ni, Pt, Au, Zn)”, *The Journal of Physical Chemistry C*, vol. 121, no. 39. American Chemical Society (ACS), pp. 21439–21448, Sep. 26, 2017. doi: 10.1021/acs.jpcc.7b06521.  
  
A. S. M. Jonayat, A. C. T. van Duinand M. J. Janik, “Discovery of Descriptors for Stable Monolayer Oxide Coatings through Machine Learning”, *ACS Applied Energy Materials*, vol. 1, no. 11. American Chemical Society (ACS), pp. 6217–6226, Oct. 23, 2018. doi: 10.1021/acsaem.8b01261.  
  
G. Kumar, E. Nikolla, S. Linic, J. W. Medlinand M. J. Janik, “Multicomponent Catalysts: Limitations and Prospects”, *ACS Catalysis*, vol. 8, no. 4. American Chemical Society (ACS), pp. 3202–3208, Mar. 06, 2018. doi: 10.1021/acscatal.8b00145.  
  
G. Kumar, “Evaluating differences in the active-site electronics of supported Au nanoparticle catalysts using Hammett and DFT studies”, *Nature Chemistry*, vol. 10, no. 3. Springer Science and Business Media LLC, pp. 268–274, Jan. 15, 2018. doi: 10.1038/nchem.2911.  
  
G. Kumar, T. Van Cleve, J. Park, A. van Duin, J. W. Medlinand M. J. Janik, “Thermodynamics of Alkanethiol Self-Assembled Monolayer Assembly on Pd Surfaces”, *Langmuir*, vol. 34, no. 22. American Chemical Society (ACS), pp. 6346–6357, May 16, 2018. doi: 10.1021/acs.langmuir.7b04351.  
  
X. Li, “Impact of Alkali Metal Cations and Iron Impurities on the Evolution of Hydrogen on Cu Electrodes in Alkaline Electrolytes”, *Journal of The Electrochemical Society*, vol. 167, no. 10. The Electrochemical Society, p. 106505, Jun. 10, 2020. doi: 10.1149/1945-7111/ab987b.  
  
Y. Li and M. J. Janik, “Recent progress on first-principles simulations of voltammograms”, *Current Opinion in Electrochemistry*, vol. 14. Elsevier BV, pp. 124–132, Apr. 2019. doi: 10.1016/j.coelec.2019.01.005.  
  
S. Maheshwari, Y. Li, N. Agrawaland M. J. Janik, “Density functional theory models for electrocatalytic reactions”, *Advances in Catalysis*. Elsevier, pp. 117–167, 2018. doi: 10.1016/bs.acat.2018.10.003.  
  
S. Maheshwari, G. Rostamikiaand M. J. Janik, “Elementary kinetics of nitrogen electroreduction on Fe surfaces”, *The Journal of Chemical Physics*, vol. 150, no. 4. AIP Publishing, p. 041708, Jan. 28, 2019. doi: 10.1063/1.5048036.  
  
L. O. Mark, N. Agrawal, A. M. Román, A. Holewinski, M. J. Janikand J. W. Medlin, “Insight into the Oxidation Mechanism of Furanic Compounds on Pt(111)”, *ACS Catalysis*, vol. 9, no. 12. American Chemical Society (ACS), pp. 11360–11370, Oct. 31, 2019. doi: 10.1021/acscatal.9b03983.  
  
I. T. McCrum, X. Chen, K. A. Schwarz, M. J. Janikand M. T. M. Koper, “Effect of Step Density and Orientation on the Apparent pH Dependence of Hydrogen and Hydroxide Adsorption on Stepped Platinum Surfaces”, *The Journal of Physical Chemistry C*, vol. 122, no. 29. American Chemical Society (ACS), pp. 16756–16764, Jul. 03, 2018. doi: 10.1021/acs.jpcc.8b03660.  
  
I. T. McCrum, M. A. Hicknerand M. J. Janik, “First-Principles Calculation of Pt Surface Energies in an Electrochemical Environment: Thermodynamic Driving Forces for Surface Faceting and Nanoparticle Reconstruction”, *Langmuir*, vol. 33, no. 28. American Chemical Society (ACS), pp. 7043–7052, Jul. 05, 2017. doi: 10.1021/acs.langmuir.7b01530.  
  
I. T. McCrum, M. A. Hicknerand M. J. Janik, “Quaternary Ammonium Cation Specific Adsorption on Platinum Electrodes: A Combined Experimental and Density Functional Theory Study”, *Journal of The Electrochemical Society*, vol. 165, no. 2. The Electrochemical Society, pp. F114–F121, 2018. doi: 10.1149/2.1351802jes.  
  
I. T. McCrum and M. J. Janik, “First Principles Simulations of Cyclic Voltammograms on Stepped Pt(553) and Pt(533) Electrode Surfaces”, *ChemElectroChem*, vol. 3, no. 10. Wiley, pp. 1609–1617, Aug. 09, 2016. doi: 10.1002/celc.201600293.  
  
I. T. McCrum and M. J. Janik, “Deconvoluting Cyclic Voltammograms To Accurately Calculate Pt Electrochemically Active Surface Area”, *The Journal of Physical Chemistry C*, vol. 121, no. 11. American Chemical Society (ACS), pp. 6237–6245, Mar. 13, 2017. doi: 10.1021/acs.jpcc.7b01617.  
  
A. G. Oshchepkov, “Nickel Metal Nanoparticles as Anode Electrocatalysts for Highly Efficient Direct Borohydride Fuel Cells”, *ACS Catalysis*, vol. 9, no. 9. American Chemical Society (ACS), pp. 8520–8528, Jul. 29, 2019. doi: 10.1021/acscatal.9b01616.  
  
Y. Qiu, “BCC-Phased PdCu Alloy as a Highly Active Electrocatalyst for Hydrogen Oxidation in Alkaline Electrolytes”, *Journal of the American Chemical Society*, vol. 140, no. 48. American Chemical Society (ACS), pp. 16580–16588, Nov. 05, 2018. doi: 10.1021/jacs.8b08356.  
  
A. M. Román, N. Agrawal, J. C. Hasse, M. J. Janik, J. W. Medlinand A. Holewinski, “Electro-oxidation of furfural on gold is limited by furoate self-assembly”, *Journal of Catalysis*, vol. 391. Elsevier BV, pp. 327–335, Nov. 2020. doi: 10.1016/j.jcat.2020.08.034.  
  
G. Rostamikia, S. Maheshwariand M. J. Janik, “Elementary kinetics of nitrogen electroreduction to ammonia on late transition metals”, *Catalysis Science & Technology*, vol. 9, no. 1. Royal Society of Chemistry (RSC), pp. 174–181, 2019. doi: 10.1039/c8cy01845f.  
  
C. S. Spanjers, “Determination of Bulk and Surface Atomic Arrangement in Ni–Zn γ-Brass Phase at Different Ni to Zn Ratios”, *Chemistry of Materials*, vol. 29, no. 2. American Chemical Society (ACS), pp. 504–512, Dec. 22, 2016. doi: 10.1021/acs.chemmater.6b01769.  
  
Y. Sun, “Defect-mediated selective hydrogenation of nitroarenes on nanostructured WS2”, *Chemical Science*, vol. 10, no. 44. Royal Society of Chemistry (RSC), pp. 10310–10317, 2019. doi: 10.1039/c9sc03337h.  
  
Z. Wang, “Enhancement of Alkyne Semi-Hydrogenation Selectivity by Electronic Modification of Platinum”, *ACS Catalysis*, vol. 10, no. 12. American Chemical Society (ACS), pp. 6763–6770, May 12, 2020. doi: 10.1021/acscatal.9b04070.  
  
J. Zhang, S. Deo, M. J. Janikand J. W. Medlin, “Control of Molecular Bonding Strength on Metal Catalysts with Organic Monolayers for CO2 Reduction”, *Journal of the American Chemical Society*, vol. 142, no. 11. American Chemical Society (ACS), pp. 5184–5193, Feb. 21, 2020. doi: 10.1021/jacs.9b12980.  
  
J. Melguizo-Gavilanes, L. R. Boeck, R. Méveland J. E. Shepherd, “Hot surface ignition of stoichiometric hydrogen-air mixtures”, *International Journal of Hydrogen Energy*, vol. 42, no. 11. Elsevier BV, pp. 7393–7403, Mar. 2017. doi: 10.1016/j.ijhydene.2016.05.095.  
  
J. Melguizo-Gavilanes, S. Coronel, R. Méveland J. E. Shepherd, “Dynamics of ignition of stoichiometric hydrogen-air mixtures by moving heated particles”, *International Journal of Hydrogen Energy*, vol. 42, no. 11. Elsevier BV, pp. 7380–7392, Mar. 2017. doi: 10.1016/j.ijhydene.2016.05.206.  
  
J. Melguizo-Gavilanes, R. Mével, S. Coroneland J. E. Shepherd, “Effects of differential diffusion on ignition of stoichiometric hydrogen-air by moving hot spheres”, *Proceedings of the Combustion Institute*, vol. 36, no. 1. Elsevier BV, pp. 1155–1163, 2017. doi: 10.1016/j.proci.2016.06.120.  
  
J. Melguizo-Gavilanes, A. Nové-Josserand, S. Coronel, R. Méveland J. E. Shepherd, “Hot Surface Ignition of *n*-Hexane Mixtures Using Simplified Kinetics”, *Combustion Science and Technology*, vol. 188, no. 11–12. Informa UK Limited, pp. 2060–2076, Oct. 28, 2016. doi: 10.1080/00102202.2016.1212577.  
  
R. Mével, U. Niedzielska, J. Melguizo-Gavilanes, S. Coroneland J. E. Shepherd, “Chemical Kinetics of *n*-Hexane-Air Atmospheres in the Boundary Layer of a Moving Hot Sphere”, *Combustion Science and Technology*, vol. 188, no. 11–12. Informa UK Limited, pp. 2267–2283, Oct. 28, 2016. doi: 10.1080/00102202.2016.1211886.  
  
S. Acharya and Y. Kanani, “Advances in Film Cooling Heat Transfer”, *Advances in Heat Transfer*. Elsevier, pp. 91–156, 2017. doi: 10.1016/bs.aiht.2017.10.001.  
  
Y. Kanani, S. Acharyaand F. Ames, “Large Eddy Simulation of the Laminar Heat Transfer Augmentation on the Pressure Side of a Turbine Vane Under Freestream Turbulence”, *Journal of Turbomachinery*, vol. 141, no. 4. ASME International, Jan. 21, 2019. doi: 10.1115/1.4041599.  
  
Y. Kanani, S. Acharyaand F. Ames, “Simulations of Slot Film-Cooling With Freestream Acceleration and Turbulence”, *Volume 5A: Heat Transfer*. American Society of Mechanical Engineers, Jun. 26, 2017. doi: 10.1115/gt2017-65050.  
  
Y. Kanani, S. Acharyaand F. Ames, “Simulations of Slot Film-Cooling With Freestream Acceleration and Turbulence”, *Journal of Turbomachinery*, vol. 140, no. 4. ASME International, Jan. 30, 2018. doi: 10.1115/1.4038877.  
  
Y. Kanani, S. Acharyaand F. Ames, “LES Study of the Laminar Heat Transfer Augmentation on the Pressure Side of a Turbine Vane Under Freestream Turbulence”, *Volume 5C: Heat Transfer*. American Society of Mechanical Engineers, Jun. 11, 2018. doi: 10.1115/gt2018-77135.  
  
Y. Kanani, S. Acharyaand F. Ames, “Large Eddy Simulation of Bypass Transition in Vane Passage With Freestream Turbulence”, *Volume 5B: Heat Transfer*. American Society of Mechanical Engineers, Jun. 17, 2019. doi: 10.1115/gt2019-91099.  
  
Y. Kanani, S. Acharyaand F. Ames, “Large Eddy Simulation of Bypass Transition in Vane Passage With Freestream Turbulence”, *Journal of Turbomachinery*, vol. 142, no. 6. ASME International, May 12, 2020. doi: 10.1115/1.4046461.  
  
A. Consiglio and Z. Tian, “Importance of the Hubbard correction on the thermal conductivity calculation of strongly correlated materials: a case study of ZnO”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Nov. 10, 2016. doi: 10.1038/srep36875.  
  
H. Ma, H. Babaeiand Z. Tian, “The importance of van der Waals interactions to thermal transport in Graphene-C60 heterostructures”, *Carbon*, vol. 148. Elsevier BV, pp. 196–203, Jul. 2019. doi: 10.1016/j.carbon.2019.03.076.  
  
H. Ma, E. O’Donneland Z. Tian, “Tunable thermal conductivity of π-conjugated two-dimensional polymers”, *Nanoscale*, vol. 10, no. 29. Royal Society of Chemistry (RSC), pp. 13924–13929, 2018. doi: 10.1039/c8nr02994f.  
  
H. Ma and Z. Tian, “Effects of polymer topology and morphology on thermal transport: A molecular dynamics study of bottlebrush polymers”, *Applied Physics Letters*, vol. 110, no. 9. AIP Publishing, p. 091903, Feb. 27, 2017. doi: 10.1063/1.4976946.  
  
H. Ma and Z. Tian, “Chain rotation significantly reduces thermal conductivity of single-chain polymers”, *Journal of Materials Research*, vol. 34, no. 1. Springer Science and Business Media LLC, pp. 126–133, Oct. 22, 2018. doi: 10.1557/jmr.2018.362.  
  
B. Fu, C. Van Dyck, S. Zaleski, R. P. Van Duyneand M. A. Ratner, “Single Molecule Electrochemistry: Impact of Surface Site Heterogeneity”, *The Journal of Physical Chemistry C*, vol. 120, no. 48. American Chemical Society (ACS), pp. 27241–27249, Nov. 22, 2016. doi: 10.1021/acs.jpcc.6b05252.  
  
C. Van Dyck, B. Fu, R. P. Van Duyne, G. C. Schatzand M. A. Ratner, “Deducing the Adsorption Geometry of Rhodamine 6G from the Surface-Induced Mode Renormalization in Surface-Enhanced Raman Spectroscopy”, *The Journal of Physical Chemistry C*, vol. 122, no. 1. American Chemical Society (ACS), pp. 465–473, Dec. 28, 2017. doi: 10.1021/acs.jpcc.7b09441.  
  
J. Wang, S. Shinand A. Hu, “Geometrical Effects on Sintering Dynamics of Cu–Ag Core–Shell Nanoparticles”, *The Journal of Physical Chemistry C*, vol. 120, no. 31. American Chemical Society (ACS), pp. 17791–17800, Aug. 02, 2016. doi: 10.1021/acs.jpcc.6b05515.  
  
A. Yousefzadi Nobakht and S. Shin, “Anisotropic control of thermal transport in graphene/Si heterostructures”, *Journal of Applied Physics*, vol. 120, no. 22. AIP Publishing, p. 225111, Dec. 14, 2016. doi: 10.1063/1.4971873.  
  
D. C. Marable, S. Shinand A. Yousefzadi Nobakht, “Investigation into the microscopic mechanisms influencing convective heat transfer of water flow in graphene nanochannels”, *International Journal of Heat and Mass Transfer*, vol. 109. Elsevier BV, pp. 28–39, Jun. 2017. doi: 10.1016/j.ijheatmasstransfer.2017.01.100.  
  
J. Wang and S. Shin, “Sintering of multiple Cu–Ag core–shell nanoparticles and properties of nanoparticle-sintered structures”, *RSC Advances*, vol. 7, no. 35. Royal Society of Chemistry (RSC), pp. 21607–21617, 2017. doi: 10.1039/c7ra02611k.  
  
J. Wang and S. Shin, “Room temperature nanojoining of Cu-Ag core-shell nanoparticles and nanowires”, *Journal of Nanoparticle Research*, vol. 19, no. 2. Springer Science and Business Media LLC, Feb. 2017. doi: 10.1007/s11051-017-3761-6.  
  
K. S. Khare and F. R. Phelan Jr., “Quantitative Comparison of Atomistic Simulations with Experiment for a Cross-Linked Epoxy: A Specific Volume–Cooling Rate Analysis”, *Macromolecules*, vol. 51, no. 2. American Chemical Society (ACS), pp. 564–575, Jan. 08, 2018. doi: 10.1021/acs.macromol.7b01303.  
  
C. García-Sánchez and C. Gorlé, “Uncertainty quantification for microscale CFD simulations based on input from mesoscale codes”, *Journal of Wind Engineering and Industrial Aerodynamics*, vol. 176. Elsevier BV, pp. 87–97, May 2018. doi: 10.1016/j.jweia.2018.03.011.  
  
C. García-Sánchez, J. van Beeckand C. Gorlé, “Predictive large eddy simulations for urban flows: Challenges and opportunities”, *Building and Environment*, vol. 139. Elsevier BV, pp. 146–156, Jul. 2018. doi: 10.1016/j.buildenv.2018.05.007.  
  
Z. Hao and C. Gorlé, “Large eddy simulations of forced heat convection in a pin-fin array with a priori examination of an eddy-viscosity turbulence model”, *International Journal of Heat and Fluid Flow*, vol. 77. Elsevier BV, pp. 73–83, Jun. 2019. doi: 10.1016/j.ijheatfluidflow.2019.03.006.  
  
G. Lamberti, C. García-Sánchez, J. Sousaand C. Gorlé, “Optimizing turbulent inflow conditions for large-eddy simulations of the atmospheric boundary layer”, *Journal of Wind Engineering and Industrial Aerodynamics*, vol. 177. Elsevier BV, pp. 32–44, Jun. 2018. doi: 10.1016/j.jweia.2018.04.004.  
  
G. Lamberti and C. Gorlé, “Sensitivity of LES predictions of wind loading on a high-rise building to the inflow boundary condition”, *Journal of Wind Engineering and Industrial Aerodynamics*, vol. 206. Elsevier BV, p. 104370, Nov. 2020. doi: 10.1016/j.jweia.2020.104370.  
  
G. Lamberti and C. Gorlé, “A multi-fidelity machine learning framework to predict wind loads on buildings”, *Journal of Wind Engineering and Industrial Aerodynamics*, vol. 214. Elsevier BV, p. 104647, Jul. 2021. doi: 10.1016/j.jweia.2021.104647.  
  
J. Yuan and M. Aghaei Jouybari, “Topographical effects of roughness on turbulence statistics in roughness sublayer”, *Physical Review Fluids*, vol. 3, no. 11. American Physical Society (APS), Nov. 09, 2018. doi: 10.1103/physrevfluids.3.114603.  
  
R. N. Salaway and L. V. Zhigilei, “Thermal conductance of carbon nanotube contacts: Molecular dynamics simulations and general description of the contact conductance”, *Physical Review B*, vol. 94, no. 1. American Physical Society (APS), Jul. 15, 2016. doi: 10.1103/physrevb.94.014308.  
  
B. K. Wittmaack, A. H. Banna, A. N. Volkovand L. V. Zhigilei, “Mesoscopic modeling of structural self-organization of carbon nanotubes into vertically aligned networks of nanotube bundles”, *Carbon*, vol. 130. Elsevier BV, pp. 69–86, Apr. 2018. doi: 10.1016/j.carbon.2017.12.078.  
  
B. K. Wittmaack, A. N. Volkovand L. V. Zhigilei, “Mesoscopic modeling of the uniaxial compression and recovery of vertically aligned carbon nanotube forests”, *Composites Science and Technology*, vol. 166. Elsevier BV, pp. 66–85, Sep. 2018. doi: 10.1016/j.compscitech.2018.03.014.  
  
A. S. Almithn and D. D. Hibbitts, “Supra-monolayer coverages on small metal clusters and their effects on H2 chemisorption particle size estimates”, *AIChE Journal*, vol. 64, no. 8. Wiley, pp. 3109–3120, Feb. 14, 2018. doi: 10.1002/aic.16110.  
  
A. Almithn and D. Hibbitts, “Effects of Catalyst Model and High Adsorbate Coverages in ab Initio Studies of Alkane Hydrogenolysis”, *ACS Catalysis*, vol. 8, no. 7. American Chemical Society (ACS), pp. 6375–6387, May 30, 2018. doi: 10.1021/acscatal.8b01114.  
  
M. DeLuca and D. Hibbitts, “Prediction of C6–C12 Interconversion Rates Using DFT and Zeolite-specific kinetic Monte Carlo Simulation Methods”, *[]*. American Chemical Society (ACS), Apr. 25, 2019. doi: 10.26434/chemrxiv.8035565.v1.  
  
M. DeLuca, C. Janesand D. Hibbitts, “Contrasting Arene, Alkene, Diene, and Formaldehyde Hydrogenation in H-ZSM-5, H-SSZ-13, and H-SAPO-34 Frameworks during MTO”, *ACS Catalysis*, vol. 10, no. 8. American Chemical Society (ACS), pp. 4593–4607, Mar. 10, 2020. doi: 10.1021/acscatal.9b04529.  
  
J. R. Di Iorio, A. J. Hoffman, C. T. Nimlos, S. Nystrom, D. Hibbittsand R. Gounder, “Mechanistic origins of the high-pressure inhibition of methanol dehydration rates in small-pore acidic zeolites”, *Journal of Catalysis*, vol. 380. Elsevier BV, pp. 161–177, Dec. 2019. doi: 10.1016/j.jcat.2019.10.012.  
  
A. J. Hoffman, “Rigid Arrangements of Ionic Charge in Zeolite Frameworks Conferred by Specific Aluminum Distributions Preferentially Stabilize Alkanol Dehydration Transition States”, *Angewandte Chemie International Edition*, vol. 59, no. 42. Wiley, pp. 18686–18694, Aug. 18, 2020. doi: 10.1002/anie.202007790.  
  
A. Hoffman, M. DeLucaand D. Hibbitts, “Restructuring of MFI Framework Zeolite Models and Their Associated Artifacts in Density Functional Theory Calculations”, *The Journal of Physical Chemistry C*, vol. 123, no. 11. American Chemical Society (ACS), pp. 6572–6585, Feb. 15, 2019. doi: 10.1021/acs.jpcc.8b12230.  
  
P. Kravchenko, V. Krishnanand D. Hibbitts, “Mechanism and Effects of Coverage and Particle Morphology on Rh-Catalyzed NO–H2 Reactions”, *The Journal of Physical Chemistry C*, vol. 124, no. 24. American Chemical Society (ACS), pp. 13291–13303, May 25, 2020. doi: 10.1021/acs.jpcc.0c04024.  
  
P. Kravchenko, C. Plaisanceand D. Hibbitts, “A New Computational Interface for Catalysis”, *[]*. American Chemical Society (ACS), Jul. 12, 2019. doi: 10.26434/chemrxiv.8040737.v4.  
  
S. Nystrom, A. Hoffmanand D. Hibbitts, “Tuning Brønsted Acid Strength by Altering Site Proximity in CHA Framework Zeolites”, *ACS Catalysis*, vol. 8, no. 9. American Chemical Society (ACS), pp. 7842–7860, Jul. 12, 2018. doi: 10.1021/acscatal.8b02049.  
  
T. Avanessian and G. Hwang, “Thermal diode using controlled capillary in heterogeneous nanopores”, *International Journal of Heat and Mass Transfer*, vol. 124. Elsevier BV, pp. 201–209, Sep. 2018. doi: 10.1016/j.ijheatmasstransfer.2018.03.039.  
  
T. Avanessian and G. Hwang, “Thermal switch using controlled capillary transition in heterogeneous nanostructures”, *International Journal of Heat and Mass Transfer*, vol. 121. Elsevier BV, pp. 127–136, Jun. 2018. doi: 10.1016/j.ijheatmasstransfer.2017.12.142.  
  
R. Dhariwal and A. D. Bragg, “Fluid particles only separate exponentially in the dissipation range of turbulence after extremely long times”, *Physical Review Fluids*, vol. 3, no. 3. American Physical Society (APS), Mar. 16, 2018. doi: 10.1103/physrevfluids.3.034604.  
  
H. Hu, M. Chakraborty, T. P. Allred, J. A. Weibeland S. V. Garimella, “Multiscale Modeling of the Three-Dimensional Meniscus Shape of a Wetting Liquid Film on Micro-/Nanostructured Surfaces”, *Langmuir*, vol. 33, no. 43. American Chemical Society (ACS), pp. 12028–12037, Oct. 11, 2017. doi: 10.1021/acs.langmuir.7b02837.  
  
S. Chen, L. A. Baumes, A. Gel, M. Adepu, H. Emadyand Y. Jiao, “Classification of particle height in a hopper bin from limited discharge data using convolutional neural network models”, *Powder Technology*, vol. 339. Elsevier BV, pp. 615–624, Nov. 2018. doi: 10.1016/j.powtec.2018.08.048.  
  
N. O. Braun, D. I. Pullinand D. I. Meiron, “Large eddy simulation investigation of the canonical shock–turbulence interaction”, *Journal of Fluid Mechanics*, vol. 858. Cambridge University Press (CUP), pp. 500–535, Nov. 06, 2018. doi: 10.1017/jfm.2018.766.  
  
N. O. Braun, D. I. Pullinand D. I. Meiron, “Regularization method for large eddy simulations of shock-turbulence interactions”, *Journal of Computational Physics*, vol. 361. Elsevier BV, pp. 231–246, May 2018. doi: 10.1016/j.jcp.2018.01.052.  
  
S. K. Iyemperumal and N. A. Deskins, “Evaluating Solvent Effects at the Aqueous/Pt(111) Interface”, *ChemPhysChem*, vol. 18, no. 16. Wiley, pp. 2171–2190, Jun. 27, 2017. doi: 10.1002/cphc.201700162.  
  
S. K. Iyemperumal and N. A. Deskins, “Activation of CO2 by supported Cu clusters”, *Physical Chemistry Chemical Physics*, vol. 19, no. 42. Royal Society of Chemistry (RSC), pp. 28788–28807, 2017. doi: 10.1039/c7cp05718k.  
  
S. K. Iyemperumal, T. D. Pham, J. Bauerand N. A. Deskins, “Quantifying Support Interactions and Reactivity Trends of Single Metal Atom Catalysts over TiO2”, *The Journal of Physical Chemistry C*, vol. 122, no. 44. American Chemical Society (ACS), pp. 25274–25289, Oct. 16, 2018. doi: 10.1021/acs.jpcc.8b05611.  
  
G. Yang, L. M. Namin, N. Aaron Deskinsand X. Teng, “Influence of ∗OH adsorbates on the potentiodynamics of the CO2 generation during the electro-oxidation of ethanol”, *Journal of Catalysis*, vol. 353. Elsevier BV, pp. 335–348, Sep. 2017. doi: 10.1016/j.jcat.2017.07.033.  
  
P. L. Barclay and J. R. Lukes, “Fluid-fluid interfacial mobility from random walks”, *The Journal of Chemical Physics*, vol. 147, no. 24. AIP Publishing, p. 244703, Dec. 28, 2017. doi: 10.1063/1.5002694.  
  
P. L. Barclay and J. R. Lukes, “Curvature Dependence of the Mass Accommodation Coefficient”, *Langmuir*, vol. 35, no. 18. American Chemical Society (ACS), pp. 6196–6202, Apr. 12, 2019. doi: 10.1021/acs.langmuir.9b00537.  
  
P. L. Barclay and J. R. Lukes, “Cahn-Hilliard mobility of fluid-fluid interfaces from molecular dynamics”, *Physics of Fluids*, vol. 31, no. 9. AIP Publishing, p. 092107, Sep. 2019. doi: 10.1063/1.5116576.  
  
R. Ma and J. R. Lukes, “Validity of the isotropic thermal conductivity assumption in supercell lattice dynamics”, *Journal of Applied Physics*, vol. 123, no. 6. AIP Publishing, p. 065106, Feb. 14, 2018. doi: 10.1063/1.5007054.  
  
M. Carbone and A. D. Bragg, “Is vortex stretching the main cause of the turbulent energy cascade?”, *Journal of Fluid Mechanics*, vol. 883. Cambridge University Press (CUP), Jan. 25, 2020. doi: 10.1017/jfm.2019.923.  
  
M. Carbone, A. D. Braggand M. Iovieno, “Multiscale fluid–particle thermal interaction in isotropic turbulence”, *Journal of Fluid Mechanics*, vol. 881. Cambridge University Press (CUP), pp. 679–721, Oct. 25, 2019. doi: 10.1017/jfm.2019.773.  
  
R. Dhariwal and A. D. Bragg, “Small-scale dynamics of settling, bidisperse particles in turbulence”, *Journal of Fluid Mechanics*, vol. 839. Cambridge University Press (CUP), pp. 594–620, Feb. 02, 2018. doi: 10.1017/jfm.2018.24.  
  
R. Dhariwal and A. D. Bragg, “Enhanced and suppressed multiscale dispersion of bidisperse inertial particles due to gravity”, *Physical Review Fluids*, vol. 4, no. 3. American Physical Society (APS), Mar. 11, 2019. doi: 10.1103/physrevfluids.4.034302.  
  
M. Momenifar, R. Dhariwaland A. D. Bragg, “Influence of Reynolds number on the motion of settling, bidisperse inertial particles in turbulence”, *Physical Review Fluids*, vol. 4, no. 5. American Physical Society (APS), May 08, 2019. doi: 10.1103/physrevfluids.4.054301.  
  
A. Yousefzadi Nobakht, “Thermal rectification via asymmetric structural defects in graphene”, *Carbon*, vol. 132. Elsevier BV, pp. 565–572, Jun. 2018. doi: 10.1016/j.carbon.2018.02.087.  
  
A. Yousefzadi Nobakht, S. Shinand J. Wang, “Asymmetric Thermal Transport by Adjusting Structural Defects”, *2018 Joint Thermophysics and Heat Transfer Conference*. American Institute of Aeronautics and Astronautics, Jun. 24, 2018. doi: 10.2514/6.2018-2949.  
  
M. A. A. Hasan, J. Wang, Y. C. Lim, A. Huand S. Shin, “Concentration dependence of hydrogen diffusion in α-iron from atomistic perspectives”, *International Journal of Hydrogen Energy*, vol. 44, no. 51. Elsevier BV, pp. 27876–27884, Oct. 2019. doi: 10.1016/j.ijhydene.2019.09.007.  
  
J. Wang, C. Li, S. Shinand H. Qi, “Accelerated Atomic Data Production in *Ab Initio* Molecular Dynamics with Recurrent Neural Network for Materials Research”, *The Journal of Physical Chemistry C*, vol. 124, no. 27. American Chemical Society (ACS), pp. 14838–14846, Jun. 08, 2020. doi: 10.1021/acs.jpcc.0c01944.  
  
J. Wang, S. Shin, A. Huand J. K. Wilt, “Diffusion kinetics of transient liquid phase bonding of Ni-based superalloy with Ni nanoparticles: A molecular dynamics perspective”, *Computational Materials Science*, vol. 152. Elsevier BV, pp. 228–235, Sep. 2018. doi: 10.1016/j.commatsci.2018.05.056.  
  
J. Wang, S. Shinand S. Lee, “Interatomic Potential Model Development: Finite‐Temperature Dynamics Machine Learning”, *Advanced Theory and Simulations*, vol. 3, no. 2. Wiley, p. 1900210, Dec. 17, 2019. doi: 10.1002/adts.201900210.  
  
J. Wang, S. Shin, A. Yousefzadi Nobakhtand A. Shyam, “Structural deformation and transformation of θ′-Al2Cu precipitate in Al matrix via interfacial diffusion”, *Computational Materials Science*, vol. 156. Elsevier BV, pp. 111–120, Jan. 2019. doi: 10.1016/j.commatsci.2018.09.024.  
  
A. Yousefzadi Nobakht, S. Shin, K. D. Kihm, D. C. Marableand W. Lee, “Heat flow diversion in supported graphene nanomesh”, *Carbon*, vol. 123. Elsevier BV, pp. 45–53, Oct. 2017. doi: 10.1016/j.carbon.2017.07.025.  
  
Z. Cheng, “Tuning Chiral Nematic Pitch of Bioresourced Photonic Films via Coupling Organic Acid Hydrolysis”, *Advanced Materials Interfaces*, vol. 6, no. 7. Wiley, p. 1802010, Feb. 27, 2019. doi: 10.1002/admi.201802010.  
  
Z. Shen, W. Baker, H. Yeand Y. Li, “pH-Dependent aggregation and pH-independent cell membrane adhesion of monolayer-protected mixed charged gold nanoparticles”, *Nanoscale*, vol. 11, no. 15. Royal Society of Chemistry (RSC), pp. 7371–7385, 2019. doi: 10.1039/c8nr09617a.  
  
Z. Shen, D. T. Loe, A. Fisher, M. Kröger, J. L. Rougeand Y. Li, “Polymer stiffness governs template mediated self-assembly of liposome-like nanoparticles: simulation, theory and experiment”, *Nanoscale*, vol. 11, no. 42. Royal Society of Chemistry (RSC), pp. 20179–20193, 2019. doi: 10.1039/c9nr07063j.  
  
Z. Shen, H. Ye, M. Krögerand Y. Li, “Aggregation of polyethylene glycol polymers suppresses receptor-mediated endocytosis of PEGylated liposomes”, *Nanoscale*, vol. 10, no. 9. Royal Society of Chemistry (RSC), pp. 4545–4560, 2018. doi: 10.1039/c7nr09011k.  
  
Z. Shen, H. Ye, M. Kröger, S. Tangand Y. Li, “Interplay between ligand mobility and nanoparticle geometry during cellular uptake of PEGylated liposomes and bicelles”, *Nanoscale*, vol. 11, no. 34. Royal Society of Chemistry (RSC), pp. 15971–15983, 2019. doi: 10.1039/c9nr02408e.  
  
Z. Shen, H. Yeand Y. Li, “Understanding receptor-mediated endocytosis of elastic nanoparticles through coarse grained molecular dynamic simulation”, *Physical Chemistry Chemical Physics*, vol. 20, no. 24. Royal Society of Chemistry (RSC), pp. 16372–16385, 2018. doi: 10.1039/c7cp08644j.  
  
Z. Shen, H. Ye, X. Yiand Y. Li, “Membrane Wrapping Efficiency of Elastic Nanoparticles during Endocytosis: Size and Shape Matter”, *ACS Nano*, vol. 13, no. 1. American Chemical Society (ACS), pp. 215–228, Dec. 17, 2018. doi: 10.1021/acsnano.8b05340.  
  
H. Ye, Z. Shenand Y. Li, “Interplay of deformability and adhesion on localization of elastic micro-particles in blood flow”, *Journal of Fluid Mechanics*, vol. 861. Cambridge University Press (CUP), pp. 55–87, Dec. 19, 2018. doi: 10.1017/jfm.2018.890.  
  
H. Ye, Z. Shenand Y. Li, “Shear rate dependent margination of sphere-like, oblate-like and prolate-like micro-particles within blood flow”, *Soft Matter*, vol. 14, no. 36. Royal Society of Chemistry (RSC), pp. 7401–7419, 2018. doi: 10.1039/c8sm01304g.  
  
H. Ye, Z. Shenand Y. Li, “Shape-Dependent Transport of Microparticles in Blood Flow: From Margination to Adhesion”, *Journal of Engineering Mechanics*, vol. 145, no. 4. American Society of Civil Engineers (ASCE), Apr. 2019. doi: 10.1061/(asce)em.1943-7889.0001597.  
  
H. Ye, Z. Shenand Y. Li, “Multiscale Modeling of Vascular Dynamics of Micro- and Nano-particles”, *[]*. Morgan & Claypool Publishers, Dec. 2019. doi: 10.1088/2053-2571/ab4124.  
  
H. Ye, Z. Shen, L. Yu, M. Weiand Y. Li, “Manipulating nanoparticle transport within blood flow through external forces: an exemplar of mechanics in nanomedicine”, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 474, no. 2211. The Royal Society, p. 20170845, Mar. 2018. doi: 10.1098/rspa.2017.0845.  
  
H. Ye, Z. Shenand Y. Li, “Cell Stiffness Governs Its Adhesion Dynamics on Substrate Under Shear Flow”, *IEEE Transactions on Nanotechnology*, vol. 17, no. 3. Institute of Electrical and Electronics Engineers (IEEE), pp. 407–411, May 2018. doi: 10.1109/tnano.2017.2786943.  
  
H. Ye, Z. Shenand Y. Li, “Computational modeling of magnetic particle margination within blood flow through LAMMPS”, *Computational Mechanics*, vol. 62, no. 3. Springer Science and Business Media LLC, pp. 457–476, Nov. 11, 2017. doi: 10.1007/s00466-017-1508-y.  
  
H. Ye, Z. Shen, L. Yu, M. Weiand Y. Li, “Anomalous Vascular Dynamics of Nanoworms within Blood Flow”, *ACS Biomaterials Science & Engineering*, vol. 4, no. 1. American Chemical Society (ACS), pp. 66–77, Dec. 05, 2017. doi: 10.1021/acsbiomaterials.7b00434.  
  
A. Zandian, W. A. Sirignanoand F. Hussain, “Understanding liquid-jet atomization cascades via vortex dynamics”, *Journal of Fluid Mechanics*, vol. 843. Cambridge University Press (CUP), pp. 293–354, Mar. 21, 2018. doi: 10.1017/jfm.2018.113.  
  
A. Zandian, W. A. Sirignanoand F. Hussain, “Vorticity dynamics in a spatially developing liquid jet inside a co-flowing gas”, *Journal of Fluid Mechanics*, vol. 877. Cambridge University Press (CUP), pp. 429–470, Aug. 27, 2019. doi: 10.1017/jfm.2019.596.  
  
I. Rahbari and G. Paniagua, “Acoustic streaming in turbulent compressible channel flow for heat transfer enhancement”, *Journal of Fluid Mechanics*, vol. 889. Cambridge University Press (CUP), Feb. 18, 2020. doi: 10.1017/jfm.2020.69.  
  
A. R. Malipeddi and K. Sarkar, “Shear-induced collective diffusivity down a concentration gradient in a viscous emulsion of drops”, *Journal of Fluid Mechanics*, vol. 868. Cambridge University Press (CUP), pp. 5–25, Apr. 03, 2019. doi: 10.1017/jfm.2019.122.  
  
A. K. Chew and R. C. Van Lehn, “Quantifying the Stability of the Hydronium Ion in Organic Solvents With Molecular Dynamics Simulations”, *Frontiers in Chemistry*, vol. 7. Frontiers Media SA, Jun. 19, 2019. doi: 10.3389/fchem.2019.00439.  
  
A. K. Chew, “Effect of Mixed-Solvent Environments on the Selectivity of Acid-Catalyzed Dehydration Reactions”, *ACS Catalysis*, vol. 10, no. 3. American Chemical Society (ACS), pp. 1679–1691, Dec. 27, 2019. doi: 10.1021/acscatal.9b03460.  
  
B. C. Dallin and R. C. Van Lehn, “Spatially Heterogeneous Water Properties at Disordered Surfaces Decrease the Hydrophobicity of Nonpolar Self-Assembled Monolayers”, *The Journal of Physical Chemistry Letters*, vol. 10, no. 14. American Chemical Society (ACS), pp. 3991–3997, Jul. 02, 2019. doi: 10.1021/acs.jpclett.9b01707.  
  
J. H. Dwyer, “Solvent-Mediated Affinity of Polymer-Wrapped Single-Walled Carbon Nanotubes for Chemically Modified Surfaces”, *Langmuir*, vol. 35, no. 38. American Chemical Society (ACS), pp. 12492–12500, Aug. 28, 2019. doi: 10.1021/acs.langmuir.9b02217.  
  
J. K. Sheavly, J. I. Gold, M. Mavrikakisand R. C. Van Lehn, “Molecular simulations of analyte partitioning and diffusion in liquid crystal sensors”, *Molecular Systems Design & Engineering*, vol. 5, no. 1. Royal Society of Chemistry (RSC), pp. 304–316, 2020. doi: 10.1039/c9me00126c.  
  
T. W. Walker, “Universal kinetic solvent effects in acid-catalyzed reactions of biomass-derived oxygenates”, *Energy & Environmental Science*, vol. 11, no. 3. Royal Society of Chemistry (RSC), pp. 617–628, 2018. doi: 10.1039/c7ee03432f.  
  
A. A. Alghafis, A. M. Alshwairekh, A. M. Alwatban, U. F. Alqsairand A. Oztekin, “The Performance Enhancement of Hemodialyzers: Computational Fluid Dynamics Study”, *Volume 1: Fluid Mechanics*. American Society of Mechanical Engineers, Jul. 28, 2019. doi: 10.1115/ajkfluids2019-4863.  
  
U. F. Alqsair, A. M. Alwatban, A. A. Alghafis, A. M. Alshwairekhand A. Oztekin, “Heat and Mass Transfer Characteristics of Vapor Permeation in Sweeping Gas Membrane Distillation Systems for Sea Water Desalination”, *ASME 2019 Heat Transfer Summer Conference*. American Society of Mechanical Engineers, Jul. 14, 2019. doi: 10.1115/ht2019-3674.  
  
U. F. Alqsair, A. M. Alwatban, A. M. Alshwairekh, R. Krysko, A. A. Alghafisand A. Oztekin, “The Effect of Mixing Promotors on Sweeping Gas Membrane Distillation System Performance”, *Volume 7: Fluids Engineering*. American Society of Mechanical Engineers, Nov. 11, 2019. doi: 10.1115/imece2019-10727.  
  
A. M. Alshwairekh, A. A. Alghafis, A. M. Alwatban, U. F. Alqsairand A. Oztekin, “The effects of membrane and channel corrugations in forward osmosis membrane modules – Numerical analyses”, *Desalination*, vol. 460. Elsevier BV, pp. 41–55, Jun. 2019. doi: 10.1016/j.desal.2019.03.003.  
  
A. M. Alshwairekh, A. A. Alghafis, A. M. Alwatban, U. F. Alqsairand A. Oztekin, “The Effect of Mixing Promoters on the Performance of Forward Osmosis Membrane Systems: Computational Fluid Dynamics Simulations”, *Volume 2: Computational Fluid Dynamics*. American Society of Mechanical Engineers, Jul. 28, 2019. doi: 10.1115/ajkfluids2019-4862.  
  
M. Altimemy, B. Attiya, C. Daskiran, I.-H. Liuand A. Oztekin, “Mitigation of flow-induced pressure fluctuations in a Francis turbine operating at the design and partial load regimes—LES simulations”, *International Journal of Heat and Fluid Flow*, vol. 79. Elsevier BV, p. 108444, Oct. 2019. doi: 10.1016/j.ijheatfluidflow.2019.108444.  
  
M. Altimemy, B. Attiya, C. Daskiran, I.-H. Liuand A. Oztekin, “Stabilizing Pump-Turbine Operations Using Water Injection Passive Control”, *Volume 3B: Fluid Applications and Systems*. American Society of Mechanical Engineers, Jul. 28, 2019. doi: 10.1115/ajkfluids2019-4866.  
  
M. Altimemy, B. Attiya, C. Daskiran, I.-H. Liuand A. Oztekin, “Mitigation of Flow-Induced Pressure Fluctuations in a Francis Turbine Using Water Injection”, *Volume 3B: Fluid Applications and Systems*. American Society of Mechanical Engineers, Jul. 28, 2019. doi: 10.1115/ajkfluids2019-4867.  
  
A. M. Alwatban, A. M. Alshwairekh, U. F. Alqsair, A. A. Alghafisand A. Oztekin, “Effect of membrane properties and operational parameters on systems for seawater desalination using computational fluid dynamics simulations”, *DESALINATION AND WATER TREATMENT*, vol. 161. Desalination Publications, pp. 92–107, 2019. doi: 10.5004/dwt.2019.24275.  
  
A. M. Alwatban, A. M. Alshwairekh, U. F. Alqsair, A. A. Alghafisand A. Oztekin, “Performance improvements by embedded spacer in direct contact membrane distillation – Computational study”, *Desalination*, vol. 470. Elsevier BV, p. 114103, Nov. 2019. doi: 10.1016/j.desal.2019.114103.  
  
A. M. Alwatban, A. M. Alshwairekh, U. F. Alqsair, A. A. Alghafisand A. Oztekin, “The Effect of Net-Type Spacer on the Performance of Direct Contact Membrane Distillation System for Seawater Desalination: Heat and Mass Transfer Analysis”, *ASME 2019 Heat Transfer Summer Conference*. American Society of Mechanical Engineers, Jul. 14, 2019. doi: 10.1115/ht2019-3673.  
  
A. M. Alwatban, A. M. Alshwairekh, U. F. Alqsair, R. Krysko, A. A. Alghafisand A. Oztekin, “The Effect of the Embedded Spacers on the Performance of Direct Contact Membrane Distillation System Operating With Different Inlet Feed Temperature”, *Volume 7: Fluids Engineering*. American Society of Mechanical Engineers, Nov. 11, 2019. doi: 10.1115/imece2019-10723.  
  
A. E. Anqi, M. Usta, R. Krysko, J.-G. Lee, N. Ghaffourand A. Oztekin, “Numerical study of desalination by vacuum membrane distillation – Transient three-dimensional analysis”, *Journal of Membrane Science*, vol. 596. Elsevier BV, p. 117609, Feb. 2020. doi: 10.1016/j.memsci.2019.117609.  
  
B. Attiya, M. Altimemy, C. Daskiran, I.-H. Liuand A. Oztekin, “Micro-Hydrokinetic Turbine Operating in the Vicinity of a Free Surface: Multiphase Large Eddy Simulations”, *Volume 7: Fluids Engineering*. American Society of Mechanical Engineers, Nov. 11, 2019. doi: 10.1115/imece2019-10899.  
  
C. Daskiran, B. Attiya, M. Altimemy, I.-H. Liuand A. Oztekin, “Oxygen dissolution via pump-turbine – Application to wastewater treatment”, *International Journal of Heat and Mass Transfer*, vol. 131. Elsevier BV, pp. 1052–1063, Mar. 2019. doi: 10.1016/j.ijheatmasstransfer.2018.11.130.  
  
C. Daskiran, B. Attiya, J. Riglinand A. Oztekin, “Large eddy simulations of ventilated micro hydrokinetic turbine at design and off-design operating conditions”, *Ocean Engineering*, vol. 169. Elsevier BV, pp. 1–18, Dec. 2018. doi: 10.1016/j.oceaneng.2018.09.008.  
  
M. Morabito, “Internal Tensile Force and A2 Domain Unfolding of von Willebrand Factor Multimers in Shear Flow”, *Biophysical Journal*, vol. 115, no. 10. Elsevier BV, pp. 1860–1871, Nov. 2018. doi: 10.1016/j.bpj.2018.09.001.  
  
Q. Ranjha, N. Vahediand A. Oztekin, “High-temperature thermochemical energy storage – heat transfer enhancements within reaction bed”, *Applied Thermal Engineering*, vol. 163. Elsevier BV, p. 114407, Dec. 2019. doi: 10.1016/j.applthermaleng.2019.114407.  
  
M. Usta, R. M. Krysko, A. E. Anqi, A. M. Alshwairekhand A. Oztekin, “The Effect of PTFE Membrane Properties on Vacuum Membrane Distillation Module Performance”, *Volume 7: Fluids Engineering*. American Society of Mechanical Engineers, Nov. 09, 2018. doi: 10.1115/imece2018-86327.  
  
M. Usta, M. Morabito, M. Alrehili, A. Hakimand A. Oztekin, “Steady three-dimensional flows past hollow fiber membrane arrays – cross flow arrangement”, *Canadian Journal of Physics*, vol. 96, no. 12. Canadian Science Publishing, pp. 1272–1287, Dec. 2018. doi: 10.1139/cjp-2017-0914.  
  
M. Usta, M. Morabito, A. Anqi, M. Alrehili, A. Hakimand A. Oztekin, “Twisted hollow fiber membrane modules for reverse osmosis-driven desalination”, *Desalination*, vol. 441. Elsevier BV, pp. 21–34, Sep. 2018. doi: 10.1016/j.desal.2018.04.027.  
  
N. Vahedi and A. Oztekin, “Split Flow Modified Packed Bed Reactor for Cobalt Oxide Based High-Temperature TCES Systems”, *Volume 6: Energy*. American Society of Mechanical Engineers, Nov. 11, 2019. doi: 10.1115/imece2019-10740.  
  
N. Vahedi and A. Oztekin, “Parametric Study of High-Temperature Thermochemical Energy Storage Using Manganese-Iron Oxide”, *ASME 2019 Heat Transfer Summer Conference*. American Society of Mechanical Engineers, Jul. 14, 2019. doi: 10.1115/ht2019-3682.  
  
N. Vahedi and A. Oztekin, “Parametric Study of Split Flow Cylindrical Packed Bed Reactor for High-Temperature Thermochemical Energy Storage Using Cobalt Oxide Redox Reaction”, *Volume 6: Energy*. American Society of Mechanical Engineers, Nov. 11, 2019. doi: 10.1115/imece2019-10956.  
  
N. Vahedi, Q. A. Ranjhaand A. Oztekin, “Numerical Study of High Temperature Thermochemical Energy Storage Using Co3O4/CoO”, *Volume 6B: Energy*. American Society of Mechanical Engineers, Nov. 09, 2018. doi: 10.1115/imece2018-86329.  
  
W. Wei, “Coarse-Grain Modeling of Shear-Induced Binding between von Willebrand Factor and Collagen”, *Biophysical Journal*, vol. 114, no. 8. Elsevier BV, pp. 1816–1829, Apr. 2018. doi: 10.1016/j.bpj.2018.02.017.  
  
N. Ashton, J. Davisand C. Brehm, “Assessment of the Elliptic Blending Reynolds Stress Model for a Rotating Turbulent Pipe Flow Using New DNS Data”, *AIAA Aviation 2019 Forum*. American Institute of Aeronautics and Astronautics, Jun. 15, 2019. doi: 10.2514/6.2019-2966.  
  
J. Davis, S. Ganju, N. Ashton, S. Baileyand C. Brehm, “A DNS Study to Investigate Turbulence Suppression in Rotating Pipe Flows”, *AIAA Aviation 2019 Forum*. American Institute of Aeronautics and Astronautics, Jun. 15, 2019. doi: 10.2514/6.2019-3639.  
  
J. Davis, S. Ganju, A. Venkatesh, N. Ashton, S. C. Baileyand C. Brehm, “Coherence Analysis of Rotating Turbulent Pipe Flow”, *AIAA Scitech 2020 Forum*. American Institute of Aeronautics and Astronautics, Jan. 05, 2020. doi: 10.2514/6.2020-1570.  
  
J. Davis, S. Ganju, A. Venkatesh, N. Ashton, S. C. Baileyand C. Brehm, “Correction: Coherence Analysis of Rotating Turbulent Pipe Flow”, *AIAA Scitech 2020 Forum*. American Institute of Aeronautics and Astronautics, Jan. 06, 2020. doi: 10.2514/6.2020-1570.c1.  
  
S. Ganju, J. Davis, S. C. Baileyand C. Brehm, “Direct Numerical Simulations of Turbulent Channel Flows with Sinusoidal Walls”, *AIAA Scitech 2019 Forum*. American Institute of Aeronautics and Astronautics, Jan. 06, 2019. doi: 10.2514/6.2019-2141.  
  
S. Ganju, J. Davis, S. Baileyand C. Brehm, “Direct Numerical Simulations of Turbulent Channel Flows with Two- and Three-Dimensional Superimposed Sinusoidal Roughness”, *AIAA Aviation 2019 Forum*. American Institute of Aeronautics and Astronautics, Jun. 15, 2019. doi: 10.2514/6.2019-3641.  
  
Z. Ghiasi, D. Li, J. Komperdaand F. Mashayek, “Near-wall resolution requirement for direct numerical simulation of turbulent flow using multidomain Chebyshev grid”, *International Journal of Heat and Mass Transfer*, vol. 126. Elsevier BV, pp. 746–760, Nov. 2018. doi: 10.1016/j.ijheatmasstransfer.2018.05.114.  
  
K. P. Iyer, J. D. Scheel, J. Schumacherand K. R. Sreenivasan, “Classical 1/3 scaling of convection holds up to Ra = 10 15”, *Proceedings of the National Academy of Sciences*, vol. 117, no. 14. Proceedings of the National Academy of Sciences, pp. 7594–7598, Mar. 25, 2020. doi: 10.1073/pnas.1922794117.  
  
J. Yao, X. Chenand F. Hussain, “Drag control in wall-bounded turbulent flows via spanwise opposed wall-jet forcing”, *Journal of Fluid Mechanics*, vol. 852. Cambridge University Press (CUP), pp. 678–709, Aug. 13, 2018. doi: 10.1017/jfm.2018.553.  
  
J. Yao, X. Chenand F. Hussain, “Reynolds number effect on drag control via spanwise wall oscillation in turbulent channel flows”, *Physics of Fluids*, vol. 31, no. 8. AIP Publishing, p. 085108, Aug. 2019. doi: 10.1063/1.5111651.  
  
J. Yao and F. Hussain, “Supersonic turbulent boundary layer drag control using spanwise wall oscillation”, *Journal of Fluid Mechanics*, vol. 880. Cambridge University Press (CUP), pp. 388–429, Oct. 09, 2019. doi: 10.1017/jfm.2019.727.  
  
A. Agarwal and M. F. Trujillo, “The effect of nozzle internal flow on spray atomization”, *International Journal of Engine Research*, vol. 21, no. 1. SAGE Publications, pp. 55–72, Sep. 20, 2019. doi: 10.1177/1468087419875843.  
  
N. Geneva and N. Zabaras, “Quantifying model form uncertainty in Reynolds-averaged turbulence models with Bayesian deep neural networks”, *Journal of Computational Physics*, vol. 383. Elsevier BV, pp. 125–147, Apr. 2019. doi: 10.1016/j.jcp.2019.01.021.  
  
N. Geneva and N. Zabaras, “Modeling the dynamics of PDE systems with physics-constrained deep auto-regressive networks”, *Journal of Computational Physics*, vol. 403. Elsevier BV, p. 109056, Feb. 2020. doi: 10.1016/j.jcp.2019.109056.  
  
S. Singha, “Mechanisms of spontaneous chain formation and subsequent microstructural evolution in shear-driven strongly confined drop monolayers”, *Soft Matter*, vol. 15, no. 24. Royal Society of Chemistry (RSC), pp. 4873–4889, 2019. doi: 10.1039/c9sm00536f.  
  
D. Morrow, A. Nairand R. M. Spearrin, “Minimizing hydraulic losses in additively manufactured swirl coaxial injectors”, *AIAA Propulsion and Energy 2019 Forum*. American Institute of Aeronautics and Astronautics, Aug. 16, 2019. doi: 10.2514/6.2019-4310.  
  
A. S. Rosen, “Tuning the Redox Activity of Metal–Organic Frameworks for Enhanced, Selective O2 Binding: Design Rules and Ambient Temperature O2 Chemisorption in a Cobalt–Triazolate Framework”, *Journal of the American Chemical Society*, vol. 142, no. 9. American Chemical Society (ACS), pp. 4317–4328, Feb. 07, 2020. doi: 10.1021/jacs.9b12401.  
  
A. S. Rosen, J. M. Notesteinand R. Q. Snurr, “Identifying promising metal–organic frameworks for heterogeneous catalysis via high‐throughput periodic density functional theory”, *Journal of Computational Chemistry*, vol. 40, no. 12. Wiley, pp. 1305–1318, Feb. 04, 2019. doi: 10.1002/jcc.25787.  
  
A. S. Rosen, J. M. Notesteinand R. Q. Snurr, “Structure–Activity Relationships That Identify Metal–Organic Framework Catalysts for Methane Activation”, *ACS Catalysis*, vol. 9, no. 4. American Chemical Society (ACS), pp. 3576–3587, Mar. 08, 2019. doi: 10.1021/acscatal.8b05178.  
  
A. S. Rosen, J. M. Notesteinand R. Q. Snurr, “High‐Valent Metal–Oxo Species at the Nodes of Metal–Triazolate Frameworks: The Effects of Ligand Exchange and Two‐State Reactivity for C−H Bond Activation”, *Angewandte Chemie International Edition*, vol. 59, no. 44. Wiley, pp. 19494–19502, May 07, 2020. doi: 10.1002/anie.202004458.  
  
M. C. Wasson, “Supramolecular Porous Assemblies of Atomically Precise Catalytically Active Cerium-Based Clusters”, *Chemistry of Materials*, vol. 32, no. 19. American Chemical Society (ACS), pp. 8522–8529, Sep. 16, 2020. doi: 10.1021/acs.chemmater.0c02740.  
  
A. H. Raffiee, A. M. Ardekaniand S. Dabiri, “Numerical investigation of elasto-inertial particle focusing patterns in viscoelastic microfluidic devices”, *Journal of Non-Newtonian Fluid Mechanics*, vol. 272. Elsevier BV, p. 104166, Oct. 2019. doi: 10.1016/j.jnnfm.2019.104166.  
  
M. J. Mercier, S. Wang, J. Péméja, P. Ernand A. M. Ardekani, “Settling disks in a linearly stratified fluid”, *Journal of Fluid Mechanics*, vol. 885. Cambridge University Press (CUP), Dec. 17, 2019. doi: 10.1017/jfm.2019.957.  
  
X. Zhang, C. Caruso, W. A. Lamand M. D. Graham, “Flow-induced segregation and dynamics of red blood cells in sickle cell disease”, *Physical Review Fluids*, vol. 5, no. 5. American Physical Society (APS), May 04, 2020. doi: 10.1103/physrevfluids.5.053101.  
  
J. Jeun and J. W. Nichols, “Wavepacket modeling of turbulent jet noise generation using input-output analysis”, *23rd AIAA/CEAS Aeroacoustics Conference*. American Institute of Aeronautics and Astronautics, Jun. 02, 2017. doi: 10.2514/6.2017-3378.  
  
J. Jeun and J. W. Nichols, “Non-compact sources of sound in high-speed turbulent jets using input-output analysis”, *2018 AIAA/CEAS Aeroacoustics Conference*. American Institute of Aeronautics and Astronautics, Jun. 24, 2018. doi: 10.2514/6.2018-3467.  
  
J. Jeun, J. W. Nicholsand M. R. Jovanovic, “Input-output analysis of heated axisymmetric turbulent jets”, *22nd AIAA/CEAS Aeroacoustics Conference*. American Institute of Aeronautics and Astronautics, May 27, 2016. doi: 10.2514/6.2016-2934.  
  
J. Jeun, J. W. Nicholsand M. R. Jovanović, “Input-output analysis of high-speed axisymmetric isothermal jet noise”, *Physics of Fluids*, vol. 28, no. 4. AIP Publishing, p. 047101, Apr. 2016. doi: 10.1063/1.4946886.  
  
J. Jeun, G. J. Wuand S. K. Lele, “Towards large-eddy simulations of twin rectangular jets including screech”, *AIAA Scitech 2020 Forum*. American Institute of Aeronautics and Astronautics, Jan. 05, 2020. doi: 10.2514/6.2020-0998.  
  
G. Wu, S. K. Leleand J. Jeun, “Towards Large Eddy Simulations of Supersonic Rectangular Jets including Screech”, *25th AIAA/CEAS Aeroacoustics Conference*. American Institute of Aeronautics and Astronautics, May 18, 2019. doi: 10.2514/6.2019-2520.  
  
I. Alshareedah, M. M. Moosa, M. Raju, D. A. Potoyanand P. R. Banerjee, “Phase transition of RNA−protein complexes into ordered hollow condensates”, *Proceedings of the National Academy of Sciences*, vol. 117, no. 27. Proceedings of the National Academy of Sciences, pp. 15650–15658, Jun. 22, 2020. doi: 10.1073/pnas.1922365117.  
  
R. Laghmach and D. A. Potoyan, “Liquid-liquid phase separation driven compartmentalization of reactive nucleoplasm”, *[]*. Cold Spring Harbor Laboratory, Jul. 14, 2020. doi: 10.1101/2020.07.13.200980.  
  
R. Laghmach, M. Di Pierroand D. A. Potoyan, “Mesoscale liquid model of chromatin recapitulates nuclear order of eukaryotes”, *[]*. Cold Spring Harbor Laboratory, May 10, 2019. doi: 10.1101/634980.  
  
J. Graña-Otero, S. Mahmoudi, E. M. Sullivanand S. Schmitt, “Kinetics of Oxidation of Carbon Materials”, *AIAA Aviation 2019 Forum*. American Institute of Aeronautics and Astronautics, Jun. 15, 2019. doi: 10.2514/6.2019-3128.  
  
S. Schmitt, J. Graña-Oteroand S. Mahmoudi, “Molecular-Scale Carbon Oxidation at Hypersonic Speeds”, *AIAA Aviation 2019 Forum*. American Institute of Aeronautics and Astronautics, Jun. 15, 2019. doi: 10.2514/6.2019-3129.  
  
J. Yao and F. Hussain, “A physical model of turbulence cascade via vortex reconnection sequence and avalanche”, *Journal of Fluid Mechanics*, vol. 883. Cambridge University Press (CUP), Nov. 28, 2019. doi: 10.1017/jfm.2019.905.  
  
J. Yao and F. Hussain, “Turbulence statistics and coherent structures in compressible channel flow”, *Physical Review Fluids*, vol. 5, no. 8. American Physical Society (APS), Aug. 07, 2020. doi: 10.1103/physrevfluids.5.084603.  
  
J. Yao and F. Hussain, “Separation scaling for viscous vortex reconnection”, *Journal of Fluid Mechanics*, vol. 900. Cambridge University Press (CUP), Aug. 06, 2020. doi: 10.1017/jfm.2020.558.  
  
J. Yao and F. Hussain, “On singularity formation via viscous vortex reconnection”, *Journal of Fluid Mechanics*, vol. 888. Cambridge University Press (CUP), Feb. 06, 2020. doi: 10.1017/jfm.2020.58.  
  
E. P. S. Baumer, “Broadening Exposure, Questioning Opinions, and Reading Patterns with Reflext: a Computational Support for Frame Reflection”, *Journal of Information Technology & Politics*, vol. 11, no. 1. Informa UK Limited, pp. 45–63, Jan. 02, 2014. doi: 10.1080/19331681.2013.872072.  
  
J. S. Borg, M.-A. Vu, C. Badea, A. Badea, G. A. Johnsonand K. Dzirasa, “Localization of Metal Electrodes in the Intact Rat Brain Using Registration of 3D Microcomputed Tomography Images to a Magnetic Resonance Histology Atlas”, *eneuro*, vol. 2, no. 4. Society for Neuroscience, pp. ENEURO.0017–15.2015, Jul. 2015. doi: 10.1523/eneuro.0017-15.2015.  
  
P. Chakraborty, J. B. Colditz, A. J. Silvestre, M. R. Friedman, K. W. Bogenand B. A. Primack, “Observation of public sentiment toward human papillomavirus vaccination on Twitter”, *Cogent Medicine*, vol. 4, no. 1. Informa UK Limited, p. 1390853, Jan. 01, 2017. doi: 10.1080/2331205x.2017.1390853.  
  
J. B. Colditz, J. Welling, N. A. Smith, A. E. Jamesand B. A. Primack, “World Vaping Day: Contextualizing Vaping Culture in Online Social Media Using a Mixed Methods Approach”, *Journal of Mixed Methods Research*, vol. 13, no. 2. SAGE Publications, pp. 196–215, Apr. 09, 2017. doi: 10.1177/1558689817702753.  
  
B. L. Hoffman, E. L. Rosenthal, J. B. Colditz, R. Mcgarryand B. A. Primack, “Use of Twitter to Assess Viewer Reactions to the Medical Drama, *Code Black*”, *Journal of Health Communication*, vol. 23, no. 3. Informa UK Limited, pp. 244–253, Feb. 16, 2018. doi: 10.1080/10810730.2018.1426660.  
  
J. B. Colditz, “Toward Real-Time Infoveillance of Twitter Health Messages”, *American Journal of Public Health*, vol. 108, no. 8. American Public Health Association, pp. 1009–1014, Aug. 2018. doi: 10.2105/ajph.2018.304497.  
  
B. Q. Geuther, “Robust mouse tracking in complex environments using neural networks”, *Communications Biology*, vol. 2, no. 1. Springer Science and Business Media LLC, Mar. 29, 2019. doi: 10.1038/s42003-019-0362-1.  
  
R. Eckart de Castilho, N. Ide, J.-D. Kim, J.-C. Klieand K. Suderman, “Towards cross-platform interoperability for machine-assisted text annotation”, *Genomics & Informatics*, vol. 17, no. 2. Korea Genome Organization, p. e19, Jun. 30, 2019. doi: 10.5808/gi.2019.17.2.e19.  
  
D. Bullock, “Associative white matter connecting the dorsal and ventral posterior human cortex”, *Brain Structure and Function*, vol. 224, no. 8. Springer Science and Business Media LLC, pp. 2631–2660, Jul. 24, 2019. doi: 10.1007/s00429-019-01907-8.  
  
T. Kaneko, H. Takemura, F. Pestilli, A. C. Silva, F. Q. Yeand D. A. Leopold, “Spatial organization of occipital white matter tracts in the common marmoset”, *Brain Structure and Function*, vol. 225, no. 4. Springer Science and Business Media LLC, pp. 1313–1326, Apr. 06, 2020. doi: 10.1007/s00429-020-02060-3.  
  
P. M. Rossini, “Methods for analysis of brain connectivity: An IFCN-sponsored review”, *Clinical Neurophysiology*, vol. 130, no. 10. Elsevier BV, pp. 1833–1858, Oct. 2019. doi: 10.1016/j.clinph.2019.06.006.  
  
P. Avesani, “The open diffusion data derivatives, brain data upcycling via integrated publishing of derivatives and reproducible open cloud services”, *Scientific Data*, vol. 6, no. 1. Springer Science and Business Media LLC, May 23, 2019. doi: 10.1038/s41597-019-0073-y.  
  
G. Berto, P. Avesani, F. Pestilli, D. Bullock, B. Caronand E. Olivetti, “Anatomically-Informed Multiple Linear Assignment Problems for White Matter Bundle Segmentation”, *2019 IEEE 16th International Symposium on Biomedical Imaging (ISBI 2019)*. IEEE, Apr. 2019. doi: 10.1109/isbi.2019.8759174.  
  
G. Berto, P. Avesani, F. Pestilli, D. Bullock, B. Caronand E. Olivetti, “Anatomically-Informed Multiple Linear Assignment Problems for White Matter Bundle Segmentation”, *2019 IEEE 16th International Symposium on Biomedical Imaging (ISBI 2019)*. IEEE, Apr. 2019. doi: 10.1109/isbi.2019.8759174.  
  
G. Bertò, “Classifyber, a robust streamline-based linear classifier for white matter bundle segmentation”, *[]*. Cold Spring Harbor Laboratory, Feb. 12, 2020. doi: 10.1101/2020.02.10.942714.  
  
B. Caron, “Advanced mapping of the human white matter microstructure better separates elite sports participation”, *[]*. Center for Open Science, Jan. 03, 2020. doi: 10.31234/osf.io/dxaqp.  
  
S. Kumar, V. Sreenivasan, P. Talukdar, F. Pestilliand D. Sridharan, “ReAl-LiFE: Accelerating the Discovery of Individualized Brain Connectomes on GPUs”, *Proceedings of the AAAI Conference on Artificial Intelligence*, vol. 33, no. 1. Association for the Advancement of Artificial Intelligence (AAAI), pp. 630–638, Jul. 17, 2019. doi: 10.1609/aaai.v33i01.3301630.  
  
J. W. Kurzawski, K. Mikellidou, M. C. Morroneand F. Pestilli, “The visual white matter connecting human area prostriata and the thalamus is retinotopically organized”, *Brain Structure and Function*, vol. 225, no. 6. Springer Science and Business Media LLC, pp. 1839–1853, Jun. 13, 2020. doi: 10.1007/s00429-020-02096-5.  
  
J. Mejia, A. Mejiaand F. Pestilli, “Open data on industry payments to healthcare providers reveal potential hidden costs to the public”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Sep. 20, 2019. doi: 10.1038/s41467-019-12317-z.  
  
R. J. Puzniak, “Quantifying nerve decussation abnormalities in the optic chiasm”, *NeuroImage: Clinical*, vol. 24. Elsevier BV, p. 102055, 2019. doi: 10.1016/j.nicl.2019.102055.  
  
R. J. Puzniak, “Quantifying nerve decussation abnormalities in the optic chiasm”, *NeuroImage: Clinical*, vol. 24. Elsevier BV, p. 102055, 2019. doi: 10.1016/j.nicl.2019.102055.  
  
F. Rheault, “Tractostorm: The what, why, and how of tractography dissection reproducibility”, *Human Brain Mapping*, vol. 41, no. 7. Wiley, pp. 1859–1874, Jan. 10, 2020. doi: 10.1002/hbm.24917.  
  
F. Rheault, “Tractostorm: The what, why, and how of tractography dissection reproducibility”, *Human Brain Mapping*, vol. 41, no. 7. Wiley, pp. 1859–1874, Jan. 10, 2020. doi: 10.1002/hbm.24917.  
  
I. Sani, B. C. McPherson, H. Stemmann, F. Pestilliand W. A. Freiwald, “Functionally defined white matter of the macaque monkey brain reveals a dorso-ventral attention network”, *eLife*, vol. 8. eLife Sciences Publications, Ltd, Jan. 02, 2019. doi: 10.7554/elife.40520.  
  
I. Sani, B. C. McPherson, H. Stemmann, F. Pestilliand W. A. Freiwald, “Functionally defined white matter of the macaque monkey brain reveals a dorso-ventral attention network”, *eLife*, vol. 8. eLife Sciences Publications, Ltd, Jan. 02, 2019. doi: 10.7554/elife.40520.  
  
H. Takemura, F. Pestilliand K. S. Weiner, “Comparative neuroanatomy: Integrating classic and modern methods to understand association fibers connecting dorsal and ventral visual cortex”, *Neuroscience Research*, vol. 146. Elsevier BV, pp. 1–12, Sep. 2019. doi: 10.1016/j.neures.2018.10.011.  
  
M. K. Eckstein and A. G. Collins, “Computational Evidence for Hierarchically-Structured Reinforcement Learning in Humans”, *[]*. Cold Spring Harbor Laboratory, Aug. 10, 2019. doi: 10.1101/731752.  
  
J. P. Howard, II, “Phonetic Spelling Algorithm Implementations for *R*”, *Journal of Statistical Software*, vol. 95, no. 8. Foundation for Open Access Statistic, 2020. doi: 10.18637/jss.v095.i08.  
  
J. M. Capriles, N. Tripcevich, A. E. Nielsen, M. D. Glascock, J. Albarracin-Jordanand C. M. Santoro, “Late Pleistocene Lithic Procurement and Geochemical Characterization of the Cerro Kaskio Obsidian Source in South-western Bolivia”, *Archaeometry*, vol. 60, no. 5. Wiley, pp. 898–914, Apr. 22, 2018. doi: 10.1111/arcm.12363.  
  
M. S. Maxwell, E. C. Ni, C. Tong, S. G. Henderson, H. Topalogluand S. R. Hunter, “A Bound on the Performance of an Optimal Ambulance Redeployment Policy”, *Operations Research*, vol. 62, no. 5. Institute for Operations Research and the Management Sciences (INFORMS), pp. 1014–1027, Oct. 2014. doi: 10.1287/opre.2014.1302.  
  
H. Zerze, J. Mittaland A. J. McHugh, “Ab Initio Crystallization of Alkanes: Structure and Kinetics of Nuclei Formation”, *Macromolecules*, vol. 46, no. 22. American Chemical Society (ACS), pp. 9151–9157, Nov. 18, 2013. doi: 10.1021/ma401836b.  
  
Z. Lyu, G. K. Kenwayand J. R. R. A. Martins, “RANS-based Aerodynamic Shape Optimization Investigations of the Common Research Model Wing”, *52nd Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 10, 2014. doi: 10.2514/6.2014-0567.  
  
Z. Lyu, G. K. Kenway, C. Paigeand J. R. R. A. Martins, “Automatic Differentiation Adjoint of the Reynolds-Averaged Navier-Stokes Equations with a Turbulence Model”, *21st AIAA Computational Fluid Dynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 22, 2013. doi: 10.2514/6.2013-2581.  
  
Z. Lyu and J. R. R. A. Martins, “RANS-based Aerodynamic Shape Optimization of a Blended-Wing-Body Aircraft”, *21st AIAA Computational Fluid Dynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 22, 2013. doi: 10.2514/6.2013-2586.  
  
B. J. Brelje and J. R. R. A. Martins, “Coupled component sizing and aerodynamic shape optimization via geometric constraints”, *AIAA Aviation 2019 Forum*. American Institute of Aeronautics and Astronautics, Jun. 15, 2019. doi: 10.2514/6.2019-3105.  
  
T. R. Brooks, G. Kennedyand J. R. R. A. Martins, “High-fidelity Multipoint Aerostructural Optimization of a High Aspect Ratio Tow-steered Composite Wing”, *58th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference*. American Institute of Aeronautics and Astronautics, Jan. 05, 2017. doi: 10.2514/6.2017-1350.  
  
T. R. Brooks, G. K. Kenwayand J. R. R. A. Martins, “Undeflected Common Research Model (uCRM): An Aerostructural Model for the Study of High Aspect Ratio Transport Aircraft Wings”, *35th AIAA Applied Aerodynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 02, 2017. doi: 10.2514/6.2017-4456.  
  
T. R. Brooks, J. R. R. A. Martinsand G. J. Kennedy, “High-fidelity aerostructural optimization of tow-steered composite wings”, *Journal of Fluids and Structures*, vol. 88. Elsevier BV, pp. 122–147, Jul. 2019. doi: 10.1016/j.jfluidstructs.2019.04.005.  
  
D. A. Burdette and J. R. R. A. Martins, “Design of a transonic wing with an adaptive morphing trailing edge via aerostructural optimization”, *Aerospace Science and Technology*, vol. 81. Elsevier BV, pp. 192–203, Oct. 2018. doi: 10.1016/j.ast.2018.08.004.  
  
D. A. Burdette and J. R. R. A. Martins, “Impact of Morphing Trailing Edges on Mission Performance for the Common Research Model”, *Journal of Aircraft*, vol. 56, no. 1. American Institute of Aeronautics and Astronautics (AIAA), pp. 369–384, Jan. 2019. doi: 10.2514/1.c034967.  
  
S. Chen, Z. Lyu, G. K. W. Kenwayand J. R. R. A. Martins, “Aerodynamic Shape Optimization of Common Research Model Wing–Body–Tail Configuration”, *Journal of Aircraft*, vol. 53, no. 1. American Institute of Aeronautics and Astronautics (AIAA), pp. 276–293, Jan. 2016. doi: 10.2514/1.c033328.  
  
G. K. W. Kenway, C. A. Mader, P. Heand J. R. R. A. Martins, “Effective adjoint approaches for computational fluid dynamics”, *Progress in Aerospace Sciences*, vol. 110. Elsevier BV, p. 100542, Oct. 2019. doi: 10.1016/j.paerosci.2019.05.002.  
  
P. He, G. Filip, J. R. R. A. Martinsand K. J. Maki, “Design optimization for self-propulsion of a bulk carrier hull using a discrete adjoint method”, *Computers & Fluids*, vol. 192. Elsevier BV, p. 104259, Oct. 2019. doi: 10.1016/j.compfluid.2019.104259.  
  
P. He, C. A. Mader, J. R. R. A. Martinsand K. J. Maki, “Aerothermal optimization of a ribbed U-bend cooling channel using the adjoint method”, *International Journal of Heat and Mass Transfer*, vol. 140. Elsevier BV, pp. 152–172, Sep. 2019. doi: 10.1016/j.ijheatmasstransfer.2019.05.075.  
  
G. K. W. Kenway and J. R. R. A. Martins, “Buffet-Onset Constraint Formulation for Aerodynamic Shape Optimization”, *AIAA Journal*, vol. 55, no. 6. American Institute of Aeronautics and Astronautics (AIAA), pp. 1930–1947, Jun. 2017. doi: 10.2514/1.j055172.  
  
Z. Lyu and J. R. R. A. Martins, “Aerodynamic Shape Optimization of an Adaptive Morphing Trailing Edge Wing”, *15th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference*. American Institute of Aeronautics and Astronautics, Jun. 13, 2014. doi: 10.2514/6.2014-3275.  
  
Z. Lyu and J. R. R. A. Martins, “Strategies for Solving High-Fidelity Aerodynamic Shape Optimization Problems”, *15th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference*. American Institute of Aeronautics and Astronautics, Jun. 13, 2014. doi: 10.2514/6.2014-2594.  
  
Z. Lyu and J. R. R. A. Martins, “Aerodynamic Shape Optimization of an Adaptive Morphing Trailing-Edge Wing”, *Journal of Aircraft*, vol. 52, no. 6. American Institute of Aeronautics and Astronautics (AIAA), pp. 1951–1970, Nov. 2015. doi: 10.2514/1.c033116.  
  
J. R. R. A. Martins, “Chapter 19: Multidisciplinary Design Optimization of Aerospace Systems”, *Advances and Trends in Optimization with Engineering Applications*. Society for Industrial and Applied Mathematics, pp. 249–257, Apr. 26, 2017. doi: 10.1137/1.9781611974683.ch19.  
  
N. R. Secco, J. Jasa, G. K. Kenwayand J. R. R. A. Martins, “Component-based Geometry Manipulation for Aerodynamic Shape Optimization with Overset Meshes”, *18th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference*. American Institute of Aeronautics and Astronautics, Jun. 02, 2017. doi: 10.2514/6.2017-3327.  
  
N. R. Secco and J. R. R. A. Martins, “RANS-based Aerodynamic Shape Optimization of a Strut-braced Wing with Overset Meshes”, *2018 AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference*. American Institute of Aeronautics and Astronautics, Jan. 07, 2018. doi: 10.2514/6.2018-0413.  
  
N. R. Secco and J. R. R. A. Martins, “RANS-Based Aerodynamic Shape Optimization of a Strut-Braced Wing with Overset Meshes”, *Journal of Aircraft*, vol. 56, no. 1. American Institute of Aeronautics and Astronautics (AIAA), pp. 217–227, Jan. 2019. doi: 10.2514/1.c034934.  
  
A. Yildirim, J. S. Gray, C. A. Maderand J. R. R. A. Martins, “Aeropropulsive Design Optimization of a Boundary Layer Ingestion System”, *AIAA Aviation 2019 Forum*. American Institute of Aeronautics and Astronautics, Jun. 14, 2019. doi: 10.2514/6.2019-3455.  
  
A. Yildirim, G. K. W. Kenway, C. A. Maderand J. R. R. A. Martins, “A Jacobian-free approximate Newton–Krylov startup strategy for RANS simulations”, *Journal of Computational Physics*, vol. 397. Elsevier BV, p. 108741, Nov. 2019. doi: 10.1016/j.jcp.2019.06.018.  
  
G. K. W. Kenway and J. R. R. A. Martins, “Multipoint Aerodynamic Shape Optimization Investigations of the Common Research Model Wing”, *AIAA Journal*, vol. 54, no. 1. American Institute of Aeronautics and Astronautics (AIAA), pp. 113–128, Jan. 2016. doi: 10.2514/1.j054154.  
  
V. Bandaru, “Economic sustainability modeling provides decision support for assessing hybrid poplar-based biofuel development in California”, *California Agriculture*, vol. 69, no. 3. University of California Agriculture and Natural Resources (UC ANR), pp. 171–176, Jul. 2015. doi: 10.3733/ca.v069n03p171.  
  
H. Yu, “Efficient Statistical Validation of Autonomous Driving Systems”, *Safe, Autonomous and Intelligent Vehicles*. Springer International Publishing, pp. 5–32, Nov. 15, 2018. doi: 10.1007/978-3-319-97301-2\_2.  
  
I. Marquetti and S. Desai, “Orientation effects on the nanoscale adsorption behavior of bone morphogenetic protein-2 on hydrophilic silicon dioxide”, *RSC Advances*, vol. 9, no. 2. Royal Society of Chemistry (RSC), pp. 906–916, 2019. doi: 10.1039/c8ra09165j.  
  
J. Rodrigues and S. Desai, “The nanoscale Leidenfrost effect”, *Nanoscale*, vol. 11, no. 25. Royal Society of Chemistry (RSC), pp. 12139–12151, 2019. doi: 10.1039/c9nr01386e.  
  
M. A. Miller, “A RESTful API for Access to Phylogenetic Tools via the CIPRES Science Gateway”, *Evolutionary Bioinformatics*, vol. 11. SAGE Publications, p. EBO.S21501, Jan. 2015. doi: 10.4137/ebo.s21501.  
  
M. A. Miller, T. Schwartzand W. Pfeiffer, “User behavior and usage patterns for a highly accessed science gateway”, *Proceedings of the XSEDE16 Conference on Diversity, Big Data, and Science at Scale*. ACM, Jul. 17, 2016. doi: 10.1145/2949550.2949658.  
  
S. Nakandala, “Apache Airavata Sharing Service”, *Proceedings of the Practice and Experience in Advanced Research Computing 2017 on Sustainability, Success and Impact*. ACM, Jul. 09, 2017. doi: 10.1145/3093338.3093359.  
  
G. C. Cardoso, B. T. Klingbeil, F. A. La Sorte, C. A. Lepczyk, D. Finkand C. H. Flather, “Exposure to noise pollution across North American passerines supports the noise filter hypothesis”, *Global Ecology and Biogeography*, vol. 29, no. 8. Wiley, pp. 1430–1434, Mar. 10, 2020. doi: 10.1111/geb.13085.  
  
N. Ferreira, “BirdVis: Visualizing and Understanding Bird Populations”, *IEEE Transactions on Visualization and Computer Graphics*, vol. 17, no. 12. Institute of Electrical and Electronics Engineers (IEEE), pp. 2374–2383, Dec. 2011. doi: 10.1109/tvcg.2011.176.  
  
W. M. Hochachka, D. Fink, R. A. Hutchinson, D. Sheldon, W.-K. Wongand S. Kelling, “Data-intensive science applied to broad-scale citizen science”, *Trends in Ecology & Evolution*, vol. 27, no. 2. Elsevier BV, pp. 130–137, Feb. 2012. doi: 10.1016/j.tree.2011.11.006.  
  
K. G. Horton, “Navigating north: how body mass and winds shape avian flight behaviours across a North American migratory flyway”, *Ecology Letters*, vol. 21, no. 7. Wiley, pp. 1055–1064, May 07, 2018. doi: 10.1111/ele.12971.  
  
S. Kelling, D. Fink, F. A. La Sorte, A. Johnston, N. E. Brunsand W. M. Hochachka, “Taking a ‘Big Data’ approach to data quality in a citizen science project”, *Ambio*, vol. 44, no. S4. Springer Science and Business Media LLC, pp. 601–611, Oct. 27, 2015. doi: 10.1007/s13280-015-0710-4.  
  
B. T. Klingbeil, F. A. La Sorte, C. A. Lepczyk, D. Finkand C. H. Flather, “Geographical associations with anthropogenic noise pollution for North American breeding birds”, *Global Ecology and Biogeography*, vol. 29, no. 1. Wiley, pp. 148–158, Oct. 11, 2019. doi: 10.1111/geb.13016.  
  
F. A. La Sorte, D. Fink, W. M. Hochachka, J. P. DeLongand S. Kelling, “Spring phenology of ecological productivity contributes to the use of looped migration strategies by birds”, *Proceedings of the Royal Society B: Biological Sciences*, vol. 281, no. 1793. The Royal Society, p. 20140984, Oct. 22, 2014. doi: 10.1098/rspb.2014.0984.  
  
F. A. La Sorte, “The role of atmospheric conditions in the seasonal dynamics of North American migration flyways”, *Journal of Biogeography*, vol. 41, no. 9. Wiley, pp. 1685–1696, May 05, 2014. doi: 10.1111/jbi.12328.  
  
F. A. La Sorte, “Migration timing and its determinants for nocturnal migratory birds during autumn migration”, *Journal of Animal Ecology*, vol. 84, no. 5. Wiley, pp. 1202–1212, Apr. 30, 2015. doi: 10.1111/1365-2656.12376.  
  
M. D. Reynolds, “Dynamic conservation for migratory species”, *Science Advances*, vol. 3, no. 8. American Association for the Advancement of Science (AAAS), Aug. 04, 2017. doi: 10.1126/sciadv.1700707.  
  
C. Wood, B. Sullivan, M. Iliff, D. Finkand S. Kelling, “eBird: Engaging Birders in Science and Conservation”, *PLoS Biology*, vol. 9, no. 12. Public Library of Science (PLoS), p. e1001220, Dec. 20, 2011. doi: 10.1371/journal.pbio.1001220.  
  
B. Zuckerberg, D. Fink, F. A. La Sorte, W. M. Hochachkaand S. Kelling, “Novel seasonal land cover associations for eastern North American forest birds identified through dynamic species distribution modelling”, *Diversity and Distributions*, vol. 22, no. 6. Wiley, pp. 717–730, Feb. 18, 2016. doi: 10.1111/ddi.12428.  
  
Y. Lan, J. C. Morrison, R. Hershbergand G. L. Rosen, “POGO-DB—a database of pairwise-comparisons of genomes and conserved orthologous genes”, *Nucleic Acids Research*, vol. 42, no. D1. Oxford University Press (OUP), pp. D625–D632, Nov. 05, 2013. doi: 10.1093/nar/gkt1094.  
  
V. Mozhayskiy and I. Tagkopoulos, “Microbial evolution in vivo and in silico: methods and applications”, *Integr. Biol.*, vol. 5, no. 2. Oxford University Press (OUP), pp. 262–277, 2013. doi: 10.1039/c2ib20095c.  
  
A. T. Clark, “Spatial convergent cross mapping to detect causal relationships from short time series”, *Ecology*, vol. 96, no. 5. Wiley, pp. 1174–1181, May 2015. doi: 10.1890/14-1479.1.  
  
K. R. Thorp, “Proximal hyperspectral sensing and data analysis approaches for field-based plant phenomics”, *Computers and Electronics in Agriculture*, vol. 118. Elsevier BV, pp. 225–236, Oct. 2015. doi: 10.1016/j.compag.2015.09.005.  
  
T. A. Contreras and K. E. Sieving, “Leadership of Winter Mixed-Species Flocks by Tufted Titmice (*Baeolophus bicolor*): Are Titmice Passive Nuclear Species?”, *International Journal of Zoology*, vol. 2011. Hindawi Limited, pp. 1–11, 2011. doi: 10.1155/2011/670548.  
  
R. J. Fletcher Jr. and K. E. Sieving, “Social-Information Use in Heterogeneous Landscapes: A Prospectus”, *The Condor*, vol. 112, no. 2. Oxford University Press (OUP), pp. 225–234, May 2010. doi: 10.1525/cond.2010.090236.  
  
S. A. Hetrick and K. E. Sieving, “Antipredator calls of tufted titmice and interspecific transfer of encoded threat information”, *Behavioral Ecology*, vol. 23, no. 1. Oxford University Press (OUP), pp. 83–92, Sep. 14, 2011. doi: 10.1093/beheco/arr160.  
  
P. Huang, K. E. Sievingand C. M. S. Mary, “Heterospecific information about predation risk influences exploratory behavior”, *Behavioral Ecology*, vol. 23, no. 3. Oxford University Press (OUP), pp. 463–472, Dec. 26, 2011. doi: 10.1093/beheco/arr212.  
  
K. E. Sieving, S. A. Hetrickand M. L. Avery, “The versatility of graded acoustic measures in classification of predation threats by the tufted titmouse*Baeolophus bicolor*: exploring a mixed framework for threat communication”, *Oikos*, vol. 119, no. 2. Wiley, pp. 264–276, Feb. 2010. doi: 10.1111/j.1600-0706.2009.17682.x.  
  
B. C. Stock and B. X. Semmens, “Unifying error structures in commonly used biotracer mixing models”, *Ecology*, vol. 97, no. 10. Wiley, pp. 2562–2569, Sep. 19, 2016. doi: 10.1002/ecy.1517.  
  
Q. J. Hart, P. W. Tittmann, V. Bandaruand B. M. Jenkins, “Modeling poplar growth as a short rotation woody crop for biofuels in the Pacific Northwest”, *Biomass and Bioenergy*, vol. 79. Elsevier BV, pp. 12–27, Aug. 2015. doi: 10.1016/j.biombioe.2015.05.004.  
  
M. Memarzadeh and C. Boettiger, “Adaptive management of ecological systems under partial observability”, *Biological Conservation*, vol. 224. Elsevier BV, pp. 9–15, Aug. 2018. doi: 10.1016/j.biocon.2018.05.009.  
  
M. Memarzadeh and C. Boettiger, “Measurement uncertainty matters: ecological management using POMDPs”, *[]*. Cold Spring Harbor Laboratory, May 30, 2016. doi: 10.1101/055319.  
  
M. Bassiouni, S. P. Good, C. J. Stilland C. W. Higgins, “Plant Water Uptake Thresholds Inferred From Satellite Soil Moisture”, *Geophysical Research Letters*, vol. 47, no. 7. American Geophysical Union (AGU), Apr. 06, 2020. doi: 10.1029/2020gl087077.  
  
H. K. White, “Examining Inputs of Biogenic and Oil-Derived Hydrocarbons in Surface Waters Following the Deepwater Horizon Oil Spill”, *ACS Earth and Space Chemistry*, vol. 3, no. 7. American Chemical Society (ACS), pp. 1329–1337, May 23, 2019. doi: 10.1021/acsearthspacechem.9b00090.  
  
B. M. Sleeter, “Effects of 21st‐century climate, land use, and disturbances on ecosystem carbon balance in California”, *Global Change Biology*, vol. 25, no. 10. Wiley, pp. 3334–3353, Jun. 24, 2019. doi: 10.1111/gcb.14677.  
  
B. Wielstra, E. McCartney-Melstad, J. W. Arntzen, R. K. Butlinand H. B. Shaffer, “Phylogenomics of the adaptive radiation of Triturus newts supports gradual ecological niche expansion towards an incrementally aquatic lifestyle”, *Molecular Phylogenetics and Evolution*, vol. 133. Elsevier BV, pp. 120–127, Apr. 2019. doi: 10.1016/j.ympev.2018.12.032.  
  
E. McCartney-Melstad, J. K. Vuand H. B. Shaffer, “Genomic Data from an Endangered Amphibian Reveal Unforeseen Consequences of Fragmentation by Roads”, *[]*. Cold Spring Harbor Laboratory, Apr. 23, 2018. doi: 10.1101/306340.  
  
Z. Cui, “Complete Genome Sequence of *Cycloclasticus* sp. Strain PY97N, Which Includes Two Heavy Metal Resistance Genomic Islands”, *Microbiology Resource Announcements*, vol. 8, no. 40. American Society for Microbiology, Oct. 03, 2019. doi: 10.1128/mra.00771-19.  
  
L. T. Sein Jr. and A. F. Lashua, “DFT and experimental study of N,N′-bis(3′-carboxy,4′-aminophenyl)-1,4-quinonediimine, a carboxyl substituted aniline trimer”, *Journal of Molecular Structure*, vol. 977, no. 1–3. Elsevier BV, pp. 220–229, Aug. 2010. doi: 10.1016/j.molstruc.2010.05.038.  
  
B. P. Burton, S. Demersand A. van de Walle, “First principles phase diagram calculations for the wurtzite-structure quasibinary systems SiC-AlN, SiC-GaN and SiC-InN”, *Journal of Applied Physics*, vol. 110, no. 2. AIP Publishing, p. 023507, Jul. 15, 2011. doi: 10.1063/1.3602149.  
  
B. P. Burton and A. van de Walle, “First principles phase diagram calculations for the octahedral-interstitial system ,”, *Calphad*, vol. 37. Elsevier BV, pp. 151–157, Jun. 2012. doi: 10.1016/j.calphad.2011.12.011.  
  
R. V. Chepulskii, W. H. Butler, A. van de Walleand S. Curtarolo, “Surface segregation in nanoparticles from first principles: The case of FePt”, *Scripta Materialia*, vol. 62, no. 4. Elsevier BV, pp. 179–182, Feb. 2010. doi: 10.1016/j.scriptamat.2009.10.019.  
  
M. de Jong, “Electronic Origins of Anomalous Twin Boundary Energies in Hexagonal Close Packed Transition Metals”, *Physical Review Letters*, vol. 115, no. 6. American Physical Society (APS), Aug. 03, 2015. doi: 10.1103/physrevlett.115.065501.  
  
M. Fyhrie, “Energetics of melting of Yb2O3 and Lu2O3 from drop and catch calorimetry and first principles computations”, *The Journal of Chemical Thermodynamics*, vol. 132. Elsevier BV, pp. 405–410, May 2019. doi: 10.1016/j.jct.2019.01.008.  
  
Q.-J. Hong, “Combined computational and experimental investigation of high temperature thermodynamics and structure of cubic ZrO2 and HfO2”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, Oct. 08, 2018. doi: 10.1038/s41598-018-32848-7.  
  
Q.-J. Hong, S. V. Ushakov, A. Navrotskyand A. van de Walle, “Combined computational and experimental investigation of the refractory properties of La2Zr2O7”, *Acta Materialia*, vol. 84. Elsevier BV, pp. 275–282, Feb. 2015. doi: 10.1016/j.actamat.2014.10.026.  
  
Q.-J. Hong and A. van de Walle, “Direct first-principles chemical potential calculations of liquids”, *The Journal of Chemical Physics*, vol. 137, no. 9. AIP Publishing, p. 094114, Sep. 07, 2012. doi: 10.1063/1.4749287.  
  
Q.-J. Hong and A. van de Walle, “Solid-liquid coexistence in small systems: A statistical method to calculate melting temperatures”, *The Journal of Chemical Physics*, vol. 139, no. 9. AIP Publishing, p. 094114, Sep. 07, 2013. doi: 10.1063/1.4819792.  
  
Q.-J. Hong and A. van de Walle, “Prediction of the material with highest known melting point from*ab initio*molecular dynamics calculations”, *Physical Review B*, vol. 92, no. 2. American Physical Society (APS), Jul. 20, 2015. doi: 10.1103/physrevb.92.020104.  
  
Q.-J. Hong and A. van de Walle, “A user guide for SLUSCHI: Solid and Liquid in Ultra Small Coexistence with Hovering Interfaces”, *Calphad*, vol. 52. Elsevier BV, pp. 88–97, Mar. 2016. doi: 10.1016/j.calphad.2015.12.003.  
  
Q.-J. Hong and A. van de Walle, “Reentrant melting of sodium, magnesium, and aluminum: General trend”, *Physical Review B*, vol. 100, no. 14. American Physical Society (APS), Oct. 25, 2019. doi: 10.1103/physrevb.100.140102.  
  
Q.-J. Hong, J. Yasiand A. van de Walle, “Tetrahedron-tiling method for crystal structure prediction”, *Physical Review Materials*, vol. 1, no. 2. American Physical Society (APS), Jul. 17, 2017. doi: 10.1103/physrevmaterials.1.020801.  
  
S. Kadkhodaei, Q.-J. Hongand A. van de Walle, “Free energy calculation of mechanically unstable but dynamically stabilized bcc titanium”, *Physical Review B*, vol. 95, no. 6. American Physical Society (APS), Feb. 02, 2017. doi: 10.1103/physrevb.95.064101.  
  
S. Kadkhodaei and A. van de Walle, “First-principles calculations of thermal properties of the mechanically unstable phases of the PtTi and NiTi shape memory alloys”, *Acta Materialia*, vol. 147. Elsevier BV, pp. 296–303, Apr. 2018. doi: 10.1016/j.actamat.2018.01.025.  
  
S. Kadkhodaei and A. van de Walle, “A simple local expression for the prefactor in transition state theory”, *The Journal of Chemical Physics*, vol. 150, no. 14. AIP Publishing, p. 144105, Apr. 14, 2019. doi: 10.1063/1.5086746.  
  
S. Kadkhodaei and A. van de Walle, “Software tools for thermodynamic calculation of mechanically unstable phases from first-principles data”, *Computer Physics Communications*, vol. 246. Elsevier BV, p. 106712, Jan. 2020. doi: 10.1016/j.cpc.2019.01.008.  
  
D. Kapush, S. V. Ushakov, A. Navrotsky, Q.-J. Hong, H. Liuand A. van de Walle, “A combined experimental and theoretical study of enthalpy of phase transition and fusion of yttria above 2000 °C using “drop-n-catch” calorimetry and first-principles calculation”, *Acta Materialia*, vol. 124. Elsevier BV, pp. 204–209, Feb. 2017. doi: 10.1016/j.actamat.2016.11.003.  
  
L. Miljacic, S. Demers, Q.-J. Hongand A. van de Walle, “Equation of state of solid, liquid and gaseous tantalum from first principles”, *Calphad*, vol. 51. Elsevier BV, pp. 133–143, Dec. 2015. doi: 10.1016/j.calphad.2015.08.005.  
  
G. S. Pomrehn, E. S. Toberer, G. J. Snyderand A. van de Walle, “Predicted Electronic and Thermodynamic Properties of a Newly Discovered Zn8Sb7 Phase”, *Journal of the American Chemical Society*, vol. 133, no. 29. American Chemical Society (ACS), pp. 11255–11261, Jul. 06, 2011. doi: 10.1021/ja202458n.  
  
R. Sun, M. Astaand A. van de Walle, “First-principles thermal compatibility between Ru-based Re-substitute alloys and Ir coatings”, *Computational Materials Science*, vol. 170. Elsevier BV, p. 109199, Dec. 2019. doi: 10.1016/j.commatsci.2019.109199.  
  
R. Sun and A. van de Walle, “Automating impurity-enhanced antiphase boundary energy calculations from ab initio Monte Carlo”, *Calphad*, vol. 53. Elsevier BV, pp. 20–24, Jun. 2016. doi: 10.1016/j.calphad.2016.02.005.  
  
S. V. Ushakov, A. Navrotsky, Q.-J. Hongand A. van de Walle, “Carbides and Nitrides of Zirconium and Hafnium”, *Materials*, vol. 12, no. 17. MDPI AG, p. 2728, Aug. 26, 2019. doi: 10.3390/ma12172728.  
  
A. van de Walle, “Invited paper: Reconciling SGTE and ab initio enthalpies of the elements”, *Calphad*, vol. 60. Elsevier BV, pp. 1–6, Mar. 2018. doi: 10.1016/j.calphad.2017.10.008.  
  
A. van de Walle and M. Asta, “High-throughput calculations in the context of alloy design”, *MRS Bulletin*, vol. 44, no. 4. Springer Science and Business Media LLC, pp. 252–256, Apr. 2019. doi: 10.1557/mrs.2019.71.  
  
A. van de Walle and Q. Hong, “Assessing Phase Diagram Accuracy”, *Journal of Phase Equilibria and Diffusion*, vol. 40, no. 2. Springer Science and Business Media LLC, pp. 170–175, Jan. 31, 2019. doi: 10.1007/s11669-019-00711-5.  
  
A. van de Walle, Q. Hong, S. Kadkhodaeiand R. Sun, “The free energy of mechanically unstable phases”, *Nature Communications*, vol. 6, no. 1. Springer Science and Business Media LLC, Jul. 01, 2015. doi: 10.1038/ncomms8559.  
  
A. van de Walle, C. Natarajand Z.-K. Liu, “The Thermodynamic Database Database”, *Calphad*, vol. 61. Elsevier BV, pp. 173–178, Jun. 2018. doi: 10.1016/j.calphad.2018.04.003.  
  
A. van de Walle, J. E. C. Sabisch, A. M. Minorand M. Asta, “Identifying rhenium substitute candidate multiprincipal-element alloys from electronic structure and thermodynamic criteria”, *Journal of Materials Research*, vol. 34, no. 19. Springer Science and Business Media LLC, pp. 3296–3304, Jun. 10, 2019. doi: 10.1557/jmr.2019.179.  
  
A. van de Walle, R. Sun, Q.-J. Hongand S. Kadkhodaei, “Software tools for high-throughput CALPHAD from first-principles data”, *Calphad*, vol. 58. Elsevier BV, pp. 70–81, Sep. 2017. doi: 10.1016/j.calphad.2017.05.005.  
  
L. G. Wang and A. van de Walle, “Ab initio calculations of the melting temperatures of refractory bcc metals”, *Phys. Chem. Chem. Phys.*, vol. 14, no. 4. Royal Society of Chemistry (RSC), pp. 1529–1534, 2012. doi: 10.1039/c1cp23036k.  
  
C. Woodward, A. van de Walle, M. Astaand D. R. Trinkle, “First-principles study of interfacial boundaries in Ni–Ni3Al”, *Acta Materialia*, vol. 75. Elsevier BV, pp. 60–70, Aug. 2014. doi: 10.1016/j.actamat.2014.04.056.  
  
F. Körmann, “Lambda transitions in materials science: Recent advances in CALPHAD and first-principles modelling”, *physica status solidi (b)*, vol. 251, no. 1. Wiley, pp. 53–80, Dec. 20, 2013. doi: 10.1002/pssb.201350136.  
  
C. H. Liebscher, “A hierarchical microstructure due to chemical ordering in the bcc lattice: Early stages of formation in a ferritic Fe–Al–Cr–Ni–Ti alloy”, *Acta Materialia*, vol. 92. Elsevier BV, pp. 220–232, Jun. 2015. doi: 10.1016/j.actamat.2015.03.043.  
  
W. J. Baumgardner, “Nanoparticle Metamorphosis: An *in Situ* High-Temperature Transmission Electron Microscopy Study of the Structural Evolution of Heterogeneous Au:Fe2O3 Nanoparticles”, *ACS Nano*, vol. 8, no. 5. American Chemical Society (ACS), pp. 5315–5322, May 05, 2014. doi: 10.1021/nn501543d.  
  
K. Bian, A. K. Singh, R. G. Hennig, Z. Wangand T. Hanrath, “The Nanocrystal Superlattice Pressure Cell: A Novel Approach To Study Molecular Bundles under Uniaxial Compression”, *Nano Letters*, vol. 14, no. 8. American Chemical Society (ACS), pp. 4763–4766, Jul. 29, 2014. doi: 10.1021/nl501905a.  
  
M. N. Blonsky, H. L. Zhuang, A. K. Singhand R. G. Hennig, “*Ab Initio* Prediction of Piezoelectricity in Two-Dimensional Materials”, *ACS Nano*, vol. 9, no. 10. American Chemical Society (ACS), pp. 9885–9891, Sep. 11, 2015. doi: 10.1021/acsnano.5b03394.  
  
J. Ditto, “Interface‐Driven Structural Distortions and Composition Segregation in Two‐Dimensional Heterostructures”, *Angewandte Chemie International Edition*, vol. 56, no. 46. Wiley, pp. 14448–14452, Oct. 02, 2017. doi: 10.1002/anie.201707270.  
  
D.-H. Ha, “Solid–Solid Phase Transformations Induced through Cation Exchange and Strain in 2D Heterostructured Copper Sulfide Nanocrystals”, *Nano Letters*, vol. 14, no. 12. American Chemical Society (ACS), pp. 7090–7099, Nov. 07, 2014. doi: 10.1021/nl5035607.  
  
K. Hernández-Burgos, S. E. Burkhardt, G. G. Rodríguez-Calero, R. G. Hennigand H. D. Abruña, “Theoretical Studies of Carbonyl-Based Organic Molecules for Energy Storage Applications: The Heteroatom and Substituent Effect”, *The Journal of Physical Chemistry C*, vol. 118, no. 12. American Chemical Society (ACS), pp. 6046–6051, Mar. 18, 2014. doi: 10.1021/jp4117613.  
  
J. Hwang, “van der Waals Epitaxial Growth of Graphene on Sapphire by Chemical Vapor Deposition without a Metal Catalyst”, *ACS Nano*, vol. 7, no. 1. American Chemical Society (ACS), pp. 385–395, Dec. 26, 2012. doi: 10.1021/nn305486x.  
  
S. Karkare, L. Boulet, A. Singh, R. Hennigand I. Bazarov, “*Ab initio*studies of Cs on GaAs (100) and (110) surfaces”, *Physical Review B*, vol. 91, no. 3. American Physical Society (APS), Jan. 12, 2015. doi: 10.1103/physrevb.91.035408.  
  
L. Ma, S. Wei, H. L. Zhuang, K. E. Hendrickson, R. G. Hennigand L. A. Archer, “Hybrid cathode architectures for lithium batteries based on TiS2 and sulfur”, *Journal of Materials Chemistry A*, vol. 3, no. 39. Royal Society of Chemistry (RSC), pp. 19857–19866, 2015. doi: 10.1039/c5ta06348e.  
  
L. Ma, H. Zhuang, Y. Lu, S. S. Moganty, R. G. Hennigand L. A. Archer, “Tethered Molecular Sorbents: Enabling Metal-Sulfur Battery Cathodes”, *Advanced Energy Materials*, vol. 4, no. 17. Wiley, p. 1400390, Jul. 29, 2014. doi: 10.1002/aenm.201400390.  
  
L. Ma, “Enhanced Li–S Batteries Using Amine-Functionalized Carbon Nanotubes in the Cathode”, *ACS Nano*, vol. 10, no. 1. American Chemical Society (ACS), pp. 1050–1059, Dec. 11, 2015. doi: 10.1021/acsnano.5b06373.  
  
K. Mathew, R. Sundararaman, K. Letchworth-Weaver, T. A. Ariasand R. G. Hennig, “Implicit solvation model for density-functional study of nanocrystal surfaces and reaction pathways”, *The Journal of Chemical Physics*, vol. 140, no. 8. AIP Publishing, p. 084106, Feb. 28, 2014. doi: 10.1063/1.4865107.  
  
A. Nelson, K. E. Fritz, S. Honrao, R. G. Hennig, R. D. Robinsonand J. Suntivich, “Increased activity in hydrogen evolution electrocatalysis for partial anionic substitution in cobalt oxysulfide nanoparticles”, *Journal of Materials Chemistry A*, vol. 4, no. 8. Royal Society of Chemistry (RSC), pp. 2842–2848, 2016. doi: 10.1039/c5ta08706f.  
  
B. C. Revard, W. W. Tiptonand R. G. Hennig, “Structure and Stability Prediction of Compounds with Evolutionary Algorithms”, *Topics in Current Chemistry*. Springer International Publishing, pp. 181–222, 2014. doi: 10.1007/128\_2013\_489.  
  
B. C. Revard, W. W. Tipton, A. Yesypenkoand R. G. Hennig, “Grand-canonical evolutionary algorithm for the prediction of two-dimensional materials”, *Physical Review B*, vol. 93, no. 5. American Physical Society (APS), Feb. 26, 2016. doi: 10.1103/physrevb.93.054117.  
  
A. K. Singh and R. G. Hennig, “Computational synthesis of single-layer GaN on refractory materials”, *Applied Physics Letters*, vol. 105, no. 5. AIP Publishing, p. 051604, Aug. 04, 2014. doi: 10.1063/1.4892351.  
  
A. K. Singh and R. G. Hennig, “Computational prediction of two-dimensional group-IV mono-chalcogenides”, *Applied Physics Letters*, vol. 105, no. 4. AIP Publishing, p. 042103, Jul. 28, 2014. doi: 10.1063/1.4891230.  
  
A. K. Singh, R. G. Hennig, A. V. Davydovand F. Tavazza, “Al2O3 as a suitable substrate and a dielectric layer for *n*-layer MoS2”, *Applied Physics Letters*, vol. 107, no. 5. AIP Publishing, p. 053106, Aug. 03, 2015. doi: 10.1063/1.4928179.  
  
A. K. Singh, K. Mathew, A. V. Davydov, R. G. Hennigand F. Tavazza, “High throughput screening of substrates for synthesis and functionalization of 2D materials”, *SPIE Proceedings*. SPIE, Aug. 26, 2015. doi: 10.1117/12.2192866.  
  
A. K. Singh, K. Mathew, H. L. Zhuangand R. G. Hennig, “Computational Screening of 2D Materials for Photocatalysis”, *The Journal of Physical Chemistry Letters*, vol. 6, no. 6. American Chemical Society (ACS), pp. 1087–1098, Mar. 12, 2015. doi: 10.1021/jz502646d.  
  
A. K. Singh, B. C. Revard, R. Ramanathan, M. Ashton, F. Tavazzaand R. G. Hennig, “Genetic algorithm prediction of two-dimensional group-IV dioxides for dielectrics”, *Physical Review B*, vol. 95, no. 15. American Physical Society (APS), Apr. 18, 2017. doi: 10.1103/physrevb.95.155426.  
  
W. W. Tipton and R. G. Hennig, “A grand canonical genetic algorithm for the prediction of multi-component phase diagrams and testing of empirical potentials”, *Journal of Physics: Condensed Matter*, vol. 25, no. 49. IOP Publishing, p. 495401, Nov. 01, 2013. doi: 10.1088/0953-8984/25/49/495401.  
  
W. W. Tipton, C. A. Matulisand R. G. Hennig, “Ab initio prediction of the Li 5 Ge 2 Zintl compound”, *Computational Materials Science*, vol. 93. Elsevier BV, pp. 133–136, Oct. 2014. doi: 10.1016/j.commatsci.2014.06.014.  
  
H. L. Zhuang, V. R. Cooper, H. Xu, P. Ganesh, R. G. Hennigand P. R. C. Kent, “Rashba effect in single-layer antimony telluroiodide SbTeI”, *Physical Review B*, vol. 92, no. 11. American Physical Society (APS), Sep. 04, 2015. doi: 10.1103/physrevb.92.115302.  
  
H. L. Zhuang and R. G. Hennig, “Computational identification of single-layer CdO for electronic and optical applications”, *Applied Physics Letters*, vol. 103, no. 21. AIP Publishing, p. 212102, Nov. 18, 2013. doi: 10.1063/1.4831972.  
  
H. L. Zhuang and R. G. Hennig, “Computational Discovery, Characterization, and Design of Single-Layer Materials”, *JOM*, vol. 66, no. 3. Springer Science and Business Media LLC, pp. 366–374, Feb. 19, 2014. doi: 10.1007/s11837-014-0885-3.  
  
H. L. Zhuang, M. D. Johannes, M. N. Blonskyand R. G. Hennig, “Computational prediction and characterization of single-layer CrS2”, *Applied Physics Letters*, vol. 104, no. 2. AIP Publishing, p. 022116, Jan. 13, 2014. doi: 10.1063/1.4861659.  
  
H. L. Zhuang, M. D. Johannes, A. K. Singhand R. G. Hennig, “Doping-controlled phase transitions in single-layer ”, *Physical Review B*, vol. 96, no. 16. American Physical Society (APS), Oct. 12, 2017. doi: 10.1103/physrevb.96.165305.  
  
Z. Chen, L. Zhao, K. Park, T. A. Garcia, M. C. Tamargoand L. Krusin-Elbaum, “Robust Topological Interfaces and Charge Transfer in Epitaxial Bi2Se3/II–VI Semiconductor Superlattices”, *Nano Letters*, vol. 15, no. 10. American Chemical Society (ACS), pp. 6365–6370, Sep. 11, 2015. doi: 10.1021/acs.nanolett.5b01358.  
  
Y.-T. Hsu, K. Parkand E.-A. Kim, “Hybridization-induced interface states in a topological-insulator–ferromagnetic-metal heterostructure”, *Physical Review B*, vol. 96, no. 23. American Physical Society (APS), Dec. 21, 2017. doi: 10.1103/physrevb.96.235433.  
  
K. Schouteden, “Annealing-Induced Bi Bilayer on Bi2Te3 Investigated *via* Quasi-Particle-Interference Mapping”, *ACS Nano*, vol. 10, no. 9. American Chemical Society (ACS), pp. 8778–8787, Sep. 07, 2016. doi: 10.1021/acsnano.6b04508.  
  
K. Schouteden, “Moiré superlattices at the topological insulator Bi2Te3”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Feb. 08, 2016. doi: 10.1038/srep20278.  
  
J. W. Villanova, E. Barnesand K. Park, “Engineering and Probing Topological Properties of Dirac Semimetal Films by Asymmetric Charge Transfer”, *Nano Letters*, vol. 17, no. 2. American Chemical Society (ACS), pp. 963–972, Jan. 04, 2017. doi: 10.1021/acs.nanolett.6b04299.  
  
J. W. Villanova and K. Park, “Spin textures of topological surface states at side surfaces offrom first principles”, *Physical Review B*, vol. 93, no. 8. American Physical Society (APS), Feb. 16, 2016. doi: 10.1103/physrevb.93.085122.  
  
E. Z. Xu, “p-Type transition-metal doping of large-area MoS2thin films grown by chemical vapor deposition”, *Nanoscale*, vol. 9, no. 10. Royal Society of Chemistry (RSC), pp. 3576–3584, 2017. doi: 10.1039/c6nr09495c.  
  
W. C. Yang, “Epitaxial thin films of pyrochlore iridate Bi2+xIr2-yO7-δ: structure, defects and transport properties”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Aug. 10, 2017. doi: 10.1038/s41598-017-06785-w.  
  
Y. Li, C. Chen, J. Burton, K. Park, J. R. Heflinand C. Tao, “Self-assembled PCBM bilayers on graphene and HOPG examined by AFM and STM”, *Nanotechnology*, vol. 29, no. 18. IOP Publishing, p. 185703, Mar. 08, 2018. doi: 10.1088/1361-6528/aab00a.  
  
A. Nicolini, “Filling the Gap in Extended Metal Atom Chains: Ferromagnetic Interactions in a Tetrairon(II) String Supported by Oligo-α-pyridylamido Ligands”, *Inorganic Chemistry*, vol. 57, no. 9. American Chemical Society (ACS), pp. 5438–5448, Apr. 18, 2018. doi: 10.1021/acs.inorgchem.8b00405.  
  
W. J. Yang, “Tuning of Topological Dirac States via Modification of van der Waals Gap in Strained Ultrathin Bi2Se3 Films”, *The Journal of Physical Chemistry C*, vol. 122, no. 41. American Chemical Society (ACS), pp. 23739–23748, Sep. 28, 2018. doi: 10.1021/acs.jpcc.8b06296.  
  
W. C. Yang, “Stoichiometry control and electronic and transport properties of pyrochlore thin films”, *Physical Review Materials*, vol. 2, no. 11. American Physical Society (APS), Nov. 21, 2018. doi: 10.1103/physrevmaterials.2.114206.  
  
F. Zhang, “Atomically Resolved Observation of Continuous Interfaces between an As-Grown MoS2 Monolayer and a WS2/MoS2 Heterobilayer on SiO2”, *ACS Applied Nano Materials*, vol. 1, no. 5. American Chemical Society (ACS), pp. 2041–2048, May 07, 2018. doi: 10.1021/acsanm.8b00385.  
  
S.-Y. Liu, S. Liu, D.-J. Li, S. Wang, J. Guoand Y. Shen, “*Ab initio* atomistic thermodynamics study on the oxidation mechanism of binary and ternary alloy surfaces”, *The Journal of Chemical Physics*, vol. 142, no. 6. AIP Publishing, p. 064705, Feb. 14, 2015. doi: 10.1063/1.4907718.  
  
V. I. Razumovskiy and G. Ghosh, “A first-principles study of cementite (Fe3C) and its alloyed counterparts: Structural properties, stability, and electronic structure”, *Computational Materials Science*, vol. 110. Elsevier BV, pp. 169–181, Dec. 2015. doi: 10.1016/j.commatsci.2015.08.006.  
  
T. Balankura, X. Qiand K. A. Fichthorn, “Solvent Effects on Molecular Adsorption on Ag Surfaces: Polyvinylpyrrolidone Oligomers”, *The Journal of Physical Chemistry C*, vol. 122, no. 26. American Chemical Society (ACS), pp. 14566–14573, Jun. 02, 2018. doi: 10.1021/acs.jpcc.8b03156.  
  
T. Balankura, T. Yan, O. Jahanmahin, J. Narukatpichai, A. Ngand K. A. Fichthorn, “Oriented attachment mechanism of triangular Ag nanoplates: a molecular dynamics study”, *Nanoscale Advances*, vol. 2, no. 6. Royal Society of Chemistry (RSC), pp. 2265–2270, 2020. doi: 10.1039/d0na00124d.  
  
G. Bélanger‐Chabot, M. Rahm, R. Haigesand K. O. Christe, “Ammonia–(Dinitramido)boranes: High‐Energy‐Density Materials”, *Angewandte Chemie International Edition*, vol. 54, no. 40. Wiley, pp. 11730–11734, Aug. 13, 2015. doi: 10.1002/anie.201505684.  
  
H. E. Maynard-Casely, R. Hodyss, M. L. Cable, T. H. Vuand M. Rahm, “A co-crystal between benzene and ethane: a potential evaporite material for Saturn’s moon Titan”, *IUCrJ*, vol. 3, no. 3. International Union of Crystallography (IUCr), pp. 192–199, Mar. 30, 2016. doi: 10.1107/s2052252516002815.  
  
M. Rahm, J. I. Lunine, D. A. Usherand D. Shalloway, “Polymorphism and electronic structure of polyimine and its potential significance for prebiotic chemistry on Titan”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 29. Proceedings of the National Academy of Sciences, pp. 8121–8126, Jul. 05, 2016. doi: 10.1073/pnas.1606634113.  
  
Y. Tsuji, P. L. V. K. Dasari, S. F. Elatresh, R. Hoffmannand N. W. Ashcroft, “Structural Diversity and Electron Confinement in Li4N: Potential for 0-D, 2-D, and 3-D Electrides”, *Journal of the American Chemical Society*, vol. 138, no. 42. American Chemical Society (ACS), pp. 14108–14120, Oct. 12, 2016. doi: 10.1021/jacs.6b09067.  
  
P. Xu and R. Hoffmann, “The Dimerization of H2NO”, *The Journal of Physical Chemistry A*, vol. 120, no. 8. American Chemical Society (ACS), pp. 1283–1296, Feb. 22, 2016. doi: 10.1021/acs.jpca.5b12674.  
  
K. AlKaabi, D. L. V. K. Prasad, P. Kroll, N. W. Ashcroftand R. Hoffmann, “Silicon Monoxide at 1 atm and Elevated Pressures: Crystalline or Amorphous?”, *Journal of the American Chemical Society*, vol. 136, no. 9. American Chemical Society (ACS), pp. 3410–3423, Feb. 24, 2014. doi: 10.1021/ja409692c.  
  
H. Y. Geng, R. Hoffmannand Q. Wu, “Lattice stability and high-pressure melting mechanism of dense hydrogen up to 1.5 TPa”, *Physical Review B*, vol. 92, no. 10. American Physical Society (APS), Sep. 02, 2015. doi: 10.1103/physrevb.92.104103.  
  
K. Sakata, B. Magyari-Köpe, S. Gupta, Y. Nishi, A. Blomand P. Deák, “The effects of uniaxial and biaxial strain on the electronic structure of germanium”, *Computational Materials Science*, vol. 112. Elsevier BV, pp. 263–268, Feb. 2016. doi: 10.1016/j.commatsci.2015.10.023.  
  
F. Körmann, “Lambda transitions in materials science: Recent advances in CALPHAD and first-principles modelling”, *physica status solidi (b)*, vol. 251, no. 1. Wiley, pp. 53–80, Dec. 20, 2013. doi: 10.1002/pssb.201350136.  
  
N. L. Adamski, Z. Zhu, D. Wickramaratneand C. G. Van de Walle, “Strategies for *p*-type doping of ZnGeN2”, *Applied Physics Letters*, vol. 114, no. 3. AIP Publishing, p. 032101, Jan. 21, 2019. doi: 10.1063/1.5063581.  
  
A. Alkauskas, B. B. Buckley, D. D. Awschalomand C. G. Van de Walle, “First-principles theory of the luminescence lineshape for the triplet transition in diamond NV centres”, *New Journal of Physics*, vol. 16, no. 7. IOP Publishing, p. 073026, Jul. 17, 2014. doi: 10.1088/1367-2630/16/7/073026.  
  
L. Bjaalie, “Band alignments between SmTiO3, GdTiO3, and SrTiO3”, *Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films*, vol. 34, no. 6. American Vacuum Society, p. 061102, Nov. 2016. doi: 10.1116/1.4963833.  
  
L. Bjaalie, B. Himmetoglu, L. Weston, A. Janottiand C. G. Van de Walle, “Oxide interfaces for novel electronic applications”, *New Journal of Physics*, vol. 16, no. 2. IOP Publishing, p. 025005, Feb. 13, 2014. doi: 10.1088/1367-2630/16/2/025005.  
  
L. Bjaalie, A. Janotti, B. Himmetogluand C. G. Van de Walle, “Turninginto a Mott insulator”, *Physical Review B*, vol. 90, no. 19. American Physical Society (APS), Nov. 11, 2014. doi: 10.1103/physrevb.90.195117.  
  
L. Bjaalie, A. Janotti, B. Himmetogluand C. G. Van de Walle, “Metal versus insulator behavior in ultrathin-based heterostructures”, *Physical Review B*, vol. 94, no. 3. American Physical Society (APS), Jul. 07, 2016. doi: 10.1103/physrevb.94.035115.  
  
L. Bjaalie, A. Janotti, K. Krishnaswamyand C. G. Van de Walle, “Point defects, impurities, and small hole polarons in”, *Physical Review B*, vol. 93, no. 11. American Physical Society (APS), Mar. 28, 2016. doi: 10.1103/physrevb.93.115316.  
  
L. Bjaalie, “Small hole polarons in rare-earth titanates”, *Applied Physics Letters*, vol. 106, no. 23. AIP Publishing, p. 232103, Jun. 08, 2015. doi: 10.1063/1.4922316.  
  
L. Bjaalie, “Determination of the Mott-Hubbard gap in”, *Physical Review B*, vol. 92, no. 8. American Physical Society (APS), Aug. 06, 2015. doi: 10.1103/physrevb.92.085111.  
  
C. Carbogno, C. G. Levi, C. G. Van de Walleand M. Scheffler, “Ferroelastic switching of doped zirconia: Modeling and understanding from first principles”, *Physical Review B*, vol. 90, no. 14. American Physical Society (APS), Oct. 31, 2014. doi: 10.1103/physrevb.90.144109.  
  
I. Chatratin, “Role of point defects in the electrical and optical properties of ”, *Physical Review Materials*, vol. 3, no. 7. American Physical Society (APS), Jul. 29, 2019. doi: 10.1103/physrevmaterials.3.074604.  
  
M. Choi, A. Janottiand C. G. Van de Walle, “Native point defects and dangling bonds in α-Al2O3”, *Journal of Applied Physics*, vol. 113, no. 4. AIP Publishing, p. 044501, Jan. 28, 2013. doi: 10.1063/1.4784114.  
  
M. Choi, A. Janottiand C. G. Van de Walle, “Hydrogen Passivation of Impurities in Al2O3”, *ACS Applied Materials & Interfaces*, vol. 6, no. 6. American Chemical Society (ACS), pp. 4149–4153, Mar. 10, 2014. doi: 10.1021/am4057997.  
  
M. Choi, J. L. Lyons, A. Janottiand C. G. Van de Walle, “Impact of carbon and nitrogen impurities in high-κ dielectrics on metal-oxide-semiconductor devices”, *Applied Physics Letters*, vol. 102, no. 14. AIP Publishing, p. 142902, Apr. 08, 2013. doi: 10.1063/1.4801497.  
  
M. Choi, J. L. Lyons, A. Janottiand C. G. Van de Walle, “Impact of native defects in high-k dielectric oxides on GaN/oxide metal-oxide-semiconductor devices”, *physica status solidi (b)*, vol. 250, no. 4. Wiley, pp. 787–791, Mar. 01, 2013. doi: 10.1002/pssb.201200628.  
  
G. Conti, “Band offsets in complex-oxide thin films and heterostructures of SrTiO3/LaNiO3 and SrTiO3/GdTiO3 by soft and hard X-ray photoelectron spectroscopy”, *Journal of Applied Physics*, vol. 113, no. 14. AIP Publishing, p. 143704, Apr. 14, 2013. doi: 10.1063/1.4795612.  
  
C. E. Dreyer, A. Janottiand C. G. Van de Walle, “Effects of strain on the electron effective mass in GaN and AlN”, *Applied Physics Letters*, vol. 102, no. 14. AIP Publishing, p. 142105, Apr. 08, 2013. doi: 10.1063/1.4801520.  
  
C. E. Dreyer, A. Janottiand C. G. Van de Walle, “Brittle fracture toughnesses of GaN and AlN from first-principles surface-energy calculations”, *Applied Physics Letters*, vol. 106, no. 21. AIP Publishing, p. 212103, May 25, 2015. doi: 10.1063/1.4921855.  
  
D. Eiteneer, “Depth-Resolved Composition and Electronic Structure of Buried Layers and Interfaces in a LaNiO3/SrTiO3 Superlattice from Soft- and Hard- X-ray Standing-Wave Angle-Resolved Photoemission”, *Journal of Electron Spectroscopy and Related Phenomena*, vol. 211. Elsevier BV, pp. 70–81, Aug. 2016. doi: 10.1016/j.elspec.2016.04.008.  
  
C. Freysoldt, “Electron and chemical reservoir corrections for point-defect formation energies”, *Physical Review B*, vol. 93, no. 16. American Physical Society (APS), Apr. 22, 2016. doi: 10.1103/physrevb.93.165206.  
  
L. Gordon, H. Abu-Farsakh, A. Janottiand C. G. Van de Walle, “Hydrogen bonds in Al2O3 as dissipative two-level systems in superconducting qubits”, *Scientific Reports*, vol. 4, no. 1. Springer Science and Business Media LLC, Dec. 23, 2014. doi: 10.1038/srep07590.  
  
L. Gordon, A. Janottiand C. G. Van de Walle, “Defects as qubits inand”, *Physical Review B*, vol. 92, no. 4. American Physical Society (APS), Jul. 20, 2015. doi: 10.1103/physrevb.92.045208.  
  
L. Gordon, J. R. Weber, J. B. Varley, A. Janotti, D. D. Awschalomand C. G. Van de Walle, “Quantum computing with defects”, *MRS Bulletin*, vol. 38, no. 10. Springer Science and Business Media LLC, pp. 802–807, Oct. 2013. doi: 10.1557/mrs.2013.206.  
  
B. Himmetoglu, A. Janotti, H. Peelaers, A. Alkauskasand C. G. Van de Walle, “First-principles study of the mobility of”, *Physical Review B*, vol. 90, no. 24. American Physical Society (APS), Dec. 23, 2014. doi: 10.1103/physrevb.90.241204.  
  
K. Hoang and C. G. Van de Walle, “LiH as a Li+ and H− ion provider”, *Solid State Ionics*, vol. 253. Elsevier BV, pp. 53–56, Dec. 2013. doi: 10.1016/j.ssi.2013.08.017.  
  
W. S. Hwang, “High-voltage field effect transistors with wide-bandgap *β*-Ga2O3 nanomembranes”, *Applied Physics Letters*, vol. 104, no. 20. AIP Publishing, p. 203111, May 19, 2014. doi: 10.1063/1.4879800.  
  
A. Janotti, L. Bjaalie, B. Himmetogluand C. G. Van de Walle, “Band alignment at band-insulator/Mott-insulator interfaces”, *physica status solidi (RRL) - Rapid Research Letters*, vol. 8, no. 6. Wiley, pp. 577–582, May 14, 2014. doi: 10.1002/pssr.201409088.  
  
A. Janotti, C. Franchini, J. B. Varley, G. Kresseand C. G. Van de Walle, “Dual behavior of excess electrons in rutile TiO2”, *physica status solidi (RRL) - Rapid Research Letters*, vol. 7, no. 3. Wiley, pp. 199–203, Jan. 07, 2013. doi: 10.1002/pssr.201206464.  
  
A. Schleife, J. B. Varley, A. Janottiand C. G. Van de Walle, “Conductivity and transparency of TiO2from first principles”, *Solar Hydrogen and Nanotechnology VIII*. SPIE, Sep. 16, 2013. doi: 10.1117/12.2024566.  
  
Y. Kang, K. Krishnaswamy, H. Peelaersand C. G. Van de Walle, “Fundamental limits on the electron mobility of*β*-Ga2O3”, *Journal of Physics: Condensed Matter*, vol. 29, no. 23. IOP Publishing, p. 234001, May 12, 2017. doi: 10.1088/1361-648x/aa6f66.  
  
Y. Kang, H. Peelaers, K. Krishnaswamyand C. G. Van de Walle, “First-principles study of direct and indirect optical absorption in BaSnO3”, *Applied Physics Letters*, vol. 112, no. 6. AIP Publishing, p. 062106, Feb. 05, 2018. doi: 10.1063/1.5013641.  
  
Y. Kang, H. Peelaersand C. G. Van de Walle, “First-principles study of electron-phonon interactions and transport in anatase ”, *Physical Review B*, vol. 100, no. 12. American Physical Society (APS), Sep. 30, 2019. doi: 10.1103/physrevb.100.121113.  
  
Y. Kang and C. G. Van de Walle, “Electrical compensation mechanism in fluorine-doped SnO2”, *Applied Physics Letters*, vol. 111, no. 15. AIP Publishing, p. 152107, Oct. 09, 2017. doi: 10.1063/1.4999479.  
  
E. Kioupakis, P. Rinke, A. Janotti, Q. Yanand C. G. Van de Walle, “Energy Conversion: Solid-State Lighting”, *Computational Approaches to Energy Materials*. John Wiley & Sons Ltd, pp. 231–259, Apr. 25, 2013. doi: 10.1002/9781118551462.ch8.  
  
K. Krishnaswamy, L. Bjaalie, B. Himmetoglu, A. Janotti, L. Gordonand C. G. Van de Walle, “BaSnO3 as a channel material in perovskite oxide heterostructures”, *Applied Physics Letters*, vol. 108, no. 8. AIP Publishing, p. 083501, Feb. 22, 2016. doi: 10.1063/1.4942366.  
  
K. Krishnaswamy, C. E. Dreyer, A. Janottiand C. G. Van de Walle, “Structure and energetics of(001) surfaces”, *Physical Review B*, vol. 90, no. 23. American Physical Society (APS), Dec. 29, 2014. doi: 10.1103/physrevb.90.235436.  
  
K. Krishnaswamy, C. E. Dreyer, A. Janottiand C. G. Van de Walle, “First-principles study of surface charging inheterostructures”, *Physical Review B*, vol. 92, no. 8. American Physical Society (APS), Aug. 19, 2015. doi: 10.1103/physrevb.92.085420.  
  
K. Krishnaswamy, B. Himmetoglu, Y. Kang, A. Janottiand C. G. Van de Walle, “First-principles analysis of electron transport in ”, *Physical Review B*, vol. 95, no. 20. American Physical Society (APS), May 15, 2017. doi: 10.1103/physrevb.95.205202.  
  
S. Limpijumnong, L. Gordon, M. Miao, A. Janottiand C. G. Van de Walle, “Alternative sources of p-type conduction in acceptor-doped ZnO”, *Applied Physics Letters*, vol. 97, no. 7. AIP Publishing, p. 072112, Aug. 16, 2010. doi: 10.1063/1.3481069.  
  
J. L. Lyons, A. Janottiand C. G. Van de Walle, “Effects of hole localization on limiting *p*-type conductivity in oxide and nitride semiconductors”, *Journal of Applied Physics*, vol. 115, no. 1. AIP Publishing, p. 012014, Jan. 07, 2014. doi: 10.1063/1.4838075.  
  
J. L. Lyons, K. Krishnaswamy, L. Gordon, A. Janottiand C. G. Van de Walle, “Identification of Microscopic Hole-Trapping Mechanisms in Nitride Semiconductors”, *IEEE Electron Device Letters*, vol. 37, no. 2. Institute of Electrical and Electronics Engineers (IEEE), pp. 154–156, Feb. 2016. doi: 10.1109/led.2015.2509068.  
  
J. L. Lyons and C. G. Van de Walle, “Computationally predicted energies and properties of defects in GaN”, *npj Computational Materials*, vol. 3, no. 1. Springer Science and Business Media LLC, Mar. 24, 2017. doi: 10.1038/s41524-017-0014-2.  
  
J. L. Lyons, J. B. Varley, D. Steiauf, A. Janottiand C. G. Van de Walle, “First-principles characterization of native-defect-related optical transitions in ZnO”, *Journal of Applied Physics*, vol. 122, no. 3. AIP Publishing, p. 035704, Jul. 21, 2017. doi: 10.1063/1.4992128.  
  
P. M. McBride, A. Janotti, C. E. Dreyer, B. Himmetogluand C. G. Van de Walle, “Effects of biaxial stress and layer thickness on octahedral tilts in LaNiO3”, *Applied Physics Letters*, vol. 107, no. 26. AIP Publishing, p. 261901, Dec. 28, 2015. doi: 10.1063/1.4939002.  
  
M.-. sheng . Miao and C. G. Van de Walle, “Nitride-based high-electron-mobility transistor with single-layer InN for mobility-enhanced channel”, *Applied Physics Express*, vol. 8, no. 2. IOP Publishing, p. 024302, Jan. 29, 2015. doi: 10.7567/apex.8.024302.  
  
M. S. Miao, Q. M. Yanand C. G. Van de Walle, “Electronic structure of a single-layer InN quantum well in a GaN matrix”, *Applied Physics Letters*, vol. 102, no. 10. AIP Publishing, p. 102103, Mar. 11, 2013. doi: 10.1063/1.4794986.  
  
P. G. Moses, A. Janotti, C. Franchini, G. Kresseand C. G. Van de Walle, “Donor defects and small polarons on the TiO2(110) surface”, *Journal of Applied Physics*, vol. 119, no. 18. AIP Publishing, p. 181503, May 14, 2016. doi: 10.1063/1.4948239.  
  
S. Nemšák, “Energetic, spatial, and momentum character of the electronic structure at a buried interface: The two-dimensional electron gas between two metal oxides”, *Physical Review B*, vol. 93, no. 24. American Physical Society (APS), Jun. 01, 2016. doi: 10.1103/physrevb.93.245103.  
  
S. Nemšák, “Observation by resonant angle-resolved photoemission of a critical thickness for 2-dimensional electron gas formation in SrTiO3 embedded in GdTiO3”, *Applied Physics Letters*, vol. 107, no. 23. AIP Publishing, p. 231602, Dec. 07, 2015. doi: 10.1063/1.4936936.  
  
J. E. Padilha, H. Peelaers, A. Janottiand C. G. Van de Walle, “Nature and evolution of the band-edge states in: From monolayer to bulk”, *Physical Review B*, vol. 90, no. 20. American Physical Society (APS), Nov. 17, 2014. doi: 10.1103/physrevb.90.205420.  
  
H. Peelaers, E. Kioupakisand C. G. Van de Walle, “Fundamental limits on optical transparency of transparent conducting oxides: Free-carrier absorption in SnO2”, *Applied Physics Letters*, vol. 100, no. 1. AIP Publishing, p. 011914, Jan. 02, 2012. doi: 10.1063/1.3671162.  
  
H. Peelaers, E. Kioupakisand C. G. Van de Walle, “Limitations of In2O3 as a transparent conducting oxide”, *Applied Physics Letters*, vol. 115, no. 8. AIP Publishing, p. 082105, Aug. 19, 2019. doi: 10.1063/1.5109569.  
  
H. Peelaers, J. L. Lyons, J. B. Varleyand C. G. Van de Walle, “Deep acceptors and their diffusion in Ga2O3”, *APL Materials*, vol. 7, no. 2. AIP Publishing, p. 022519, Feb. 2019. doi: 10.1063/1.5063807.  
  
H. Peelaers, D. Steiauf, J. B. Varley, A. Janottiand C. G. Van de Walle, “alloys for transparent electronics”, *Physical Review B*, vol. 92, no. 8. American Physical Society (APS), Aug. 31, 2015. doi: 10.1103/physrevb.92.085206.  
  
H. Peelaers and C. G. Van de Walle, “Elastic Constants and Pressure-Induced Effects in MoS2”, *The Journal of Physical Chemistry C*, vol. 118, no. 22. American Chemical Society (ACS), pp. 12073–12076, May 23, 2014. doi: 10.1021/jp503683h.  
  
H. Peelaers and C. G. Van de Walle, “First-principles study of van der Waals interactions in MoS2and MoO3”, *Journal of Physics: Condensed Matter*, vol. 26, no. 30. IOP Publishing, p. 305502, Jul. 10, 2014. doi: 10.1088/0953-8984/26/30/305502.  
  
H. Peelaers and C. G. Van de Walle, “Brillouin zone and band structure of β-Ga2O3”, *physica status solidi (b)*, vol. 252, no. 4. Wiley, pp. 828–832, Jan. 20, 2015. doi: 10.1002/pssb.201451551.  
  
H. Peelaers and C. G. Van de Walle, “Doping of with transition metals”, *Physical Review B*, vol. 94, no. 19. American Physical Society (APS), Nov. 10, 2016. doi: 10.1103/physrevb.94.195203.  
  
H. Peelaers and C. G. Van de Walle, “Lack of quantum confinement in nanolayers”, *Physical Review B*, vol. 96, no. 8. American Physical Society (APS), Aug. 25, 2017. doi: 10.1103/physrevb.96.081409.  
  
H. Peelaers and C. G. Van de Walle, “Sub-band-gap absorption in Ga2O3”, *Applied Physics Letters*, vol. 111, no. 18. AIP Publishing, p. 182104, Oct. 30, 2017. doi: 10.1063/1.5001323.  
  
H. Peelaers and C. G. Van de Walle, “Phonon- and charged-impurity-assisted indirect free-carrier absorption in ”, *Physical Review B*, vol. 100, no. 8. American Physical Society (APS), Aug. 05, 2019. doi: 10.1103/physrevb.100.081202.  
  
H. Peelaers, J. B. Varley, J. S. Speckand C. G. Van de Walle, “Structural and electronic properties of Ga2O3-Al2O3 alloys”, *Applied Physics Letters*, vol. 112, no. 24. AIP Publishing, p. 242101, Jun. 11, 2018. doi: 10.1063/1.5036991.  
  
J. M. Sander, L. Ismerand C. G. Van de Walle, “Point-defect kinetics in α- and γ-MgH2”, *International Journal of Hydrogen Energy*, vol. 41, no. 13. Elsevier BV, pp. 5688–5692, Apr. 2016. doi: 10.1016/j.ijhydene.2016.01.156.  
  
J.-X. Shen, A. Schleife, A. Janottiand C. G. Van de Walle, “Effects of La and states on the electronic and optical properties of ”, *Physical Review B*, vol. 94, no. 20. American Physical Society (APS), Nov. 22, 2016. doi: 10.1103/physrevb.94.205203.  
  
J.-X. Shen, D. Wickramaratneand C. G. Van de Walle, “Band bowing and the direct-to-indirect crossover in random BAlN alloys”, *Physical Review Materials*, vol. 1, no. 6. American Physical Society (APS), Nov. 13, 2017. doi: 10.1103/physrevmaterials.1.065001.  
  
D. Steiauf, J. L. Lyons, A. Janottiand C. G. Van de Walle, “First-principles study of vacancy-assisted impurity diffusion in ZnO”, *APL Materials*, vol. 2, no. 9. AIP Publishing, p. 096101, Sep. 2014. doi: 10.1063/1.4894195.  
  
M. Swift, A. Janottiand C. G. Van de Walle, “Small polarons and point defects in barium cerate”, *Physical Review B*, vol. 92, no. 21. American Physical Society (APS), Dec. 28, 2015. doi: 10.1103/physrevb.92.214114.  
  
M. W. Swift, Z. Porter, S. D. Wilsonand C. G. Van de Walle, “Electron doping in : Collapse of band gap and magnetic order”, *Physical Review B*, vol. 98, no. 8. American Physical Society (APS), Aug. 10, 2018. doi: 10.1103/physrevb.98.081106.  
  
M. W. Swift and C. G. Van de Walle, “Conditions for T2 resistivity from electron-electron scattering”, *The European Physical Journal B*, vol. 90, no. 8. Springer Science and Business Media LLC, Aug. 2017. doi: 10.1140/epjb/e2017-80367-1.  
  
M. W. Swift, C. G. Van de Walleand M. P. A. Fisher, “Posner molecules: from atomic structure to nuclear spins”, *Physical Chemistry Chemical Physics*, vol. 20, no. 18. Royal Society of Chemistry (RSC), pp. 12373–12380, 2018. doi: 10.1039/c7cp07720c.  
  
M. E. Turiansky, A. Alkauskas, L. C. Bassettand C. G. Van de Walle, “Dangling Bonds in Hexagonal Boron Nitride as Single-Photon Emitters”, *Physical Review Letters*, vol. 123, no. 12. American Physical Society (APS), Sep. 16, 2019. doi: 10.1103/physrevlett.123.127401.  
  
M. E. Turiansky, J.-X. Shen, D. Wickramaratneand C. G. Van de Walle, “First-principles study of bandgap bowing in BGaN alloys”, *Journal of Applied Physics*, vol. 126, no. 9. AIP Publishing, p. 095706, Sep. 07, 2019. doi: 10.1063/1.5111414.  
  
C. G. Van de Walle, M. Choi, J. R. Weber, J. L. Lyonsand A. Janotti, “Defects at Ge/oxide and III–V/oxide interfaces”, *Microelectronic Engineering*, vol. 109. Elsevier BV, pp. 211–215, Sep. 2013. doi: 10.1016/j.mee.2013.03.151.  
  
J. B. Varley, A. Janottiand C. G. Van de Walle, “Defects in AlN as candidates for solid-state qubits”, *Physical Review B*, vol. 93, no. 16. American Physical Society (APS), Apr. 01, 2016. doi: 10.1103/physrevb.93.161201.  
  
J. Varley, A. Janotti, C. G. Van de Walleand J. L. Lyons, “First-principles calculations of optical transitions at native defects and impurities in ZnO”, *Oxide-based Materials and Devices IX*. SPIE, Feb. 23, 2018. doi: 10.1117/12.2303687.  
  
J. B. Varley, A. Schleife, A. Janottiand C. G. Van de Walle, “Ambipolar doping in SnO”, *Applied Physics Letters*, vol. 103, no. 8. AIP Publishing, p. 082118, Aug. 19, 2013. doi: 10.1063/1.4819068.  
  
W. Wang, A. Janottiand C. G. Van de Walle, “Phase transformations upon doping in WO3”, *The Journal of Chemical Physics*, vol. 146, no. 21. AIP Publishing, p. 214504, Jun. 07, 2017. doi: 10.1063/1.4984581.  
  
W. Wang, H. Peelaers, J.-X. Shenand C. G. Van de Walle, “Carrier-induced absorption as a mechanism for electrochromism in tungsten trioxide”, *MRS Communications*, vol. 8, no. 3. Springer Science and Business Media LLC, pp. 926–931, Jun. 29, 2018. doi: 10.1557/mrc.2018.115.  
  
L. Weston, L. Bjaalie, K. Krishnaswamyand C. G. Van de Walle, “Origins of -type doping difficulties in perovskite stannates”, *Physical Review B*, vol. 97, no. 5. American Physical Society (APS), Feb. 26, 2018. doi: 10.1103/physrevb.97.054112.  
  
L. Weston, A. Janotti, X. Y. Cui, B. Himmetoglu, C. Stampfland C. G. Van de Walle, “Structural and electronic properties ofand Sr(Ti,Zr)alloys”, *Physical Review B*, vol. 92, no. 8. American Physical Society (APS), Aug. 11, 2015. doi: 10.1103/physrevb.92.085201.  
  
L. Weston, H. Tailor, K. Krishnaswamy, L. Bjaalieand C. G. Van de Walle, “Accurate and efficient band-offset calculations from density functional theory”, *Computational Materials Science*, vol. 151. Elsevier BV, pp. 174–180, Aug. 2018. doi: 10.1016/j.commatsci.2018.05.002.  
  
L. Weston, D. Wickramaratne, M. Mackoit, A. Alkauskasand C. G. Van de Walle, “Native point defects and impurities in hexagonal boron nitride”, *Physical Review B*, vol. 97, no. 21. American Physical Society (APS), Jun. 18, 2018. doi: 10.1103/physrevb.97.214104.  
  
L. Weston, D. Wickramaratneand C. G. Van de Walle, “Hole polarons and -type doping in boron nitride polymorphs”, *Physical Review B*, vol. 96, no. 10. American Physical Society (APS), Sep. 29, 2017. doi: 10.1103/physrevb.96.100102.  
  
D. Wickramaratne, “Defect identification based on first-principles calculations for deep level transient spectroscopy”, *Applied Physics Letters*, vol. 113, no. 19. AIP Publishing, p. 192106, Nov. 05, 2018. doi: 10.1063/1.5047808.  
  
D. Wickramaratne, L. Westonand C. G. Van de Walle, “Monolayer to Bulk Properties of Hexagonal Boron Nitride”, *The Journal of Physical Chemistry C*, vol. 122, no. 44. American Chemical Society (ACS), pp. 25524–25529, Oct. 11, 2018. doi: 10.1021/acs.jpcc.8b09087.  
  
Q. Yan, A. Janotti, M. Schefflerand C. G. Van de Walle, “Origins of optical absorption and emission lines in AlN”, *Applied Physics Letters*, vol. 105, no. 11. AIP Publishing, p. 111104, Sep. 15, 2014. doi: 10.1063/1.4895786.  
  
Q. Yan, “Strain effects and band parameters in MgO, ZnO, and CdO”, *Applied Physics Letters*, vol. 101, no. 15. AIP Publishing, p. 152105, Oct. 08, 2012. doi: 10.1063/1.4759107.  
  
L. Zhang, A. Janotti, A. C. Meng, K. Tang, C. G. Van de Walleand P. C. McIntyre, “Interfacial Cation-Defect Charge Dipoles in Stacked TiO2/Al2O3 Gate Dielectrics”, *ACS Applied Materials & Interfaces*, vol. 10, no. 6. American Chemical Society (ACS), pp. 5140–5146, Jan. 30, 2018. doi: 10.1021/acsami.7b19619.  
  
L. N. Bartlett, D. C. Van Aken, J. Medvedeva, D. Isheim, N. Medvedevaand K. Song, “An Atom Probe Study of κ-carbide Precipitation in Austenitic Lightweight Steel and the Effect of Phosphorus”, *Metallurgical and Materials Transactions A*, vol. 48, no. 11. Springer Science and Business Media LLC, pp. 5500–5515, Aug. 31, 2017. doi: 10.1007/s11661-017-4287-3.  
  
S. M. Islam, “Multistates and Polyamorphism in Phase-Change K2Sb8Se13”, *Journal of the American Chemical Society*, vol. 140, no. 29. American Chemical Society (ACS), pp. 9261–9268, Jun. 29, 2018. doi: 10.1021/jacs.8b05542.  
  
C. Kurter, “Conductance Spectroscopy of Exfoliated Thin Flakes of Nb*x*Bi2Se3”, *Nano Letters*, vol. 19, no. 1. American Chemical Society (ACS), pp. 38–45, Nov. 27, 2018. doi: 10.1021/acs.nanolett.8b02954.  
  
T. A. Safeera, R. Khanal, J. E. Medvedeva, A. I. Martinez, G. Vinithaand E. I. Anila, “Low temperature synthesis and characterization of zinc gallate quantum dots for optoelectronic applications”, *Journal of Alloys and Compounds*, vol. 740. Elsevier BV, pp. 567–573, Apr. 2018. doi: 10.1016/j.jallcom.2018.01.035.  
  
X. Zhang, “Synergistic Boron Doping of Semiconductor and Dielectric Layers for High-Performance Metal Oxide Transistors: Interplay of Experiment and Theory”, *Journal of the American Chemical Society*, vol. 140, no. 39. American Chemical Society (ACS), pp. 12501–12510, Sep. 05, 2018. doi: 10.1021/jacs.8b06395.  
  
J. Salfi, “Spatially resolving valley quantum interference of a donor in silicon”, *Nature Materials*, vol. 13, no. 6. Springer Science and Business Media LLC, pp. 605–610, Apr. 06, 2014. doi: 10.1038/nmat3941.  
  
D. G. Fleming, S. P. Cottrell, I. McKenzieand R. M. Macrae, “New results for the formation of a muoniated radical in the Mu + Br2 system: a van der Waals complex or evidence for vibrational bonding in Br–Mu–Br?”, *Physical Chemistry Chemical Physics*, vol. 14, no. 31. Royal Society of Chemistry (RSC), p. 10953, 2012. doi: 10.1039/c2cp41366c.  
  
A. F. Baldwin, “Rational Design of Organotin Polyesters”, *Macromolecules*, vol. 48, no. 8. American Chemical Society (ACS), pp. 2422–2428, Apr. 15, 2015. doi: 10.1021/ma502424r.  
  
A. F. Baldwin, “Poly(dimethyltin glutarate) as a Prospective Material for High Dielectric Applications”, *Advanced Materials*, vol. 27, no. 2. Wiley, pp. 346–351, Nov. 25, 2014. doi: 10.1002/adma.201404162.  
  
R. Batra, T. D. Huan, J. L. Jones, G. Rossetti Jr.and R. Ramprasad, “Factors Favoring Ferroelectricity in Hafnia: A First-Principles Computational Study”, *The Journal of Physical Chemistry C*, vol. 121, no. 8. American Chemical Society (ACS), pp. 4139–4145, Feb. 16, 2017. doi: 10.1021/acs.jpcc.6b11972.  
  
R. Batra, T. D. Huan, G. A. Rossetti Jr.and R. Ramprasad, “Dopants Promoting Ferroelectricity in Hafnia: Insights from a comprehensive Chemical Space Exploration”, *Chemistry of Materials*, vol. 29, no. 21. American Chemical Society (ACS), pp. 9102–9109, Oct. 26, 2017. doi: 10.1021/acs.chemmater.7b02835.  
  
R. Batra, “General Atomic Neighborhood Fingerprint for Machine Learning-Based Methods”, *The Journal of Physical Chemistry C*, vol. 123, no. 25. American Chemical Society (ACS), pp. 15859–15866, Jun. 06, 2019. doi: 10.1021/acs.jpcc.9b03925.  
  
R. Batra, H. D. Tranand R. Ramprasad, “Stabilization of metastable phases in hafnia owing to surface energy effects”, *Applied Physics Letters*, vol. 108, no. 17. AIP Publishing, p. 172902, Apr. 25, 2016. doi: 10.1063/1.4947490.  
  
R. Batra, H. D. Tranand R. Ramprasad, “Stabilization of metastable phases in hafnia owing to surface energy effects”, *Applied Physics Letters*, vol. 108, no. 17. AIP Publishing, p. 172902, Apr. 25, 2016. doi: 10.1063/1.4947490.  
  
V. Botu, R. Batra, J. Chapmanand R. Ramprasad, “Machine Learning Force Fields: Construction, Validation, and Outlook”, *The Journal of Physical Chemistry C*, vol. 121, no. 1. American Chemical Society (ACS), pp. 511–522, Dec. 29, 2016. doi: 10.1021/acs.jpcc.6b10908.  
  
V. Botu, J. Chapmanand R. Ramprasad, “A study of adatom ripening on an Al (1 1 1) surface with machine learning force fields”, *Computational Materials Science*, vol. 129. Elsevier BV, pp. 332–335, Mar. 2017. doi: 10.1016/j.commatsci.2016.12.007.  
  
A. Chandrasekaran, D. Kamal, R. Batra, C. Kim, L. Chenand R. Ramprasad, “Solving the electronic structure problem with machine learning”, *npj Computational Materials*, vol. 5, no. 1. Springer Science and Business Media LLC, Feb. 18, 2019. doi: 10.1038/s41524-019-0162-7.  
  
J. Chapman, R. Batra, B. P. Uberuaga, G. Pilaniaand R. Ramprasad, “A comprehensive computational study of adatom diffusion on the aluminum (1 0 0) surface”, *Computational Materials Science*, vol. 158. Elsevier BV, pp. 353–358, Feb. 2019. doi: 10.1016/j.commatsci.2018.11.032.  
  
L. Chen, H. D. Tranand R. Ramprasad, “Atomistic mechanisms for chemical defects formation in polyethylene”, *The Journal of Chemical Physics*, vol. 149, no. 23. AIP Publishing, p. 234902, Dec. 21, 2018. doi: 10.1063/1.5063944.  
  
D. Das, A. Chandrasekaran, S. Venkatramand R. Ramprasad, “Effect of Crystallinity on Li Adsorption in Polyethylene Oxide”, *Chemistry of Materials*, vol. 30, no. 24. American Chemical Society (ACS), pp. 8804–8810, Dec. 02, 2018. doi: 10.1021/acs.chemmater.8b03434.  
  
T. D. Huan, “Advanced polymeric dielectrics for high energy density applications”, *Progress in Materials Science*, vol. 83. Elsevier BV, pp. 236–269, Oct. 2016. doi: 10.1016/j.pmatsci.2016.05.001.  
  
T. D. Huan, V. Sharma, G. A. Rossettiand R. Ramprasad, “Pathways towards ferroelectricity in hafnia”, *Physical Review B*, vol. 90, no. 6. American Physical Society (APS), Aug. 27, 2014. doi: 10.1103/physrevb.90.064111.  
  
D. Kamal, “Computable Bulk and Interfacial Electronic Structure Features as Proxies for Dielectric Breakdown of Polymers”, *ACS Applied Materials & Interfaces*, vol. 12, no. 33. American Chemical Society (ACS), pp. 37182–37187, Jul. 24, 2020. doi: 10.1021/acsami.0c09555.  
  
C. Kim, A. Chandrasekaran, T. D. Huan, D. Dasand R. Ramprasad, “Polymer Genome: A Data-Powered Polymer Informatics Platform for Property Predictions”, *The Journal of Physical Chemistry C*, vol. 122, no. 31. American Chemical Society (ACS), pp. 17575–17585, Jul. 13, 2018. doi: 10.1021/acs.jpcc.8b02913.  
  
C. Kim, G. Pilaniaand R. Ramprasad, “From Organized High-Throughput Data to Phenomenological Theory using Machine Learning: The Example of Dielectric Breakdown”, *Chemistry of Materials*, vol. 28, no. 5. American Chemical Society (ACS), pp. 1304–1311, Feb. 12, 2016. doi: 10.1021/acs.chemmater.5b04109.  
  
C. Kim, G. Pilaniaand R. Ramprasad, “Machine Learning Assisted Predictions of Intrinsic Dielectric Breakdown Strength of ABX3 Perovskites”, *The Journal of Physical Chemistry C*, vol. 120, no. 27. American Chemical Society (ACS), pp. 14575–14580, Jul. 01, 2016. doi: 10.1021/acs.jpcc.6b05068.  
  
C. Kim and R. Ramprasad, “Dielectric breakdown field of strained silicon under hydrostatic pressure”, *Applied Physics Letters*, vol. 111, no. 11. AIP Publishing, p. 112904, Sep. 11, 2017. doi: 10.1063/1.5003344.  
  
S. Krishnan, M. K. Mahapatra, P. Singhand R. Ramprasad, “First principles study of Cr poisoning in solid oxide fuel cell cathodes: Application to (La,Sr) CoO3”, *Computational Materials Science*, vol. 137. Elsevier BV, pp. 6–9, Sep. 2017. doi: 10.1016/j.commatsci.2017.04.020.  
  
A. Mannodi-Kanakkithodi, T. D. Huanand R. Ramprasad, “Mining Materials Design Rules from Data: The Example of Polymer Dielectrics”, *Chemistry of Materials*, vol. 29, no. 21. American Chemical Society (ACS), pp. 9001–9010, Oct. 18, 2017. doi: 10.1021/acs.chemmater.7b02027.  
  
A. Mannodi-Kanakkithodi, G. Pilania, T. D. Huan, T. Lookmanand R. Ramprasad, “Machine Learning Strategy for Accelerated Design of Polymer Dielectrics”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Feb. 15, 2016. doi: 10.1038/srep20952.  
  
A. Mannodi-Kanakkithodi, G. Pilaniaand R. Ramprasad, “Critical assessment of regression-based machine learning methods for polymer dielectrics”, *Computational Materials Science*, vol. 125. Elsevier BV, pp. 123–135, Dec. 2016. doi: 10.1016/j.commatsci.2016.08.039.  
  
A. Mannodi-Kanakkithodi, G. Pilaniaand R. Ramprasad, “Critical assessment of regression-based machine learning methods for polymer dielectrics”, *Computational Materials Science*, vol. 125. Elsevier BV, pp. 123–135, Dec. 2016. doi: 10.1016/j.commatsci.2016.08.039.  
  
A. Mannodi-Kanakkithodi, G. Pilania, R. Ramprasad, T. Lookmanand J. E. Gubernatis, “Multi-objective optimization techniques to design the Pareto front of organic dielectric polymers”, *Computational Materials Science*, vol. 125. Elsevier BV, pp. 92–99, Dec. 2016. doi: 10.1016/j.commatsci.2016.08.018.  
  
A. Mannodi-Kanakkithodi, G. Pilania, R. Ramprasad, T. Lookmanand J. E. Gubernatis, “Multi-objective optimization techniques to design the Pareto front of organic dielectric polymers”, *Computational Materials Science*, vol. 125. Elsevier BV, pp. 92–99, Dec. 2016. doi: 10.1016/j.commatsci.2016.08.018.  
  
A. Mannodi-Kanakkithodi, “Rational Co-Design of Polymer Dielectrics for Energy Storage”, *Advanced Materials*, vol. 28, no. 30. Wiley, pp. 6277–6291, May 11, 2016. doi: 10.1002/adma.201600377.  
  
A. Mannodi-Kanakkithodi, C. C. Wangand R. Ramprasad, “Compounds based on Group 14 elements: building blocks for advanced insulator dielectrics design”, *Journal of Materials Science*, vol. 50, no. 2. Springer Science and Business Media LLC, pp. 801–807, Oct. 10, 2014. doi: 10.1007/s10853-014-8640-2.  
  
R. Ma, “Rational design and synthesis of polythioureas as capacitor dielectrics”, *Journal of Materials Chemistry A*, vol. 3, no. 28. Royal Society of Chemistry (RSC), pp. 14845–14852, 2015. doi: 10.1039/c5ta01252j.  
  
M. Misra, A. Mannodi-Kanakkithodi, T. C. Chung, R. Ramprasadand S. K. Kumar, “Critical role of morphology on the dielectric constant of semicrystalline polyolefins”, *The Journal of Chemical Physics*, vol. 144, no. 23. AIP Publishing, p. 234905, Jun. 21, 2016. doi: 10.1063/1.4953182.  
  
G. Pilania, A. Mannodi-Kanakkithodi, B. P. Uberuaga, R. Ramprasad, J. E. Gubernatisand T. Lookman, “Machine learning bandgaps of double perovskites”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Jan. 19, 2016. doi: 10.1038/srep19375.  
  
H. N. Sharma, V. Sharma, T. Hamzehlouyan, W. Epling, A. B. Mhadeshwarand R. Ramprasad, “SO*x* Oxidation Kinetics on Pt(111) and Pd(111): First-Principles Computations Meet Microkinetic Modeling”, *The Journal of Physical Chemistry C*, vol. 118, no. 13. American Chemical Society (ACS), pp. 6934–6940, Mar. 21, 2014. doi: 10.1021/jp501538v.  
  
V. Sharma, A. McDannald, M. Staruch, R. Ramprasadand M. Jain, “Dopant-mediated structural and magnetic properties of TbMnO3”, *Applied Physics Letters*, vol. 107, no. 1. AIP Publishing, p. 012901, Jul. 06, 2015. doi: 10.1063/1.4926369.  
  
V. Sharma, G. Pilania, G. A. Rossetti, K. Slenesand R. Ramprasad, “Comprehensive examination of dopants and defects in BaTiOfrom first principles”, *Physical Review B*, vol. 87, no. 13. American Physical Society (APS), Apr. 30, 2013. doi: 10.1103/physrevb.87.134109.  
  
V. Sharma, “Rational design of all organic polymer dielectrics”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, Sep. 17, 2014. doi: 10.1038/ncomms5845.  
  
T. D. Huan, A. Mannodi-Kanakkithodi, C. Kim, V. Sharma, G. Pilaniaand R. Ramprasad, “A polymer dataset for accelerated property prediction and design”, *Scientific Data*, vol. 3, no. 1. Springer Science and Business Media LLC, Mar. 01, 2016. doi: 10.1038/sdata.2016.12.  
  
T. D. Huan and R. Ramprasad, “Polymer Structure Prediction from First Principles”, *The Journal of Physical Chemistry Letters*, vol. 11, no. 15. American Chemical Society (ACS), pp. 5823–5829, Jul. 01, 2020. doi: 10.1021/acs.jpclett.0c01553.  
  
G. M. Treich, “Optimization of Organotin Polymers for Dielectric Applications”, *ACS Applied Materials & Interfaces*, vol. 8, no. 33. American Chemical Society (ACS), pp. 21270–21277, Aug. 09, 2016. doi: 10.1021/acsami.6b04091.  
  
G. M. Treich, “A rational co-design approach to the creation of new dielectric polymers with high energy density”, *IEEE Transactions on Dielectrics and Electrical Insulation*, vol. 24, no. 2. Institute of Electrical and Electronics Engineers (IEEE), pp. 732–743, Apr. 2017. doi: 10.1109/tdei.2017.006329.  
  
Q. Zhu, V. Sharma, A. R. Oganovand R. Ramprasad, “Predicting polymeric crystal structures by evolutionary algorithms”, *The Journal of Chemical Physics*, vol. 141, no. 15. AIP Publishing, p. 154102, Oct. 21, 2014. doi: 10.1063/1.4897337.  
  
V. Sharma, M. K. Mahapatra, P. Singhand R. Ramprasad, “Cationic surface segregation in doped LaMnO3”, *Journal of Materials Science*, vol. 50, no. 8. Springer Science and Business Media LLC, pp. 3051–3056, Feb. 04, 2015. doi: 10.1007/s10853-015-8861-z.  
  
S. Krishnan, V. Sharma, P. Singhand R. Ramprasad, “Dopants in Lanthanum Manganite: Insights from First-Principles Chemical Space Exploration”, *The Journal of Physical Chemistry C*, vol. 120, no. 39. American Chemical Society (ACS), pp. 22126–22133, Sep. 22, 2016. doi: 10.1021/acs.jpcc.6b04524.  
  
L. Chen, R. Batra, R. Ranganathan, G. Sotzing, Y. Caoand R. Ramprasad, “Electronic Structure of Polymer Dielectrics: The Role of Chemical and Morphological Complexity”, *Chemistry of Materials*, vol. 30, no. 21. American Chemical Society (ACS), pp. 7699–7706, Oct. 17, 2018. doi: 10.1021/acs.chemmater.8b02997.  
  
M. Dutt, M. J. Nayhouse, O. Kuksenok, S. R. Littleand A. C. Balazs, “Interactions of End-functionalized Nanotubes with Lipid Vesicles: Spontaneous Insertion and Nanotube Self-Organization”, *Current Nanoscience*, vol. 7, no. 5. Bentham Science Publishers Ltd., pp. 699–715, Oct. 01, 2011. doi: 10.2174/157341311797483772.  
  
M. Dutt, O. Kuksenokand A. C. Balazs, “Nano-pipette directed transport of nanotube transmembrane channels and hybrid vesicles”, *Nanoscale*, vol. 5, no. 20. Royal Society of Chemistry (RSC), p. 9773, 2013. doi: 10.1039/c3nr33991b.  
  
R. Agarwal and D. R. Trinkle, “Light-element diffusion in Mg using first-principles calculations: Anisotropy and elastodiffusion”, *Physical Review B*, vol. 94, no. 5. American Physical Society (APS), Aug. 12, 2016. doi: 10.1103/physrevb.94.054106.  
  
R. Agarwal and D. R. Trinkle, “Exact Model of Vacancy-Mediated Solute Transport in Magnesium”, *Physical Review Letters*, vol. 118, no. 10. American Physical Society (APS), Mar. 07, 2017. doi: 10.1103/physrevlett.118.105901.  
  
R. Agarwal and D. R. Trinkle, “Ab initio magnesium-solute transport database using exact diffusion theory”, *Acta Materialia*, vol. 150. Elsevier BV, pp. 339–350, May 2018. doi: 10.1016/j.actamat.2018.03.025.  
  
M. R. Fellinger, L. G. Hector Jr.and D. R. Trinkle, “Effect of solutes on the lattice parameters and elastic stiffness coefficients of body-centered tetragonal Fe”, *Computational Materials Science*, vol. 152. Elsevier BV, pp. 308–323, Sep. 2018. doi: 10.1016/j.commatsci.2018.05.021.  
  
M. R. Fellinger, A. M. Z. Tan, L. G. Hectorand D. R. Trinkle, “Geometries of edge and mixed dislocations in bcc Fe from first-principles calculations”, *Physical Review Materials*, vol. 2, no. 11. American Physical Society (APS), Nov. 26, 2018. doi: 10.1103/physrevmaterials.2.113605.  
  
M. Ghazisaeidi and D. R. Trinkle, “Core structure of a screw dislocation in Ti from density functional theory and classical potentials”, *Acta Materialia*, vol. 60, no. 3. Elsevier BV, pp. 1287–1292, Feb. 2012. doi: 10.1016/j.actamat.2011.11.024.  
  
M. Ghazisaeidi and D. R. Trinkle, “Interaction of oxygen interstitials with lattice faults in Ti”, *Acta Materialia*, vol. 76. Elsevier BV, pp. 82–86, Sep. 2014. doi: 10.1016/j.actamat.2014.05.025.  
  
G. T. Hohensee, M. R. Fellinger, D. R. Trinkleand D. G. Cahill, “Thermal transport across high-pressure semiconductor-metal transition in Si and”, *Physical Review B*, vol. 91, no. 20. American Physical Society (APS), May 07, 2015. doi: 10.1103/physrevb.91.205104.  
  
H. Kim and D. R. Trinkle, “Effect of charge on point defect size misfits from ab initio: Aliovalently doped ”, *Computational Materials Science*, vol. 119. Elsevier BV, pp. 41–45, Jun. 2016. doi: 10.1016/j.commatsci.2016.02.040.  
  
H. Kim and D. R. Trinkle, “Mechanical properties and phase stability of monoborides using density functional theory calculations”, *Physical Review Materials*, vol. 1, no. 1. American Physical Society (APS), Jun. 26, 2017. doi: 10.1103/physrevmaterials.1.013601.  
  
B. Lee and D. R. Trinkle, “Energetics of Rutile TiO2 Vicinal Surfaces with ⟨001⟩ Steps from the Energy Density Method”, *The Journal of Physical Chemistry C*, vol. 119, no. 32. American Chemical Society (ACS), pp. 18203–18209, Aug. 05, 2015. doi: 10.1021/acs.jpcc.5b03623.  
  
T. Nogaret, W. A. Curtin, J. A. Yasi, L. G. Hector Jrand D. R. Trinkle, “Atomistic study of edge and screw 〈c+a〉 dislocations in magnesium”, *Acta Materialia*, vol. 58, no. 13. Elsevier BV, pp. 4332–4343, Aug. 2010. doi: 10.1016/j.actamat.2010.04.022.  
  
E. J. Schiavone and D. R. Trinkle, “*Ab initio*modeling of quasielastic neutron scattering of hydrogen pipe diffusion in palladium”, *Physical Review B*, vol. 94, no. 5. American Physical Society (APS), Aug. 26, 2016. doi: 10.1103/physrevb.94.054114.  
  
H. H. Wu and D. R. Trinkle, “Solute effect on oxygen diffusion in α-titanium”, *Journal of Applied Physics*, vol. 113, no. 22. AIP Publishing, p. 223504, Jun. 14, 2013. doi: 10.1063/1.4808283.  
  
J. A. Yasi, L. G. Hector Jr.and D. R. Trinkle, “First-principles data for solid-solution strengthening of magnesium: From geometry and chemistry to properties”, *Acta Materialia*, vol. 58, no. 17. Elsevier BV, pp. 5704–5713, Oct. 2010. doi: 10.1016/j.actamat.2010.06.045.  
  
J. A. Yasi, L. G. Hector Jr.and D. R. Trinkle, “Prediction of thermal cross-slip stress in magnesium alloys from direct first-principles data”, *Acta Materialia*, vol. 59, no. 14. Elsevier BV, pp. 5652–5660, Aug. 2011. doi: 10.1016/j.actamat.2011.05.040.  
  
J. A. Yasi, L. G. Hector Jr.and D. R. Trinkle, “Prediction of thermal cross-slip stress in magnesium alloys from a geometric interaction model”, *Acta Materialia*, vol. 60, no. 5. Elsevier BV, pp. 2350–2358, Mar. 2012. doi: 10.1016/j.actamat.2012.01.004.  
  
M. Yu and D. R. Trinkle, “Au/TiO2(110) Interfacial Reconstruction Stability from ab Initio”, *The Journal of Physical Chemistry C*, vol. 115, no. 36. American Chemical Society (ACS), pp. 17799–17805, Aug. 23, 2011. doi: 10.1021/jp2017133.  
  
U. Lienert, “High-energy diffraction microscopy at the advanced photon source”, *JOM*, vol. 63, no. 7. Springer Science and Business Media LLC, pp. 70–77, Jul. 2011. doi: 10.1007/s11837-011-0116-0.  
  
S. Maddali, S. Ta’asanand R. M. Suter, “Topology-faithful nonparametric estimation and tracking of bulk interface networks”, *Computational Materials Science*, vol. 125. Elsevier BV, pp. 328–340, Dec. 2016. doi: 10.1016/j.commatsci.2016.08.021.  
  
L. Barnard, N. Cunningham, G. R. Odette, I. Szlufarskaand D. Morgan, “Thermodynamic and kinetic modeling of oxide precipitation in nanostructured ferritic alloys”, *Acta Materialia*, vol. 91. Elsevier BV, pp. 340–354, Jun. 2015. doi: 10.1016/j.actamat.2015.03.014.  
  
L. Barnard, “Atomistic modeling of the order–disorder phase transformation in the Ni2Cr model alloy”, *Acta Materialia*, vol. 81. Elsevier BV, pp. 258–271, Dec. 2014. doi: 10.1016/j.actamat.2014.08.017.  
  
A. Bengtson, H. O. Nam, S. Saha, R. Sakidjaand D. Morgan, “First-principles molecular dynamics modeling of the LiCl–KCl molten salt system”, *Computational Materials Science*, vol. 83. Elsevier BV, pp. 362–370, Feb. 2014. doi: 10.1016/j.commatsci.2013.10.043.  
  
L. Jamison, M.-J. Zheng, S. Shannon, T. Allen, D. Morganand I. Szlufarska, “Experimental and ab initio study of enhanced resistance to amorphization of nanocrystalline silicon carbide under electron irradiation”, *Journal of Nuclear Materials*, vol. 445, no. 1–3. Elsevier BV, pp. 181–189, Feb. 2014. doi: 10.1016/j.jnucmat.2013.11.010.  
  
H. Jiang, C. Jiang, D. Morganand I. Szlufarska, “Accelerated atomistic simulation study on the stability and mobility of carbon tri-interstitial cluster in cubic SiC”, *Computational Materials Science*, vol. 89. Elsevier BV, pp. 182–188, Jun. 2014. doi: 10.1016/j.commatsci.2014.03.051.  
  
H. Kim, “Strain-compensated GaAs1−*y*P*y*/GaAs1−*z*Bi*z*/GaAs1−*y*P*y*quantum wells for laser applications”, *Semiconductor Science and Technology*, vol. 30, no. 9. IOP Publishing, p. 094011, Jul. 07, 2015. doi: 10.1088/0268-1242/30/9/094011.  
  
D. Lee, “Enhanced Oxygen Surface Exchange Kinetics and Stability on Epitaxial La0.8Sr0.2CoO3−δ Thin Films by La0.8Sr0.2MnO3−δ Decoration”, *The Journal of Physical Chemistry C*, vol. 118, no. 26. American Chemical Society (ACS), pp. 14326–14334, Jun. 18, 2014. doi: 10.1021/jp502192m.  
  
D. Lee, “Strontium influence on the oxygen electrocatalysis of La2−xSrxNiO4±δ (0.0 ≤ xSr ≤ 1.0) thin films”, *J. Mater. Chem. A*, vol. 2, no. 18. Royal Society of Chemistry (RSC), pp. 6480–6487, 2014. doi: 10.1039/c3ta14918h.  
  
Y.-L. Lee and D. Morgan, “*Ab initio*defect energetics of perovskite (001) surfaces for solid oxide fuel cells: A comparative study ofversusand”, *Physical Review B*, vol. 91, no. 19. American Physical Society (APS), May 21, 2015. doi: 10.1103/physrevb.91.195430.  
  
G. Luo, K. Forghani, T. F. Kuechand D. Morgan, “First-principles predictions of electronic properties of GaAs1-*x*-*y*P*y*Bi*x* and GaAs1-*x*-*y*P*y*Bi*x*-based heterojunctions”, *Applied Physics Letters*, vol. 109, no. 11. AIP Publishing, p. 112104, Sep. 12, 2016. doi: 10.1063/1.4962729.  
  
G. Luo, T. F. Kuechand D. Morgan, “Transition state redox during dynamical processes in semiconductors and insulators”, *NPG Asia Materials*, vol. 10, no. 4. Springer Science and Business Media LLC, pp. 45–51, Apr. 2018. doi: 10.1038/s41427-018-0010-0.  
  
G. Luo, S. Yang, G. R. Jenness, Z. Song, T. F. Kuechand D. Morgan, “Understanding and reducing deleterious defects in the metastable alloy GaAsBi”, *NPG Asia Materials*, vol. 9, no. 1. Springer Science and Business Media LLC, pp. e345–e345, Jan. 2017. doi: 10.1038/am.2016.201.  
  
G. Luo, “First-principles studies on molecular beam epitaxy growth of”, *Physical Review B*, vol. 92, no. 3. American Physical Society (APS), Jul. 14, 2015. doi: 10.1103/physrevb.92.035415.  
  
T. Mayeshiba and D. Morgan, “Strain effects on oxygen migration in perovskites”, *Physical Chemistry Chemical Physics*, vol. 17, no. 4. Royal Society of Chemistry (RSC), pp. 2715–2721, 2015. doi: 10.1039/c4cp05554c.  
  
H. O. Nam, A. Bengtson, K. Vörtler, S. Saha, R. Sakidjaand D. Morgan, “First-principles molecular dynamics modeling of the molten fluoride salt with Cr solute”, *Journal of Nuclear Materials*, vol. 449, no. 1–3. Elsevier BV, pp. 148–157, Jun. 2014. doi: 10.1016/j.jnucmat.2014.03.014.  
  
H. O. Nam and D. Morgan, “Redox condition in molten salts and solute behavior: A first-principles molecular dynamics study”, *Journal of Nuclear Materials*, vol. 465. Elsevier BV, pp. 224–235, Oct. 2015. doi: 10.1016/j.jnucmat.2015.05.028.  
  
I.-C. Tung, “Polarity-driven oxygen vacancy formation in ultrathin films on ”, *Physical Review Materials*, vol. 1, no. 5. American Physical Society (APS), Oct. 18, 2017. doi: 10.1103/physrevmaterials.1.053404.  
  
F. Wang, “Nanometre-thick single-crystalline nanosheets grown at the water–air interface”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Jan. 20, 2016. doi: 10.1038/ncomms10444.  
  
W. Xie, Y.-L. Lee, Y. Shao-Hornand D. Morgan, “Oxygen Point Defect Chemistry in Ruddlesden–Popper Oxides (La1–*x*Sr*x*)2MO4±δ (M = Co, Ni, Cu)”, *The Journal of Physical Chemistry Letters*, vol. 7, no. 10. American Chemical Society (ACS), pp. 1939–1944, May 11, 2016. doi: 10.1021/acs.jpclett.6b00739.  
  
W. Xie, C. A. Marianettiand D. Morgan, “Reply to “Comment on ‘Correlation and relativistic effects in U metal and U-Zr alloy: Validation of*ab initio*approaches’ ””, *Physical Review B*, vol. 93, no. 15. American Physical Society (APS), Apr. 25, 2016. doi: 10.1103/physrevb.93.157101.  
  
W. Xie, C. A. Marianettiand D. Morgan, “Response to letter “Electron correlation and relativity of the 5f electrons in the U Zr alloy system””, *Journal of Nuclear Materials*, vol. 476. Elsevier BV, pp. 110–112, Aug. 2016. doi: 10.1016/j.jnucmat.2016.04.043.  
  
W. Xie and D. Morgan, “CALPHAD modeling and ab initio calculations of the Np-U-Zr system”, *Computational Materials Science*, vol. 143. Elsevier BV, pp. 505–514, Feb. 2018. doi: 10.1016/j.commatsci.2017.11.042.  
  
W. Xie, W. Xiong, C. A. Marianettiand D. Morgan, “Correlation and relativistic effects in U metal and U-Zr alloy: Validation of*ab initio*approaches”, *Physical Review B*, vol. 88, no. 23. American Physical Society (APS), Dec. 26, 2013. doi: 10.1103/physrevb.88.235128.  
  
W. Xiong, W. Xieand D. Morgan, “Thermodynamic evaluation of the Np–Zr system using CALPHAD and ab initio methods”, *Journal of Nuclear Materials*, vol. 452, no. 1–3. Elsevier BV, pp. 569–577, Sep. 2014. doi: 10.1016/j.jnucmat.2014.06.023.  
  
W. Xiong, W. Xie, C. Shenand D. Morgan, “Thermodynamic modeling of the U–Zr system – A revisit”, *Journal of Nuclear Materials*, vol. 443, no. 1–3. Elsevier BV, pp. 331–341, Nov. 2013. doi: 10.1016/j.jnucmat.2013.07.034.  
  
S. Xu, S.-H. Shimand D. Morgan, “Origin of Fe 3+ in Fe-containing, Al-free mantle silicate perovskite”, *Earth and Planetary Science Letters*, vol. 409. Elsevier BV, pp. 319–328, Jan. 2015. doi: 10.1016/j.epsl.2014.11.006.  
  
M.-J. Zheng, I. Szlufarskaand D. Morgan, “Defect kinetics and resistance to amorphization in zirconium carbide”, *Journal of Nuclear Materials*, vol. 457. Elsevier BV, pp. 343–351, Feb. 2015. doi: 10.1016/j.jnucmat.2014.11.059.  
  
N. S. Bobbitt, N. Sai, N. Marom, M. Kimand J. R. Chelikowsky, “Real space pseudopotential calculations for size trends in Ga- and Al-doped zinc oxide nanocrystals with wurtzite and zincblende structures”, *The Journal of Chemical Physics*, vol. 141, no. 9. AIP Publishing, p. 094309, Sep. 07, 2014. doi: 10.1063/1.4893478.  
  
T.-L. Chan, A. J. Leeand J. R. Chelikowsky, “Ionization of a P-doped Si(111) nanofilm using two-dimensional periodic boundary conditions”, *Physical Review B*, vol. 91, no. 23. American Physical Society (APS), Jun. 25, 2015. doi: 10.1103/physrevb.91.235445.  
  
T.-L. Chan, A. J. Lee, A. W. K. Mokand J. R. Chelikowsky, “Interaction Range of P-Dopants in Si[110] Nanowires: Determining the Nondegenerate Limit”, *Nano Letters*, vol. 14, no. 11. American Chemical Society (ACS), pp. 6306–6313, Nov. 03, 2014. doi: 10.1021/nl502703z.  
  
T.-L. Chan, J. Souto-Casares, J. R. Chelikowsky, K.-M. Ho, C.-Z. Wangand S. B. Zhang, “The role of quantum confinement in the formation of Schottky barriers in Pb–Si interfaces”, *Solid State Communications*, vol. 217. Elsevier BV, pp. 43–46, Sep. 2015. doi: 10.1016/j.ssc.2015.05.014.  
  
J. R. Chelikowsky, D. Fan, A. J. Leeand Y. Sakai, “Simulating noncontact atomic force microscopy images”, *Physical Review Materials*, vol. 3, no. 11. American Physical Society (APS), Nov. 27, 2019. doi: 10.1103/physrevmaterials.3.110302.  
  
J.-H. Eom, T.-L. Chanand J. R. Chelikowsky, “Vacancies and B doping in Si nanocrystals”, *Solid State Communications*, vol. 150, no. 1–2. Elsevier BV, pp. 130–132, Jan. 2010. doi: 10.1016/j.ssc.2009.09.033.  
  
D. Fan, Y. Sakaiand J. R. Chelikowsky, “Real-space pseudopotential calculations for simulating noncontact atomic force microscopy images”, *Journal of Vacuum Science & Technology B*, vol. 36, no. 4. American Vacuum Society, pp. 04H102, Jul. 2018. doi: 10.1116/1.5029827.  
  
D. Fan, Y. Sakaiand J. R. Chelikowsky, “Discrimination of Bond Order in Organic Molecules Using Noncontact Atomic Force Microscopy”, *Nano Letters*, vol. 19, no. 8. American Chemical Society (ACS), pp. 5562–5567, Jul. 25, 2019. doi: 10.1021/acs.nanolett.9b02097.  
  
A. J. Lee, Y. Sakai, M. Kimand J. R. Chelikowsky, “Repulsive tip tilting as the dominant mechanism for hydrogen bond-like features in atomic force microscopy imaging”, *Applied Physics Letters*, vol. 108, no. 19. AIP Publishing, p. 193102, May 09, 2016. doi: 10.1063/1.4948600.  
  
J. E. Moussa, P. A. Schultzand J. R. Chelikowsky, “Analysis of the Heyd-Scuseria-Ernzerhof density functional parameter space”, *The Journal of Chemical Physics*, vol. 136, no. 20. AIP Publishing, p. 204117, May 28, 2012. doi: 10.1063/1.4722993.  
  
Y. Saad, J. R. Chelikowskyand S. M. Shontz, “Numerical Methods for Electronic Structure Calculations of Materials”, *SIAM Review*, vol. 52, no. 1. Society for Industrial & Applied Mathematics (SIAM), pp. 3–54, Jan. 2010. doi: 10.1137/060651653.  
  
Y. Sakai, A. J. Leeand J. R. Chelikowsky, “First-Principles Atomic Force Microscopy Image Simulations with Density Embedding Theory”, *Nano Letters*, vol. 16, no. 5. American Chemical Society (ACS), pp. 3242–3246, Apr. 11, 2016. doi: 10.1021/acs.nanolett.6b00741.  
  
M. Sakurai and J. R. Chelikowsky, “Real-space pseudopotential method for calculating magnetocrystalline anisotropy”, *Physical Review Materials*, vol. 2, no. 8. American Physical Society (APS), Aug. 24, 2018. doi: 10.1103/physrevmaterials.2.084411.  
  
M. Sakurai, J. R. Chelikowsky, S. G. Louieand S. Saito, “Quasiparticle energies and dielectric functions of diamond polytypes”, *Physical Review Materials*, vol. 1, no. 5. American Physical Society (APS), Oct. 25, 2017. doi: 10.1103/physrevmaterials.1.054603.  
  
M. Sakurai, J. Souto-Casaresand J. R. Chelikowsky, “Size dependence of structural stability and magnetization of nickel clusters from real-space pseudopotentials”, *Physical Review B*, vol. 94, no. 2. American Physical Society (APS), Jul. 29, 2016. doi: 10.1103/physrevb.94.024437.  
  
M. Sakurai, “Magnetocrystalline anisotropy in and compounds from first-principles real-space pseudopotentials calculations”, *Physical Review Materials*, vol. 2, no. 8. American Physical Society (APS), Aug. 24, 2018. doi: 10.1103/physrevmaterials.2.084410.  
  
M. Sakurai, X. Zhao, C.-Z. Wang, K.-M. Hoand J. R. Chelikowsky, “Influence of nitrogen dopants on the magnetization of clusters”, *Physical Review Materials*, vol. 2, no. 2. American Physical Society (APS), Feb. 06, 2018. doi: 10.1103/physrevmaterials.2.024401.  
  
J. Souto-Casares, M. Sakuraiand J. R. Chelikowsky, “Structural and magnetic properties of large cobalt clusters”, *Physical Review B*, vol. 93, no. 17. American Physical Society (APS), May 20, 2016. doi: 10.1103/physrevb.93.174418.  
  
A. J. Lee, Y. Sakaiand J. R. Chelikowsky, “Simulating contrast inversion in atomic force microscopy imaging with real-space pseudopotentials”, *Physical Review B*, vol. 95, no. 8. American Physical Society (APS), Feb. 01, 2017. doi: 10.1103/physrevb.95.081401.  
  
Y. Sakai, J. R. Chelikowskyand M. L. Cohen, “Magnetism in amorphous carbon”, *Physical Review Materials*, vol. 2, no. 7. American Physical Society (APS), Jul. 13, 2018. doi: 10.1103/physrevmaterials.2.074403.  
  
Y. Sakai, J. R. Chelikowskyand M. L. Cohen, “Simulating the effect of boron doping in superconducting carbon”, *Physical Review B*, vol. 97, no. 5. American Physical Society (APS), Feb. 01, 2018. doi: 10.1103/physrevb.97.054501.  
  
N. M. Bardhan, “Enhanced Cell Capture on Functionalized Graphene Oxide Nanosheets through Oxygen Clustering”, *ACS Nano*, vol. 11, no. 2. American Chemical Society (ACS), pp. 1548–1558, Jan. 24, 2017. doi: 10.1021/acsnano.6b06979.  
  
P. R. Brown, “Energy Level Modification in Lead Sulfide Quantum Dot Thin Films through Ligand Exchange”, *ACS Nano*, vol. 8, no. 6. American Chemical Society (ACS), pp. 5863–5872, Jun. 03, 2014. doi: 10.1021/nn500897c.  
  
J. Choi, L.-C. Linand J. C. Grossman, “Role of Structural Defects in the Water Adsorption Properties of MOF-801”, *The Journal of Physical Chemistry C*, vol. 122, no. 10. American Chemical Society (ACS), pp. 5545–5552, Feb. 21, 2018. doi: 10.1021/acs.jpcc.8b00014.  
  
D. Cohen-Tanugi, L.-C. Linand J. C. Grossman, “Multilayer Nanoporous Graphene Membranes for Water Desalination”, *Nano Letters*, vol. 16, no. 2. American Chemical Society (ACS), pp. 1027–1033, Jan. 25, 2016. doi: 10.1021/acs.nanolett.5b04089.  
  
E. Durgun, H. Manzano, P. V. Kumarand J. C. Grossman, “The Characterization, Stability, and Reactivity of Synthetic Calcium Silicate Surfaces from First Principles”, *The Journal of Physical Chemistry C*, vol. 118, no. 28. American Chemical Society (ACS), pp. 15214–15219, Jul. 03, 2014. doi: 10.1021/jp408325f.  
  
N. Ferralis, Y. Liu, K. D. Bake, A. E. Pomerantzand J. C. Grossman, “Direct correlation between aromatization of carbon-rich organic matter and its visible electronic absorption edge”, *Carbon*, vol. 88. Elsevier BV, pp. 139–147, Jul. 2015. doi: 10.1016/j.carbon.2015.02.075.  
  
R. H. Gilmore, “Epitaxial Dimers and Auger-Assisted Detrapping in PbS Quantum Dot Solids”, *Matter*, vol. 1, no. 1. Elsevier BV, pp. 250–265, Jul. 2019. doi: 10.1016/j.matt.2019.05.015.  
  
M. Gong, “Polychiral Semiconducting Carbon Nanotube–Fullerene Solar Cells”, *Nano Letters*, vol. 14, no. 9. American Chemical Society (ACS), pp. 5308–5314, Aug. 11, 2014. doi: 10.1021/nl5027452.  
  
G. W. Hwang, “Identifying and Eliminating Emissive Sub-bandgap States in Thin Films of PbS Nanocrystals”, *Advanced Materials*, vol. 27, no. 30. Wiley, pp. 4481–4486, Jul. 01, 2015. doi: 10.1002/adma.201501156.  
  
J. Y. Kim and J. C. Grossman, “High-Efficiency Thermoelectrics with Functionalized Graphene”, *Nano Letters*, vol. 15, no. 5. American Chemical Society (ACS), pp. 2830–2835, Apr. 13, 2015. doi: 10.1021/nl504257q.  
  
A. L. Koh, S. Wang, C. Ataca, J. C. Grossman, R. Sinclairand J. H. Warner, “Torsional Deformations in Subnanometer MoS Interconnecting Wires”, *Nano Letters*, vol. 16, no. 2. American Chemical Society (ACS), pp. 1210–1217, Jan. 19, 2016. doi: 10.1021/acs.nanolett.5b04507.  
  
P. V. Kumar, N. M. Bardhan, G.-Y. Chen, Z. Li, A. M. Belcherand J. C. Grossman, “New insights into the thermal reduction of graphene oxide: Impact of oxygen clustering”, *Carbon*, vol. 100. Elsevier BV, pp. 90–98, Apr. 2016. doi: 10.1016/j.carbon.2015.12.087.  
  
H. Li, D. A. Strubbeand J. C. Grossman, “Functionalized Graphene Superlattice as a Single-Sheet Solar Cell”, *Advanced Functional Materials*, vol. 25, no. 32. Wiley, pp. 5199–5205, Jul. 14, 2015. doi: 10.1002/adfm.201501906.  
  
H. Li, D. Zhitomirsky, S. Daveand J. C. Grossman, “Toward the Ultimate Limit of Connectivity in Quantum Dots with High Mobility and Clean Gaps”, *ACS Nano*, vol. 10, no. 1. American Chemical Society (ACS), pp. 606–614, Jan. 12, 2016. doi: 10.1021/acsnano.5b05626.  
  
H. Li, D. Zhitomirskyand J. C. Grossman, “Tunable and Energetically Robust PbS Nanoplatelets for Optoelectronic Applications”, *Chemistry of Materials*, vol. 28, no. 6. American Chemical Society (ACS), pp. 1888–1896, Mar. 09, 2016. doi: 10.1021/acs.chemmater.6b00167.  
  
L.-C. Lin, J. Choiand J. C. Grossman, “Two-dimensional covalent triazine framework as an ultrathin-film nanoporous membrane for desalination”, *Chemical Communications*, vol. 51, no. 80. Royal Society of Chemistry (RSC), pp. 14921–14924, 2015. doi: 10.1039/c5cc05969k.  
  
L.-C. Lin and J. C. Grossman, “Atomistic understandings of reduced graphene oxide as an ultrathin-film nanoporous membrane for separations”, *Nature Communications*, vol. 6, no. 1. Springer Science and Business Media LLC, Sep. 23, 2015. doi: 10.1038/ncomms9335.  
  
Y. Liu, N. Ferralis, L. T. Bryndziaand J. C. Grossman, “Genome-inspired molecular identification in organic matter via Raman spectroscopy”, *Carbon*, vol. 101. Elsevier BV, pp. 361–367, May 2016. doi: 10.1016/j.carbon.2016.02.017.  
  
Y. Liu and J. C. Grossman, “Accelerating the Design of Solar Thermal Fuel Materials through High Throughput Simulations”, *Nano Letters*, vol. 14, no. 12. American Chemical Society (ACS), pp. 7046–7050, Nov. 17, 2014. doi: 10.1021/nl5034073.  
  
Y. Liu, D. Kim, O. P. Morris, D. Zhitomirskyand J. C. Grossman, “Origins of the Stokes Shift in PbS Quantum Dots: Impact of Polydispersity, Ligands, and Defects”, *ACS Nano*, vol. 12, no. 3. American Chemical Society (ACS), pp. 2838–2845, Mar. 07, 2018. doi: 10.1021/acsnano.8b00132.  
  
Y. Liu, N. Peardand J. C. Grossman, “Bandlike Transport in PbS Quantum Dot Superlattices with Quantum Confinement”, *The Journal of Physical Chemistry Letters*, vol. 10, no. 13. American Chemical Society (ACS), pp. 3756–3762, Jun. 12, 2019. doi: 10.1021/acs.jpclett.9b01282.  
  
R. Raghunathan, E. Johlinand J. C. Grossman, “Grain Boundary Engineering for Improved Thin Silicon Photovoltaics”, *Nano Letters*, vol. 14, no. 9. American Chemical Society (ACS), pp. 4943–4950, Aug. 18, 2014. doi: 10.1021/nl501020q.  
  
F. Risplendi, M. Bernardi, G. Ciceroand J. C. Grossman, “Structure-property relations in amorphous carbon for photovoltaics”, *Applied Physics Letters*, vol. 105, no. 4. AIP Publishing, p. 043903, Jul. 28, 2014. doi: 10.1063/1.4891498.  
  
F. Risplendi, G. Ciceroand J. C. Grossman, “Nanostructured Bulk-Heterojunction Solar Cells Based on Amorphous Carbon”, *ACS Energy Letters*, vol. 2, no. 4. American Chemical Society (ACS), pp. 882–888, Mar. 20, 2017. doi: 10.1021/acsenergylett.7b00166.  
  
D. A. Strubbe, E. C. Johlin, T. R. Kirkpatrick, T. Buonassisiand J. C. Grossman, “Stress effects on the Raman spectrum of an amorphous material: Theory and experiment on-Si:H”, *Physical Review B*, vol. 92, no. 24. American Physical Society (APS), Dec. 18, 2015. doi: 10.1103/physrevb.92.241202.  
  
T. Xie, A. France-Lanord, Y. Wang, Y. Shao-Hornand J. C. Grossman, “Graph dynamical networks for unsupervised learning of atomic scale dynamics in materials”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Jun. 17, 2019. doi: 10.1038/s41467-019-10663-6.  
  
T. Xie and J. C. Grossman, “Hierarchical visualization of materials space with graph convolutional neural networks”, *The Journal of Chemical Physics*, vol. 149, no. 17. AIP Publishing, p. 174111, Nov. 07, 2018. doi: 10.1063/1.5047803.  
  
T. Xie and J. C. Grossman, “Crystal Graph Convolutional Neural Networks for an Accurate and Interpretable Prediction of Material Properties”, *Physical Review Letters*, vol. 120, no. 14. American Physical Society (APS), Apr. 06, 2018. doi: 10.1103/physrevlett.120.145301.  
  
S. Yang, “Self-Driven Photodetector and Ambipolar Transistor in Atomically Thin GaTe-MoS2 p–n vdW Heterostructure”, *ACS Applied Materials & Interfaces*, vol. 8, no. 4. American Chemical Society (ACS), pp. 2533–2539, Jan. 21, 2016. doi: 10.1021/acsami.5b10001.  
  
A. Bajpai, “The effect of centred versus offset interpenetration on C2H2 sorption in hybrid ultramicroporous materials”, *Chem. Commun.*, vol. 53, no. 84. Royal Society of Chemistry (RSC), pp. 11592–11595, 2017. doi: 10.1039/c7cc05882a.  
  
A. Bajpai, “Towards an understanding of the propensity for crystalline hydrate formation by molecular compounds”, *IUCrJ*, vol. 3, no. 6. International Union of Crystallography (IUCr), pp. 430–439, Oct. 18, 2016. doi: 10.1107/s2052252516015633.  
  
K. Chen, “Tuning Pore Size in Square‐Lattice Coordination Networks for Size‐Selective Sieving of CO 2”, *Angewandte Chemie International Edition*, vol. 55, no. 35. Wiley, pp. 10268–10272, Jul. 21, 2016. doi: 10.1002/anie.201603934.  
  
K.-J. Chen, “Benchmark C2H2/CO2 and CO2/C2H2 Separation by Two Closely Related Hybrid Ultramicroporous Materials”, *Chem*, vol. 1, no. 5. Elsevier BV, pp. 753–765, Nov. 2016. doi: 10.1016/j.chempr.2016.10.009.  
  
K. Chen, “Efficient CO 2 Removal for Ultra **‐** Pure CO Production by Two Hybrid Ultramicroporous Materials”, *Angewandte Chemie International Edition*, vol. 57, no. 13. Wiley, pp. 3332–3336, Feb. 22, 2018. doi: 10.1002/anie.201706090.  
  
C. R. Cioce, K. McLaughlin, J. L. Belofand B. Space, “A Polarizable and Transferable PHAST N2 Potential for Use in Materials Simulation”, *Journal of Chemical Theory and Computation*, vol. 9, no. 12. American Chemical Society (ACS), pp. 5550–5557, Nov. 22, 2013. doi: 10.1021/ct400526a.  
  
S. K. Elsaidi, “Crystal Engineering of a 4,6-c fsc Platform That Can Serve as a Carbon Dioxide Single-Molecule Trap”, *Crystal Growth & Design*, vol. 16, no. 2. American Chemical Society (ACS), pp. 1071–1080, Jan. 06, 2016. doi: 10.1021/acs.cgd.5b01632.  
  
S. K. Elsaidi, “Hydrophobic pillared square grids for selective removal of CO2 from simulated flue gas”, *Chemical Communications*, vol. 51, no. 85. Royal Society of Chemistry (RSC), pp. 15530–15533, 2015. doi: 10.1039/c5cc06577a.  
  
S. K. Elsaidi, “Effect of ring rotation upon gas adsorption in SIFSIX-3-M (M = Fe, Ni) pillared square grid networks”, *Chemical Science*, vol. 8, no. 3. Royal Society of Chemistry (RSC), pp. 2373–2380, 2017. doi: 10.1039/c6sc05012c.  
  
S. K. Elsaidi, “Putting the Squeeze on CH4 and CO2 through Control over Interpenetration in Diamondoid Nets”, *Journal of the American Chemical Society*, vol. 136, no. 13. American Chemical Society (ACS), pp. 5072–5077, Mar. 24, 2014. doi: 10.1021/ja500005k.  
  
K. A. Forrest, D. M. Franz, T. Phamand B. Space, “Investigating C2H2 Sorption in α-[M3(O2CH)6] (M = Mg, Mn) Through Theoretical Studies”, *Crystal Growth & Design*, vol. 18, no. 9. American Chemical Society (ACS), pp. 5342–5352, Aug. 06, 2018. doi: 10.1021/acs.cgd.8b00770.  
  
K. A. Forrest, “Investigating CO2 Sorption in SIFSIX-3-M (M = Fe, Co, Ni, Cu, Zn) through Computational Studies”, *Crystal Growth & Design*, vol. 19, no. 7. American Chemical Society (ACS), pp. 3732–3743, May 31, 2019. doi: 10.1021/acs.cgd.9b00086.  
  
K. A. Forrest, “Inelastic Neutron Scattering and Theoretical Studies of H2 Sorption in a Dy(III)-Based Phosphine Coordination Material”, *Chemistry of Materials*, vol. 27, no. 22. American Chemical Society (ACS), pp. 7619–7626, Nov. 04, 2015. doi: 10.1021/acs.chemmater.5b02747.  
  
K. A. Forrest, “Investigating H2 Sorption in a Fluorinated Metal–Organic Framework with Small Pores Through Molecular Simulation and Inelastic Neutron Scattering”, *Langmuir*, vol. 31, no. 26. American Chemical Society (ACS), pp. 7328–7336, Jun. 24, 2015. doi: 10.1021/acs.langmuir.5b01664.  
  
K. A. Forrest, “Computational Studies of CO2Sorption and Separation in an Ultramicroporous Metal–Organic Material”, *The Journal of Physical Chemistry C*, vol. 117, no. 34. American Chemical Society (ACS), pp. 17687–17698, Aug. 14, 2013. doi: 10.1021/jp405781c.  
  
K. A. Forrest, “Simulation of the Mechanism of Gas Sorption in a Metal–Organic Framework with Open Metal Sites: Molecular Hydrogen in PCN-61”, *The Journal of Physical Chemistry C*, vol. 116, no. 29. American Chemical Society (ACS), pp. 15538–15549, Jul. 12, 2012. doi: 10.1021/jp306084t.  
  
K. A. Forrest, “Examining the Effects of Different Ring Configurations and Equatorial Fluorine Atom Positions on CO2Sorption in [Cu(bpy)2SiF6]”, *Crystal Growth & Design*, vol. 13, no. 10. American Chemical Society (ACS), pp. 4542–4548, Sep. 10, 2013. doi: 10.1021/cg401034s.  
  
K. A. Forrest, T. Phamand B. Space, “Investigating gas sorption in an **rht**-metal–organic framework with 1,2,3-triazole groups”, *Physical Chemistry Chemical Physics*, vol. 19, no. 43. Royal Society of Chemistry (RSC), pp. 29204–29221, 2017. doi: 10.1039/c7cp06128e.  
  
K. A. Forrest, T. Phamand B. Space, “Comparing the mechanism and energetics of CO2 sorption in the SIFSIX series”, *CrystEngComm*, vol. 19, no. 24. Royal Society of Chemistry (RSC), pp. 3338–3347, 2017. doi: 10.1039/c7ce00594f.  
  
D. M. Franz, Z. E. Dyott, K. A. Forrest, A. Hogan, T. Phamand B. Space, “Simulations of hydrogen, carbon dioxide, and small hydrocarbon sorption in a nitrogen-rich *rht*-metal–organic framework”, *Physical Chemistry Chemical Physics*, vol. 20, no. 3. Royal Society of Chemistry (RSC), pp. 1761–1777, 2018. doi: 10.1039/c7cp06885a.  
  
D. Franz, K. A. Forrest, T. Phamand B. Space, “Accurate H2 Sorption Modeling in the *rht*-MOF NOTT-112 Using Explicit Polarization”, *Crystal Growth & Design*, vol. 16, no. 10. American Chemical Society (ACS), pp. 6024–6032, Sep. 01, 2016. doi: 10.1021/acs.cgd.6b01058.  
  
L. Han, “Molecular Sieving and Direct Visualization of CO2 in Binding Pockets of an Ultramicroporous Lanthanide Metal–Organic Framework Platform”, *ACS Applied Materials & Interfaces*, vol. 11, no. 26. American Chemical Society (ACS), pp. 23192–23197, Jun. 11, 2019. doi: 10.1021/acsami.9b04619.  
  
H. He, “A Stable Metal–Organic Framework Featuring a Local Buffer Environment for Carbon Dioxide Fixation”, *Angewandte Chemie International Edition*, vol. 57, no. 17. Wiley, pp. 4657–4662, Mar. 15, 2018. doi: 10.1002/anie.201801122.  
  
B. Li, “Introduction of π-Complexation into Porous Aromatic Framework for Highly Selective Adsorption of Ethylene over Ethane”, *Journal of the American Chemical Society*, vol. 136, no. 24. American Chemical Society (ACS), pp. 8654–8660, Jun. 05, 2014. doi: 10.1021/ja502119z.  
  
D. G. Madden, “Highly selective CO2 removal for one-step liquefied natural gas processing by physisorbents”, *Chemical Communications*, vol. 55, no. 22. Royal Society of Chemistry (RSC), pp. 3219–3222, 2019. doi: 10.1039/c9cc00626e.  
  
K. McLaughlin, C. R. Cioce, J. L. Belofand B. Space, “A molecular H2 potential for heterogeneous simulations including polarization and many-body van der Waals interactions”, *The Journal of Chemical Physics*, vol. 136, no. 19. AIP Publishing, p. 194302, May 21, 2012. doi: 10.1063/1.4717705.  
  
K. McLaughlin, C. R. Cioce, T. Pham, J. L. Belofand B. Space, “Efficient calculation of many-body induced electrostatics in molecular systems”, *The Journal of Chemical Physics*, vol. 139, no. 18. AIP Publishing, p. 184112, Nov. 14, 2013. doi: 10.1063/1.4829144.  
  
M. H. Mohamed, “Highly Selective CO2 Uptake in Uninodal 6-Connected “mmo” Nets Based upon MO42– (M = Cr, Mo) Pillars”, *Journal of the American Chemical Society*, vol. 134, no. 48. American Chemical Society (ACS), pp. 19556–19559, Nov. 21, 2012. doi: 10.1021/ja309452y.  
  
A. L. Mullen, T. Pham, K. A. Forrest, C. R. Cioce, K. McLaughlinand B. Space, “A Polarizable and Transferable PHAST CO2 Potential for Materials Simulation”, *Journal of Chemical Theory and Computation*, vol. 9, no. 12. American Chemical Society (ACS), pp. 5421–5429, Nov. 22, 2013. doi: 10.1021/ct400549q.  
  
Z. Niu, “A Metal–Organic Framework Based Methane Nano‐trap for the Capture of Coal‐Mine Methane”, *Angewandte Chemie International Edition*, vol. 58, no. 30. Wiley, pp. 10138–10141, May 22, 2019. doi: 10.1002/anie.201904507.  
  
P. Nugent, “Porous materials with optimal adsorption thermodynamics and kinetics for CO2 separation”, *Nature*, vol. 495, no. 7439. Springer Science and Business Media LLC, pp. 80–84, Feb. 27, 2013. doi: 10.1038/nature11893.  
  
P. S. Nugent, “A Robust Molecular Porous Material with High CO2 Uptake and Selectivity”, *Journal of the American Chemical Society*, vol. 135, no. 30. American Chemical Society (ACS), pp. 10950–10953, Jul. 22, 2013. doi: 10.1021/ja4054948.  
  
P. Nugent, “Enhancement of CO2 selectivity in a pillared pcu MOM platform through pillar substitution”, *Chemical Communications*, vol. 49, no. 16. Royal Society of Chemistry (RSC), p. 1606, 2013. doi: 10.1039/c3cc37695h.  
  
D. O’Nolan, “Impact of partial interpenetration in a hybrid ultramicroporous material on C2H2/C2H4 separation performance”, *Chemical Communications*, vol. 54, no. 28. Royal Society of Chemistry (RSC), pp. 3488–3491, 2018. doi: 10.1039/c8cc01627e.  
  
Y. Peng, “Robust Microporous Metal–Organic Frameworks for Highly Efficient and Simultaneous Removal of Propyne and Propadiene from Propylene”, *Angewandte Chemie International Edition*, vol. 58, no. 30. Wiley, pp. 10209–10214, Jun. 24, 2019. doi: 10.1002/anie.201904312.  
  
Y.-L. Peng, “Robust Ultramicroporous Metal-Organic Frameworks with Benchmark Affinity for Acetylene”, *Angewandte Chemie International Edition*, vol. 57, no. 34. Wiley, pp. 10971–10975, Jul. 20, 2018. doi: 10.1002/anie.201806732.  
  
T. Pham, K. A. Forrest, K.-J. Chen, A. Kumar, M. J. Zaworotkoand B. Space, “Theoretical Investigations of CO2 and H2 Sorption in Robust Molecular Porous Materials”, *Langmuir*, vol. 32, no. 44. American Chemical Society (ACS), pp. 11492–11505, Oct. 24, 2016. doi: 10.1021/acs.langmuir.6b03161.  
  
T. Pham, “Investigating the Gas Sorption Mechanism in an *rht*-Metal–Organic Framework through Computational Studies”, *The Journal of Physical Chemistry C*, vol. 118, no. 1. American Chemical Society (ACS), pp. 439–456, Dec. 27, 2013. doi: 10.1021/jp409950r.  
  
T. Pham, K. A. Forrest, J. Eckertand B. Space, “Dramatic Effect of the Electrostatic Parameters on H2 Sorption in an M-MOF-74 Analogue”, *Crystal Growth & Design*, vol. 16, no. 2. American Chemical Society (ACS), pp. 867–874, Dec. 30, 2015. doi: 10.1021/acs.cgd.5b01434.  
  
T. Pham, K. A. Forrest, E. H. L. Falcão, J. Eckertand B. Space, “Exceptional H2 sorption characteristics in a Mg2+-based metal–organic framework with small pores: insights from experimental and theoretical studies”, *Physical Chemistry Chemical Physics*, vol. 18, no. 3. Royal Society of Chemistry (RSC), pp. 1786–1796, 2016. doi: 10.1039/c5cp05906b.  
  
T. Pham, K. A. Forrest, D. M. Franz, Z. Guo, B. Chenand B. Space, “Predictive models of gas sorption in a metal–organic framework with open-metal sites and small pore sizes”, *Physical Chemistry Chemical Physics*, vol. 19, no. 28. Royal Society of Chemistry (RSC), pp. 18587–18602, 2017. doi: 10.1039/c7cp02767b.  
  
T. Pham, K. A. Forrest, D. M. Franzand B. Space, “Experimental and theoretical investigations of the gas adsorption sites in rht-metal–organic frameworks”, *CrystEngComm*, vol. 19, no. 32. Royal Society of Chemistry (RSC), pp. 4646–4665, 2017. doi: 10.1039/c7ce01032j.  
  
T. Pham, K. A. Forrest, H. Furukawa, J. Eckertand B. Space, “Hydrogen Adsorption in a Zeolitic Imidazolate Framework with lta Topology”, *The Journal of Physical Chemistry C*, vol. 122, no. 27. American Chemical Society (ACS), pp. 15435–15445, Jun. 14, 2018. doi: 10.1021/acs.jpcc.8b04027.  
  
T. Pham, “High H2 Sorption Energetics in Zeolitic Imidazolate Frameworks”, *The Journal of Physical Chemistry C*, vol. 121, no. 3. American Chemical Society (ACS), pp. 1723–1733, Jan. 12, 2017. doi: 10.1021/acs.jpcc.6b11466.  
  
T. Pham, K. A. Forrest, W.-Y. Gao, S. Maand B. Space, “Theoretical Insights into the Tuning of Metal Binding Sites of Paddlewheels in*rht*-Metal-Organic Frameworks”, *ChemPhysChem*, vol. 16, no. 15. Wiley, pp. 3170–3179, Aug. 25, 2015. doi: 10.1002/cphc.201500504.  
  
T. Pham, “Theoretical Investigations of CO2 and H2 Sorption in an Interpenetrated Square-Pillared Metal–Organic Material”, *The Journal of Physical Chemistry C*, vol. 117, no. 19. American Chemical Society (ACS), pp. 9970–9982, May 06, 2013. doi: 10.1021/jp402764s.  
  
T. Pham, “The rotational dynamics of H2 adsorbed in covalent organic frameworks”, *Physical Chemistry Chemical Physics*, vol. 19, no. 20. Royal Society of Chemistry (RSC), pp. 13075–13082, 2017. doi: 10.1039/c7cp00924k.  
  
T. Pham, “Understanding Hydrogen Sorption in a Metal–Organic Framework with Open-Metal Sites and Amide Functional Groups”, *The Journal of Physical Chemistry C*, vol. 117, no. 18. American Chemical Society (ACS), pp. 9340–9354, Apr. 25, 2013. doi: 10.1021/jp402304a.  
  
T. Pham, K. A. Forrestand B. Space, “An unusual H2 sorption mechanism in PCN-14: insights from molecular simulation”, *Physical Chemistry Chemical Physics*, vol. 18, no. 31. Royal Society of Chemistry (RSC), pp. 21421–21430, 2016. doi: 10.1039/c6cp02650h.  
  
T. Pham, K. A. Forrest, B. Spaceand J. Eckert, “Dynamics of H2 adsorbed in porous materials as revealed by computational analysis of inelastic neutron scattering spectra”, *Physical Chemistry Chemical Physics*, vol. 18, no. 26. Royal Society of Chemistry (RSC), pp. 17141–17158, 2016. doi: 10.1039/c6cp01863g.  
  
T. Pham, “Theoretical Investigations of CO2 and CH4 Sorption in an Interpenetrated Diamondoid Metal–Organic Material”, *Langmuir*, vol. 30, no. 22. American Chemical Society (ACS), pp. 6454–6462, May 29, 2014. doi: 10.1021/la500967w.  
  
H. S. Scott, “Novel mode of 2-fold interpenetration observed in a primitive cubic network of formula [Ni(1,2-bis(4-pyridyl)acetylene)2(Cr2O7)]n”, *Chemical Communications*, vol. 51, no. 80. Royal Society of Chemistry (RSC), pp. 14832–14835, 2015. doi: 10.1039/c5cc05866j.  
  
H. S. Scott, “Crystal engineering of a family of hybrid ultramicroporous materials based upon interpenetration and dichromate linkers”, *Chemical Science*, vol. 7, no. 8. Royal Society of Chemistry (RSC), pp. 5470–5476, 2016. doi: 10.1039/c6sc01385f.  
  
M. Shivanna, “Readily accessible shape-memory effect in a porous interpenetrated coordination network”, *Science Advances*, vol. 4, no. 4. American Association for the Advancement of Science (AAAS), Apr. 06, 2018. doi: 10.1126/sciadv.aaq1636.  
  
S. Suepaul, K. A. Forrest, T. Phamand B. Space, “Investigating the Effects of Linker Extension on H2 Sorption in the rht-Metal–Organic Framework NU-111 by Molecular Simulations”, *Crystal Growth & Design*, vol. 18, no. 12. American Chemical Society (ACS), pp. 7599–7610, Oct. 24, 2018. doi: 10.1021/acs.cgd.8b01398.  
  
Q. Yang, “Reversible Switching between Highly Porous and Nonporous Phases of an Interpenetrated Diamondoid Coordination Network That Exhibits Gate‐Opening at Methane Storage Pressures”, *Angewandte Chemie International Edition*, vol. 57, no. 20. Wiley, pp. 5684–5689, Apr. 17, 2018. doi: 10.1002/anie.201800820.  
  
M. Zhang, “Fine Tuning of MOF-505 Analogues To Reduce Low-Pressure Methane Uptake and Enhance Methane Working Capacity”, *Angewandte Chemie International Edition*, vol. 56, no. 38. Wiley, pp. 11426–11430, Aug. 09, 2017. doi: 10.1002/anie.201704974.  
  
W.-Y. Gao, “Remote Stabilization of Copper Paddlewheel Based Molecular Building Blocks in Metal–Organic Frameworks”, *Chemistry of Materials*, vol. 27, no. 6. American Chemical Society (ACS), pp. 2144–2151, Mar. 13, 2015. doi: 10.1021/acs.chemmater.5b00084.  
  
W.-Y. Gao, “The local electric field favours more than exposed nitrogen atoms on CO2 capture: a case study on the **rht**-type MOF platform”, *Chemical Communications*, vol. 51, no. 47. Royal Society of Chemistry (RSC), pp. 9636–9639, 2015. doi: 10.1039/c5cc02573g.  
  
T. Pham, K. A. Forrest, R. Banerjee, G. Orcajo, J. Eckertand B. Space, “Understanding the H2 Sorption Trends in the M-MOF-74 Series (M = Mg, Ni, Co, Zn)”, *The Journal of Physical Chemistry C*, vol. 119, no. 2. American Chemical Society (ACS), pp. 1078–1090, Dec. 30, 2014. doi: 10.1021/jp510253m.  
  
T. Pham, “Understanding Hydrogen Sorption in In-*soc*-MOF: A Charged Metal-Organic Framework with Open-Metal Sites, Narrow Channels, and Counterions”, *Crystal Growth & Design*, vol. 15, no. 3. American Chemical Society (ACS), pp. 1460–1471, Feb. 06, 2015. doi: 10.1021/cg5018104.  
  
T. Pham, K. A. Forrest, K. McDonaldand B. Space, “Modeling PCN-61 and PCN-66: Isostructural *rht*-Metal–Organic Frameworks with Distinct CO2 Sorption Mechanisms”, *Crystal Growth & Design*, vol. 14, no. 11. American Chemical Society (ACS), pp. 5599–5607, Oct. 09, 2014. doi: 10.1021/cg500860t.  
  
T. Pham, K. A. Forrest, K. McLaughlin, J. Eckertand B. Space, “Capturing the H2–Metal Interaction in Mg-MOF-74 Using Classical Polarization”, *The Journal of Physical Chemistry C*, vol. 118, no. 39. American Chemical Society (ACS), pp. 22683–22690, Sep. 17, 2014. doi: 10.1021/jp508249c.  
  
L. Basurto, F. Amerikheirabadi, R. Zopeand T. Baruah, “The electronic structure and charge transfer excited states of the endohedral trimetallic nitride C80 (Ih) fullerenes–Zn-tetraphenyl porphyrin dyads”, *Physical Chemistry Chemical Physics*, vol. 17, no. 8. Royal Society of Chemistry (RSC), pp. 5832–5839, 2015. doi: 10.1039/c4cp04583a.  
  
M. Olguin, L. Basurto, R. R. Zopeand T. Baruah, “The effect of structural changes on charge transfer states in a light-harvesting carotenoid-diaryl-porphyrin-C60 molecular triad”, *The Journal of Chemical Physics*, vol. 140, no. 20. AIP Publishing, p. 204309, May 28, 2014. doi: 10.1063/1.4876075.  
  
C. M. Ramos-Castillo, J. U. Reveles, R. R. Zopeand R. de Coss, “Palladium Clusters Supported on Graphene Monovacancies for Hydrogen Storage”, *The Journal of Physical Chemistry C*, vol. 119, no. 15. American Chemical Society (ACS), pp. 8402–8409, Apr. 02, 2015. doi: 10.1021/acs.jpcc.5b02358.  
  
A. Y. Zamora, J. U. Reveles, R. Mejia-Olvera, T. Baruahand R. R. Zope, “FeO2/MgO(1 0 0) supported cluster: Computational pursual for a low-cost and low-temperature CO nanocatalyst”, *Chemical Physics Letters*, vol. 612. Elsevier BV, pp. 117–123, Sep. 2014. doi: 10.1016/j.cplett.2014.07.061.  
  
L. Xiong, X. Chen, N. Zhang, D. L. McDowelland Y. Chen, “Prediction of phonon properties of 1D polyatomic systems using concurrent atomistic–continuum simulation”, *Archive of Applied Mechanics*, vol. 84, no. 9–11. Springer Science and Business Media LLC, pp. 1665–1675, Jul. 03, 2014. doi: 10.1007/s00419-014-0880-8.  
  
L. Xiong and Y. Chen, “Coarse-grained atomistic modeling and simulation of inelastic material behavior”, *Acta Mechanica Solida Sinica*, vol. 25, no. 3. Springer Science and Business Media LLC, pp. 244–261, Jun. 2012. doi: 10.1016/s0894-9166(12)60023-8.  
  
B. K. Nikolić, K. K. Saha, T. Markussenand K. S. Thygesen, “First-principles quantum transport modeling of thermoelectricity in single-molecule nanojunctions with graphene nanoribbon electrodes”, *Journal of Computational Electronics*, vol. 11, no. 1. Springer Science and Business Media LLC, pp. 78–92, Jan. 31, 2012. doi: 10.1007/s10825-012-0386-y.  
  
K. K. Saha, M. Drndićand B. K. Nikolić, “DNA Base-Specific Modulation of Microampere Transverse Edge Currents through a Metallic Graphene Nanoribbon with a Nanopore”, *Nano Letters*, vol. 12, no. 1. American Chemical Society (ACS), pp. 50–55, Dec. 15, 2011. doi: 10.1021/nl202870y.  
  
N. J. Borys, “Anomalous Above-Gap Photoexcitations and Optical Signatures of Localized Charge Puddles in Monolayer Molybdenum Disulfide”, *ACS Nano*, vol. 11, no. 2. American Chemical Society (ACS), pp. 2115–2123, Feb. 01, 2017. doi: 10.1021/acsnano.6b08278.  
  
B. Deng, “Efficient electrical control of thin-film black phosphorus bandgap”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Apr. 19, 2017. doi: 10.1038/ncomms14474.  
  
R. Fei, A. Faghaninia, R. Soklaski, J.-A. Yan, C. Loand L. Yang, “Enhanced Thermoelectric Efficiency via Orthogonal Electrical and Thermal Conductances in Phosphorene”, *Nano Letters*, vol. 14, no. 11. American Chemical Society (ACS), pp. 6393–6399, Sep. 30, 2014. doi: 10.1021/nl502865s.  
  
R. Fei, W. Kangand L. Yang, “Ferroelectricity and Phase Transitions in Monolayer Group-IV Monochalcogenides”, *Physical Review Letters*, vol. 117, no. 9. American Physical Society (APS), Aug. 23, 2016. doi: 10.1103/physrevlett.117.097601.  
  
R. Fei, V. Tranand L. Yang, “Topologically protected Dirac cones in compressed bulk black phosphorus”, *Physical Review B*, vol. 91, no. 19. American Physical Society (APS), May 27, 2015. doi: 10.1103/physrevb.91.195319.  
  
R. Fei and L. Yang, “Strain-Engineering the Anisotropic Electrical Conductance of Few-Layer Black Phosphorus”, *Nano Letters*, vol. 14, no. 5. American Chemical Society (ACS), pp. 2884–2889, May 02, 2014. doi: 10.1021/nl500935z.  
  
R. Fei and L. Yang, “Lattice vibrational modes and Raman scattering spectra of strained phosphorene”, *Applied Physics Letters*, vol. 105, no. 8. AIP Publishing, p. 083120, Aug. 25, 2014. doi: 10.1063/1.4894273.  
  
A. K. Gangopadhyay, “Anomalous thermal contraction of the first coordination shell in metallic alloy liquids”, *The Journal of Chemical Physics*, vol. 140, no. 4. AIP Publishing, p. 044505, Jan. 28, 2014. doi: 10.1063/1.4861666.  
  
S. Gao, Y. Liang, C. D. Spataruand L. Yang, “Dynamical Excitonic Effects in Doped Two-Dimensional Semiconductors”, *Nano Letters*, vol. 16, no. 9. American Chemical Society (ACS), pp. 5568–5573, Aug. 04, 2016. doi: 10.1021/acs.nanolett.6b02118.  
  
S. Gao and L. Yang, “Renormalization of the quasiparticle band gap in doped two-dimensional materials from many-body calculations”, *Physical Review B*, vol. 96, no. 15. American Physical Society (APS), Oct. 05, 2017. doi: 10.1103/physrevb.96.155410.  
  
S. Gao and L. Yang, “Edge-insensitive magnetism and half metallicity in graphene nanoribbons”, *Journal of Physics: Condensed Matter*, vol. 30, no. 48. IOP Publishing, pp. 48LT01, Nov. 08, 2018. doi: 10.1088/1361-648x/aae9cb.  
  
J. Guan, W. Song, L. Yangand D. Tománek, “Strain-controlled fundamental gap and structure of bulk black phosphorus”, *Physical Review B*, vol. 94, no. 4. American Physical Society (APS), Jul. 11, 2016. doi: 10.1103/physrevb.94.045414.  
  
R. W. Havener, Y. Liang, L. Brown, L. Yangand J. Park, “Van Hove Singularities and Excitonic Effects in the Optical Conductivity of Twisted Bilayer Graphene”, *Nano Letters*, vol. 14, no. 6. American Chemical Society (ACS), pp. 3353–3357, May 07, 2014. doi: 10.1021/nl500823k.  
  
J. Koo, S. Gao, H. Leeand L. Yang, “Vertical dielectric screening of few-layer van der Waals semiconductors”, *Nanoscale*, vol. 9, no. 38. Royal Society of Chemistry (RSC), pp. 14540–14547, 2017. doi: 10.1039/c7nr04134a.  
  
B. Lei, “Direct Observation of Semiconductor–Metal Phase Transition in Bilayer Tungsten Diselenide Induced by Potassium Surface Functionalization”, *ACS Nano*, vol. 12, no. 2. American Chemical Society (ACS), pp. 2070–2077, Jan. 30, 2018. doi: 10.1021/acsnano.8b00398.  
  
B. Lei, “Direct Observation of Semiconductor–Metal Phase Transition in Bilayer Tungsten Diselenide Induced by Potassium Surface Functionalization”, *ACS Nano*, vol. 12, no. 2. American Chemical Society (ACS), pp. 2070–2077, Jan. 30, 2018. doi: 10.1021/acsnano.8b00398.  
  
L. Li, “Quantum oscillations in a two-dimensional electron gas in black phosphorus thin films”, *Nature Nanotechnology*, vol. 10, no. 7. Springer Science and Business Media LLC, pp. 608–613, May 18, 2015. doi: 10.1038/nnano.2015.91.  
  
X. Lu and L. Yang, “Stark effect of doped two-dimensional transition metal dichalcogenides”, *Applied Physics Letters*, vol. 111, no. 19. AIP Publishing, p. 193104, Nov. 06, 2017. doi: 10.1063/1.5004413.  
  
G. Moody, “Microsecond Valley Lifetime of Defect-Bound Excitons in Monolayer ”, *Physical Review Letters*, vol. 121, no. 5. American Physical Society (APS), Aug. 02, 2018. doi: 10.1103/physrevlett.121.057403.  
  
G. Moody, “Microsecond Valley Lifetime of Defect-Bound Excitons in Monolayer ”, *Physical Review Letters*, vol. 121, no. 5. American Physical Society (APS), Aug. 02, 2018. doi: 10.1103/physrevlett.121.057403.  
  
Y. Pan, “Schottky Barriers in Bilayer Phosphorene Transistors”, *ACS Applied Materials & Interfaces*, vol. 9, no. 14. American Chemical Society (ACS), pp. 12694–12705, Mar. 30, 2017. doi: 10.1021/acsami.6b16826.  
  
Y. Pan, S. Gao, L. Yangand J. Lu, “Dependence of excited-state properties of tellurium on dimensionality: From bulk to two dimensions to one dimensions”, *Physical Review B*, vol. 98, no. 8. American Physical Society (APS), Aug. 22, 2018. doi: 10.1103/physrevb.98.085135.  
  
H. Patel, “Tunable Optical Excitations in Twisted Bilayer Graphene Form Strongly Bound Excitons”, *Nano Letters*, vol. 15, no. 9. American Chemical Society (ACS), pp. 5932–5937, Aug. 03, 2015. doi: 10.1021/acs.nanolett.5b02035.  
  
Z. Qiu, “Giant gate-tunable bandgap renormalization and excitonic effects in a 2D semiconductor”, *Science Advances*, vol. 5, no. 7. American Association for the Advancement of Science (AAAS), Jul. 05, 2019. doi: 10.1126/sciadv.aaw2347.  
  
K. L. Seyler, “Ligand-field helical luminescence in a 2D ferromagnetic insulator”, *Nature Physics*, vol. 14, no. 3. Springer Science and Business Media LLC, pp. 277–281, Dec. 04, 2017. doi: 10.1038/s41567-017-0006-7.  
  
R. Soklaski, Y. Liangand L. Yang, “Temperature effect on optical spectra of monolayer molybdenum disulfide”, *Applied Physics Letters*, vol. 104, no. 19. AIP Publishing, p. 193110, May 12, 2014. doi: 10.1063/1.4878098.  
  
R. Soklaski, V. Tran, Z. Nussinov, K. F. Keltonand L. Yang, “A locally preferred structure characterises all dynamical regimes of a supercooled liquid”, *Philosophical Magazine*, vol. 96, no. 12. Informa UK Limited, pp. 1212–1227, Mar. 11, 2016. doi: 10.1080/14786435.2016.1158427.  
  
W. Song and L. Yang, “Quasiparticle band gaps and optical spectra of strained monolayer transition-metal dichalcogenides”, *Physical Review B*, vol. 96, no. 23. American Physical Society (APS), Dec. 26, 2017. doi: 10.1103/physrevb.96.235441.  
  
J. Wang, T. Yang, Z. Zhangand L. Yang, “Enhanced doping effect on tuning structural phases of monolayer antimony”, *Applied Physics Letters*, vol. 112, no. 21. AIP Publishing, p. 213104, May 21, 2018. doi: 10.1063/1.5028265.  
  
X. Wang, “Highly anisotropic and robust excitons in monolayer black phosphorus”, *Nature Nanotechnology*, vol. 10, no. 6. Springer Science and Business Media LLC, pp. 517–521, Apr. 27, 2015. doi: 10.1038/nnano.2015.71.  
  
H. Zhong, “Interfacial Properties of Monolayer and Bilayer MoS2 Contacts with Metals: Beyond the Energy Band Calculations”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Mar. 01, 2016. doi: 10.1038/srep21786.  
  
X. Shen, “High On/Off Ratio Memristive Switching of Manganite/Cuprate Bilayer by Interfacial Magnetoelectricity”, *Advanced Materials Interfaces*, vol. 3, no. 16. Wiley, p. 1600086, May 27, 2016. doi: 10.1002/admi.201600086.  
  
X. Shen, Y. S. Puzyrev, C. Combsand S. T. Pantelides, “Variability of structural and electronic properties of bulk and monolayer Si2Te3”, *Applied Physics Letters*, vol. 109, no. 11. AIP Publishing, p. 113104, Sep. 12, 2016. doi: 10.1063/1.4962826.  
  
Y. K. Sharma, “Phosphorous passivation of the SiO2/4H–SiC interface”, *Solid-State Electronics*, vol. 68. Elsevier BV, pp. 103–107, Feb. 2012. doi: 10.1016/j.sse.2011.10.030.  
  
M. Bierbaum, B. D. Leahy, A. A. Alemi, I. Cohenand J. P. Sethna, “Light Microscopy at Maximal Precision”, *Physical Review X*, vol. 7, no. 4. American Physical Society (APS), Oct. 13, 2017. doi: 10.1103/physrevx.7.041007.  
  
Y. S. Chen, W. Choi, S. Papanikolaou, M. Bierbaumand J. P. Sethna, “Scaling theory of continuum dislocation dynamics in three dimensions: Self-organized fractal pattern formation”, *International Journal of Plasticity*, vol. 46. Elsevier BV, pp. 94–129, Jul. 2013. doi: 10.1016/j.ijplas.2013.02.011.  
  
B. Tang, E. Khatamiand M. Rigol, “A short introduction to numerical linked-cluster expansions”, *Computer Physics Communications*, vol. 184, no. 3. Elsevier BV, pp. 557–564, Mar. 2013. doi: 10.1016/j.cpc.2012.10.008.  
  
D. Ebrahimi, R. J.-M. Pellenqand A. J. Whittle, “Nanoscale Elastic Properties of Montmorillonite upon Water Adsorption”, *Langmuir*, vol. 28, no. 49. American Chemical Society (ACS), pp. 16855–16863, Nov. 26, 2012. doi: 10.1021/la302997g.  
  
D. Ebrahimi, R. J.-M. Pellenqand A. J. Whittle, “Mesoscale simulation of clay aggregate formation and mechanical properties”, *Granular Matter*, vol. 18, no. 3. Springer Science and Business Media LLC, Jun. 21, 2016. doi: 10.1007/s10035-016-0655-8.  
  
D. Ebrahimi, A. J. Whittleand R. J.-M. Pellenq, “Mesoscale properties of clay aggregates from potential of mean force representation of interactions between nanoplatelets”, *The Journal of Chemical Physics*, vol. 140, no. 15. AIP Publishing, p. 154309, Apr. 21, 2014. doi: 10.1063/1.4870932.  
  
V. I. Artyukhov, E. S. Penevand B. I. Yakobson, “Why nanotubes grow chiral”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, Sep. 16, 2014. doi: 10.1038/ncomms5892.  
  
Y. Liu, E. S. Penevand B. I. Yakobson, “Probing the Synthesis of Two-Dimensional Boron by First-Principles Computations”, *Angewandte Chemie International Edition*, vol. 52, no. 11. Wiley, pp. 3156–3159, Jan. 28, 2013. doi: 10.1002/anie.201207972.  
  
Y. Liu, F. Xu, Z. Zhang, E. S. Penevand B. I. Yakobson, “Two-Dimensional Mono-Elemental Semiconductor with Electronically Inactive Defects: The Case of Phosphorus”, *Nano Letters*, vol. 14, no. 12. American Chemical Society (ACS), pp. 6782–6786, Aug. 27, 2014. doi: 10.1021/nl5021393.  
  
S. Ozden, “Indentation Tests Reveal Geometry-Regulated Stiffening of Nanotube Junctions”, *Nano Letters*, vol. 16, no. 1. American Chemical Society (ACS), pp. 232–236, Dec. 07, 2015. doi: 10.1021/acs.nanolett.5b03607.  
  
E. S. Penev, V. I. Artyukhovand B. I. Yakobson, “Extensive Energy Landscape Sampling of Nanotube End-Caps Reveals No Chiral-Angle Bias for Their Nucleation”, *ACS Nano*, vol. 8, no. 2. American Chemical Society (ACS), pp. 1899–1906, Jan. 28, 2014. doi: 10.1021/nn406462e.  
  
E. S. Penev, V. I. Artyukhovand B. I. Yakobson, “Basic structural units in carbon fibers: Atomistic models and tensile behavior”, *Carbon*, vol. 85. Elsevier BV, pp. 72–78, Apr. 2015. doi: 10.1016/j.carbon.2014.12.067.  
  
E. S. Penev, K. V. Bets, N. Guptaand B. I. Yakobson, “Transient Kinetic Selectivity in Nanotubes Growth on Solid Co–W Catalyst”, *Nano Letters*, vol. 18, no. 8. American Chemical Society (ACS), pp. 5288–5293, Jul. 06, 2018. doi: 10.1021/acs.nanolett.8b02283.  
  
E. S. Penev, S. Bhowmick, A. Sadrzadehand B. I. Yakobson, “Polymorphism of Two-Dimensional Boron”, *Nano Letters*, vol. 12, no. 5. American Chemical Society (ACS), pp. 2441–2445, Apr. 20, 2012. doi: 10.1021/nl3004754.  
  
Z. Zhang, Y. Liu, Y. Yangand B. I. Yakobson, “Growth Mechanism and Morphology of Hexagonal Boron Nitride”, *Nano Letters*, vol. 16, no. 2. American Chemical Society (ACS), pp. 1398–1403, Feb. 01, 2016. doi: 10.1021/acs.nanolett.5b04874.  
  
Z. Zhang, S. N. Shirodkar, Y. Yangand B. I. Yakobson, “Gate‐Voltage Control of Borophene Structure Formation”, *Angewandte Chemie*, vol. 129, no. 48. Wiley, pp. 15623–15628, Oct. 25, 2017. doi: 10.1002/ange.201705459.  
  
Z. Zhang, Y. Yang, E. S. Penevand B. I. Yakobson, “Elasticity, Flexibility, and Ideal Strength of Borophenes”, *Advanced Functional Materials*, vol. 27, no. 9. Wiley, p. 1605059, Jan. 11, 2017. doi: 10.1002/adfm.201605059.  
  
Z. Shi, A. Kutanaand B. I. Yakobson, “How Much N-Doping Can Graphene Sustain?”, *The Journal of Physical Chemistry Letters*, vol. 6, no. 1. American Chemical Society (ACS), pp. 106–112, Dec. 17, 2014. doi: 10.1021/jz502093c.  
  
L. Wang, A. Kutanaand B. I. Yakobson, “Many-body and spin-orbit effects on direct-indirect band gap transition of strained monolayer MoS2and WS2”, *Annalen der Physik*, vol. 526, no. 9–10. Wiley, pp. L7–L12, Aug. 04, 2014. doi: 10.1002/andp.201400098.  
  
T. P. Yadav, “Chromiteen: A New 2D Oxide Magnetic Material from Natural Ore”, *Advanced Materials Interfaces*, vol. 5, no. 19. Wiley, p. 1800549, Jul. 08, 2018. doi: 10.1002/admi.201800549.  
  
W. Zan, Z. Zhang, Y. Yang, X. Yao, S. Liand B. I. Yakobson, “Width-dependent phase crossover in transition metal dichalcogenide nanoribbons”, *Nanotechnology*, vol. 30, no. 7. IOP Publishing, p. 075701, Dec. 14, 2018. doi: 10.1088/1361-6528/aaf25b.  
  
A. Ramasubramaniam, D. Navehand E. Towe, “Tunable Band Gaps in Bilayer Graphene−BN Heterostructures”, *Nano Letters*, vol. 11, no. 3. American Chemical Society (ACS), pp. 1070–1075, Jan. 28, 2011. doi: 10.1021/nl1039499.  
  
J. K. Bindra, “Evidence of Ferrimagnetism in Fe-Doped CdSe Quantum Dots”, *Chemistry of Materials*, vol. 30, no. 23. American Chemical Society (ACS), pp. 8446–8456, Oct. 26, 2018. doi: 10.1021/acs.chemmater.8b02505.  
  
G. Kurian and M. Mochena, “First principles investigations of Fe3+ impurity and Fe3+ + V−Cd complex in strongly confined CdSe quantum dot”, *Journal of Applied Physics*, vol. 128, no. 17. AIP Publishing, p. 173901, Nov. 07, 2020. doi: 10.1063/5.0026895.  
  
K. L. Holladay, J. M. Sharpand M. Janssens, “Automatic pyrolysis mass loss modeling from thermo-gravimetric analysis data using genetic programming”, *Proceedings of the 13th annual conference companion on Genetic and evolutionary computation*. ACM, Jul. 12, 2011. doi: 10.1145/2001858.2002063.  
  
S. Kattel, P. Atanassovand B. Kiefer, “Stability, Electronic and Magnetic Properties of In-Plane Defects in Graphene: A First-Principles Study”, *The Journal of Physical Chemistry C*, vol. 116, no. 14. American Chemical Society (ACS), pp. 8161–8166, Mar. 30, 2012. doi: 10.1021/jp2121609.  
  
S. Kattel, P. Atanassovand B. Kiefer, “Density Functional Theory Study of Ni–N*x*/C Electrocatalyst for Oxygen Reduction in Alkaline and Acidic Media”, *The Journal of Physical Chemistry C*, vol. 116, no. 33. American Chemical Society (ACS), pp. 17378–17383, Aug. 10, 2012. doi: 10.1021/jp3044708.  
  
X. Yang, V. H. Chhasatia, J. Shahand Y. Sun, “Coalescence, evaporation and particle deposition of consecutively printed colloidal drops”, *Soft Matter*, vol. 8, no. 35. Royal Society of Chemistry (RSC), p. 9205, 2012. doi: 10.1039/c2sm25906k.  
  
X. Yang, V. H. Chhasatiaand Y. Sun, “Oscillation and Recoil of Single and Consecutively Printed Droplets”, *Langmuir*, vol. 29, no. 7. American Chemical Society (ACS), pp. 2185–2192, Feb. 07, 2013. doi: 10.1021/la303980j.  
  
L. Mandeltort, P. Choudhury, J. K. Johnsonand J. T. Yates Jr., “Methyl Radical Reactivity on the Basal Plane of Graphite”, *The Journal of Physical Chemistry C*, vol. 116, no. 34. American Chemical Society (ACS), pp. 18347–18357, Aug. 17, 2012. doi: 10.1021/jp3063367.  
  
L. Mandeltort, P. Choudhury, J. K. Johnsonand J. T. Yates Jr., “Reaction of the Basal Plane of Graphite with the Methyl Radical”, *The Journal of Physical Chemistry Letters*, vol. 3, no. 12. American Chemical Society (ACS), pp. 1680–1683, Jun. 07, 2012. doi: 10.1021/jz300578x.  
  
M. Büttner, P. Choudhury, J. Karl Johnsonand J. T. Yates Jr., “Vacancy clusters as entry ports for cesium intercalation in graphite”, *Carbon*, vol. 49, no. 12. Elsevier BV, pp. 3937–3952, Oct. 2011. doi: 10.1016/j.carbon.2011.05.032.  
  
P. Choudhury and J. K. Johnson, “Methyl Chloride Reactions on Lithiated Carbon Nanotubes: Lithium as Both Reactant and Catalyst”, *The Journal of Physical Chemistry C*, vol. 115, no. 23. American Chemical Society (ACS), pp. 11694–11700, May 24, 2011. doi: 10.1021/jp202688k.  
  
W. Zhang, “Unexpected Stable Stoichiometries of Sodium Chlorides”, *Science*, vol. 342, no. 6165. American Association for the Advancement of Science (AAAS), pp. 1502–1505, Dec. 20, 2013. doi: 10.1126/science.1244989.  
  
X. Dong, “A stable compound of helium and sodium at high pressure”, *Nature Chemistry*, vol. 9, no. 5. Springer Science and Business Media LLC, pp. 440–445, Feb. 06, 2017. doi: 10.1038/nchem.2716.  
  
M. Burbano, “A dipole polarizable potential for reduced and doped CeO2obtained from first principles”, *Journal of Physics: Condensed Matter*, vol. 23, no. 25. IOP Publishing, p. 255402, Jun. 09, 2011. doi: 10.1088/0953-8984/23/25/255402.  
  
A. Krishnamoorthy, F. W. Herbert, S. Yip, K. J. Van Vlietand B. Yildiz, “Electronic states of intrinsic surface and bulk vacancies in FeS2”, *Journal of Physics: Condensed Matter*, vol. 25, no. 4. IOP Publishing, p. 045004, Dec. 10, 2012. doi: 10.1088/0953-8984/25/4/045004.  
  
Y. Kuru, D. Marrocchelli, S. R. Bishop, D. Chen, B. Yildizand H. L. Tuller, “Anomalous Chemical Expansion Behavior of Pr0.2Ce0.8O2-δThin Films Grown by Pulsed Laser Deposition”, *Journal of The Electrochemical Society*, vol. 159, no. 11. The Electrochemical Society, pp. F799–F803, 2012. doi: 10.1149/2.016212jes.  
  
W. Lee, J. W. Han, Y. Chen, Z. Caiand B. Yildiz, “Cation Size Mismatch and Charge Interactions Drive Dopant Segregation at the Surfaces of Manganite Perovskites”, *Journal of the American Chemical Society*, vol. 135, no. 21. American Chemical Society (ACS), pp. 7909–7925, May 17, 2013. doi: 10.1021/ja3125349.  
  
D. Marrocchelli, S. R. Bishopand J. Kilner, “Chemical expansion and its dependence on the host cation radius”, *Journal of Materials Chemistry A*, vol. 1, no. 26. Royal Society of Chemistry (RSC), p. 7673, 2013. doi: 10.1039/c3ta11020f.  
  
D. Marrocchelli, S. R. Bishop, H. L. Tullerand B. Yildiz, “Understanding Chemical Expansion in Non-Stoichiometric Oxides: Ceria and Zirconia Case Studies”, *Advanced Functional Materials*, vol. 22, no. 9. Wiley, pp. 1958–1965, Feb. 16, 2012. doi: 10.1002/adfm.201102648.  
  
D. Marrocchelli and B. Yildiz, “First-Principles Assessment of H2S and H2O Reaction Mechanisms and the Subsequent Hydrogen Absorption on the CeO2(111) Surface”, *The Journal of Physical Chemistry C*, vol. 116, no. 3. American Chemical Society (ACS), pp. 2411–2424, Jan. 11, 2012. doi: 10.1021/jp205573v.  
  
J. L. M. Rupp, “Scalable Oxygen-Ion Transport Kinetics in Metal-Oxide Films: Impact of Thermally Induced Lattice Compaction in Acceptor Doped Ceria Films”, *Advanced Functional Materials*, vol. 24, no. 11. Wiley, pp. 1562–1574, Jan. 03, 2014. doi: 10.1002/adfm.201302117.  
  
S. D. Ghadge, P. P. Patel, M. K. Datta, O. I. Velikokhatnyi, P. M. Shanthiand P. N. Kumta, “First report of vertically aligned (Sn,Ir)O2:F solid solution nanotubes: Highly efficient and robust oxygen evolution electrocatalysts for proton exchange membrane based water electrolysis”, *Journal of Power Sources*, vol. 392. Elsevier BV, pp. 139–149, Jul. 2018. doi: 10.1016/j.jpowsour.2018.04.065.  
  
S. D. Ghadge, O. I. Velikokhatnyi, M. K. Datta, P. M. Shanthi, S. Tanand P. N. Kumta, “Computational and Experimental Study of Fluorine Doped (Mn1–*x*Nb*x*)O2 Nanorod Electrocatalysts for Acid-Mediated Oxygen Evolution Reaction”, *ACS Applied Energy Materials*, vol. 3, no. 1. American Chemical Society (ACS), pp. 541–557, Dec. 18, 2019. doi: 10.1021/acsaem.9b01796.  
  
P. J. Hanumantha, B. Gattu, O. Velikokhatnyi, M. K. Datta, S. S. Damleand P. N. Kumta, “Heterostructures for Improved Stability of Lithium Sulfur Batteries”, *Journal of The Electrochemical Society*, vol. 161, no. 6. The Electrochemical Society, pp. A1173–A1180, 2014. doi: 10.1149/2.107406jes.  
  
D. Hong, “Binder-jetting 3D printing and alloy development of new biodegradable Fe-Mn-Ca/Mg alloys”, *Acta Biomaterialia*, vol. 45. Elsevier BV, pp. 375–386, Nov. 2016. doi: 10.1016/j.actbio.2016.08.032.  
  
K. S. Kadakia, “A Complexed Sol-Gel (CSG) Approach to High Surface Area (HSA) Durable Ultra Active Platinum-Ruthenium Electro-Catalysts for Direct Methanol Fuel Cells”, *Journal of The Electrochemical Society*, vol. 161, no. 10. The Electrochemical Society, pp. F1053–F1060, 2014. doi: 10.1149/2.0711410jes.  
  
K. S. Kadakia, “Nanostructured (Ir,Sn)O2:F – Oxygen Evolution Reaction Anode Electro-Catalyst Powders for PEM Based Water Electrolysis”, *Journal of The Electrochemical Society*, vol. 161, no. 9. The Electrochemical Society, pp. F868–F875, 2014. doi: 10.1149/2.0381409jes.  
  
K. S. Kadakia, “Nanostructured F doped IrO2 electro-catalyst powders for PEM based water electrolysis”, *Journal of Power Sources*, vol. 269. Elsevier BV, pp. 855–865, Dec. 2014. doi: 10.1016/j.jpowsour.2014.07.045.  
  
K. S. Kadakia, “Study of fluorine doped (Nb,Ir)O2 solid solution electro-catalyst powders for proton exchange membrane based oxygen evolution reaction”, *Materials Science and Engineering: B*, vol. 212. Elsevier BV, pp. 101–108, Oct. 2016. doi: 10.1016/j.mseb.2016.06.015.  
  
P. P. Patel, “Nanostructured robust cobalt metal alloy based anode electro-catalysts exhibiting remarkably high performance and durability for proton exchange membrane fuel cells”, *Journal of Materials Chemistry A*, vol. 3, no. 26. Royal Society of Chemistry (RSC), pp. 14015–14032, 2015. doi: 10.1039/c5ta01362c.  
  
P. P. Patel, “Noble metal-free bifunctional oxygen evolution and oxygen reduction acidic media electro-catalysts”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Jul. 06, 2016. doi: 10.1038/srep28367.  
  
P. P. Patel, “Cobalt based nanostructured alloys: Versatile high performance robust hydrogen evolution reaction electro-catalysts for electrolytic and photo-electrochemical water splitting”, *International Journal of Hydrogen Energy*, vol. 42, no. 27. Elsevier BV, pp. 17049–17062, Jul. 2017. doi: 10.1016/j.ijhydene.2017.05.175.  
  
P. P. Patel, “Vertically aligned nitrogen doped (Sn,Nb)O2 nanotubes – Robust photoanodes for hydrogen generation by photoelectrochemical water splitting”, *Materials Science and Engineering: B*, vol. 208. Elsevier BV, pp. 1–14, Jun. 2016. doi: 10.1016/j.mseb.2016.02.001.  
  
P. P. Patel, “Electrochemically active and robust cobalt doped copper phosphosulfide electro-catalysts for hydrogen evolution reaction in electrolytic and photoelectrochemical water splitting”, *International Journal of Hydrogen Energy*, vol. 43, no. 16. Elsevier BV, pp. 7855–7871, Apr. 2018. doi: 10.1016/j.ijhydene.2018.02.147.  
  
P. P. Patel, “Highly active robust oxide solid solution electro-catalysts for oxygen reduction reaction for proton exchange membrane fuel cell and direct methanol fuel cell cathodes”, *International Journal of Hydrogen Energy*, vol. 42, no. 38. Elsevier BV, pp. 24079–24089, Sep. 2017. doi: 10.1016/j.ijhydene.2017.07.139.  
  
P. M. Shanthi, “Theoretical and Experimental Strategies for New Heterostructures with Improved Stability for Rechargeable Lithium Sulfur Batteries”, *Journal of The Electrochemical Society*, vol. 167, no. 4. The Electrochemical Society, p. 040513, Feb. 20, 2020. doi: 10.1149/1945-7111/ab7220.  
  
O. I. Velikokhatnyi and P. N. Kumta, “First principles study of the elastic properties of magnesium and iron based bio-resorbable alloys”, *Materials Science and Engineering: B*, vol. 230. Elsevier BV, pp. 20–23, Apr. 2018. doi: 10.1016/j.mseb.2017.12.024.  
  
P. P. Patel, “Nitrogen and cobalt co-doped zinc oxide nanowires – Viable photoanodes for hydrogen generation via photoelectrochemical water splitting”, *Journal of Power Sources*, vol. 299. Elsevier BV, pp. 11–24, Dec. 2015. doi: 10.1016/j.jpowsour.2015.08.027.  
  
P. P. Patel, “WO3 based solid solution oxide – promising proton exchange membrane fuel cell anode electro-catalyst”, *Journal of Materials Chemistry A*, vol. 3, no. 35. Royal Society of Chemistry (RSC), pp. 18296–18309, 2015. doi: 10.1039/c5ta03792a.  
  
L. K. Aagesen, M. E. Coltrin, J. Hanand K. Thornton, “Phase-field simulations of GaN growth by selective area epitaxy from complex mask geometries”, *Journal of Applied Physics*, vol. 117, no. 19. AIP Publishing, p. 194302, May 15, 2015. doi: 10.1063/1.4921053.  
  
A. Abdellahi, O. Akyildiz, R. Malik, K. Thorntonand G. Ceder, “Particle-size and morphology dependence of the preferred interface orientation in LiFePO4 nano-particles”, *J. Mater. Chem. A*, vol. 2, no. 37. Royal Society of Chemistry (RSC), pp. 15437–15447, 2014. doi: 10.1039/c4ta02935f.  
  
A. Abdellahi, O. Akyildiz, R. Malik, K. Thorntonand G. Ceder, “The thermodynamic stability of intermediate solid solutions in LiFePO4 nanoparticles”, *Journal of Materials Chemistry A*, vol. 4, no. 15. Royal Society of Chemistry (RSC), pp. 5436–5447, 2016. doi: 10.1039/c5ta10498j.  
  
W. B. Andrews, P. W. Voorheesand K. Thornton, “Simulation of coarsening in two-phase systems with dissimilar mobilities”, *Computational Materials Science*, vol. 173. Elsevier BV, p. 109418, Feb. 2020. doi: 10.1016/j.commatsci.2019.109418.  
  
A. F. Chadwick, J. A. Stewart, R. A. Enrique, S. Duand K. Thornton, “Numerical Modeling of Localized Corrosion Using Phase-Field and Smoothed Boundary Methods”, *Journal of The Electrochemical Society*, vol. 165, no. 10. The Electrochemical Society, pp. C633–C646, 2018. doi: 10.1149/2.0701810jes.  
  
V. W. L. Chan, N. Pisutha-Arnondand K. Thornton, “Phase-field crystal model for a diamond-cubic structure”, *Physical Review E*, vol. 91, no. 5. American Physical Society (APS), May 14, 2015. doi: 10.1103/physreve.91.053305.  
  
V. W. L. Chan, N. Pisutha-Arnondand K. Thornton, “Thermodynamic relationships for homogeneous crystalline and liquid phases in the phase-field crystal model”, *Computational Materials Science*, vol. 135. Elsevier BV, pp. 205–213, Jul. 2017. doi: 10.1016/j.commatsci.2017.04.017.  
  
H.-Y. Chen, H.-C. Yu, J. Scott Cronin, J. R. Wilson, S. A. Barnettand K. Thornton, “Simulation of coarsening in three-phase solid oxide fuel cell anodes”, *Journal of Power Sources*, vol. 196, no. 3. Elsevier BV, pp. 1333–1337, Feb. 2011. doi: 10.1016/j.jpowsour.2010.08.010.  
  
S. DeWitt and K. Thornton, “Model for Anodic Film Growth on Aluminum with Coupled Bulk Transport and Interfacial Reactions”, *Langmuir*, vol. 30, no. 18. American Chemical Society (ACS), pp. 5314–5325, Apr. 28, 2014. doi: 10.1021/la500782d.  
  
S. DeWitt and K. Thornton, “Simulations of Anodic Nanopore Growth Using the Smoothed Boundary and Level Set Methods”, *The Journal of Physical Chemistry C*, vol. 120, no. 4. American Chemical Society (ACS), pp. 2419–2431, Jan. 27, 2016. doi: 10.1021/acs.jpcc.5b09983.  
  
J. L. Fife, J. W. Gibbs, E. B. Gulsoy, C.-L. Park, K. Thorntonand P. W. Voorhees, “The dynamics of interfaces during coarsening in solid–liquid systems”, *Acta Materialia*, vol. 70. Elsevier BV, pp. 66–78, May 2014. doi: 10.1016/j.actamat.2014.01.024.  
  
C. M. Funkhouser, M. Mayer, F. J. Solisand K. Thornton, “Effects of interleaflet coupling on the morphologies of multicomponent lipid bilayer membranes”, *The Journal of Chemical Physics*, vol. 138, no. 2. AIP Publishing, p. 024909, Jan. 14, 2013. doi: 10.1063/1.4773856.  
  
C. M. Funkhouser, F. J. Solisand K. Thornton, “Dynamics of coarsening in multicomponent lipid vesicles with non-uniform mechanical properties”, *The Journal of Chemical Physics*, vol. 140, no. 14. AIP Publishing, p. 144908, Apr. 14, 2014. doi: 10.1063/1.4870478.  
  
S. P. Gentry and K. Thornton, “Simulating recrystallization in titanium using the phase field method”, *IOP Conference Series: Materials Science and Engineering*, vol. 89. IOP Publishing, p. 012024, Aug. 07, 2015. doi: 10.1088/1757-899x/89/1/012024.  
  
S. P. Gentry and K. Thornton, “Sensitivity analysis of a phase field model for static recrystallization of deformed microstructures”, *Modelling and Simulation in Materials Science and Engineering*, vol. 28, no. 6. IOP Publishing, p. 065002, Jun. 22, 2020. doi: 10.1088/1361-651x/ab9751.  
  
J. Kim, “Template-Directed Directionally Solidified 3D Mesostructured AgCl-KCl Eutectic Photonic Crystals”, *Advanced Materials*, vol. 27, no. 31. Wiley, pp. 4551–4559, Jul. 14, 2015. doi: 10.1002/adma.201502265.  
  
S. Kobayashi, C. A. J. Fisher, T. Kato, Y. Ukyo, T. Hirayamaand Y. Ikuhara, “Atomic-Scale Observations of (010) LiFePO4 Surfaces Before and After Chemical Delithiation”, *Nano Letters*, vol. 16, no. 9. American Chemical Society (ACS), pp. 5409–5414, Aug. 03, 2016. doi: 10.1021/acs.nanolett.6b01689.  
  
L. K. Lee, L. K. Aagesen, K. Thorntonand P.-C. Ku, “Origin of broad luminescence from site-controlled InGaN nanodots fabricated by selective-area epitaxy”, *physica status solidi (a)*, vol. 211, no. 3. Wiley, pp. 531–535, Jan. 31, 2014. doi: 10.1002/pssa.201330362.  
  
H. Liu, “Effects of Antisite Defects on Li Diffusion in LiFePO4 Revealed by Li Isotope Exchange”, *The Journal of Physical Chemistry C*, vol. 121, no. 22. American Chemical Society (ACS), pp. 12025–12036, May 30, 2017. doi: 10.1021/acs.jpcc.7b02819.  
  
Y. Lu, “Performance Variability and Degradation in Porous La1-xSrxCoO3-δElectrodes”, *Journal of The Electrochemical Society*, vol. 161, no. 4. The Electrochemical Society, pp. F561–F568, 2014. doi: 10.1149/2.101404jes.  
  
J. D. Madison, L. K. Aagesen, V. W. Chanand K. Thornton, “Advancing quantitative description of porosity in autogenous laser-welds of 304L stainless steel”, *Integrating Materials and Manufacturing Innovation*, vol. 3, no. 1. Springer Science and Business Media LLC, pp. 141–157, Apr. 29, 2014. doi: 10.1186/2193-9772-3-11.  
  
B. Orvananos, T. R. Ferguson, H.-C. Yu, M. Z. Bazantand K. Thornton, “Particle-Level Modeling of the Charge-Discharge Behavior of Nanoparticulate Phase-Separating Li-Ion Battery Electrodes”, *Journal of The Electrochemical Society*, vol. 161, no. 4. The Electrochemical Society, pp. A535–A546, 2014. doi: 10.1149/2.024404jes.  
  
B. Orvananos, “Architecture Dependence on the Dynamics of Nano-LiFePO4 Electrodes”, *Electrochimica Acta*, vol. 137. Elsevier BV, pp. 245–257, Aug. 2014. doi: 10.1016/j.electacta.2014.06.029.  
  
B. Orvananos, “Kinetics of Nanoparticle Interactions in Battery Electrodes”, *Journal of The Electrochemical Society*, vol. 162, no. 6. The Electrochemical Society, pp. A965–A973, 2015. doi: 10.1149/2.0481506jes.  
  
B. Orvananos, “Effect of a Size-Dependent Equilibrium Potential on Nano-LiFePO4Particle Interactions”, *Journal of The Electrochemical Society*, vol. 162, no. 9. The Electrochemical Society, pp. A1718–A1724, 2015. doi: 10.1149/2.0161509jes.  
  
C.-L. Park, J. W. Gibbs, P. W. Voorheesand K. Thornton, “Coarsening of complex microstructures following spinodal decomposition”, *Acta Materialia*, vol. 132. Elsevier BV, pp. 13–24, Jun. 2017. doi: 10.1016/j.actamat.2017.03.020.  
  
C.-L. Park, P. W. Voorheesand K. Thornton, “Application of the level-set method to the analysis of an evolving microstructure”, *Computational Materials Science*, vol. 85. Elsevier BV, pp. 46–58, Apr. 2014. doi: 10.1016/j.commatsci.2013.12.022.  
  
C.-L. Park, P. W. Voorheesand K. Thornton, “Evolution of interfacial curvatures of a bicontinuous structure generated via nonconserved dynamics”, *Acta Materialia*, vol. 90. Elsevier BV, pp. 182–193, May 2015. doi: 10.1016/j.actamat.2015.02.037.  
  
N. O. Shanti, V. W. L. Chan, S. R. Stock, F. De Carlo, K. Thorntonand K. T. Faber, “X-ray micro-computed tomography and tortuosity calculations of percolating pore networks”, *Acta Materialia*, vol. 71. Elsevier BV, pp. 126–135, Jun. 2014. doi: 10.1016/j.actamat.2014.03.003.  
  
F. C. Strobridge, “Mapping the Inhomogeneous Electrochemical Reaction Through Porous LiFePO4-Electrodes in a Standard Coin Cell Battery”, *Chemistry of Materials*, vol. 27, no. 7. American Chemical Society (ACS), pp. 2374–2386, Mar. 18, 2015. doi: 10.1021/cm504317a.  
  
Y. Sun, W. B. Andrews, K. Thorntonand P. W. Voorhees, “Self-Similarity and the Dynamics of Coarsening in Materials”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, Dec. 18, 2018. doi: 10.1038/s41598-018-36354-8.  
  
F. Wang, “Tracking lithium transport and electrochemical reactions in nanoparticles”, *Nature Communications*, vol. 3, no. 1. Springer Science and Business Media LLC, Nov. 13, 2012. doi: 10.1038/ncomms2185.  
  
H.-C. Yu, S. B. Adler, S. A. Barnettand K. Thornton, “Simulation of the diffusional impedance and application to the characterization of electrodes with complex microstructures”, *Electrochimica Acta*, vol. 354. Elsevier BV, p. 136534, Sep. 2020. doi: 10.1016/j.electacta.2020.136534.  
  
H.-C. Yu, H.-Y. Chenand K. Thornton, “Extended smoothed boundary method for solving partial differential equations with general boundary conditions on complex boundaries”, *Modelling and Simulation in Materials Science and Engineering*, vol. 20, no. 7. IOP Publishing, p. 075008, Sep. 14, 2012. doi: 10.1088/0965-0393/20/7/075008.  
  
H.-C. Yu, M.-J. Choe, G. G. Amatucci, Y.-M. Chiangand K. Thornton, “Smoothed Boundary Method for simulating bulk and grain boundary transport in complex polycrystalline microstructures”, *Computational Materials Science*, vol. 121. Elsevier BV, pp. 14–22, Aug. 2016. doi: 10.1016/j.commatsci.2016.04.028.  
  
H.-C. Yu, C. Ling, J. Bhattacharya, J. C. Thomas, K. Thorntonand A. Van der Ven, “Designing the next generation high capacity battery electrodes”, *Energy & Environmental Science*, vol. 7, no. 5. Royal Society of Chemistry (RSC), p. 1760, 2014. doi: 10.1039/c3ee43154a.  
  
H.-C. Yu, “Deformation and stresses in solid-state composite battery cathodes”, *Journal of Power Sources*, vol. 440. Elsevier BV, p. 227116, Nov. 2019. doi: 10.1016/j.jpowsour.2019.227116.  
  
H.-C. Yu, F. Wang, G. G. Amatucciand K. Thornton, “A Phase-Field Model and Simulation of Kinetically Asymmetric Ternary Conversion-Reconversion Transformation in Battery Electrodes”, *Journal of Phase Equilibria and Diffusion*, vol. 37, no. 1. Springer Science and Business Media LLC, pp. 86–99, Jan. 04, 2016. doi: 10.1007/s11669-015-0440-0.  
  
W. Zhang, “Localized concentration reversal of lithium during intercalation into nanoparticles”, *Science Advances*, vol. 4, no. 1. American Association for the Advancement of Science (AAAS), Jan. 05, 2018. doi: 10.1126/sciadv.aao2608.  
  
J. K. Seo, J. Shin, H. Chung, P. Y. Meng, X. Wangand Y. S. Meng, “Intercalation and Conversion Reactions of Nanosized β-MnO2 Cathode in the Secondary Zn/MnO2 Alkaline Battery”, *The Journal of Physical Chemistry C*, vol. 122, no. 21. American Chemical Society (ACS), pp. 11177–11185, May 03, 2018. doi: 10.1021/acs.jpcc.7b11685.  
  
A. Singer, “Nucleation of dislocations and their dynamics in layered oxide cathode materials during battery charging”, *Nature Energy*, vol. 3, no. 8. Springer Science and Business Media LLC, pp. 641–647, Jul. 16, 2018. doi: 10.1038/s41560-018-0184-2.  
  
T. A. Wynn, “Mitigating oxygen release in anionic-redox-active cathode materials by cationic substitution through rational design”, *Journal of Materials Chemistry A*, vol. 6, no. 47. Royal Society of Chemistry (RSC), pp. 24651–24659, 2018. doi: 10.1039/c8ta06296j.  
  
H. Xia, “A monoclinic polymorph of sodium birnessite for ultrafast and ultrastable sodium ion storage”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Nov. 30, 2018. doi: 10.1038/s41467-018-07595-y.  
  
Q. Zhang, M. G. Verde, J. K. Seo, X. Liand Y. S. Meng, “Structural and electrochemical properties of Gd-doped Li4Ti5O12 as anode material with improved rate capability for lithium-ion batteries”, *Journal of Power Sources*, vol. 280. Elsevier BV, pp. 355–362, Apr. 2015. doi: 10.1016/j.jpowsour.2015.01.124.  
  
X. Chen, “*In situ*atomic-scale observation of inhomogeneous oxide reduction”, *Chemical Communications*, vol. 54, no. 53. Royal Society of Chemistry (RSC), pp. 7342–7345, 2018. doi: 10.1039/c8cc03822h.  
  
C. Li, P. Zhang, J. Wang, J. A. Boscoboinikand G. Zhou, “Tuning the Deoxygenation of Bulk-Dissolved Oxygen in Copper”, *The Journal of Physical Chemistry C*, vol. 122, no. 15. American Chemical Society (ACS), pp. 8254–8261, Apr. 05, 2018. doi: 10.1021/acs.jpcc.7b12030.  
  
J. Li, L. Liand G. Zhou, “The onset of sub-surface oxidation induced by defects in a chemisorbed oxygen layer”, *The Journal of Chemical Physics*, vol. 142, no. 8. AIP Publishing, p. 084701, Feb. 24, 2015. doi: 10.1063/1.4913237.  
  
J. Li and G. Zhou, “Density functional theory study of O–H and C–H bond scission of methanol catalyzed by a chemisorbed oxygen layer on Cu(111)”, *Surface Science*, vol. 646. Elsevier BV, pp. 288–297, Apr. 2016. doi: 10.1016/j.susc.2015.11.012.  
  
L. Li, N. Cai, W. A. Saidiand G. Zhou, “Role of oxygen in Cu(1 1 0) surface restructuring in the vicinity of step edges”, *Chemical Physics Letters*, vol. 613. Elsevier BV, pp. 64–69, Oct. 2014. doi: 10.1016/j.cplett.2014.08.050.  
  
L. Li, Q. Liu, J. Li, W. A. Saidiand G. Zhou, “Kinetic Barriers of the Phase Transition in the Oxygen Chemisorbed Cu(110)-(2 × 1)-O as a Function of Oxygen Coverage”, *The Journal of Physical Chemistry C*, vol. 118, no. 36. American Chemical Society (ACS), pp. 20858–20866, Aug. 29, 2014. doi: 10.1021/jp503757k.  
  
L. Li and G. Zhou, “Oxygen subsurface adsorption on the Cu(110)-c(6×2) surface”, *Surface Science*, vol. 615. Elsevier BV, pp. 57–64, Sep. 2013. doi: 10.1016/j.susc.2013.04.005.  
  
Q. Liu, J. Li, X. Tongand G. Zhou, “Enhancing Dissociative Adsorption of Water on Cu(111) via Chemisorbed Oxygen”, *The Journal of Physical Chemistry C*, vol. 121, no. 22. American Chemical Society (ACS), pp. 12117–12126, May 30, 2017. doi: 10.1021/acs.jpcc.6b12897.  
  
Q. Liu, L. Li, N. Cai, W. A. Saidiand G. Zhou, “Oxygen chemisorption-induced surface phase transitions on Cu(110)”, *Surface Science*, vol. 627. Elsevier BV, pp. 75–84, Sep. 2014. doi: 10.1016/j.susc.2014.04.017.  
  
H. Qin, X. Chen, L. Li, P. W. Sutterand G. Zhou, “Oxidation-driven surface dynamics on NiAl(100)”, *Proceedings of the National Academy of Sciences*, vol. 112, no. 2. Proceedings of the National Academy of Sciences, Dec. 29, 2014. doi: 10.1073/pnas.1420690112.  
  
W. Shan, Q. Liu, J. Li, N. Cai, W. A. Saidiand G. Zhou, “Hydrogen-induced atomic structure evolution of the oxygen-chemisorbed Cu(110) surface”, *The Journal of Chemical Physics*, vol. 145, no. 23. AIP Publishing, p. 234704, Dec. 21, 2016. doi: 10.1063/1.4972070.  
  
Y. Wang, C. Cai, L. Li, L. Yang, Y. Zhouand G. Zhou, “Oxygen vacancy ordering induced displacements of cations in yttria-stabilized zirconia”, *AIP Advances*, vol. 6, no. 9. AIP Publishing, p. 095113, Sep. 2016. doi: 10.1063/1.4963202.  
  
D. Wu, J. Liand G. Zhou, “Oxygen adsorption at heterophase boundaries of the oxygenated Cu(110)”, *Surface Science*, vol. 666. Elsevier BV, pp. 28–43, Dec. 2017. doi: 10.1016/j.susc.2017.08.017.  
  
D. Wu, Q. Liu, J. Li, J. T. Sadowskiand G. Zhou, “Visualizing Reversible Two-Dimensional Phase Transitions in Oxygen Chemisorbed Layers”, *The Journal of Physical Chemistry C*, vol. 122, no. 49. American Chemical Society (ACS), pp. 28233–28244, Nov. 16, 2018. doi: 10.1021/acs.jpcc.8b10892.  
  
Q. Zhu, L. Zou, G. Zhou, W. A. Saidiand J. C. Yang, “Early and transient stages of Cu oxidation: Atomistic insights from theoretical simulations and in situ experiments”, *Surface Science*, vol. 652. Elsevier BV, pp. 98–113, Oct. 2016. doi: 10.1016/j.susc.2016.03.003.  
  
L. Zou, J. Li, D. Zakharov, E. A. Stachand G. Zhou, “In situ atomic-scale imaging of the metal/oxide interfacial transformation”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Aug. 21, 2017. doi: 10.1038/s41467-017-00371-4.  
  
L. Zou, “Segregation induced order-disorder transition in Cu(Au) surface alloys”, *Acta Materialia*, vol. 154. Elsevier BV, pp. 220–227, Aug. 2018. doi: 10.1016/j.actamat.2018.05.040.  
  
L. Zou, “Dislocation nucleation facilitated by atomic segregation”, *Nature Materials*, vol. 17, no. 1. Springer Science and Business Media LLC, pp. 56–63, Nov. 27, 2017. doi: 10.1038/nmat5034.  
  
B. Rasulev, M. Watkins, M. Theodore, J. Jackmanand J. Leszczynski, “Structures and Stabilities: Quantum-Chemical Study of Aun (n = 2-2016) Nanoclusters by Extended Huckel and DFT Approaches”, *Nanoscience &Nanotechnology-Asia*, vol. 2, no. 1. Bentham Science Publishers Ltd., pp. 2–10, Jun. 01, 2012. doi: 10.2174/2210681211202010002.  
  
M. Wang, A. Alexander-Katzand B. D. Olsen, “Diffusion of Entangled Rod–Coil Block Copolymers”, *ACS Macro Letters*, vol. 1, no. 6. American Chemical Society (ACS), pp. 676–680, May 16, 2012. doi: 10.1021/mz300127s.  
  
R. N. Gunasinghe, “Resonant orbitals in fluorinated epitaxial graphene”, *Physical Chemistry Chemical Physics*, vol. 16, no. 35. Royal Society of Chemistry (RSC), p. 18902, Jul. 25, 2014. doi: 10.1039/c4cp03163f.  
  
U. K. Wijewardena, S. E. Brownand X.-Q. Wang, “Epoxy-Carbonyl Conformation of Graphene Oxides”, *The Journal of Physical Chemistry C*, vol. 120, no. 39. American Chemical Society (ACS), pp. 22739–22743, Sep. 21, 2016. doi: 10.1021/acs.jpcc.6b07648.  
  
D. Chang, “Selectively Deuterated Poly(ε-caprolactone)s: Synthesis and Isotope Effects on the Crystal Structures and Properties”, *Macromolecules*, vol. 51, no. 22. American Chemical Society (ACS), pp. 9393–9404, Nov. 14, 2018. doi: 10.1021/acs.macromol.8b01851.  
  
N. T. Ekanayake, J. Huang, J. Jakowski, B. G. Sumpterand S. Garashchuk, “Relevance of the Nuclear Quantum Effects on the Proton/Deuteron Transmission through Hexagonal Boron Nitride and Graphene Monolayers”, *The Journal of Physical Chemistry C*, vol. 121, no. 43. American Chemical Society (ACS), pp. 24335–24344, Oct. 20, 2017. doi: 10.1021/acs.jpcc.7b08152.  
  
S. Garashchuk, J. Jakowskiand V. A. Rassolov, “Approximate quantum trajectory dynamics for reactive processes in condensed phase”, *Molecular Simulation*, vol. 41, no. 1–3. Informa UK Limited, pp. 86–106, Apr. 24, 2014. doi: 10.1080/08927022.2014.907493.  
  
B. Gu and S. Garashchuk, “Molecular dynamics of large systems with quantum corrections for the nuclei”, *AIP Conference Proceedings*. AIP Publishing LLC, 2015. doi: 10.1063/1.4938822.  
  
B. Gu and S. Garashchuk, “Determination of the collective modes from the quantum-mechanical time-correlation functions”, *Theoretical Chemistry Accounts*, vol. 134, no. 11. Springer Science and Business Media LLC, Oct. 14, 2015. doi: 10.1007/s00214-015-1736-1.  
  
B. Gu and S. Garashchuk, “Quantum Dynamics with Gaussian Bases Defined by the Quantum Trajectories”, *The Journal of Physical Chemistry A*, vol. 120, no. 19. American Chemical Society (ACS), pp. 3023–3031, Jan. 13, 2016. doi: 10.1021/acs.jpca.5b10029.  
  
B. Gu, R. J. Hinde, V. A. Rassolovand S. Garashchuk, “Estimation of the Ground State Energy of an Atomic Solid by Employing Quantum Trajectory Dynamics with Friction”, *Journal of Chemical Theory and Computation*, vol. 11, no. 7. American Chemical Society (ACS), pp. 2891–2899, Jun. 03, 2015. doi: 10.1021/ct501176m.  
  
J. A. Hachtel, “Damage-Free Nanoscale Isotopic Analysis of Biological Materials with Vibrational Electron Spectroscopy”, *Microscopy and Microanalysis*, vol. 25, no. S2. Oxford University Press (OUP), pp. 1088–1089, Aug. 2019. doi: 10.1017/s1431927619006172.  
  
J. A. Hachtel, “Identification of site-specific isotopic labels by vibrational spectroscopy in the electron microscope”, *Science*, vol. 363, no. 6426. American Association for the Advancement of Science (AAAS), pp. 525–528, Jan. 31, 2019. doi: 10.1126/science.aav5845.  
  
C. Hu, “Effects of partial La filling and Sb vacancy defects on skutterudites”, *Physical Review B*, vol. 95, no. 16. American Physical Society (APS), Apr. 25, 2017. doi: 10.1103/physrevb.95.165204.  
  
Z. Hu, “An experimental and computational study of donor–linker–acceptor block copolymers for organic photovoltaics”, *Journal of Polymer Science Part B: Polymer Physics*, vol. 56, no. 16. Wiley, pp. 1135–1143, Aug. 15, 2018. doi: 10.1002/polb.24633.  
  
A. V. Ievlev, “Building with ions: towards direct write of platinum nanostructures using in situ liquid cell helium ion microscopy”, *Nanoscale*, vol. 9, no. 35. Royal Society of Chemistry (RSC), pp. 12949–12956, 2017. doi: 10.1039/c7nr04417h.  
  
Y. Ihm, “Assessing the Predictive Power of Density Functional Theory in Finite-Temperature Hydrogen Adsorption/Desorption Thermodynamics”, *The Journal of Physical Chemistry C*, vol. 122, no. 45. American Chemical Society (ACS), pp. 26189–26195, Oct. 09, 2018. doi: 10.1021/acs.jpcc.8b00793.  
  
J. Jakowski, “Deuteration as a Means to Tune Crystallinity of Conducting Polymers”, *The Journal of Physical Chemistry Letters*, vol. 8, no. 18. American Chemical Society (ACS), pp. 4333–4340, Aug. 30, 2017. doi: 10.1021/acs.jpclett.7b01803.  
  
J. Jakowski, J. Huang, B. G. Sumpterand S. Garashchuk, “Theoretical assessment of the nuclear quantum effects on polymer crystallinity via perturbation theory and dynamics”, *International Journal of Quantum Chemistry*, vol. 118, no. 20. Wiley, Sep. 22, 2018. doi: 10.1002/qua.25712.  
  
S. Kim, “Multi-purposed Ar gas cluster ion beam processing for graphene engineering”, *Carbon*, vol. 131. Elsevier BV, pp. 142–148, May 2018. doi: 10.1016/j.carbon.2018.01.098.  
  
D. Lingerfelt, J. Jakowski, P. Ganeshand B. Sumpter, “A TD-DFT Treatment of Electronic Excitations in the STEM Spanning Dipole and Impact Scattering Regimes”, *Microscopy and Microanalysis*, vol. 25, no. S2. Oxford University Press (OUP), pp. 2300–2301, Aug. 2019. doi: 10.1017/s1431927619012236.  
  
J. W. Mazzuca, S. Garashchukand J. Jakowski, “The effect of local substrate motion on quantum hydrogen transfer in soybean lipoxygenase-1 modeled with QTES-DFTB dynamics”, *Chemical Physics Letters*, vol. 613. Elsevier BV, pp. 104–109, Oct. 2014. doi: 10.1016/j.cplett.2014.08.006.  
  
D. Nugawela, S. J. Stuartand J. Jakowski, “Highly Energetic Collisions of Xe with Fullerene Clusters”, *Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment*. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616514.  
  
M. Shao, “The isotopic effects of deuteration on optoelectronic properties of conducting polymers”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, Jan. 24, 2014. doi: 10.1038/ncomms4180.  
  
Y.-H. Tian, “Non-Transition-Metal Catalytic System for N2 Reduction to NH3: A Density Functional Theory Study of Al-Doped Graphene”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 3. American Chemical Society (ACS), pp. 570–576, Jan. 19, 2018. doi: 10.1021/acs.jpclett.7b03094.  
  
L. Wang, J. Jakowskiand S. Garashchuk, “Adsorption of a Hydrogen Atom on a Graphene Flake Examined with Quantum Trajectory/Electronic Structure Dynamics”, *The Journal of Physical Chemistry C*, vol. 118, no. 29. American Chemical Society (ACS), pp. 16175–16187, Jul. 14, 2014. doi: 10.1021/jp503261k.  
  
L. Wang, J. Jakowski, S. Garashchukand B. G. Sumpter, “Understanding How Isotopes Affect Charge Transfer in P3HT/PCBM: A Quantum Trajectory-Electronic Structure Study with Nonlinear Quantum Corrections”, *Journal of Chemical Theory and Computation*, vol. 12, no. 9. American Chemical Society (ACS), pp. 4487–4500, Aug. 31, 2016. doi: 10.1021/acs.jctc.6b00126.  
  
L. Wang, J. W. Mazzuca, S. Garashchukand J. Jakowski, “The hybrid Quantum Trajectory/Electronic Structure DFTB-based approach to Molecular Dynamics”, *Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment*. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616503.  
  
B. Yang, “Enhancing Ion Migration in Grain Boundaries of Hybrid Organic–Inorganic Perovskites by Chlorine”, *Advanced Functional Materials*, vol. 27, no. 26. Wiley, p. 1700749, May 26, 2017. doi: 10.1002/adfm.201700749.  
  
T. Yu, F. Fabunmi, J. Huang, B. G. Sumpterand J. Jakowski, “A fast scheme to calculate electronic couplings between P3HT polymer units using diabatic orbitals for charge transfer dynamics simulations”, *Journal of Computational Chemistry*, vol. 40, no. 2. Wiley, pp. 532–542, Dec. 12, 2018. doi: 10.1002/jcc.25749.  
  
W. A. Saidi, H. Fengand K. A. Fichthorn, “Binding of Polyvinylpyrrolidone to Ag Surfaces: Insight into a Structure-Directing Agent from Dispersion-Corrected Density Functional Theory”, *The Journal of Physical Chemistry C*, vol. 117, no. 2. American Chemical Society (ACS), pp. 1163–1171, Jan. 07, 2013. doi: 10.1021/jp309867n.  
  
T. Balankura, X. Qi, Y. Zhouand K. A. Fichthorn, “Predicting kinetic nanocrystal shapes through multi-scale theory and simulation: Polyvinylpyrrolidone-mediated growth of Ag nanocrystals”, *The Journal of Chemical Physics*, vol. 145, no. 14. AIP Publishing, p. 144106, Oct. 13, 2016. doi: 10.1063/1.4964297.  
  
K. A. Fichthorn, “Molecular phenomena in colloidal nanostructure synthesis”, *Molecular Simulation*, vol. 40, no. 1–3. Informa UK Limited, pp. 134–140, Dec. 24, 2013. doi: 10.1080/08927022.2013.840899.  
  
K. A. Fichthorn, “Atomic-Scale Theory and Simulations for Colloidal Metal Nanocrystal Growth”, *Journal of Chemical & Engineering Data*, vol. 59, no. 10. American Chemical Society (ACS), pp. 3113–3119, May 27, 2014. doi: 10.1021/je500189s.  
  
S.-H. Liu, T. Balankuraand K. A. Fichthorn, “Self-assembled monolayer structures of hexadecylamine on Cu surfaces: density-functional theory”, *Physical Chemistry Chemical Physics*, vol. 18, no. 48. Royal Society of Chemistry (RSC), pp. 32753–32761, 2016. doi: 10.1039/c6cp07030b.  
  
S.-H. Liu and K. A. Fichthorn, “Interaction of Alkylamines with Cu Surfaces: A Metal–Organic Many-Body Force Field”, *The Journal of Physical Chemistry C*, vol. 121, no. 40. American Chemical Society (ACS), pp. 22531–22541, Sep. 29, 2017. doi: 10.1021/acs.jpcc.7b07861.  
  
X. Qi, T. Balankura, Y. Zhouand K. A. Fichthorn, “How Structure-Directing Agents Control Nanocrystal Shape: Polyvinylpyrrolidone-Mediated Growth of Ag Nanocubes”, *Nano Letters*, vol. 15, no. 11. American Chemical Society (ACS), pp. 7711–7717, Nov. 02, 2015. doi: 10.1021/acs.nanolett.5b04204.  
  
X. Qi and K. A. Fichthorn, “Theory of the thermodynamic influence of solution-phase additives in shape-controlled nanocrystal synthesis”, *Nanoscale*, vol. 9, no. 40. Royal Society of Chemistry (RSC), pp. 15635–15642, 2017. doi: 10.1039/c7nr05765b.  
  
X. Qi, Y. Zhouand K. A. Fichthorn, “Obtaining the solid-liquid interfacial free energy via multi-scheme thermodynamic integration: Ag-ethylene glycol interfaces”, *The Journal of Chemical Physics*, vol. 145, no. 19. AIP Publishing, p. 194108, Nov. 21, 2016. doi: 10.1063/1.4967521.  
  
Y. Zhou and K. A. Fichthorn, “Internal Stress-Induced Orthorhombic Phase in 5-Fold-Twinned Noble Metal Nanowires”, *The Journal of Physical Chemistry C*, vol. 118, no. 32. American Chemical Society (ACS), pp. 18746–18755, Aug. 01, 2014. doi: 10.1021/jp505334x.  
  
Y. Zhou, W. A. Saidiand K. A. Fichthorn, “Comparison of the Binding of Polyvinylpyrrolidone and Polyethylene Oxide to Ag Surfaces: Elements of a Successful Structure-Directing Agent”, *The Journal of Physical Chemistry C*, vol. 117, no. 21. American Chemical Society (ACS), pp. 11444–11448, May 17, 2013. doi: 10.1021/jp403318h.  
  
Y. Zhou, W. A. Saidiand K. A. Fichthorn, “A Force Field for Describing the Polyvinylpyrrolidone-Mediated Solution-Phase Synthesis of Shape-Selective Ag Nanoparticles”, *The Journal of Physical Chemistry C*, vol. 118, no. 6. American Chemical Society (ACS), pp. 3366–3374, Jan. 31, 2014. doi: 10.1021/jp412098n.  
  
S.-H. Liu, W. A. Saidi, Y. Zhouand K. A. Fichthorn, “Synthesis of {111}-Faceted Au Nanocrystals Mediated by Polyvinylpyrrolidone: Insights from Density-Functional Theory and Molecular Dynamics”, *The Journal of Physical Chemistry C*, vol. 119, no. 21. American Chemical Society (ACS), pp. 11982–11990, May 15, 2015. doi: 10.1021/acs.jpcc.5b01867.  
  
A. Cammarata and J. M. Rondinelli, “Spin-assisted covalent bond mechanism in “charge-ordering” perovskite oxides”, *Physical Review B*, vol. 86, no. 19. American Physical Society (APS), Nov. 30, 2012. doi: 10.1103/physrevb.86.195144.  
  
A. Cammarata and J. M. Rondinelli, “Octahedral engineering of orbital polarizations in charge transfer oxides”, *Physical Review B*, vol. 87, no. 15. American Physical Society (APS), Apr. 19, 2013. doi: 10.1103/physrevb.87.155135.  
  
A. Cammarata and J. M. Rondinelli, “Covalent dependence of octahedral rotations in orthorhombic perovskite oxides”, *The Journal of Chemical Physics*, vol. 141, no. 11. AIP Publishing, p. 114704, Sep. 21, 2014. doi: 10.1063/1.4895967.  
  
A. Cammarata and J. M. Rondinelli, “Ferroelectricity from coupled cooperative Jahn-Teller distortions and octahedral rotations in ordered Ruddlesden-Popper manganates”, *Physical Review B*, vol. 92, no. 1. American Physical Society (APS), Jul. 02, 2015. doi: 10.1103/physrevb.92.014102.  
  
A. Cammarata and J. Rondinelli, “Microscopic interactions governing phase matchability in nonlinear optical materials”, *Journal of Materials Chemistry C*, vol. 4, no. 24. Royal Society of Chemistry (RSC), pp. 5858–5863, 2016. doi: 10.1039/c6tc01633b.  
  
A. Cammarata and J. M. Rondinelli, “Electronic doping of transition metal oxide perovskites”, *Applied Physics Letters*, vol. 108, no. 21. AIP Publishing, p. 213109, May 23, 2016. doi: 10.1063/1.4953041.  
  
N. Charles and J. M. Rondinelli, “Microscopic origin of pressure-induced isosymmetric transitions in fluoromanganate cryolites”, *Physical Review B*, vol. 90, no. 9. American Physical Society (APS), Sep. 24, 2014. doi: 10.1103/physrevb.90.094114.  
  
K. A. Collins, R. J. Saballos, M. S. Fataftah, D. Puggioni, J. M. Rondinelliand D. E. Freedman, “Synthetic investigation of competing magnetic interactions in 2D metal–chloranilate radical frameworks”, *Chemical Science*, vol. 11, no. 23. Royal Society of Chemistry (RSC), pp. 5922–5928, 2020. doi: 10.1039/d0sc01994a.  
  
F. Ding, “Multimodal Structure Solution with 19F NMR Crystallography of Spin Singlet Molybdenum Oxyfluorides”, *Journal of the American Chemical Society*, vol. 142, no. 28. American Chemical Society (ACS), pp. 12288–12298, Jun. 12, 2020. doi: 10.1021/jacs.0c04019.  
  
G. Giovannetti, D. Puggioni, P. Barone, S. Picozzi, J. M. Rondinelliand M. Capone, “Magnetoelectric coupling in the type-I multiferroic ”, *Physical Review B*, vol. 94, no. 19. American Physical Society (APS), Nov. 09, 2016. doi: 10.1103/physrevb.94.195116.  
  
G. Giovannetti, D. Puggioni, J. M. Rondinelliand M. Capone, “Interplay between electron correlations and polar displacements in metallic”, *Physical Review B*, vol. 93, no. 11. American Physical Society (APS), Mar. 30, 2016. doi: 10.1103/physrevb.93.115147.  
  
G. Gou, M. Zhao, J. Shi, J. K. Haradaand J. M. Rondinelli, “Anion Ordered and Ferroelectric Ruddlesden–Popper Oxynitride Ca3Nb2N2O5 for Visible-Light-Active Photocatalysis”, *Chemistry of Materials*, vol. 32, no. 7. American Chemical Society (ACS), pp. 2815–2823, Mar. 05, 2020. doi: 10.1021/acs.chemmater.9b04429.  
  
M. Gu and J. M. Rondinelli, “Role of orbital filling on nonlinear ionic Raman scattering in perovskite titanates”, *Physical Review B*, vol. 95, no. 2. American Physical Society (APS), Jan. 11, 2017. doi: 10.1103/physrevb.95.024109.  
  
M. Gu and J. M. Rondinelli, “Coupled Raman-Raman modes in the ionic Raman scattering process”, *Applied Physics Letters*, vol. 113, no. 11. AIP Publishing, p. 112903, Sep. 10, 2018. doi: 10.1063/1.5048037.  
  
S. S. Hong, “Extreme tensile strain states in La 0.7 Ca 0.3 MnO 3 membranes”, *Science*, vol. 368, no. 6486. American Association for the Advancement of Science (AAAS), pp. 71–76, Apr. 03, 2020. doi: 10.1126/science.aax9753.  
  
F.-T. Huang, “Domain topology and domain switching kinetics in a hybrid improper ferroelectric”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, May 24, 2016. doi: 10.1038/ncomms11602.  
  
L.-F. Huang, M. J. Hutchison, R. J. Santucci Jr., J. R. Scullyand J. M. Rondinelli, “Improved Electrochemical Phase Diagrams from Theory and Experiment: The Ni–Water System and Its Complex Compounds”, *The Journal of Physical Chemistry C*, vol. 121, no. 18. American Chemical Society (ACS), pp. 9782–9789, May 01, 2017. doi: 10.1021/acs.jpcc.7b02771.  
  
L.-F. Huang, N. Z. Koocher, M. Guand J. M. Rondinelli, “Structure Dependent Phase Stability and Thermal Expansion of Ruddlesden–Popper Strontium Titanates”, *Chemistry of Materials*, vol. 30, no. 20. American Chemical Society (ACS), pp. 7100–7110, Sep. 26, 2018. doi: 10.1021/acs.chemmater.8b02944.  
  
L.-F. Huang and J. M. Rondinelli, “Reliable electrochemical phase diagrams of magnetic transition metals and related compounds from high-throughput ab initio calculations”, *npj Materials Degradation*, vol. 3, no. 1. Springer Science and Business Media LLC, Jun. 21, 2019. doi: 10.1038/s41529-019-0088-z.  
  
F. Jin, “Uniaxial Strain-Controlled Ground States in Manganite Films”, *Nano Letters*, vol. 20, no. 2. American Chemical Society (ACS), pp. 1131–1140, Jan. 24, 2020. doi: 10.1021/acs.nanolett.9b04506.  
  
T. H. Kim, “Polar metals by geometric design”, *Nature*, vol. 533, no. 7601. Springer Science and Business Media LLC, pp. 68–72, Apr. 20, 2016. doi: 10.1038/nature17628.  
  
R. A. Klein, “High-pressure synthesis of the perovskite”, *Physical Review Materials*, vol. 3, no. 6. American Physical Society (APS), Jun. 20, 2019. doi: 10.1103/physrevmaterials.3.064411.  
  
X.-Z. Lu and J. M. Rondinelli, “Epitaxial-strain-induced polar-to-nonpolar transitions in layered oxides”, *Nature Materials*, vol. 15, no. 9. Springer Science and Business Media LLC, pp. 951–955, Jun. 13, 2016. doi: 10.1038/nmat4664.  
  
X. Lu and J. M. Rondinelli, “Room Temperature Electric‐Field Control of Magnetism in Layered Oxides with Cation Order”, *Advanced Functional Materials*, vol. 27, no. 4. Wiley, p. 1604312, Dec. 12, 2016. doi: 10.1002/adfm.201604312.  
  
X.-Z. Lu and J. M. Rondinelli, “Discovery Principles and Materials for Symmetry-Protected Persistent Spin Textures with Long Spin Lifetimes”, *Matter*, vol. 3, no. 4. Elsevier BV, pp. 1211–1225, Oct. 2020. doi: 10.1016/j.matt.2020.08.028.  
  
A. S. McLeod, “Multi-messenger nanoprobes of hidden magnetism in a strained manganite”, *Nature Materials*, vol. 19, no. 4. Springer Science and Business Media LLC, pp. 397–404, Dec. 16, 2019. doi: 10.1038/s41563-019-0533-y.  
  
M. D. Scafetta, A. M. Cordi, J. M. Rondinelliand S. J. May, “Band structure and optical transitions in LaFeO3: theory and experiment”, *Journal of Physics: Condensed Matter*, vol. 26, no. 50. IOP Publishing, p. 505502, Nov. 19, 2014. doi: 10.1088/0953-8984/26/50/505502.  
  
E. C. Schueller, “Structural signatures of the insulator-to-metal transition in ”, *Physical Review Materials*, vol. 4, no. 10. American Physical Society (APS), Oct. 01, 2020. doi: 10.1103/physrevmaterials.4.104401.  
  
Y. Shin and J. M. Rondinelli, “Pressure effects on magnetism in -type ferrites and manganites”, *Physical Review B*, vol. 102, no. 10. American Physical Society (APS), Sep. 21, 2020. doi: 10.1103/physrevb.102.104426.  
  
G. Stone, “Atomic and electronic structure of domains walls in a polar metal”, *Physical Review B*, vol. 99, no. 1. American Physical Society (APS), Jan. 09, 2019. doi: 10.1103/physrevb.99.014105.  
  
C. C. Stoumpos, “Ruddlesden–Popper Hybrid Lead Iodide Perovskite 2D Homologous Semiconductors”, *Chemistry of Materials*, vol. 28, no. 8. American Chemical Society (ACS), pp. 2852–2867, Apr. 15, 2016. doi: 10.1021/acs.chemmater.6b00847.  
  
A. D. Tamerius, “Discovery of Cu 3 Pb”, *Angewandte Chemie International Edition*, vol. 57, no. 39. Wiley, pp. 12809–12813, Sep. 04, 2018. doi: 10.1002/anie.201807934.  
  
N. Wagner, D. Puggioniand J. M. Rondinelli, “Learning from Correlations Based on Local Structure: Rare-Earth Nickelates Revisited”, *Journal of Chemical Information and Modeling*, vol. 58, no. 12. American Chemical Society (ACS), pp. 2491–2501, Aug. 16, 2018. doi: 10.1021/acs.jcim.8b00411.  
  
J. Wang, “Physical properties of epitaxial SrMnO2.5−*δ* F *γ* oxyfluoride films”, *Journal of Physics: Condensed Matter*, vol. 31, no. 36. IOP Publishing, p. 365602, Jun. 19, 2019. doi: 10.1088/1361-648x/ab2414.  
  
J. Young and J. M. Rondinelli, “Improper ferroelectricity and piezoelectric responses in rhombohedral (,)perovskite oxides”, *Physical Review B*, vol. 89, no. 17. American Physical Society (APS), May 23, 2014. doi: 10.1103/physrevb.89.174110.  
  
J. Young and J. M. Rondinelli, “Inducing spontaneous electric polarizations in double perovskite iodide superlattices for ferroelectric photovoltaic materials”, *Physical Review Materials*, vol. 2, no. 6. American Physical Society (APS), Jun. 22, 2018. doi: 10.1103/physrevmaterials.2.065406.  
  
J. Young, A. Stroppa, S. Picozziand J. M. Rondinelli, “Tuning the ferroelectric polarization in AA′MnWO6 double perovskites through A cation substitution”, *Dalton Transactions*, vol. 44, no. 23. Royal Society of Chemistry (RSC), pp. 10644–10653, 2015. doi: 10.1039/c4dt03521f.  
  
D. Duncan, B. Magyari-Kopeand Y. Nishi, “Ab-Initio Modeling of the Resistance Switching Mechanism in RRAM Devices: Case Study of Hafnium Oxide (HfO2)”, *MRS Proceedings*, vol. 1430. Springer Science and Business Media LLC, 2012. doi: 10.1557/opl.2012.980.  
  
D. Duncan, B. Magyari-Kopeand Y. Nishi, “Filament-Induced Anisotropic Oxygen Vacancy Diffusion and Charge Trapping Effects in Hafnium Oxide RRAM”, *IEEE Electron Device Letters*, vol. 37, no. 4. Institute of Electrical and Electronics Engineers (IEEE), pp. 400–403, Apr. 2016. doi: 10.1109/led.2016.2524450.  
  
D. Duncan, B. Magyari-Köpeand Y. Nishi, “Hydrogen doping in HfO2 resistance change random access memory”, *Applied Physics Letters*, vol. 108, no. 4. AIP Publishing, p. 043501, Jan. 25, 2016. doi: 10.1063/1.4940369.  
  
L. Goux, J. Y. Kim, B. Magyari-Kope, Y. Nishi, A. Redolfiand M. Jurczak, “H-treatment impact on conductive-filament formation and stability in Ta2O5-based resistive-switching memory cells”, *Journal of Applied Physics*, vol. 117, no. 12. AIP Publishing, p. 124501, Mar. 23, 2015. doi: 10.1063/1.4915946.  
  
K. Kamiya, M. Y. Yang, B. Magyari-Köpe, Y. Nishiand K. Shiraishi, “Modeling of resistive random access memory (RRAM) switching mechanisms and memory structures”, *Advances in Non-volatile Memory and Storage Technology*. Elsevier, pp. 262–284e, 2014. doi: 10.1533/9780857098092.2.262.  
  
K. Kamiya, M. Y. Yang, B. Magyari-Kope, M. Niwa, Y. Nishiand K. Shiraishi, “Physics in designing desirable ReRAM stack structure &#x2014; Atomistic recipes based on oxygen chemical potential control and charge injection/removal”, *2012 International Electron Devices Meeting*. IEEE, Dec. 2012. doi: 10.1109/iedm.2012.6479078.  
  
K. Kamiya, M. Y. Yang, B. Magyari-Kope, M. Niwa, Y. Nishiand K. Shiraishi, “Vacancy Cohesion-Isolation Phase Transition Upon Charge Injection and Removal in Binary Oxide-Based RRAM Filamentary-Type Switching”, *IEEE Transactions on Electron Devices*, vol. 60, no. 10. Institute of Electrical and Electronics Engineers (IEEE), pp. 3400–3406, Oct. 2013. doi: 10.1109/ted.2013.2279397.  
  
J. Y. Kim, “First-Principles Study of Oxygen Vacancy and Hydrogen Impurity Effects in the Pseudo-Hexagonal Ta2O5”, *ECS Transactions*, vol. 58, no. 5. The Electrochemical Society, pp. 41–44, Aug. 31, 2013. doi: 10.1149/05805.0041ecst.  
  
J.-Y. Kim, B. Magyari-Köpe, K.-J. Lee, H.-S. Kim, S.-H. Leeand Y. Nishi, “Electronic structure and stability of low symmetry Ta2 O5 polymorphs”, *physica status solidi (RRL) - Rapid Research Letters*, vol. 8, no. 6. Wiley, pp. 560–565, May 20, 2014. doi: 10.1002/pssr.201409018.  
  
J.-Y. Kim, B. Magyari-Köpe, Y. Nishiand J.-H. Ahn, “First-principles study of carbon impurity effects in the pseudo-hexagonal Ta2O5”, *Current Applied Physics*, vol. 16, no. 6. Elsevier BV, pp. 638–643, Jun. 2016. doi: 10.1016/j.cap.2016.03.014.  
  
B. Magyari-Köpe and Y. Nishi, “Resistive Switching in Transition Metal Oxide ReRAM Devices”, *Extended Abstracts of the 2012 International Conference on Solid State Devices and Materials*. The Japan Society of Applied Physics, Sep. 27, 2012. doi: 10.7567/ssdm.2012.b-7-1.  
  
B. Magyari-Köpe, S. G. Park, H.-D. Leeand Y. Nishi, “First principles calculations of oxygen vacancy-ordering effects in resistance change memory materials incorporating binary transition metal oxides”, *Journal of Materials Science*, vol. 47, no. 21. Springer Science and Business Media LLC, pp. 7498–7514, Jun. 22, 2012. doi: 10.1007/s10853-012-6638-1.  
  
B. Magyari-Kope, “(Invited) The Interplay between Electronic and Ionic Transport in the Resistive Switching Process of Random Access Memory Devices”, *ECS Transactions*, vol. 64, no. 8. The Electrochemical Society, pp. 153–158, Aug. 09, 2014. doi: 10.1149/06408.0153ecst.  
  
B. Magyari-Kope, L. Zhao, Y. Nishi, K. Kamiya, M. Y. Yangand K. Shiraishi, “Ab initio modeling of resistive switching mechanism in binary metal oxides”, *2014 IEEE International Symposium on Circuits and Systems (ISCAS)*. IEEE, Jun. 2014. doi: 10.1109/iscas.2014.6865561.  
  
M. J. Mleczko, “Atomically-thin HfSe<inf>2</inf> transistors with native metal oxides”, *2016 74th Annual Device Research Conference (DRC)*. IEEE, Jun. 2016. doi: 10.1109/drc.2016.7548474.  
  
O. Pirrotta, A. Padovani, L. Larcher, L. Zhao, B. Magyari-Kopeand Y. Nishi, “Multi-scale modeling of oxygen vacancies assisted charge transport in sub-stoichiometric TiO<inf>x</inf> for RRAM application”, *2014 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)*. IEEE, Sep. 2014. doi: 10.1109/sispad.2014.6931557.  
  
L. Zhao, S. Clima, B. Magyari-Köpe, M. Jurczakand Y. Nishi, “*Ab initio* modeling of oxygen-vacancy formation in doped-HfOx RRAM: Effects of oxide phases, stoichiometry, and dopant concentrations”, *Applied Physics Letters*, vol. 107, no. 1. AIP Publishing, p. 013504, Jul. 06, 2015. doi: 10.1063/1.4926337.  
  
L. Zhao, S. G. Park, B. M. Kopeand Y. Nishi, “First-Principles Investigations of the Metal Doping Effects in TiO2 ReRAM”, *Extended Abstracts of the 2012 International Conference on Solid State Devices and Materials*. The Japan Society of Applied Physics, 2012. doi: 10.7567/ssdm.2012.ps-4-3.  
  
L. Zhao, S.-G. Park, B. Magyari-Köpeand Y. Nishi, “First-principles investigation of the conductive filament configuration in rutile TiO2-x ReRAM”, *MRS Proceedings*, vol. 1430. Springer Science and Business Media LLC, 2012. doi: 10.1557/opl.2012.1103.  
  
L. Zhao, S.-G. Park, B. Magyari-Köpeand Y. Nishi, “Dopant selection rules for desired electronic structure and vacancy formation characteristics of TiO2 resistive memory”, *Applied Physics Letters*, vol. 102, no. 8. AIP Publishing, p. 083506, Feb. 25, 2013. doi: 10.1063/1.4794083.  
  
L. Zhao, S.-G. Park, B. Magyari-Köpeand Y. Nishi, “First principles modeling of charged oxygen vacancy filaments in reduced TiO 2 –implications to the operation of non-volatile memory devices”, *Mathematical and Computer Modelling*, vol. 58, no. 1–2. Elsevier BV, pp. 275–281, Jul. 2013. doi: 10.1016/j.mcm.2012.11.009.  
  
L. Zhao, “Ultrathin (&#x223C;2nm) HfO<inf>x</inf> as the fundamental resistive switching element: Thickness scaling limit, stack engineering and 3D integration”, *2014 IEEE International Electron Devices Meeting*. IEEE, Dec. 2014. doi: 10.1109/iedm.2014.7046998.  
  
T. C. Asmara, “Tunable and low-loss correlated plasmons in Mott-like insulating oxides”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, May 12, 2017. doi: 10.1038/ncomms15271.  
  
M. de Jong, I. Winter, D. C. Chrzanand M. Asta, “Ideal strength and ductility in metals from second- and third-order elastic constants”, *Physical Review B*, vol. 96, no. 1. American Physical Society (APS), Jul. 10, 2017. doi: 10.1103/physrevb.96.014105.  
  
T. Frolov and M. Asta, “Step free energies at faceted solid-liquid interfaces from equilibrium molecular dynamics simulations”, *The Journal of Chemical Physics*, vol. 137, no. 21. AIP Publishing, p. 214108, Dec. 07, 2012. doi: 10.1063/1.4769381.  
  
D. Y. Wan, “Electron transport and visible light absorption in a plasmonic photocatalyst based on strontium niobate”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Apr. 19, 2017. doi: 10.1038/ncomms15070.  
  
L. Ahmed, B. Rasulev, M. Turabekova, D. Leszczynskaand J. Leszczynski, “Receptor- and ligand-based study of fullerene analogues: comprehensive computational approach including quantum-chemical, QSAR and molecular docking simulations”, *Organic & Biomolecular Chemistry*, vol. 11, no. 35. Royal Society of Chemistry (RSC), p. 5798, 2013. doi: 10.1039/c3ob40878g.  
  
S. J. Capuzzi, R. Politi, O. Isayev, S. Faragand A. Tropsha, “QSAR Modeling of Tox21 Challenge Stress Response and Nuclear Receptor Signaling Toxicity Assays”, *Frontiers in Environmental Science*, vol. 4. Frontiers Media SA, Feb. 04, 2016. doi: 10.3389/fenvs.2016.00003.  
  
A. Golbamaki, N. Golbamaki, N. Sizochenko, B. Rasulev, J. Leszczynskiand E. Benfenati, “Genotoxicity induced by metal oxide nanoparticles: a weight of evidence study and effect of particle surface and electronic properties”, *Nanotoxicology*, vol. 12, no. 10. Informa UK Limited, pp. 1113–1129, Jun. 09, 2018. doi: 10.1080/17435390.2018.1478999.  
  
A. Golbamaki, N. Golbamaki, N. Sizochenko, B. Rasulev, J. Leszczynskiand E. Benfenati, “Genotoxicity induced by metal oxide nanoparticles: a weight of evidence study and effect of particle surface and electronic properties”, *Nanotoxicology*, vol. 12, no. 10. Informa UK Limited, pp. 1113–1129, Jun. 09, 2018. doi: 10.1080/17435390.2018.1478999.  
  
A. Golius, L. Gorb, O. Isayevand J. Leszczynski, “Diffusion of energetic compounds through biological membrane: Application of classical MD and COSMOmic approximations”, *Journal of Biomolecular Structure and Dynamics*, vol. 37, no. 1. Informa UK Limited, pp. 247–255, Jan. 19, 2018. doi: 10.1080/07391102.2018.1424037.  
  
A. Golius, “Experimental and computational study of membrane affinity for selected energetic compounds”, *Chemosphere*, vol. 148. Elsevier BV, pp. 322–327, Apr. 2016. doi: 10.1016/j.chemosphere.2016.01.010.  
  
A. Gooch, N. Sizochenko, L. Sviatenko, L. Gorband J. Leszczynski, “A quantum chemical based toxicity study of estimated reduction potential and hydrophobicity in series of nitroaromatic compounds”, *SAR and QSAR in Environmental Research*, vol. 28, no. 2. Informa UK Limited, pp. 133–150, Feb. 01, 2017. doi: 10.1080/1062936x.2017.1286687.  
  
L. Gorb, M. Ilchenkoand J. Leszczynski, “A density functional theory study of simplest nanocomposites formed by graphene oxide and polyvinyl alcohol: geometry, interaction energy and vibrational spectrum”, *Journal of Molecular Modeling*, vol. 26, no. 7. Springer Science and Business Media LLC, Jun. 25, 2020. doi: 10.1007/s00894-020-04447-9.  
  
J. Gu, J. Wangand J. Leszczynski, “Electron interaction with a DNA duplex: dCpdC:dGpdG”, *Physical Chemistry Chemical Physics*, vol. 18, no. 19. Royal Society of Chemistry (RSC), pp. 13657–13665, 2016. doi: 10.1039/c6cp01408a.  
  
O. Isayev, C. Oses, C. Toher, E. Gossett, S. Curtaroloand A. Tropsha, “Universal fragment descriptors for predicting properties of inorganic crystals”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Jun. 05, 2017. doi: 10.1038/ncomms15679.  
  
C. P. Johnston, “Catalytic enantioselective synthesis of indanes by a cation-directed 5-endo-trig cyclization”, *Nature Chemistry*, vol. 7, no. 2. Springer Science and Business Media LLC, pp. 171–177, Jan. 12, 2015. doi: 10.1038/nchem.2150.  
  
K. Kapusta, N. Sizochenko, S. Karabulut, S. Okovytyy, E. Voronkovand J. Leszczynski, “QSPR modeling of optical rotation of amino acids using specific quantum chemical descriptors”, *Journal of Molecular Modeling*, vol. 24, no. 3. Springer Science and Business Media LLC, Feb. 17, 2018. doi: 10.1007/s00894-018-3593-z.  
  
K. Kapusta, N. Sizochenko, S. Karabulut, S. Okovytyy, E. Voronkovand J. Leszczynski, “QSPR modeling of optical rotation of amino acids using specific quantum chemical descriptors”, *Journal of Molecular Modeling*, vol. 24, no. 3. Springer Science and Business Media LLC, Feb. 17, 2018. doi: 10.1007/s00894-018-3593-z.  
  
K. Kapusta, E. Voronkov, S. Okovytyy, V. Korobovand J. Leszczynski, “Reconstruction of STO-3G Family Basis Set for the Accurate Calculation of Magnetic Properties”, *Russian Journal of Physical Chemistry A*, vol. 92, no. 13. Pleiades Publishing Ltd, pp. 2827–2834, Dec. 2018. doi: 10.1134/s0036024418130174.  
  
K. Kapusta, E. Voronkov, S. Okovytyy, V. Korobovand J. Leszczynski, “Reconstruction of STO-3G Family Basis Set for the Accurate Calculation of Magnetic Properties”, *Russian Journal of Physical Chemistry A*, vol. 92, no. 13. Pleiades Publishing Ltd, pp. 2827–2834, Dec. 2018. doi: 10.1134/s0036024418130174.  
  
S. Kar, J. Roy, D. Leszczynskaand J. Leszczynski, “Power Conversion Efficiency of Arylamine Organic Dyes for Dye-Sensitized Solar Cells (DSSCs) Explicit to Cobalt Electrolyte: Understanding the Structural Attributes Using a Direct QSPR Approach”, *Computation*, vol. 5, no. 4. MDPI AG, p. 2, Dec. 23, 2016. doi: 10.3390/computation5010002.  
  
S. Kar, J. K. Royand J. Leszczynski, “In silico designing of power conversion efficient organic lead dyes for solar cells using todays innovative approaches to assure renewable energy for future”, *npj Computational Materials*, vol. 3, no. 1. Springer Science and Business Media LLC, Jun. 21, 2017. doi: 10.1038/s41524-017-0025-z.  
  
M. Khan, S. Kar, J. Wangand J. Leszczynski, “Theoretical study of formate, tartrate, tartronate, and glycolate production from 6-carbon trioxylate intermediate in the citric acid cycle”, *Journal of Molecular Modeling*, vol. 25, no. 12. Springer Science and Business Media LLC, Nov. 15, 2019. doi: 10.1007/s00894-019-4240-z.  
  
E. Kiss, “A Counterion-Directed Approach to the Diels-Alder Paradigm: Cascade Synthesis of Tricyclic Fused Cyclopropanes”, *Angewandte Chemie International Edition*, vol. 55, no. 44. Wiley, pp. 13813–13817, Oct. 07, 2016. doi: 10.1002/anie.201608534.  
  
K. Klimenko, “Novel enhanced applications of QSPR models: Temperature dependence of aqueous solubility”, *Journal of Computational Chemistry*, vol. 37, no. 22. Wiley, pp. 2045–2051, Jun. 24, 2016. doi: 10.1002/jcc.24424.  
  
P. Mazierski, “Systematic and detailed examination of NaYF4-Er-Yb-TiO2 photocatalytic activity under Vis–NIR irradiation: Experimental and theoretical analyses”, *Applied Surface Science*, vol. 536. Elsevier BV, p. 147805, Jan. 2021. doi: 10.1016/j.apsusc.2020.147805.  
  
A. Mikolajczyk, H. P. Pinto, A. Gajewicz, T. Puzynand J. Leszczynski, “<i>Ab Initio</i> Studies of Anatase TiO<sub>2</sub> (101) Surface-supported Au<sub>8</sub> Clusters”, *Current Topics in Medicinal Chemistry*, vol. 15, no. 18. Bentham Science Publishers Ltd., pp. 1859–1867, Jun. 16, 2015. doi: 10.2174/1568026615666150506151826.  
  
A. Mirchi, N. Sizochenkoand J. Leszczynski, “Fullerene quinazolinone conjugates targeting Mycobacterium tuberculosis: a combined molecular docking, QSAR, and ONIOM approach”, *Structural Chemistry*, vol. 29, no. 3. Springer Science and Business Media LLC, pp. 765–775, Mar. 10, 2018. doi: 10.1007/s11224-018-1100-x.  
  
A. Mirchi, N. Sizochenkoand J. Leszczynski, “Fullerene quinazolinone conjugates targeting Mycobacterium tuberculosis: a combined molecular docking, QSAR, and ONIOM approach”, *Structural Chemistry*, vol. 29, no. 3. Springer Science and Business Media LLC, pp. 765–775, Mar. 10, 2018. doi: 10.1007/s11224-018-1100-x.  
  
T. Moot, “Material informatics driven design and experimental validation of lead titanate as an aqueous solar photocathode”, *Materials Discovery*, vol. 6. Elsevier BV, pp. 9–16, Oct. 2016. doi: 10.1016/j.md.2017.04.001.  
  
M. Popova, O. Isayevand A. Tropsha, “Deep reinforcement learning for de novo drug design”, *Science Advances*, vol. 4, no. 7. American Association for the Advancement of Science (AAAS), Jul. 06, 2018. doi: 10.1126/sciadv.aap7885.  
  
M. Popova, O. Isayevand A. Tropsha, “Deep reinforcement learning for de novo drug design”, *Science Advances*, vol. 4, no. 7. American Association for the Advancement of Science (AAAS), Jul. 06, 2018. doi: 10.1126/sciadv.aap7885.  
  
H. Reis, B. Rasulev, M. G. Papadopoulosand J. Leszczynski, “Reliable but Timesaving: In Search of an Efficient Quantum-chemical Method for the Description of Functional Fullerenes”, *Current Topics in Medicinal Chemistry*, vol. 15, no. 18. Bentham Science Publishers Ltd., pp. 1845–1858, Jun. 16, 2015. doi: 10.2174/1568026615666150506150601.  
  
J. K. Roy, S. Karand J. Leszczynski, “Electronic Structure and Optical Properties of Designed Photo-Efficient Indoline-Based Dye-Sensitizers with D–A−π–A Framework”, *The Journal of Physical Chemistry C*, vol. 123, no. 6. American Chemical Society (ACS), pp. 3309–3320, Jan. 18, 2019. doi: 10.1021/acs.jpcc.8b10708.  
  
J. K. Roy, S. Karand J. Leszczynski, “Optoelectronic Properties of C60 and C70 Fullerene Derivatives: Designing and Evaluating Novel Candidates for Efficient P3HT Polymer Solar Cells”, *Materials*, vol. 12, no. 14. MDPI AG, p. 2282, Jul. 16, 2019. doi: 10.3390/ma12142282.  
  
J. K. Roy, S. Karand J. Leszczynski, “Revealing the Photophysical Mechanism of *N*,*N*′-Diphenyl-aniline Based Sensitizers with the D–D−π–A Framework: Theoretical Insights”, *ACS Sustainable Chemistry & Engineering*, vol. 8, no. 35. American Chemical Society (ACS), pp. 13328–13341, Aug. 10, 2020. doi: 10.1021/acssuschemeng.0c04061.  
  
J. K. Roy, E. S. Vasquez, H. P. Pinto, S. Kumari, K. B. Waltersand J. Leszczynski, “Computational and experimental approach to understanding the structural interplay of self-assembled end-terminated alkanethiolates on gold surfaces”, *Physical Chemistry Chemical Physics*, vol. 21, no. 42. Royal Society of Chemistry (RSC), pp. 23320–23328, 2019. doi: 10.1039/c9cp03613j.  
  
T. Sergeieva, “Origin of Substituent Effect on Tautomeric Behavior of 1,2,4-Triazole Derivatives: Combined Spectroscopic and Theoretical Study”, *The Journal of Physical Chemistry A*, vol. 120, no. 51. American Chemical Society (ACS), pp. 10116–10122, Dec. 15, 2016. doi: 10.1021/acs.jpca.6b08317.  
  
T. Y. Sergeieva, “Hydrazinolysis of 3-*R*-[1,2,4]Triazino[2,3-c]quinazolin-2-ones. Synthetic and Theoretical Aspects”, *The Journal of Physical Chemistry A*, vol. 118, no. 10. American Chemical Society (ACS), pp. 1895–1905, Feb. 26, 2014. doi: 10.1021/jp4052616.  
  
J. S. Smith, O. Isayevand A. E. Roitberg, “ANI-1: an extensible neural network potential with DFT accuracy at force field computational cost”, *Chemical Science*, vol. 8, no. 4. Royal Society of Chemistry (RSC), pp. 3192–3203, 2017. doi: 10.1039/c6sc05720a.  
  
J. S. Smith, O. Isayevand A. E. Roitberg, “ANI-1, A data set of 20 million calculated off-equilibrium conformations for organic molecules”, *Scientific Data*, vol. 4, no. 1. Springer Science and Business Media LLC, Dec. 19, 2017. doi: 10.1038/sdata.2017.193.  
  
J. S. Smith, B. Nebgen, N. Lubbers, O. Isayevand A. E. Roitberg, “Less is more: Sampling chemical space with active learning”, *The Journal of Chemical Physics*, vol. 148, no. 24. AIP Publishing, p. 241733, Jun. 28, 2018. doi: 10.1063/1.5023802.  
  
J. S. Smith, B. Nebgen, N. Lubbers, O. Isayevand A. E. Roitberg, “Less is more: Sampling chemical space with active learning”, *The Journal of Chemical Physics*, vol. 148, no. 24. AIP Publishing, p. 241733, Jun. 28, 2018. doi: 10.1063/1.5023802.  
  
L. K. Sviatenko, L. Gorb, F. C. Hill, D. Leszczynskaand J. Leszczynski, “Structure and electrochemical properties for complexes of nitrocompounds with inorganic ions: A theoretical approach”, *Journal of Computational Chemistry*, vol. 37, no. 13. Wiley, pp. 1206–1213, Jan. 26, 2016. doi: 10.1002/jcc.24310.  
  
L. K. Sviatenko, L. Gorb, F. C. Hill, D. Leszczynska, S. I. Okovytyyand J. Leszczynski, “Alkaline hydrolysis of hexahydro-1,3,5-trinitro-1,3,5-triazine: M06-2X investigation”, *Chemosphere*, vol. 134. Elsevier BV, pp. 31–38, Sep. 2015. doi: 10.1016/j.chemosphere.2015.03.064.  
  
L. K. Sviatenko, “In Silico Alkaline Hydrolysis of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine: Density Functional Theory Investigation”, *Environmental Science & Technology*, vol. 50, no. 18. American Chemical Society (ACS), pp. 10039–10046, Aug. 29, 2016. doi: 10.1021/acs.est.5b06130.  
  
L. K. Sviatenko, L. Gorb, D. Leszczynska, S. I. Okovytyy, M. K. Shuklaand J. Leszczynski, “In silico kinetics of alkaline hydrolysis of 1,3,5-trinitro-1,3,5-triazinane (RDX): M06-2X investigation”, *Environmental Science: Processes & Impacts*, vol. 19, no. 3. Royal Society of Chemistry (RSC), pp. 388–394, 2017. doi: 10.1039/c6em00565a.  
  
L. K. Sviatenko, L. Gorb, J. Leszczynski, D. Leszczynska, S. I. Okovytyyand M. K. Shukla, “A density functional theory investigation of degradation of Nitroguanidine in the photoactivated triplet state”, *Journal of Molecular Modeling*, vol. 25, no. 12. Springer Science and Business Media LLC, Dec. 2019. doi: 10.1007/s00894-019-4252-8.  
  
L. K. Sviatenko, L. Gorb, M. K. Shukla, J. M. Seiter, D. Leszczynskaand J. Leszczynski, “Adsorption of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20) on a soil organic matter. A DFT M05 computational study”, *Chemosphere*, vol. 148. Elsevier BV, pp. 294–299, Apr. 2016. doi: 10.1016/j.chemosphere.2016.01.011.  
  
L. K. Sviatenko, O. Isayev, L. Gorb, F. C. Hill, D. Leszczynskaand J. Leszczynski, “Are the reduction and oxidation properties of nitrocompounds dissolved in water different from those produced when adsorbed on a silica surface? A DFT M05-2X computational study”, *Journal of Computational Chemistry*, vol. 36, no. 14. Wiley, pp. 1029–1035, Mar. 03, 2015. doi: 10.1002/jcc.23878.  
  
L. Sviatenko, “Comprehensive Investigations of Kinetics of Alkaline Hydrolysis of TNT (2,4,6-Trinitrotoluene), DNT (2,4-Dinitrotoluene), and DNAN (2,4-Dinitroanisole)”, *Environmental Science & Technology*, vol. 48, no. 17. American Chemical Society (ACS), pp. 10465–10474, Aug. 15, 2014. doi: 10.1021/es5026678.  
  
V. Vargaljuk, S. Okovytyy, V. Polonskyy, O. Kramska, A. Shchukinand J. Leszczynski, “Copper Crystallization from Aqueous Solution: Initiation and Evolution of the Polynuclear Clusters”, *Journal of Cluster Science*, vol. 28, no. 5. Springer Science and Business Media LLC, pp. 2517–2528, May 20, 2017. doi: 10.1007/s10876-017-1239-4.  
  
J. Wang, J. Gu, M. Hossainand J. Leszczynski, “Theoretical Studies on Hydrogen Bonds in Anions Encapsulated by an Azamacrocyclic Receptor”, *Crystals*, vol. 6, no. 3. MDPI AG, p. 31, Mar. 22, 2016. doi: 10.3390/cryst6030031.  
  
M. Yengui, H. P. Pinto, J. Leszczynskiand D. Riedel, “Atomic scale study of corrugating and anticorrugating states on the bare Si(1 0 0) surface”, *Journal of Physics: Condensed Matter*, vol. 27, no. 4. IOP Publishing, p. 045001, Dec. 19, 2014. doi: 10.1088/0953-8984/27/4/045001.  
  
H. Yilmaz, B. Rasulevand J. Leszczynski, “Modeling the Dispersibility of Single Walled Carbon Nanotubes in Organic Solvents by Quantitative Structure-Activity Relationship Approach”, *Nanomaterials*, vol. 5, no. 2. MDPI AG, pp. 778–791, May 12, 2015. doi: 10.3390/nano5020778.  
  
T. Zubatiuk, G. Hill, D. Leszczynska, M. Fan, A. H. Ronyand J. Leszczynski, “Insight into mechanism of iron-oxides reduction in atmospheres of CH4 and CO”, *Chemical Physics Letters*, vol. 706. Elsevier BV, pp. 708–714, Aug. 2018. doi: 10.1016/j.cplett.2018.07.027.  
  
T. Zubatiuk, G. Hill, D. Leszczynska, M. Fan, A. H. Ronyand J. Leszczynski, “Insight into mechanism of iron-oxides reduction in atmospheres of CH4 and CO”, *Chemical Physics Letters*, vol. 706. Elsevier BV, pp. 708–714, Aug. 2018. doi: 10.1016/j.cplett.2018.07.027.  
  
T. Zubatiuk, “Structure and Binding Energy of Double-Stranded A-DNA Mini-helices: Quantum-Chemical Study”, *The Journal of Physical Chemistry B*, vol. 119, no. 40. American Chemical Society (ACS), pp. 12741–12749, Sep. 24, 2015. doi: 10.1021/acs.jpcb.5b04644.  
  
T. Zubatiuk, O. Shishkin, L. Gorb, D. Hovorunand J. Leszczynski, “Structural Waters in the Minor and Major Grooves of DNA—A Major Factor Governing Structural Adjustments of the A–T Mini-Helix”, *The Journal of Physical Chemistry B*, vol. 119, no. 2. American Chemical Society (ACS), pp. 381–391, Dec. 29, 2014. doi: 10.1021/jp5075225.  
  
E. T. Karim, M. Shugaev, C. Wu, Z. Lin, R. F. Hainseyand L. V. Zhigilei, “Atomistic simulation study of short pulse laser interactions with a metal target under conditions of spatial confinement by a transparent overlayer”, *Journal of Applied Physics*, vol. 115, no. 18. AIP Publishing, p. 183501, May 14, 2014. doi: 10.1063/1.4872245.  
  
E. T. Karim, C. Wuand L. V. Zhigilei, “Molecular Dynamics Simulations of Laser-Materials Interactions: General and Material-Specific Mechanisms of Material Removal and Generation of Crystal Defects”, *Fundamentals of Laser-Assisted Micro- and Nanotechnologies*. Springer International Publishing, pp. 27–49, 2014. doi: 10.1007/978-3-319-05987-7\_2.  
  
A. Abou-Saleh, “Spallation-induced roughness promoting high spatial frequency nanostructure formation on Cr”, *Applied Physics A*, vol. 124, no. 4. Springer Science and Business Media LLC, Mar. 14, 2018. doi: 10.1007/s00339-018-1716-0.  
  
M. He, C. Wu, M. V. Shugaev, G. D. Samolyukand L. V. Zhigilei, “Computational Study of Short-Pulse Laser-Induced Generation of Crystal Defects in Ni-Based Single-Phase Binary Solid–Solution Alloys”, *The Journal of Physical Chemistry C*, vol. 123, no. 4. American Chemical Society (ACS), pp. 2202–2215, Jan. 04, 2019. doi: 10.1021/acs.jpcc.8b09922.  
  
E. T. Karim, Z. Linand L. V. Zhigilei, “Molecular dynamics study of femtosecond laser interactions with Cr targets”, *AIP Conference Proceedings*. American Institute of Physics, 2012. doi: 10.1063/1.4739881.  
  
E. T. Karim, “Experimental characterization and atomistic modeling of interfacial void formation and detachment in short pulse laser processing of metal surfaces covered by solid transparent overlayers”, *Applied Physics A*, vol. 122, no. 4. Springer Science and Business Media LLC, Mar. 16, 2016. doi: 10.1007/s00339-016-9944-7.  
  
A. Naghilou, M. He, J. S. Schubert, L. V. Zhigileiand W. Kautek, “Femtosecond laser generation of microbumps and nanojets on single and bilayer Cu/Ag thin films”, *Physical Chemistry Chemical Physics*, vol. 21, no. 22. Royal Society of Chemistry (RSC), pp. 11846–11860, 2019. doi: 10.1039/c9cp02174d.  
  
C. M. Rouleau, C.-Y. Shih, C. Wu, L. V. Zhigilei, A. A. Puretzkyand D. B. Geohegan, “Nanoparticle generation and transport resulting from femtosecond laser ablation of ultrathin metal films: Time-resolved measurements and molecular dynamics simulations”, *Applied Physics Letters*, vol. 104, no. 19. AIP Publishing, p. 193106, May 12, 2014. doi: 10.1063/1.4876601.  
  
R. N. Salaway and L. V. Zhigilei, “Molecular dynamics simulations of thermal conductivity of carbon nanotubes: Resolving the effects of computational parameters”, *International Journal of Heat and Mass Transfer*, vol. 70. Elsevier BV, pp. 954–964, Mar. 2014. doi: 10.1016/j.ijheatmasstransfer.2013.11.065.  
  
X. Sedao, “Growth Twinning and Generation of High-Frequency Surface Nanostructures in Ultrafast Laser-Induced Transient Melting and Resolidification”, *ACS Nano*, vol. 10, no. 7. American Chemical Society (ACS), pp. 6995–7007, Jul. 12, 2016. doi: 10.1021/acsnano.6b02970.  
  
C.-Y. Shih, I. Gnilitskyi, M. V. Shugaev, E. Skoulas, E. Stratakisand L. V. Zhigilei, “Effect of a liquid environment on single-pulse generation of laser induced periodic surface structures and nanoparticles”, *Nanoscale*, vol. 12, no. 14. Royal Society of Chemistry (RSC), pp. 7674–7687, 2020. doi: 10.1039/d0nr00269k.  
  
C.-Y. Shih, M. V. Shugaev, C. Wuand L. V. Zhigilei, “Generation of Subsurface Voids, Incubation Effect, and Formation of Nanoparticles in Short Pulse Laser Interactions with Bulk Metal Targets in Liquid: Molecular Dynamics Study”, *The Journal of Physical Chemistry C*, vol. 121, no. 30. American Chemical Society (ACS), pp. 16549–16567, Jun. 22, 2017. doi: 10.1021/acs.jpcc.7b02301.  
  
C.-Y. Shih, M. V. Shugaev, C. Wuand L. V. Zhigilei, “The effect of pulse duration on nanoparticle generation in pulsed laser ablation in liquids: insights from large-scale atomistic simulations”, *Physical Chemistry Chemical Physics*, vol. 22, no. 13. Royal Society of Chemistry (RSC), pp. 7077–7099, 2020. doi: 10.1039/d0cp00608d.  
  
C.-Y. Shih, “Two mechanisms of nanoparticle generation in picosecond laser ablation in liquids: the origin of the bimodal size distribution”, *Nanoscale*, vol. 10, no. 15. Royal Society of Chemistry (RSC), pp. 6900–6910, 2018. doi: 10.1039/c7nr08614h.  
  
C.-Y. Shih, C. Wu, M. V. Shugaevand L. V. Zhigilei, “Atomistic modeling of nanoparticle generation in short pulse laser ablation of thin metal films in water”, *Journal of Colloid and Interface Science*, vol. 489. Elsevier BV, pp. 3–17, Mar. 2017. doi: 10.1016/j.jcis.2016.10.029.  
  
M. V. Shugaev, “Insights into Laser-Materials Interaction Through Modeling on Atomic and Macroscopic Scales”, *Advances in the Application of Lasers in Materials Science*. Springer International Publishing, pp. 107–148, 2018. doi: 10.1007/978-3-319-96845-2\_5.  
  
M. V. Shugaev, A. J. Manzo, C. Wu, V. Y. Zaitsev, H. Helvajianand L. V. Zhigilei, “Strong enhancement of surface diffusion by nonlinear surface acoustic waves”, *Physical Review B*, vol. 91, no. 23. American Physical Society (APS), Jun. 30, 2015. doi: 10.1103/physrevb.91.235450.  
  
M. V. Shugaev, C.-Y. Shih, E. T. Karim, C. Wuand L. V. Zhigilei, “Generation of nanocrystalline surface layer in short pulse laser processing of metal targets under conditions of spatial confinement by solid or liquid overlayer”, *Applied Surface Science*, vol. 417. Elsevier BV, pp. 54–63, Sep. 2017. doi: 10.1016/j.apsusc.2017.02.030.  
  
M. V. Shugaev, “Fundamentals of ultrafast laser–material interaction”, *MRS Bulletin*, vol. 41, no. 12. Springer Science and Business Media LLC, pp. 960–968, Dec. 2016. doi: 10.1557/mrs.2016.274.  
  
M. V. Shugaev, C. Wu, V. Y. Zaitsevand L. V. Zhigilei, “Molecular dynamics modeling of nonlinear propagation of surface acoustic waves”, *Journal of Applied Physics*, vol. 128, no. 4. AIP Publishing, p. 045117, Jul. 28, 2020. doi: 10.1063/5.0013302.  
  
M. V. Shugaev and L. V. Zhigilei, “Thermodynamic analysis and atomistic modeling of subsurface cavitation in photomechanical spallation”, *Computational Materials Science*, vol. 166. Elsevier BV, pp. 311–317, Aug. 2019. doi: 10.1016/j.commatsci.2019.05.017.  
  
A. N. Volkov, T. Shiga, D. Nicholson, J. Shiomiand L. V. Zhigilei, “Effect of bending buckling of carbon nanotubes on thermal conductivity of carbon nanotube materials”, *Journal of Applied Physics*, vol. 111, no. 5. AIP Publishing, p. 053501, Mar. 2012. doi: 10.1063/1.3687943.  
  
A. N. Volkov and L. V. Zhigilei, “Heat conduction in carbon nanotube materials: Strong effect of intrinsic thermal conductivity of carbon nanotubes”, *Applied Physics Letters*, vol. 101, no. 4. AIP Publishing, p. 043113, Jul. 23, 2012. doi: 10.1063/1.4737903.  
  
A. N. Volkov and L. V. Zhigilei, “Computational study of the role of gas-phase oxidation in CW laser ablation of Al target in an external supersonic air flow”, *Applied Physics A*, vol. 110, no. 3. Springer Science and Business Media LLC, pp. 537–546, Oct. 12, 2012. doi: 10.1007/s00339-012-7290-y.  
  
C. Wu, M. S. Christensen, J.-M. Savolainen, P. Ballingand L. V. Zhigilei, “Generation of subsurface voids and a nanocrystalline surface layer in femtosecond laser irradiation of a single-crystal Ag target”, *Physical Review B*, vol. 91, no. 3. American Physical Society (APS), Jan. 12, 2015. doi: 10.1103/physrevb.91.035413.  
  
C. Wu, E. T. Karim, A. N. Volkovand L. V. Zhigilei, “Atomic Movies of Laser-Induced Structural and Phase Transformations from Molecular Dynamics Simulations”, *Lasers in Materials Science*. Springer International Publishing, pp. 67–100, 2014. doi: 10.1007/978-3-319-02898-9\_4.  
  
C. Wu, V. Y. Zaitsevand L. V. Zhigilei, “Mechanism of acoustically induced diffusional structuring of surface adatoms”, *Applied Physics Letters*, vol. 103, no. 22. AIP Publishing, p. 221601, Nov. 25, 2013. doi: 10.1063/1.4832996.  
  
C. Wu, V. Y. Zaitsevand L. V. Zhigilei, “Acoustic Enhancement of Surface Diffusion”, *The Journal of Physical Chemistry C*, vol. 117, no. 18. American Chemical Society (ACS), pp. 9252–9258, May 01, 2013. doi: 10.1021/jp400884d.  
  
C. Wu and L. V. Zhigilei, “Microscopic mechanisms of laser spallation and ablation of metal targets from large-scale molecular dynamics simulations”, *Applied Physics A*, vol. 114, no. 1. Springer Science and Business Media LLC, pp. 11–32, Dec. 17, 2013. doi: 10.1007/s00339-013-8086-4.  
  
C. Wu and L. V. Zhigilei, “Nanocrystalline and Polyicosahedral Structure of a Nanospike Generated on Metal Surface Irradiated by a Single Femtosecond Laser Pulse”, *The Journal of Physical Chemistry C*, vol. 120, no. 8. American Chemical Society (ACS), pp. 4438–4447, Feb. 24, 2016. doi: 10.1021/acs.jpcc.6b00013.  
  
H. Wu, C. Wu, N. Zhang, X. Zhu, X. Maand L. V. Zhigilei, “Experimental and computational study of the effect of 1 atm background gas on nanoparticle generation in femtosecond laser ablation of metals”, *Applied Surface Science*, vol. 435. Elsevier BV, pp. 1114–1119, Mar. 2018. doi: 10.1016/j.apsusc.2017.11.190.  
  
L. V. Zhigilei, R. N. Salaway, B. K. Wittmaackand A. N. Volkov, “Computational Studies of Thermal Transport Properties of Carbon Nanotube Materials”, *Carbon Nanotubes for Interconnects*. Springer International Publishing, pp. 129–161, Jul. 10, 2016. doi: 10.1007/978-3-319-29746-0\_5.  
  
A. Bagusetty, P. Choudhury, W. A. Saidi, B. Derksen, E. Gattoand J. K. Johnson, “Facile Anhydrous Proton Transport on Hydroxyl Functionalized Graphane”, *Physical Review Letters*, vol. 118, no. 18. American Physical Society (APS), May 03, 2017. doi: 10.1103/physrevlett.118.186101.  
  
A. Bagusetty and J. K. Johnson, “Unraveling Anhydrous Proton Conduction in Hydroxygraphane”, *The Journal of Physical Chemistry Letters*, vol. 10, no. 3. American Chemical Society (ACS), pp. 518–523, Jan. 16, 2019. doi: 10.1021/acs.jpclett.8b03627.  
  
A. Bagusetty, J. Livingstonand J. K. Johnson, “Graphamine: Amine-Functionalized Graphane for Intrinsic Anhydrous Proton Conduction”, *The Journal of Physical Chemistry C*, vol. 123, no. 3. American Chemical Society (ACS), pp. 1566–1571, Dec. 27, 2018. doi: 10.1021/acs.jpcc.8b09001.  
  
T. Cai, J. K. Johnson, Y. Wuand X. Chen, “Toward Understanding the Kinetics of CO2 Capture on Sodium Carbonate”, *ACS Applied Materials & Interfaces*, vol. 11, no. 9. American Chemical Society (ACS), pp. 9033–9041, Feb. 07, 2019. doi: 10.1021/acsami.8b20000.  
  
L. Li, S. Zhang, J. P. Ruffleyand J. K. Johnson, “Energy Efficient Formaldehyde Synthesis by Direct Hydrogenation of Carbon Monoxide in Functionalized Metal–Organic Frameworks”, *ACS Sustainable Chemistry & Engineering*, vol. 7, no. 2. American Chemical Society (ACS), pp. 2508–2515, Dec. 15, 2018. doi: 10.1021/acssuschemeng.8b05413.  
  
J. Ye, L. Liand J. K. Johnson, “The effect of topology in Lewis pair functionalized metal organic frameworks on CO2 adsorption and hydrogenation”, *Catalysis Science & Technology*, vol. 8, no. 18. Royal Society of Chemistry (RSC), pp. 4609–4617, 2018. doi: 10.1039/c8cy01018h.  
  
J. H. Park, P. Choudhuryand A. C. Kummel, “NO Adsorption on Copper Phthalocyanine Functionalized Graphite”, *The Journal of Physical Chemistry C*, vol. 118, no. 19. American Chemical Society (ACS), pp. 10076–10082, May 01, 2014. doi: 10.1021/jp5002258.  
  
M. Wang, A. E. Likhtmanand B. D. Olsen, “Crossover between activated reptation and arm retraction mechanisms in entangled rod-coil block copolymers”, *The Journal of Chemical Physics*, vol. 143, no. 18. AIP Publishing, p. 184904, Nov. 14, 2015. doi: 10.1063/1.4933427.  
  
M. Wang, A. E. Likhtmanand B. D. Olsen, “Tube Curvature Slows the Motion of Rod–Coil Block Copolymers through Activated Reptation”, *ACS Macro Letters*, vol. 4, no. 2. American Chemical Society (ACS), pp. 242–246, Jan. 29, 2015. doi: 10.1021/mz5007377.  
  
M. Wang, K. Timachovaand B. D. Olsen, “Diffusion Mechanisms of Entangled Rod–Coil Diblock Copolymers”, *Macromolecules*, vol. 46, no. 14. American Chemical Society (ACS), pp. 5694–5701, Jul. 12, 2013. doi: 10.1021/ma400653g.  
  
M. Wang, K. Timachovaand B. D. Olsen, “Self-Diffusion and Constraint Release in Isotropic Entangled Rod–Coil Block Copolymers”, *Macromolecules*, vol. 48, no. 9. American Chemical Society (ACS), pp. 3121–3129, Apr. 28, 2015. doi: 10.1021/ma501954k.  
  
R. Dutta, B. Kiefer, E. Greenberg, V. B. Prakapenkaand T. S. Duffy, “Ultrahigh-Pressure Behavior of AO2 (A = Sn, Pb, Hf) Compounds”, *The Journal of Physical Chemistry C*, vol. 123, no. 45. American Chemical Society (ACS), pp. 27735–27741, Oct. 08, 2019. doi: 10.1021/acs.jpcc.9b06856.  
  
S. Ghazisaeed, J. Majzlan, J. Plášiland B. Kiefer, “A simple method for the prediction of the orientation of H2O molecules in ionic crystals”, *Journal of Applied Crystallography*, vol. 51, no. 4. International Union of Crystallography (IUCr), pp. 1116–1124, Jul. 13, 2018. doi: 10.1107/s1600576718008567.  
  
S. Ghazisaeed, M. Minuddin, H. Nakotteand B. Kiefer, “Density-functional-theory-predicted symmetry lowering from cubic to tetragonal in nickel hexacyanoferrate”, *Journal of Applied Crystallography*, vol. 53, no. 1. International Union of Crystallography (IUCr), pp. 117–126, Feb. 01, 2020. doi: 10.1107/s1600576719016492.  
  
G. R. Haripriya, “Contrasting the magnetism in double perovskites: The role of electronic and cationic disorder”, *Physical Review B*, vol. 99, no. 18. American Physical Society (APS), May 13, 2019. doi: 10.1103/physrevb.99.184411.  
  
J. Majzlan, “Thermodynamics and crystal chemistry of rhomboclase, (H5O2)Fe(SO4)2·2H2O, and the phase (H3O)Fe(SO4)2and implications for acid mine drainage”, *American Mineralogist*, vol. 102, no. 3. Mineralogical Society of America, pp. 643–654, Mar. 2017. doi: 10.2138/am-2017-5909.  
  
G. Steciuk, S. Ghazisaeed, B. Kieferand J. Plášil, “Crystal structure of vyacheslavite, U(PO4)(OH), solved from natural nanocrystal: a precession electron diffraction tomography (PEDT) study and DFT calculations”, *RSC Advances*, vol. 9, no. 34. Royal Society of Chemistry (RSC), pp. 19657–19661, 2019. doi: 10.1039/c9ra03694f.  
  
M. Dutt, O. Kuksenok, M. J. Nayhouse, S. R. Littleand A. C. Balazs, “Modeling the Self-Assembly of Lipids and Nanotubes in Solution: Forming Vesicles and Bicelles with Transmembrane Nanotube Channels”, *ACS Nano*, vol. 5, no. 6. American Chemical Society (ACS), pp. 4769–4782, May 31, 2011. doi: 10.1021/nn201260r.  
  
S. Lin, A. J. Hilmer, J. D. Mendenhall, M. S. Stranoand D. Blankschtein, “Molecular Perspective on Diazonium Adsorption for Controllable Functionalization of Single-Walled Carbon Nanotubes in Aqueous Surfactant Solutions”, *Journal of the American Chemical Society*, vol. 134, no. 19. American Chemical Society (ACS), pp. 8194–8204, May 04, 2012. doi: 10.1021/ja301635e.  
  
S. Lin, C.-J. Shih, M. S. Stranoand D. Blankschtein, “Molecular Insights into the Surface Morphology, Layering Structure, and Aggregation Kinetics of Surfactant-Stabilized Graphene Dispersions”, *Journal of the American Chemical Society*, vol. 133, no. 32. American Chemical Society (ACS), pp. 12810–12823, Jul. 22, 2011. doi: 10.1021/ja2048013.  
  
R. J. Lang and D. S. Simmons, “Interfacial Dynamic Length Scales in the Glass Transition of a Model Freestanding Polymer Film and Their Connection to Cooperative Motion”, *Macromolecules*, vol. 46, no. 24. American Chemical Society (ACS), pp. 9818–9825, Dec. 12, 2013. doi: 10.1021/ma401525q.  
  
M. E. Mackura and D. S. Simmons, “Enhancing heterogenous crystallization resistance in a bead-spring polymer model by modifying bond length”, *Journal of Polymer Science Part B: Polymer Physics*, vol. 52, no. 2. Wiley, pp. 134–140, Oct. 20, 2013. doi: 10.1002/polb.23398.  
  
B. K. Chu, I. W. Fu, C. B. Markegard, S. E. Choiand H. D. Nguyen, “A Tail of Two Peptide Amphiphiles: Effect of Conjugation with Hydrophobic Polymer on Folding of Peptide Sequences”, *Biomacromolecules*, vol. 15, no. 9. American Chemical Society (ACS), pp. 3313–3320, Aug. 08, 2014. doi: 10.1021/bm500733h.  
  
Y. Cote, I. W. Fu, E. T. Dobson, J. E. Goldberger, H. D. Nguyenand J. K. Shen, “Mechanism of the pH-Controlled Self-Assembly of Nanofibers from Peptide Amphiphiles”, *The Journal of Physical Chemistry C*, vol. 118, no. 29. American Chemical Society (ACS), pp. 16272–16278, Jul. 15, 2014. doi: 10.1021/jp5048024.  
  
I. W. Fu, C. B. Markegard, B. K. Chuand H. D. Nguyen, “The Role of Electrostatics and Temperature on Morphological Transitions of Hydrogel Nanostructures Self-Assembled by Peptide Amphiphiles Via Molecular Dynamics Simulations”, *Advanced Healthcare Materials*, vol. 2, no. 10. Wiley, pp. 1388–1400, Apr. 04, 2013. doi: 10.1002/adhm.201200400.  
  
I. W. Fu, C. B. Markegard, B. K. Chuand H. D. Nguyen, “Role of Hydrophobicity on Self-Assembly by Peptide Amphiphiles via Molecular Dynamics Simulations”, *Langmuir*, vol. 30, no. 26. American Chemical Society (ACS), pp. 7745–7754, Jun. 25, 2014. doi: 10.1021/la5012988.  
  
I. W. Fu, C. B. Markegardand H. D. Nguyen, “Solvent Effects on Kinetic Mechanisms of Self-Assembly by Peptide Amphiphiles via Molecular Dynamics Simulations”, *Langmuir*, vol. 31, no. 1. American Chemical Society (ACS), pp. 315–324, Dec. 22, 2014. doi: 10.1021/la503399x.  
  
I. W. Fu and H. D. Nguyen, “Sequence-Dependent Structural Stability of Self-Assembled Cylindrical Nanofibers by Peptide Amphiphiles”, *Biomacromolecules*, vol. 16, no. 7. American Chemical Society (ACS), pp. 2209–2219, Jun. 30, 2015. doi: 10.1021/acs.biomac.5b00595.  
  
C. B. Markegard, I. W. Fu, K. A. Reddyand H. D. Nguyen, “Coarse-Grained Simulation Study of Sequence Effects on DNA Hybridization in a Concentrated Environment”, *The Journal of Physical Chemistry B*, vol. 119, no. 5. American Chemical Society (ACS), pp. 1823–1834, Jan. 26, 2015. doi: 10.1021/jp509857k.  
  
C. B. Markegard, “Molecular Dynamics Simulations of Perylenediimide DNA Base Surrogates”, *The Journal of Physical Chemistry B*, vol. 119, no. 35. American Chemical Society (ACS), pp. 11459–11465, Aug. 21, 2015. doi: 10.1021/acs.jpcb.5b03874.  
  
A. Aryanfar, “Integrated Computational Modeling of Water Side Corrosion in Zirconium Metal Clad Under Nominal LWR Operating Conditions”, *JOM*, vol. 68, no. 11. Springer Science and Business Media LLC, pp. 2900–2911, Oct. 07, 2016. doi: 10.1007/s11837-016-2129-1.  
  
F. W. Herbert, A. Krishnamoorthy, K. J. Van Vlietand B. Yildiz, “Quantification of electronic band gap and surface states on FeS2(100)”, *Surface Science*, vol. 618. Elsevier BV, pp. 53–61, Dec. 2013. doi: 10.1016/j.susc.2013.08.014.  
  
F. W. Herbert, A. Krishnamoorthy, B. Yildizand K. J. Van Vliet, “Diffusion-limited kinetics of the antiferromagnetic to ferrimagnetic *λ*-transition in Fe1−xS”, *Applied Physics Letters*, vol. 106, no. 9. AIP Publishing, p. 092402, Mar. 02, 2015. doi: 10.1063/1.4913201.  
  
F. Hess and B. Yildiz, “Polar or not polar? The interplay between reconstruction, Sr enrichment, and reduction at the (001) surface”, *Physical Review Materials*, vol. 4, no. 1. American Physical Society (APS), Jan. 31, 2020. doi: 10.1103/physrevmaterials.4.015801.  
  
D. Kim, R. Bliem, F. Hess, J.-J. Galletand B. Yildiz, “Electrochemical Polarization Dependence of the Elastic and Electrostatic Driving Forces to Aliovalent Dopant Segregation on LaMnO3”, *Journal of the American Chemical Society*, vol. 142, no. 7. American Chemical Society (ACS), pp. 3548–3563, Jan. 14, 2020. doi: 10.1021/jacs.9b13040.  
  
A. Krishnamoorthy, M. A. Dinhand B. Yildiz, “Hydrogen weakens interlayer bonding in layered transition metal sulfide Fe1+xS”, *Journal of Materials Chemistry A*, vol. 5, no. 10. Royal Society of Chemistry (RSC), pp. 5030–5035, 2017. doi: 10.1039/c6ta10538f.  
  
A. Krishnamoorthy and B. Yildiz, “Quantifying the origin of inter-adsorbate interactions on reactive surfaces for catalyst screening and design”, *Physical Chemistry Chemical Physics*, vol. 17, no. 34. Royal Society of Chemistry (RSC), pp. 22227–22234, 2015. doi: 10.1039/c5cp03143e.  
  
Q. Lu, “Bi-directional tuning of thermal transport in SrCoOx with electrochemically induced phase transitions”, *Nature Materials*, vol. 19, no. 6. Springer Science and Business Media LLC, pp. 655–662, Feb. 24, 2020. doi: 10.1038/s41563-020-0612-0.  
  
D. Marrocchelli, L. Sunand B. Yildiz, “Dislocations in SrTiO3: Easy To Reduce but Not so Fast for Oxygen Transport”, *Journal of the American Chemical Society*, vol. 137, no. 14. American Chemical Society (ACS), pp. 4735–4748, Apr. 03, 2015. doi: 10.1021/ja513176u.  
  
U. Otgonbaatar, W. Ma, M. Youssefand B. Yildiz, “Effect of Niobium on the Defect Chemistry and Oxidation Kinetics of Tetragonal ZrO2”, *The Journal of Physical Chemistry C*, vol. 118, no. 35. American Chemical Society (ACS), pp. 20122–20131, Aug. 25, 2014. doi: 10.1021/jp504874v.  
  
N. Tsvetkov, Q. Lu, L. Sun, E. J. Crumlinand B. Yildiz, “Improved chemical and electrochemical stability of perovskite oxides with less reducible cations at the surface”, *Nature Materials*, vol. 15, no. 9. Springer Science and Business Media LLC, pp. 1010–1016, Jun. 13, 2016. doi: 10.1038/nmat4659.  
  
F. William Herbert, A. Krishnamoorthy, L. Rands, K. J. Van Vlietand B. Yildiz, “Magnetic diffusion anomaly at the Néel temperature of pyrrhotite, Fe1−xS”, *Physical Chemistry Chemical Physics*, vol. 17, no. 16. Royal Society of Chemistry (RSC), pp. 11036–11041, 2015. doi: 10.1039/c4cp05389c.  
  
J. Yang, M. Youssefand B. Yildiz, “Predicting point defect equilibria across oxide hetero-interfaces: model system of ZrO2/Cr2O3”, *Physical Chemistry Chemical Physics*, vol. 19, no. 5. Royal Society of Chemistry (RSC), pp. 3869–3883, 2017. doi: 10.1039/c6cp04997d.  
  
J. Yang, M. Youssefand B. Yildiz, “Oxygen self-diffusion mechanisms in monoclinic revealed and quantified by density functional theory, random walk analysis, and kinetic Monte Carlo calculations”, *Physical Review B*, vol. 97, no. 2. American Physical Society (APS), Jan. 29, 2018. doi: 10.1103/physrevb.97.024114.  
  
M. Youssef, M. Yangand B. Yildiz, “Doping in the Valley of Hydrogen Solubility: A Route to Designing Hydrogen-Resistant Zirconium Alloys”, *Physical Review Applied*, vol. 5, no. 1. American Physical Society (APS), Jan. 26, 2016. doi: 10.1103/physrevapplied.5.014008.  
  
M. Youssef and B. Yildiz, “Predicting self-diffusion in metal oxides from first principles: The case of oxygen in tetragonal ZrO”, *Physical Review B*, vol. 89, no. 2. American Physical Society (APS), Jan. 16, 2014. doi: 10.1103/physrevb.89.024105.  
  
J. Liu, E. Wang, Y. Zhao, X. Xu, J.-S. Moonand M. P. Anantram, “Impact of doping on bonding energy hierarchy and melting of phase change materials”, *Journal of Applied Physics*, vol. 124, no. 9. AIP Publishing, p. 094503, Sep. 07, 2018. doi: 10.1063/1.5039831.  
  
J. Liu, X. Xuand M. P. Anantram, “Role of inelastic electron–phonon scattering in electron transport through ultra-scaled amorphous phase change material nanostructures”, *Journal of Computational Electronics*, vol. 13, no. 3. Springer Science and Business Media LLC, pp. 620–626, May 16, 2014. doi: 10.1007/s10825-014-0579-7.  
  
J. Liu, X. Xu, L. Brushand M. P. Anantram, “A multi-scale analysis of the crystallization of amorphous germanium telluride using *ab initio* simulations and classical crystallization theory”, *Journal of Applied Physics*, vol. 115, no. 2. AIP Publishing, p. 023513, Jan. 14, 2014. doi: 10.1063/1.4861721.  
  
A. Aghaei and K. Dayal, “Symmetry-adapted non-equilibrium molecular dynamics of chiral carbon nanotubes under tensile loading”, *Journal of Applied Physics*, vol. 109, no. 12. AIP Publishing, p. 123501, Jun. 15, 2011. doi: 10.1063/1.3596827.  
  
A. Aghaei and K. Dayal, “Tension and twist of chiral nanotubes: torsional buckling, mechanical response and indicators of failure”, *Modelling and Simulation in Materials Science and Engineering*, vol. 20, no. 8. IOP Publishing, p. 085001, Oct. 02, 2012. doi: 10.1088/0965-0393/20/8/085001.  
  
A. Aghaei, K. Dayaland R. S. Elliott, “Anomalous phonon behavior of carbon nanotubes: First-order influence of external load”, *Journal of Applied Physics*, vol. 113, no. 2. AIP Publishing, p. 023503, Jan. 14, 2013. doi: 10.1063/1.4774077.  
  
A. Aghaei, K. Dayaland R. S. Elliott, “Symmetry-adapted phonon analysis of nanotubes”, *Journal of the Mechanics and Physics of Solids*, vol. 61, no. 2. Elsevier BV, pp. 557–578, Feb. 2013. doi: 10.1016/j.jmps.2012.09.008.  
  
V. Agrawal and K. Dayal, “A dynamic phase-field model for structural transformations and twinning: Regularized interfaces with transparent prescription of complex kinetics and nucleation. Part I: Formulation and one-dimensional characterization”, *Journal of the Mechanics and Physics of Solids*, vol. 85. Elsevier BV, pp. 270–290, Dec. 2015. doi: 10.1016/j.jmps.2015.04.010.  
  
V. Agrawal and K. Dayal, “A dynamic phase-field model for structural transformations and twinning: Regularized interfaces with transparent prescription of complex kinetics and nucleation. Part II: Two-dimensional characterization and boundary kinetics”, *Journal of the Mechanics and Physics of Solids*, vol. 85. Elsevier BV, pp. 291–307, Dec. 2015. doi: 10.1016/j.jmps.2015.05.001.  
  
V. Agrawal and K. Dayal, “Dependence of equilibrium Griffith surface energy on crack speed in phase-field models for fracture coupled to elastodynamics”, *International Journal of Fracture*, vol. 207, no. 2. Springer Science and Business Media LLC, pp. 243–249, Jul. 20, 2017. doi: 10.1007/s10704-017-0234-y.  
  
T. Breitzman and K. Dayal, “Bond-level deformation gradients and energy averaging in peridynamics”, *Journal of the Mechanics and Physics of Solids*, vol. 110. Elsevier BV, pp. 192–204, Jan. 2018. doi: 10.1016/j.jmps.2017.09.015.  
  
K. Dayal, “Leading-order nonlocal kinetic energy in peridynamics for consistent energetics and wave dispersion”, *Journal of the Mechanics and Physics of Solids*, vol. 105. Elsevier BV, pp. 235–253, Aug. 2017. doi: 10.1016/j.jmps.2017.05.002.  
  
K. Dayal and R. D. James, “Nonequilibrium molecular dynamics for bulk materials and nanostructures”, *Journal of the Mechanics and Physics of Solids*, vol. 58, no. 2. Elsevier BV, pp. 145–163, Feb. 2010. doi: 10.1016/j.jmps.2009.10.008.  
  
K. Dayal and R. D. James, “Design of viscometers corresponding to a universal molecular simulation method”, *Journal of Fluid Mechanics*, vol. 691. Cambridge University Press (CUP), pp. 461–486, Dec. 05, 2011. doi: 10.1017/jfm.2011.483.  
  
R. B. de Macedo, H. Pourmatin, T. Breitzmanand K. Dayal, “Disclinations without gradients: A nonlocal model for topological defects in liquid crystals”, *Extreme Mechanics Letters*, vol. 23. Elsevier BV, pp. 29–40, Sep. 2018. doi: 10.1016/j.eml.2018.07.005.  
  
M. Grasinger and K. Dayal, “Architected elastomer networks for optimal electromechanical response”, *Journal of the Mechanics and Physics of Solids*, vol. 146. Elsevier BV, p. 104171, Jan. 2021. doi: 10.1016/j.jmps.2020.104171.  
  
M. Grasinger and K. Dayal, “Statistical mechanical analysis of the electromechanical coupling in an electrically-responsive polymer chain”, *Soft Matter*, vol. 16, no. 27. Royal Society of Chemistry (RSC), pp. 6265–6284, 2020. doi: 10.1039/d0sm00845a.  
  
C.-T. Lu and K. Dayal, “Linear instability signals the initiation of motion of a twin plane under load”, *Philosophical Magazine Letters*, vol. 91, no. 4. Informa UK Limited, pp. 264–271, Apr. 2011. doi: 10.1080/09500839.2011.552448.  
  
J. Marshall and K. Dayal, “Atomistic-to-continuum multiscale modeling with long-range electrostatic interactions in ionic solids”, *Journal of the Mechanics and Physics of Solids*, vol. 62. Elsevier BV, pp. 137–162, Jan. 2014. doi: 10.1016/j.jmps.2013.09.025.  
  
X. Peng, N. Mathew, I. J. Beyerlein, K. Dayaland A. Hunter, “A 3D phase field dislocation dynamics model for body-centered cubic crystals”, *Computational Materials Science*, vol. 171. Elsevier BV, p. 109217, Jan. 2020. doi: 10.1016/j.commatsci.2019.109217.  
  
X. Peng, D. Nepaland K. Dayal, “Effective response of heterogeneous materials using the recursive projection method”, *Computer Methods in Applied Mechanics and Engineering*, vol. 364. Elsevier BV, p. 112946, Jun. 2020. doi: 10.1016/j.cma.2020.112946.  
  
H. Pourmatin and K. Dayal, “Multiscale real-space quantum-mechanical tight-binding calculations of electronic structure in crystals with defects using perfectly matched layers”, *Journal of Computational Physics*, vol. 323. Elsevier BV, pp. 115–125, Oct. 2016. doi: 10.1016/j.jcp.2016.07.024.  
  
E. Rosenbaum, M. Massoudiand K. Dayal, “Effects of Polydispersity on Structuring and Rheology in Flowing Suspensions”, *Journal of Applied Mechanics*, vol. 86, no. 8. ASME International, Apr. 19, 2019. doi: 10.1115/1.4043094.  
  
E. Rosenbaum, M. Massoudiand K. Dayal, “The Influence of Bubbles on Foamed Cement Viscosity Using an Extended Stokesian Dynamics Approach”, *Fluids*, vol. 4, no. 3. MDPI AG, p. 166, Sep. 06, 2019. doi: 10.3390/fluids4030166.  
  
E. Rosenbaum, M. Massoudiand K. Dayal, “Surfactant stabilized bubbles flowing in a Newtonian fluid”, *Mathematics and Mechanics of Solids*, vol. 24, no. 12. SAGE Publications, pp. 3823–3842, Jun. 26, 2019. doi: 10.1177/1081286519854508.  
  
E. Rosenbaum, M. Massoudiand K. Dayal, “The Influence of Bubbles on Foamed Cement Viscosity Using an Extended Stokesian Dynamics Approach”, *Fluids*, vol. 4, no. 3. MDPI AG, p. 166, Sep. 06, 2019. doi: 10.3390/fluids4030166.  
  
E. Rosenbaum, M. Massoudiand K. Dayal, “Effects of Polydispersity on Structuring and Rheology in Flowing Suspensions”, *Journal of Applied Mechanics*, vol. 86, no. 8. ASME International, Apr. 19, 2019. doi: 10.1115/1.4043094.  
  
E. Rosenbaum, M. Massoudiand K. Dayal, “Surfactant stabilized bubbles flowing in a Newtonian fluid”, *Mathematics and Mechanics of Solids*, vol. 24, no. 12. SAGE Publications, pp. 3823–3842, Jun. 26, 2019. doi: 10.1177/1081286519854508.  
  
L. Yang and K. Dayal, “Effect of lattice orientation, surface modulation, and applied fields on free-surface domain microstructure in ferroelectrics”, *Acta Materialia*, vol. 59, no. 17. Elsevier BV, pp. 6594–6603, Oct. 2011. doi: 10.1016/j.actamat.2011.07.014.  
  
L. Yang and K. Dayal, “A completely iterative method for the infinite domain electrostatic problem with nonlinear dielectric media”, *Journal of Computational Physics*, vol. 230, no. 21. Elsevier BV, pp. 7821–7829, Sep. 2011. doi: 10.1016/j.jcp.2011.07.001.  
  
L. Yang and K. Dayal, “Influence of strain on space-charge distribution at ferroelectric thin-film free surfaces”, *Acta Materialia*, vol. 60, no. 19. Elsevier BV, pp. 6457–6463, Nov. 2012. doi: 10.1016/j.actamat.2012.07.050.  
  
L. Yang and K. Dayal, “Microstructure and stray electric fields at surface cracks in ferroelectrics”, *International Journal of Fracture*, vol. 174, no. 1. Springer Science and Business Media LLC, pp. 17–27, Jan. 17, 2012. doi: 10.1007/s10704-011-9670-2.  
  
L. Yang and K. Dayal, “Real-space phase-field simulation of piezoresponse force microscopy accounting for stray electric fields”, *Modelling and Simulation in Materials Science and Engineering*, vol. 20, no. 3. IOP Publishing, p. 035021, Mar. 23, 2012. doi: 10.1088/0965-0393/20/3/035021.  
  
L. Yang and K. Dayal, “Free surface domain nucleation in a ferroelectric under an electrically charged tip”, *Journal of Applied Physics*, vol. 111, no. 1. AIP Publishing, p. 014106, Jan. 2012. doi: 10.1063/1.3674320.  
  
J. Glaser, J. Qin, P. Medapuramand D. C. Morse, “Collective and Single-Chain Correlations in Disordered Melts of Symmetric Diblock Copolymers: Quantitative Comparison of Simulations and Theory”, *Macromolecules*, vol. 47, no. 2. American Chemical Society (ACS), pp. 851–869, Jan. 13, 2014. doi: 10.1021/ma401694u.  
  
J. Glaser, J. Qin, P. Medapuram, M. Müllerand D. C. Morse, “Test of a scaling hypothesis for the structure factor of disordered diblock copolymer melts”, *Soft Matter*, vol. 8, no. 44. Royal Society of Chemistry (RSC), p. 11310, 2012. doi: 10.1039/c2sm26536b.  
  
E. J. G. Santos and E. Kaxiras, “Electric-Field Dependence of the Effective Dielectric Constant in Graphene”, *Nano Letters*, vol. 13, no. 3. American Chemical Society (ACS), pp. 898–902, Feb. 15, 2013. doi: 10.1021/nl303611v.  
  
W. L. Wang, “Direct Observation of a Long-Lived Single-Atom Catalyst Chiseling Atomic Structures in Graphene”, *Nano Letters*, vol. 14, no. 2. American Chemical Society (ACS), pp. 450–455, Feb. 03, 2014. doi: 10.1021/nl403327u.  
  
C. Backes, “Production of Highly Monolayer Enriched Dispersions of Liquid-Exfoliated Nanosheets by Liquid Cascade Centrifugation”, *ACS Nano*, vol. 10, no. 1. American Chemical Society (ACS), pp. 1589–1601, Jan. 12, 2016. doi: 10.1021/acsnano.5b07228.  
  
K. Kim, “Structural and Electrical Investigation of C60–Graphene Vertical Heterostructures”, *ACS Nano*, vol. 9, no. 6. American Chemical Society (ACS), pp. 5922–5928, Jun. 08, 2015. doi: 10.1021/acsnano.5b00581.  
  
S. Kumar, “Efficient Blue Electroluminescence Using Quantum-Confined Two-Dimensional Perovskites”, *ACS Nano*, vol. 10, no. 10. American Chemical Society (ACS), pp. 9720–9729, Oct. 03, 2016. doi: 10.1021/acsnano.6b05775.  
  
E. J. G. Santos and W. L. Wang, “Ultrafast charge-transfer in organic photovoltaic interfaces: geometrical and functionalization effects”, *Nanoscale*, vol. 8, no. 35. Royal Society of Chemistry (RSC), pp. 15902–15910, 2016. doi: 10.1039/c6nr02857h.  
  
T. Tian, P. Rice, E. J. G. Santosand C.-J. Shih, “Multiscale Analysis for Field-Effect Penetration through Two-Dimensional Materials”, *Nano Letters*, vol. 16, no. 8. American Chemical Society (ACS), pp. 5044–5052, Jul. 15, 2016. doi: 10.1021/acs.nanolett.6b01876.  
  
L. Yu, “High-Performance WSe2 Complementary Metal Oxide Semiconductor Technology and Integrated Circuits”, *Nano Letters*, vol. 15, no. 8. American Chemical Society (ACS), pp. 4928–4934, Jul. 28, 2015. doi: 10.1021/acs.nanolett.5b00668.  
  
E. J. G. Santos, “Electrical Spin Switch in Hydrogenated Multilayer Graphene”, *The Journal of Physical Chemistry C*, vol. 117, no. 12. American Chemical Society (ACS), pp. 6420–6425, Mar. 15, 2013. doi: 10.1021/jp310463k.  
  
E. J. G. Santos and E. Kaxiras, “Electrically Driven Tuning of the Dielectric Constant in MoS2 Layers”, *ACS Nano*, vol. 7, no. 12. American Chemical Society (ACS), pp. 10741–10746, Nov. 25, 2013. doi: 10.1021/nn403738b.  
  
E. J. G. Santos, “Carrier-Mediated Magnetoelectric Coupling in Functionalized Graphene”, *ACS Nano*, vol. 7, no. 11. American Chemical Society (ACS), pp. 9927–9932, Nov. 11, 2013. doi: 10.1021/nn4037877.  
  
K. Kim, E. J. G. Santos, T. H. Lee, Y. Nishiand Z. Bao, “Epitaxially Grown Strained Pentacene Thin Film on Graphene Membrane”, *Small*, vol. 11, no. 17. Wiley, pp. 2037–2043, Jan. 07, 2015. doi: 10.1002/smll.201403006.  
  
C.-H. Lee, “Epitaxial Growth of Molecular Crystals on van der Waals Substrates for High-Performance Organic Electronics”, *Advanced Materials*, vol. 26, no. 18. Wiley, pp. 2812–2817, Jan. 23, 2014. doi: 10.1002/adma.201304973.  
  
L. H. Li, “Dielectric Screening in Atomically Thin Boron Nitride Nanosheets”, *Nano Letters*, vol. 15, no. 1. American Chemical Society (ACS), pp. 218–223, Dec. 05, 2014. doi: 10.1021/nl503411a.  
  
D. Balamurugan, K. Plazonic, K. Abbey, S. Husainand N. Syed, “Building an Interactive Workbench Environment for Single Cell Genomics Applications”, *Practice and Experience in Advanced Research Computing*. ACM, Jul. 26, 2020. doi: 10.1145/3311790.3396634.  
  
G. A. Tritsaris, E. Kaxiras, S. Mengand E. Wang, “Adsorption and Diffusion of Lithium on Layered Silicon for Li-Ion Storage”, *Nano Letters*, vol. 13, no. 5. American Chemical Society (ACS), pp. 2258–2263, Apr. 23, 2013. doi: 10.1021/nl400830u.  
  
G. A. Tritsaris, K. Zhao, O. U. Okekeand E. Kaxiras, “Diffusion of Lithium in Bulk Amorphous Silicon: A Theoretical Study”, *The Journal of Physical Chemistry C*, vol. 116, no. 42. American Chemical Society (ACS), pp. 22212–22216, Oct. 10, 2012. doi: 10.1021/jp307221q.  
  
B. O. Alawode and A. M. Kolpak, “PbTiO3(001) Capped with ZnO(112̅0): An ab Initio Study of Effect of Substrate Polarization on Interface Composition and CO2 Dissociation”, *The Journal of Physical Chemistry Letters*, vol. 7, no. 7. American Chemical Society (ACS), pp. 1310–1314, Mar. 23, 2016. doi: 10.1021/acs.jpclett.6b00305.  
  
N. Artrith and A. M. Kolpak, “Grand canonical molecular dynamics simulations of Cu–Au nanoalloys in thermal equilibrium using reactive ANN potentials”, *Computational Materials Science*, vol. 110. Elsevier BV, pp. 20–28, Dec. 2015. doi: 10.1016/j.commatsci.2015.07.046.  
  
N. Artrith, W. Sailuam, S. Limpijumnongand A. M. Kolpak, “Reduced overpotentials for electrocatalytic water splitting over Fe- and Ni-modified BaTiO3”, *Physical Chemistry Chemical Physics*, vol. 18, no. 42. Royal Society of Chemistry (RSC), pp. 29561–29570, 2016. doi: 10.1039/c6cp06031e.  
  
J. S. Elias, “Elucidating the Nature of the Active Phase in Copper/Ceria Catalysts for CO Oxidation”, *ACS Catalysis*, vol. 6, no. 3. American Chemical Society (ACS), pp. 1675–1679, Feb. 09, 2016. doi: 10.1021/acscatal.5b02666.  
  
B. Kolb, L. C. Lentzand A. M. Kolpak, “Discovering charge density functionals and structure-property relationships with PROPhet: A general framework for coupling machine learning and first-principles methods”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Apr. 26, 2017. doi: 10.1038/s41598-017-01251-z.  
  
L. C. Lentz, B. Kolband A. M. Kolpak, “Control of valence and conduction band energies in layered transition metal phosphates via surface functionalization”, *Physical Chemistry Chemical Physics*, vol. 18, no. 20. Royal Society of Chemistry (RSC), pp. 14122–14128, 2016. doi: 10.1039/c6cp00994h.  
  
L. C. Lentz and A. M. Kolpak, “First-principles design of nanostructured hybrid photovoltaics based on layered transition metal phosphates”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Apr. 28, 2017. doi: 10.1038/s41598-017-01296-0.  
  
J. T. Mefford, “Water electrolysis on La1−xSrxCoO3−δ perovskite electrocatalysts”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Mar. 23, 2016. doi: 10.1038/ncomms11053.  
  
X. Rong and A. M. Kolpak, “Ab Initio Approach for Prediction of Oxide Surface Structure, Stoichiometry, and Electrocatalytic Activity in Aqueous Solution”, *The Journal of Physical Chemistry Letters*, vol. 6, no. 9. American Chemical Society (ACS), pp. 1785–1789, Apr. 28, 2015. doi: 10.1021/acs.jpclett.5b00509.  
  
X. Rong, J. Parolinand A. M. Kolpak, “A Fundamental Relationship between Reaction Mechanism and Stability in Metal Oxide Catalysts for Oxygen Evolution”, *ACS Catalysis*, vol. 6, no. 2. American Chemical Society (ACS), pp. 1153–1158, Jan. 19, 2016. doi: 10.1021/acscatal.5b02432.  
  
S. Wannakao, N. Artrith, J. Limtrakuland A. M. Kolpak, “Engineering Transition-Metal-Coated Tungsten Carbides for Efficient and Selective Electrochemical Reduction of CO2to Methane”, *ChemSusChem*, vol. 8, no. 16. Wiley, pp. 2745–2751, Jul. 17, 2015. doi: 10.1002/cssc.201500245.  
  
D. K. Bediako, “Heterointerface effects in the electrointercalation of van der Waals heterostructures”, *Nature*, vol. 558, no. 7710. Springer Science and Business Media LLC, pp. 425–429, Jun. 2018. doi: 10.1038/s41586-018-0205-0.  
  
W. Chen, “Effect of Frustrated Rotations on the Pre-Exponential Factor for Unimolecular Reactions on Surfaces: A Case Study of Alkoxy Dehydrogenation”, *The Journal of Physical Chemistry C*, vol. 124, no. 2. American Chemical Society (ACS), pp. 1429–1437, Dec. 23, 2019. doi: 10.1021/acs.jpcc.9b10017.  
  
R. K. Defo, S. Fang, S. N. Shirodkar, G. A. Tritsaris, A. Dimoulasand E. Kaxiras, “Strain dependence of band gaps and exciton energies in pure and mixed transition-metal dichalcogenides”, *Physical Review B*, vol. 94, no. 15. American Physical Society (APS), Oct. 27, 2016. doi: 10.1103/physrevb.94.155310.  
  
S. Fang, S. Carr, M. A. Cazalillaand E. Kaxiras, “Electronic structure theory of strained two-dimensional materials with hexagonal symmetry”, *Physical Review B*, vol. 98, no. 7. American Physical Society (APS), Aug. 06, 2018. doi: 10.1103/physrevb.98.075106.  
  
S. Fang and E. Kaxiras, “Electronic structure theory of weakly interacting bilayers”, *Physical Review B*, vol. 93, no. 23. American Physical Society (APS), Jun. 27, 2016. doi: 10.1103/physrevb.93.235153.  
  
S. Fang, R. Kuate Defo, S. N. Shirodkar, S. Lieu, G. A. Tritsarisand E. Kaxiras, “*Ab initio* tight-binding Hamiltonian for transition metal dichalcogenides”, *Physical Review B*, vol. 92, no. 20. American Physical Society (APS), Nov. 05, 2015. doi: 10.1103/physrevb.92.205108.  
  
M. M. Islam, G. Kolesov, T. Verstraelen, E. Kaxirasand A. C. T. van Duin, “eReaxFF: A Pseudoclassical Treatment of Explicit Electrons within Reactive Force Field Simulations”, *Journal of Chemical Theory and Computation*, vol. 12, no. 8. American Chemical Society (ACS), pp. 3463–3472, Jul. 25, 2016. doi: 10.1021/acs.jctc.6b00432.  
  
G. Kolesov, E. Kaxirasand E. Manousakis, “Density functional theory beyond the Born-Oppenheimer approximation: Accurate treatment of the ionic zero-point motion”, *Physical Review B*, vol. 98, no. 19. American Physical Society (APS), Nov. 12, 2018. doi: 10.1103/physrevb.98.195112.  
  
G. Kolesov, D. Vinichenko, G. A. Tritsaris, C. M. Friendand E. Kaxiras, “Anatomy of the Photochemical Reaction: Excited-State Dynamics Reveals the C–H Acidity Mechanism of Methoxy Photo-oxidation on Titania”, *The Journal of Physical Chemistry Letters*, vol. 6, no. 9. American Chemical Society (ACS), pp. 1624–1627, Apr. 15, 2015. doi: 10.1021/acs.jpclett.5b00429.  
  
R. Kuate Defo, E. Kaxirasand S. L. Richardson, “How carbon vacancies can affect the properties of group IV color centers in diamond: A study of thermodynamics and kinetics”, *Journal of Applied Physics*, vol. 126, no. 19. AIP Publishing, p. 195103, Nov. 21, 2019. doi: 10.1063/1.5123227.  
  
R. Kuate Defo, X. Zhang, D. Bracher, G. Kim, E. Huand E. Kaxiras, “Energetics and kinetics of vacancy defects in -SiC”, *Physical Review B*, vol. 98, no. 10. American Physical Society (APS), Sep. 04, 2018. doi: 10.1103/physrevb.98.104103.  
  
D. T. Larson, S. Carr, G. A. Tritsarisand E. Kaxiras, “Effects of lithium intercalation in twisted bilayer graphene”, *Physical Review B*, vol. 101, no. 7. American Physical Society (APS), Feb. 05, 2020. doi: 10.1103/physrevb.101.075407.  
  
D. T. Larson, I. Fampiou, G. Kimand E. Kaxiras, “Lithium Intercalation in Graphene–MoS2 Heterostructures”, *The Journal of Physical Chemistry C*, vol. 122, no. 43. American Chemical Society (ACS), pp. 24535–24541, Oct. 09, 2018. doi: 10.1021/acs.jpcc.8b07548.  
  
I. Lovchinsky, “Magnetic resonance spectroscopy of an atomically thin material using a single-spin qubit”, *Science*, vol. 355, no. 6324. American Association for the Advancement of Science (AAAS), pp. 503–507, Feb. 03, 2017. doi: 10.1126/science.aal2538.  
  
A. Nourbakhsh, “MoS2 Field-Effect Transistor with Sub-10 nm Channel Length”, *Nano Letters*, vol. 16, no. 12. American Chemical Society (ACS), pp. 7798–7806, Nov. 10, 2016. doi: 10.1021/acs.nanolett.6b03999.  
  
B. Onat, E. D. Cubuk, B. D. Maloneand E. Kaxiras, “Implanted neural network potentials: Application to Li-Si alloys”, *Physical Review B*, vol. 97, no. 9. American Physical Society (APS), Mar. 20, 2018. doi: 10.1103/physrevb.97.094106.  
  
T. D. Rhone, “Data-driven studies of magnetic two-dimensional materials”, *Scientific Reports*, vol. 10, no. 1. Springer Science and Business Media LLC, Sep. 25, 2020. doi: 10.1038/s41598-020-72811-z.  
  
M. G. Sensoy, D. Vinichenko, W. Chen, C. M. Friendand E. Kaxiras, “Strain effects on the behavior of isolated and paired sulfur vacancy defects in monolayer ”, *Physical Review B*, vol. 95, no. 1. American Physical Society (APS), Jan. 17, 2017. doi: 10.1103/physrevb.95.014106.  
  
S. N. Shirodkar and E. Kaxiras, “Li intercalation at graphene/hexagonal boron nitride interfaces”, *Physical Review B*, vol. 93, no. 24. American Physical Society (APS), Jun. 30, 2016. doi: 10.1103/physrevb.93.245438.  
  
G. A. Tritsaris, B. D. Maloneand E. Kaxiras, “Structural stability and electronic properties of low-index surfaces of SnS”, *Journal of Applied Physics*, vol. 115, no. 17. AIP Publishing, p. 173702, May 07, 2014. doi: 10.1063/1.4874775.  
  
G. A. Tritsaris, M. G. Şensoy, S. N. Shirodkarand E. Kaxiras, “First-principles study of coupled effect of ripplocations and S-vacancies in MoS2”, *Journal of Applied Physics*, vol. 126, no. 8. AIP Publishing, p. 084303, Aug. 28, 2019. doi: 10.1063/1.5099496.  
  
G. A. Tritsaris, “Perturbation theory for weakly coupled two-dimensional layers”, *Journal of Materials Research*, vol. 31, no. 7. Springer Science and Business Media LLC, pp. 959–966, Mar. 28, 2016. doi: 10.1557/jmr.2016.99.  
  
D. Vinichenko, M. G. Sensoy, C. M. Friendand E. Kaxiras, “Accurate formation energies of charged defects in solids: A systematic approach”, *Physical Review B*, vol. 95, no. 23. American Physical Society (APS), Jun. 30, 2017. doi: 10.1103/physrevb.95.235310.  
  
M. Wen, S. N. Shirodkar, P. Plecháč, E. Kaxiras, R. S. Elliottand E. B. Tadmor, “A force-matching Stillinger-Weber potential for MoS2: Parameterization and Fisher information theory based sensitivity analysis”, *Journal of Applied Physics*, vol. 122, no. 24. AIP Publishing, p. 244301, Dec. 28, 2017. doi: 10.1063/1.5007842.  
  
Y. Yang, “Enhanced superconductivity upon weakening of charge density wave transport in in the two-dimensional limit”, *Physical Review B*, vol. 98, no. 3. American Physical Society (APS), Jul. 20, 2018. doi: 10.1103/physrevb.98.035203.  
  
G. Kolesov, O. Grånäs, R. Hoyt, D. Vinichenkoand E. Kaxiras, “Real-Time TD-DFT with Classical Ion Dynamics: Methodology and Applications”, *Journal of Chemical Theory and Computation*, vol. 12, no. 2. American Chemical Society (ACS), pp. 466–476, Dec. 29, 2015. doi: 10.1021/acs.jctc.5b00969.  
  
P. Yi, C. R. Lockerand G. C. Rutledge, “Molecular Dynamics Simulation of Homogeneous Crystal Nucleation in Polyethylene”, *Macromolecules*, vol. 46, no. 11. American Chemical Society (ACS), pp. 4723–4733, May 20, 2013. doi: 10.1021/ma4004659.  
  
J. Botana and M.-S. Miao, “Pressure-stabilized lithium caesides with caesium anions beyond the −1 state”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, Sep. 10, 2014. doi: 10.1038/ncomms5861.  
  
J. Botana, “Mercury under Pressure acts as a Transition Metal: Calculated from First Principles”, *Angewandte Chemie International Edition*, vol. 54, no. 32. Wiley, pp. 9280–9283, Jul. 01, 2015. doi: 10.1002/anie.201503870.  
  
W. Liu, J.-. yao . Liuand M.-. sheng . Miao, “Macrocycles inserted in graphene: from coordination chemistry on graphene to graphitic carbon oxide”, *Nanoscale*, vol. 8, no. 41. Royal Society of Chemistry (RSC), pp. 17976–17983, 2016. doi: 10.1039/c6nr04178g.  
  
W. Liu, M. Miaoand J.-. yao . Liu, “A novel two-dimensional material B2S3and its structural implication to new carbon and boron nitride allotropes”, *Journal of Materials Chemistry C*, vol. 3, no. 38. Royal Society of Chemistry (RSC), pp. 9921–9927, 2015. doi: 10.1039/c5tc01079a.  
  
M. Miao, J. Brgoch, A. Krishnapriyan, A. Goldman, J. A. Kurzmanand R. Seshadri, “On the Stereochemical Inertness of the Auride Lone Pair: Ab Initio Studies of AAu (A = K, Rb, Cs)”, *Inorganic Chemistry*, vol. 52, no. 14. American Chemical Society (ACS), pp. 8183–8189, Jul. 03, 2013. doi: 10.1021/ic400947p.  
  
M.-S. Miao and R. Hoffmann, “High Pressure Electrides: A Predictive Chemical and Physical Theory”, *Accounts of Chemical Research*, vol. 47, no. 4. American Chemical Society (ACS), pp. 1311–1317, Apr. 05, 2014. doi: 10.1021/ar4002922.  
  
M.-. sheng . Miao and R. Hoffmann, “High-Pressure Electrides: The Chemical Nature of Interstitial Quasiatoms”, *Journal of the American Chemical Society*, vol. 137, no. 10. American Chemical Society (ACS), pp. 3631–3637, Mar. 05, 2015. doi: 10.1021/jacs.5b00242.  
  
M.-. sheng . Miao, R. Hoffmann, J. Botana, I. I. Naumovand R. J. Hemley, “Quasimolecules in Compressed Lithium”, *Angewandte Chemie International Edition*, vol. 56, no. 4. Wiley, pp. 972–975, Dec. 21, 2016. doi: 10.1002/anie.201608490.  
  
M.-. sheng . Miao, “Anionic Chemistry of Noble Gases: Formation of Mg–NG (NG = Xe, Kr, Ar) Compounds under Pressure”, *Journal of the American Chemical Society*, vol. 137, no. 44. American Chemical Society (ACS), pp. 14122–14128, Nov. 03, 2015. doi: 10.1021/jacs.5b08162.  
  
F. Peng, J. Botana, Y. Wang, Y. Maand M. Miao, “Unexpected Trend in Stability of Xe–F Compounds under Pressure Driven by Xe–Xe Covalent Bonds”, *The Journal of Physical Chemistry Letters*, vol. 7, no. 22. American Chemical Society (ACS), pp. 4562–4567, Nov. 01, 2016. doi: 10.1021/acs.jpclett.6b01922.  
  
X. Sui, T. Hu, J. Wang, B.-L. Gu, W. Duanand M.-. sheng . Miao, “Voltage-controllable colossal magnetocrystalline anisotropy in single-layer transition metal dichalcogenides”, *Physical Review B*, vol. 96, no. 4. American Physical Society (APS), Jul. 26, 2017. doi: 10.1103/physrevb.96.041410.  
  
W.-. cai . Yi, T. Hu, T. Su, R. Islam, M.-. sheng . Miaoand J.-. yao . Liu, “A CNH monolayer: a direct gap 2D semiconductor with anisotropic electronic and optical properties”, *Journal of Materials Chemistry C*, vol. 5, no. 33. Royal Society of Chemistry (RSC), pp. 8498–8503, 2017. doi: 10.1039/c7tc02287e.  
  
W.-. cai . Yi, “Honeycomb Boron Allotropes with Dirac Cones: A True Analogue to Graphene”, *The Journal of Physical Chemistry Letters*, vol. 8, no. 12. American Chemical Society (ACS), pp. 2647–2653, Jun. 01, 2017. doi: 10.1021/acs.jpclett.7b00891.  
  
W.-. cai . Yi, W. Liu, L. Zhao, R. Islam, M.-. sheng . Miaoand J.-. yao . Liu, “Asymmetric passivation of edges: a route to make magnetic graphene nanoribbons”, *RSC Advances*, vol. 7, no. 45. Royal Society of Chemistry (RSC), pp. 27932–27937, 2017. doi: 10.1039/c7ra03461j.  
  
Y. Zheng, “A Solid‐State Effect Responsible for an Organic Quintet State at Room Temperature and Ambient Pressure”, *Advanced Materials*, vol. 27, no. 10. Wiley, pp. 1718–1723, Jan. 23, 2015. doi: 10.1002/adma.201405093.  
  
Y. Zheng, M.-. sheng . Miao, Y. Zhang, T.-Q. Nguyenand F. Wudl, “Striking Effect of Intra- versus Intermolecular Hydrogen Bonding on Zwitterions: Physical and Electronic Properties”, *Journal of the American Chemical Society*, vol. 136, no. 33. American Chemical Society (ACS), pp. 11614–11617, Aug. 07, 2014. doi: 10.1021/ja506803y.  
  
S. P. Coleman, D. E. Spearotand L. Capolungo, “Virtual diffraction analysis of Ni [0 1 0] symmetric tilt grain boundaries”, *Modelling and Simulation in Materials Science and Engineering*, vol. 21, no. 5. IOP Publishing, p. 055020, Jun. 11, 2013. doi: 10.1088/0965-0393/21/5/055020.  
  
S.-Y. Liu, “Oxidation of the two-phase Nb/Nb5Si3 composite: The role of energetics, thermodynamics, segregation, and interfaces”, *The Journal of Chemical Physics*, vol. 138, no. 1. AIP Publishing, p. 014708, Jan. 07, 2013. doi: 10.1063/1.4773447.  
  
Z. Hooshmand, D. Leand T. S. Rahman, “CO adsorption on Pd(111) at 0.5ML: A first principles study”, *Surface Science*, vol. 655. Elsevier BV, pp. 7–11, Jan. 2017. doi: 10.1016/j.susc.2016.09.002.  
  
D. Le and T. S. Rahman, “Joined edges in MoS2: metallic and half-metallic wires”, *Journal of Physics: Condensed Matter*, vol. 25, no. 31. IOP Publishing, p. 312201, Jul. 09, 2013. doi: 10.1088/0953-8984/25/31/312201.  
  
D. Le and T. S. Rahman, “Pt–dipyridyl tetrazine metal–organic network on the Au(100) surface: insights from first principles calculations”, *Faraday Discussions*, vol. 204. Royal Society of Chemistry (RSC), pp. 83–95, 2017. doi: 10.1039/c7fd00097a.  
  
D. Le, T. B. Rawaland T. S. Rahman, “Single-Layer MoS2 with Sulfur Vacancies: Structure and Catalytic Application”, *The Journal of Physical Chemistry C*, vol. 118, no. 10. American Chemical Society (ACS), pp. 5346–5351, Mar. 03, 2014. doi: 10.1021/jp411256g.  
  
D. Le, “Growth of aligned Mo6S6 nanowires on Cu(111)”, *Surface Science*, vol. 611. Elsevier BV, pp. 1–4, May 2013. doi: 10.1016/j.susc.2012.12.016.  
  
J. Mann, “2-Dimensional Transition Metal Dichalcogenides with Tunable Direct Band Gaps: MoS2(1-x)Se2xMonolayers”, *Advanced Materials*, vol. 26, no. 9. Wiley, pp. 1399–1404, Dec. 12, 2013. doi: 10.1002/adma.201304389.  
  
Q. Ma, “Controlled argon beam-induced desulfurization of monolayer molybdenum disulfide”, *Journal of Physics: Condensed Matter*, vol. 25, no. 25. IOP Publishing, p. 252201, May 24, 2013. doi: 10.1088/0953-8984/25/25/252201.  
  
D. J. Nash, “Heterogeneous Metal-Free Hydrogenation over Defect-Laden Hexagonal Boron Nitride”, *ACS Omega*, vol. 1, no. 6. American Chemical Society (ACS), pp. 1343–1354, Dec. 21, 2016. doi: 10.1021/acsomega.6b00315.  
  
C. D. Tempas, “Redox-active ligand controlled selectivity of vanadium oxidation on Au(100)”, *Chemical Science*, vol. 9, no. 6. Royal Society of Chemistry (RSC), pp. 1674–1685, 2018. doi: 10.1039/c7sc04752e.  
  
C. D. Tempas, “Redox Isomeric Surface Structures Are Preferred over Odd‐Electron Pt 1+”, *Chemistry – A European Journal*, vol. 24, no. 59. Wiley, pp. 15852–15858, Sep. 20, 2018. doi: 10.1002/chem.201802943.  
  
A. N. Volkov, “Effects of exit boundary conditions on results of kinetic simulations of spherical expansion of mon- and diatomic gases in a gravitational field”, *Vacuum*, vol. 109. Elsevier BV, pp. 308–318, Nov. 2014. doi: 10.1016/j.vacuum.2014.05.022.  
  
A. N. Volkov, R. N. Salawayand L. V. Zhigilei, “Atomistic simulations, mesoscopic modeling, and theoretical analysis of thermal conductivity of bundles composed of carbon nanotubes”, *Journal of Applied Physics*, vol. 114, no. 10. AIP Publishing, p. 104301, Sep. 14, 2013. doi: 10.1063/1.4819911.  
  
C. Wu, E. T. Karim, A. N. Volkovand L. V. Zhigilei, “Atomic Movies of Laser-Induced Structural and Phase Transformations from Molecular Dynamics Simulations”, *Lasers in Materials Science*. Springer International Publishing, pp. 67–100, 2014. doi: 10.1007/978-3-319-02898-9\_4.  
  
R. J. Lang, W. L. Merlingand D. S. Simmons, “Combined Dependence of Nanoconfined *T*g on Interfacial Energy and Softness of Confinement”, *ACS Macro Letters*, vol. 3, no. 8. American Chemical Society (ACS), pp. 758–762, Jul. 23, 2014. doi: 10.1021/mz500361v.  
  
D. Balamurugan, A. J. A. Aquino, F. de Dios, L. Flores Jr., H. Lischkaand M. S. Cheung, “Multiscale Simulation of the Ground and Photo-Induced Charge-Separated States of a Molecular Triad in Polar Organic Solvent: Exploring the Conformations, Fluctuations, and Free Energy Landscapes”, *The Journal of Physical Chemistry B*, vol. 117, no. 40. American Chemical Society (ACS), pp. 12065–12075, Oct. 01, 2013. doi: 10.1021/jp4026927.  
  
R. H. Coridan, K. A. Arpin, B. S. Brunschwig, P. V. Braunand N. S. Lewis, “Photoelectrochemical Behavior of Hierarchically Structured Si/WO3 Core–Shell Tandem Photoanodes”, *Nano Letters*, vol. 14, no. 5. American Chemical Society (ACS), pp. 2310–2317, Apr. 21, 2014. doi: 10.1021/nl404623t.  
  
T. Lu, C. Chen, K. Zhao, W. Zhangand T. J. Wang, “Bulge test at nano-scale: The surface effects”, *Applied Physics Letters*, vol. 103, no. 5. AIP Publishing, p. 053110, Jul. 29, 2013. doi: 10.1063/1.4817298.  
  
K.-J. Zhao, Y.-G. Liand L. Brassart, “Pressure-sensitive plasticity of lithiated silicon in Li-ion batteries”, *Acta Mechanica Sinica*, vol. 29, no. 3. Springer Science and Business Media LLC, pp. 379–387, Jun. 2013. doi: 10.1007/s10409-013-0041-2.  
  
S. Almeida, E. Ochoa, J. J. Chavez, X. W. Zhouand D. Zubia, “Calculation of surface diffusivity and residence time by molecular dynamics with application to nanoscale selective-area growth”, *Journal of Crystal Growth*, vol. 423. Elsevier BV, pp. 55–60, Aug. 2015. doi: 10.1016/j.jcrysgro.2015.04.036.  
  
A. E. Antipov, J. P. F. LeBlancand E. Gull, “Opendf - An Implementation of the Dual Fermion Method for Strongly Correlated Systems”, *Physics Procedia*, vol. 68. Elsevier BV, pp. 43–51, 2015. doi: 10.1016/j.phpro.2015.07.107.  
  
X. Chen, J. P. F. LeBlancand E. Gull, “Superconducting Fluctuations in the Normal State of the Two-Dimensional Hubbard Model”, *Physical Review Letters*, vol. 115, no. 11. American Physical Society (APS), Sep. 09, 2015. doi: 10.1103/physrevlett.115.116402.  
  
X. Dong, X. Chenand E. Gull, “Dynamical charge susceptibility in the Hubbard model”, *Physical Review B*, vol. 100, no. 23. American Physical Society (APS), Dec. 05, 2019. doi: 10.1103/physrevb.100.235107.  
  
A. Gaenko, “Updated core libraries of the ALPS project”, *Computer Physics Communications*, vol. 213. Elsevier BV, pp. 235–251, Apr. 2017. doi: 10.1016/j.cpc.2016.12.009.  
  
D. Hirschmeier, H. Hafermann, E. Gull, A. I. Lichtensteinand A. E. Antipov, “Mechanisms of finite-temperature magnetism in the three-dimensional Hubbard model”, *Physical Review B*, vol. 92, no. 14. American Physical Society (APS), Oct. 09, 2015. doi: 10.1103/physrevb.92.144409.  
  
A. A. Kananenka, E. Gulland D. Zgid, “Systematically improvable multiscale solver for correlated electron systems”, *Physical Review B*, vol. 91, no. 12. American Physical Society (APS), Mar. 23, 2015. doi: 10.1103/physrevb.91.121111.  
  
S. Li and E. Gull, “Magnetic and charge susceptibilities in the half-filled triangular lattice Hubbard model”, *Physical Review Research*, vol. 2, no. 1. American Physical Society (APS), Mar. 11, 2020. doi: 10.1103/physrevresearch.2.013295.  
  
H. Shinaoka, E. Gulland P. Werner, “Continuous-time hybridization expansion quantum impurity solver for multi-orbital systems with complex hybridizations”, *Computer Physics Communications*, vol. 215. Elsevier BV, pp. 128–136, Jun. 2017. doi: 10.1016/j.cpc.2017.01.003.  
  
D. Zgid and E. Gull, “Finite temperature quantum embedding theories for correlated systems”, *New Journal of Physics*, vol. 19, no. 2. IOP Publishing, p. 023047, Feb. 23, 2017. doi: 10.1088/1367-2630/aa5d34.  
  
X. Chen, J. P. F. LeBlancand E. Gull, “Simulation of the NMR response in the pseudogap regime of the cuprates”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Apr. 07, 2017. doi: 10.1038/ncomms14986.  
  
S. Iskakov, H. Terletskaand E. Gull, “Momentum-space cluster dual-fermion method”, *Physical Review B*, vol. 97, no. 12. American Physical Society (APS), Mar. 12, 2018. doi: 10.1103/physrevb.97.125114.  
  
T. Ribic, “Role of three-particle vertex within dual fermion calculations”, *Physical Review B*, vol. 96, no. 23. American Physical Society (APS), Dec. 18, 2017. doi: 10.1103/physrevb.96.235127.  
  
H. Terletska, T. Chen, J. Pakiand E. Gull, “Charge ordering and nonlocal correlations in the doped extended Hubbard model”, *Physical Review B*, vol. 97, no. 11. American Physical Society (APS), Mar. 09, 2018. doi: 10.1103/physrevb.97.115117.  
  
J. Niu, “In Situ Observation of Random Solid Solution Zone in LiFePO4 Electrode”, *Nano Letters*, vol. 14, no. 7. American Chemical Society (ACS), pp. 4005–4010, Jun. 09, 2014. doi: 10.1021/nl501415b.  
  
M. Wu, X. Qianand J. Li, “Tunable Exciton Funnel Using Moiré Superlattice in Twisted van der Waals Bilayer”, *Nano Letters*, vol. 14, no. 9. American Chemical Society (ACS), pp. 5350–5357, Aug. 19, 2014. doi: 10.1021/nl502414t.  
  
J. Huang, L. Valenzanoand G. Sant, “Framework and Channel Modifications in Mayenite (12CaO·7Al2O3) Nanocages By Cationic Doping”, *Chemistry of Materials*, vol. 27, no. 13. American Chemical Society (ACS), pp. 4731–4741, Jun. 25, 2015. doi: 10.1021/acs.chemmater.5b01360.  
  
J. Huang, L. Valenzano, T. V. Singh, R. Pandeyand G. Sant, “Influence of (Al, Fe, Mg) Impurities on Triclinic Ca3SiO5: Interpretations from DFT Calculations”, *Crystal Growth & Design*, vol. 14, no. 5. American Chemical Society (ACS), pp. 2158–2171, Apr. 21, 2014. doi: 10.1021/cg401647f.  
  
M. S. Block, J. D’Emidioand R. K. Kaul, “Kagome model for a quantum spin liquid”, *Physical Review B*, vol. 101, no. 2. American Physical Society (APS), Jan. 09, 2020. doi: 10.1103/physrevb.101.020402.  
  
J. D’Emidio, “Entanglement Entropy from Nonequilibrium Work”, *Physical Review Letters*, vol. 124, no. 11. American Physical Society (APS), Mar. 16, 2020. doi: 10.1103/physrevlett.124.110602.  
  
J. D’Emidio, M. S. Blockand R. K. Kaul, “Rényi entanglement entropy of criticalspin chains”, *Physical Review B*, vol. 92, no. 5. American Physical Society (APS), Aug. 06, 2015. doi: 10.1103/physrevb.92.054411.  
  
R. K. Kaul and M. S. Block, “Numerical studies of various Néel-VBS transitions in SU(*N*) anti-ferromagnets”, *Journal of Physics: Conference Series*, vol. 640. IOP Publishing, p. 012041, Sep. 28, 2015. doi: 10.1088/1742-6596/640/1/012041.  
  
W. A. Saidi, “Effects of Topological Defects and Diatom Vacancies on Characteristic Vibration Modes and Raman Intensities of Zigzag Single-Walled Carbon Nanotubes”, *The Journal of Physical Chemistry A*, vol. 118, no. 35. American Chemical Society (ACS), pp. 7235–7241, Dec. 18, 2013. doi: 10.1021/jp409209s.  
  
Y. Tang, S. C. Burkert, Y. Zhao, W. A. Saidiand A. Star, “The Effect of Metal Catalyst on the Electrocatalytic Activity of Nitrogen-Doped Carbon Nanotubes”, *The Journal of Physical Chemistry C*, vol. 117, no. 48. American Chemical Society (ACS), pp. 25213–25221, Nov. 22, 2013. doi: 10.1021/jp403033x.  
  
W. A. Saidi, “Oxygen Reduction Electrocatalysis Using N-Doped Graphene Quantum-Dots”, *The Journal of Physical Chemistry Letters*, vol. 4, no. 23. American Chemical Society (ACS), pp. 4160–4165, Nov. 22, 2013. doi: 10.1021/jz402090d.  
  
W. A. Saidi, “Influence of strain and metal thickness on metal-MoS2 contacts”, *The Journal of Chemical Physics*, vol. 141, no. 9. AIP Publishing, p. 094707, Sep. 07, 2014. doi: 10.1063/1.4893875.  
  
W. A. Saidi, “Density Functional Theory Study of Nucleation and Growth of Pt Nanoparticles on MoS2(001) Surface”, *Crystal Growth & Design*, vol. 15, no. 2. American Chemical Society (ACS), pp. 642–652, Jan. 14, 2015. doi: 10.1021/cg5013395.  
  
W. A. Saidi, “Trends in the Adsorption and Growth Morphology of Metals on the MoS2(001) Surface”, *Crystal Growth & Design*, vol. 15, no. 7. American Chemical Society (ACS), pp. 3190–3200, Jun. 10, 2015. doi: 10.1021/acs.cgd.5b00269.  
  
Q. Zhu, C. Fleck, W. A. Saidi, A. McGaugheyand J. C. Yang, “TFOx: A versatile kinetic Monte Carlo program for simulations of island growth in three dimensions”, *Computational Materials Science*, vol. 91. Elsevier BV, pp. 292–302, Aug. 2014. doi: 10.1016/j.commatsci.2014.04.053.  
  
Q. Zhu, W. A. Saidiand J. C. Yang, “Step-Induced Oxygen Upward Diffusion on Stepped Cu(100) Surface”, *The Journal of Physical Chemistry C*, vol. 119, no. 1. American Chemical Society (ACS), pp. 251–261, Dec. 18, 2014. doi: 10.1021/jp507914r.  
  
R. C. Van Lehn and A. Alexander-Katz, “Fusion of Ligand-Coated Nanoparticles with Lipid Bilayers: Effect of Ligand Flexibility”, *The Journal of Physical Chemistry A*, vol. 118, no. 31. American Chemical Society (ACS), pp. 5848–5856, May 07, 2014. doi: 10.1021/jp411662c.  
  
R. C. Van Lehn and A. Alexander-Katz, “Membrane-Embedded Nanoparticles Induce Lipid Rearrangements Similar to Those Exhibited by Biological Membrane Proteins”, *The Journal of Physical Chemistry B*, vol. 118, no. 44. American Chemical Society (ACS), pp. 12586–12598, Oct. 27, 2014. doi: 10.1021/jp506239p.  
  
R. C. Van Lehn and A. Alexander-Katz, “Pathway for insertion of amphiphilic nanoparticles into defect-free lipid bilayers from atomistic molecular dynamics simulations”, *Soft Matter*, vol. 11, no. 16. Royal Society of Chemistry (RSC), pp. 3165–3175, 2015. doi: 10.1039/c5sm00287g.  
  
R. C. Van Lehn, “Lipid tail protrusions mediate the insertion of nanoparticles into model cell membranes”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, Jul. 21, 2014. doi: 10.1038/ncomms5482.  
  
C. Bommier, W. Luo, W.-Y. Gao, A. Greaney, S. Maand X. Ji, “Predicting capacity of hard carbon anodes in sodium-ion batteries using porosity measurements”, *Carbon*, vol. 76. Elsevier BV, pp. 165–174, Sep. 2014. doi: 10.1016/j.carbon.2014.04.064.  
  
L. Han, M. Budgeand P. Alex Greaney, “Relationship between thermal conductivity and framework architecture in MOF-5”, *Computational Materials Science*, vol. 94. Elsevier BV, pp. 292–297, Nov. 2014. doi: 10.1016/j.commatsci.2014.06.008.  
  
C. Hu and P. Alex Greaney, “Role of seta angle and flexibility in the gecko adhesion mechanism”, *Journal of Applied Physics*, vol. 116, no. 7. AIP Publishing, p. 074302, Aug. 21, 2014. doi: 10.1063/1.4892628.  
  
L. de S. Oliveira and P. A. Greaney, “Thermal resistance from irradiation defects in graphite”, *Computational Materials Science*, vol. 103. Elsevier BV, pp. 68–76, Jun. 2015. doi: 10.1016/j.commatsci.2015.03.001.  
  
W. Qian, P. A. Greaney, S. Fowler, S.-K. Chiu, A. M. Goforthand J. Jiao, “Low-Temperature Nitrogen Doping in Ammonia Solution for Production of N-Doped TiO2-Hybridized Graphene as a Highly Efficient Photocatalyst for Water Treatment”, *ACS Sustainable Chemistry & Engineering*, vol. 2, no. 7. American Chemical Society (ACS), pp. 1802–1810, Jun. 20, 2014. doi: 10.1021/sc5001176.  
  
S. R. Sklan, P. Alex Greaneyand J. C. Grossman, “Resonant behavior in heat transfer across weak molecular interfaces”, *Journal of Applied Physics*, vol. 114, no. 23. AIP Publishing, p. 234308, Dec. 21, 2013. doi: 10.1063/1.4851035.  
  
A. Truszkowska, P. Alex Greaneyand G. Jovanovic, “Multiscale lattice Boltzmann modeling of two-phase flow and retention times in micro-patterned fluidic devices”, *Computers & Chemical Engineering*, vol. 95. Elsevier BV, pp. 249–259, Dec. 2016. doi: 10.1016/j.compchemeng.2016.08.016.  
  
T.-L. Cheng and Y.-H. Wen, “Toward a Quantitative Understanding of the Electric Field in Thermal Metal Oxidation and a Self-Consistent Wagner Theory”, *The Journal of Physical Chemistry Letters*, vol. 5, no. 13. American Chemical Society (ACS), pp. 2289–2294, Jun. 19, 2014. doi: 10.1021/jz5008627.  
  
T.-L. Cheng and Y.-H. Wen, “Iterative spectral method for solving electrostatic or magnetostatic problems in complex and evolving heterostructures”, *Physical Review E*, vol. 91, no. 5. American Physical Society (APS), May 22, 2015. doi: 10.1103/physreve.91.053307.  
  
T.-L. Cheng, Y.-H. Wenand J. A. Hawk, “Diffuse-Interface Modeling and Multiscale-Relay Simulation of Metal Oxidation Kinetics—With Revisit on Wagner’s Theory”, *The Journal of Physical Chemistry C*, vol. 118, no. 2. American Chemical Society (ACS), pp. 1269–1284, Jan. 03, 2014. doi: 10.1021/jp409811e.  
  
T.-L. Cheng, Y.-H. Wenand J. A. Hawk, “Modeling elasto-viscoplasticity in a consistent phase field framework”, *International Journal of Plasticity*, vol. 96. Elsevier BV, pp. 242–263, Sep. 2017. doi: 10.1016/j.ijplas.2017.05.006.  
  
K. Zhang, X. Zhu, F. Jia, E. Auyeungand C. A. Mirkin, “Temperature-Activated Nucleic Acid Nanostructures”, *Journal of the American Chemical Society*, vol. 135, no. 38. American Chemical Society (ACS), pp. 14102–14105, Sep. 16, 2013. doi: 10.1021/ja408465t.  
  
J. G. Azadani, “Anisotropy in layered half-metallic Heusler alloy superlattices”, *Journal of Applied Physics*, vol. 119, no. 4. AIP Publishing, p. 043904, Jan. 28, 2016. doi: 10.1063/1.4940878.  
  
J. Ma, “Computational investigation of half-Heusler compounds for spintronics applications”, *Physical Review B*, vol. 95, no. 2. American Physical Society (APS), Jan. 11, 2017. doi: 10.1103/physrevb.95.024411.  
  
A. R. Head, R. Tsyshevsky, L. Trotochaud, B. Eichhorn, M. M. Kukljaand H. Bluhm, “Electron Spectroscopy and Computational Studies of Dimethyl Methylphosphonate”, *The Journal of Physical Chemistry A*, vol. 120, no. 12. American Chemical Society (ACS), pp. 1985–1991, Mar. 22, 2016. doi: 10.1021/acs.jpca.6b01098.  
  
A. R. Head, “Adsorption of Dimethyl Methylphosphonate on MoO3: The Role of Oxygen Vacancies”, *The Journal of Physical Chemistry C*, vol. 120, no. 51. American Chemical Society (ACS), pp. 29077–29088, Dec. 20, 2016. doi: 10.1021/acs.jpcc.6b07340.  
  
S. Holdren, “Adsorption and Destruction of the G-Series Nerve Agent Simulant Dimethyl Methylphosphonate on Zinc Oxide”, *ACS Catalysis*, vol. 9, no. 2. American Chemical Society (ACS), pp. 902–911, Dec. 14, 2018. doi: 10.1021/acscatal.8b02999.  
  
M. M. Kuklja, O. Shariaand R. Tsyshevsky, “Manifestations of two-dimensional electron gas in molecular crystals”, *Surface Science*, vol. 657. Elsevier BV, pp. 20–27, Mar. 2017. doi: 10.1016/j.susc.2016.11.001.  
  
M. M. Kuklja, R. V. Tsyshevskyand S. Rashkeev, “Achieving tunable sensitivity in composite high-energy density materials”, *AIP Conference Proceedings*. Author(s), 2017. doi: 10.1063/1.4971519.  
  
M. M. Kuklja, R. V. Tsyshevskyand O. Sharia, “Effect of Polar Surfaces on Decomposition of Molecular Materials”, *Journal of the American Chemical Society*, vol. 136, no. 38. American Chemical Society (ACS), pp. 13289–13302, Sep. 15, 2014. doi: 10.1021/ja506297e.  
  
M. M. Kuklja, R. V. Tsyshevskyand O. Sharia, “Elucidation of high sensitivity of δ-HMX: New insight from first principles simulations”, *AIP Conference Proceedings*. Author(s), 2017. doi: 10.1063/1.4971595.  
  
M. M. Kuklja, “Achieving tunable chemical reactivity through photo-initiation of energetic materials at metal oxide surfaces”, *Physical Chemistry Chemical Physics*, vol. 22, no. 43. Royal Society of Chemistry (RSC), pp. 25284–25296, 2020. doi: 10.1039/d0cp04069j.  
  
P. Pagoria, M. Zhang, A. Racoveanu, A. DeHope, R. Tsyshevskyand M. Kuklja, “3-(4-Amino-1,2,5-oxadiazol-3-yl)-4-(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole”, *Molbank*, vol. 2014, no. 2. MDPI AG, p. M824, May 22, 2014. doi: 10.3390/m824.  
  
L. Trotochaud, “Room temperature decomposition of dimethyl methylphosphonate on cuprous oxide yields atomic phosphorus”, *Surface Science*, vol. 680. Elsevier BV, pp. 75–87, Feb. 2019. doi: 10.1016/j.susc.2018.10.003.  
  
L. Trotochaud, “Spectroscopic and Computational Investigation of Room-Temperature Decomposition of a Chemical Warfare Agent Simulant on Polycrystalline Cupric Oxide”, *Chemistry of Materials*, vol. 29, no. 17. American Chemical Society (ACS), pp. 7483–7496, Aug. 31, 2017. doi: 10.1021/acs.chemmater.7b02489.  
  
R. Tsyshevsky, A. R. Head, L. Trotochaud, H. Bluhmand M. M. Kuklja, “Mechanisms of Degradation of Toxic Nerve Agents: Quantum-chemical Insight into Interactions of Sarin and Soman with Molybdenum Dioxide”, *Surface Science*, vol. 700. Elsevier BV, p. 121639, Oct. 2020. doi: 10.1016/j.susc.2020.121639.  
  
R. Tsyshevsky, S. Holdren, B. W. Eichhorn, M. R. Zachariahand M. M. Kuklja, “Sarin Decomposition on Pristine and Hydroxylated ZnO: Quantum-Chemical Modeling”, *The Journal of Physical Chemistry C*, vol. 123, no. 43. American Chemical Society (ACS), pp. 26432–26441, Oct. 07, 2019. doi: 10.1021/acs.jpcc.9b07974.  
  
R. Tsyshevsky and M. Kuklja, “Decomposition Mechanisms and Kinetics of Novel Energetic Molecules BNFF-1 and ANFF-1: Quantum-Chemical Modeling”, *Molecules*, vol. 18, no. 7. MDPI AG, pp. 8500–8517, Jul. 18, 2013. doi: 10.3390/molecules18078500.  
  
R. V. Tsyshevsky, P. Pagoriaand M. M. Kuklja, “Computational Design of Novel Energetic Materials: Dinitro-bis-triazolo-tetrazine”, *The Journal of Physical Chemistry C*, vol. 119, no. 16. American Chemical Society (ACS), pp. 8512–8521, Apr. 08, 2015. doi: 10.1021/acs.jpcc.5b01086.  
  
R. V. Tsyshevsky, P. Pagoriaand M. M. Kuklja, “Searching for new energetic materials: Computational design of novel nitro-substituted heterocyclic explosives”, *AIP Conference Proceedings*. Author(s), 2017. doi: 10.1063/1.4971486.  
  
R. Tsyshevsky, P. Pagoria, A. S. Smirnovand M. M. Kuklja, “Comprehensive End-to-End Design of Novel High Energy Density Materials: II. Computational Modeling and Predictions”, *The Journal of Physical Chemistry C*, vol. 121, no. 43. American Chemical Society (ACS), pp. 23865–23874, Oct. 18, 2017. doi: 10.1021/acs.jpcc.7b07585.  
  
R. Tsyshevsky, “Searching for Low-Sensitivity Cast-Melt High-Energy-Density Materials: Synthesis, Characterization, and Decomposition Kinetics of 3,4-Bis(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole-2-oxide”, *The Journal of Physical Chemistry C*, vol. 119, no. 7. American Chemical Society (ACS), pp. 3509–3521, Feb. 05, 2015. doi: 10.1021/jp5118008.  
  
R. Tsyshevsky, “Comprehensive End-to-End Design of Novel High Energy Density Materials: I. Synthesis and Characterization of Oxadiazole Based Heterocycles”, *The Journal of Physical Chemistry C*, vol. 121, no. 43. American Chemical Society (ACS), pp. 23853–23864, Oct. 17, 2017. doi: 10.1021/acs.jpcc.7b07584.  
  
R. V. Tsyshevsky, S. N. Rashkeevand M. M. Kuklja, “Defect states at organic–inorganic interfaces: Insight from first principles calculations for pentaerythritol tetranitrate on MgO surface”, *Surface Science*, vol. 637–638. Elsevier BV, pp. 19–28, Jul. 2015. doi: 10.1016/j.susc.2015.01.021.  
  
R. V. Tsyshevsky, O. Shariaand M. M. Kuklja, “Energies of Electronic Transitions of Pentaerythritol Tetranitrate Molecules and Crystals”, *The Journal of Physical Chemistry C*, vol. 118, no. 18. American Chemical Society (ACS), pp. 9324–9335, Apr. 29, 2014. doi: 10.1021/jp500011a.  
  
R. V. Tsyshevsky, O. Shariaand M. M. Kuklja, “Optical Absorption Energies of Molecular Defects in Pentaerythritol Tetranitrate Crystals: Quantum Chemical Modeling”, *The Journal of Physical Chemistry C*, vol. 118, no. 46. American Chemical Society (ACS), pp. 26530–26542, Nov. 05, 2014. doi: 10.1021/jp508271k.  
  
R. Tsyshevsky, O. Shariaand M. Kuklja, “Molecular Theory of Detonation Initiation: Insight from First Principles Modeling of the Decomposition Mechanisms of Organic Nitro Energetic Materials”, *Molecules*, vol. 21, no. 2. MDPI AG, p. 236, Feb. 19, 2016. doi: 10.3390/molecules21020236.  
  
R. Tsyshevsky, “Role of Hydrogen Abstraction Reaction in Photocatalytic Decomposition of High Energy Density Materials”, *The Journal of Physical Chemistry C*, vol. 120, no. 43. American Chemical Society (ACS), pp. 24835–24846, Oct. 21, 2016. doi: 10.1021/acs.jpcc.6b08042.  
  
R. Tsyshevsky, A. Zverev, A. Mitrofanov, S. Rashkeevand M. Kuklja, “Photochemistry of the α-Al2O3-PETN Interface”, *Molecules*, vol. 21, no. 3. MDPI AG, p. 289, Feb. 29, 2016. doi: 10.3390/molecules21030289.  
  
F. Wang, R. Tsyshevsky, A. Zverev, A. Mitrofanovand M. M. Kuklja, “Can a Photosensitive Oxide Catalyze Decomposition of Energetic Materials?”, *The Journal of Physical Chemistry C*, vol. 121, no. 2. American Chemical Society (ACS), pp. 1153–1161, Jan. 05, 2017. doi: 10.1021/acs.jpcc.6b10127.  
  
C. Iacob, “Polymerized Ionic Liquids: Correlation of Ionic Conductivity with Nanoscale Morphology and Counterion Volume”, *ACS Macro Letters*, vol. 6, no. 9. American Chemical Society (ACS), pp. 941–946, Aug. 16, 2017. doi: 10.1021/acsmacrolett.7b00335.  
  
H. Liu, S. Cavaliere, D. J. Jones, J. Rozièreand S. J. Paddison, “Scaling Behavior of Nafion with Different Model Parameterizations in Dissipative Particle Dynamics Simulations”, *Macromolecular Theory and Simulations*, vol. 27, no. 4. Wiley, p. 1800003, Apr. 24, 2018. doi: 10.1002/mats.201800003.  
  
H. Liu, S. Cavaliere, D. J. Jones, J. Rozièreand S. J. Paddison, “Morphology of Hydrated Nafion through a Quantitative Cluster Analysis: A Case Study Based on Dissipative Particle Dynamics Simulations”, *The Journal of Physical Chemistry C*, vol. 122, no. 24. American Chemical Society (ACS), pp. 13130–13139, May 09, 2018. doi: 10.1021/acs.jpcc.8b01842.  
  
H. Liu and S. J. Paddison, “Alkyl Chain Length Dependence of Backbone-to-Backbone Distance in Polymerized Ionic Liquids: An Atomistic Simulation Perspective on Scattering”, *Macromolecules*, vol. 50, no. 7. American Chemical Society (ACS), pp. 2889–2895, Mar. 21, 2017. doi: 10.1021/acs.macromol.6b02708.  
  
X. Luo and S. J. Paddison, “DPD simulations of anion exchange membrane: The effect of an alkyl spacer on the hydrated morphology”, *Solid State Ionics*, vol. 339. Elsevier BV, p. 115012, Oct. 2019. doi: 10.1016/j.ssi.2019.115012.  
  
Z. Zhu, X. Luoand S. J. Paddison, “DPD simulations of anion exchange membranes functionalized with various cationic groups and associated anions”, *Solid State Ionics*, vol. 340. Elsevier BV, p. 115011, Nov. 2019. doi: 10.1016/j.ssi.2019.115011.  
  
H. Liu and S. J. Paddison, “Direct Comparison of Atomistic Molecular Dynamics Simulations and X-ray Scattering of Polymerized Ionic Liquids”, *ACS Macro Letters*, vol. 5, no. 4. American Chemical Society (ACS), pp. 537–543, Apr. 08, 2016. doi: 10.1021/acsmacrolett.6b00061.  
  
H. Liu and S. J. Paddison, “Direct calculation of the X-ray structure factor of ionic liquids”, *Physical Chemistry Chemical Physics*, vol. 18, no. 16. Royal Society of Chemistry (RSC), pp. 11000–11007, 2016. doi: 10.1039/c5cp06199g.  
  
K. Bashyal, C. K. Pyles, S. Afroosheh, A. Lamichhaneand A. T. Zayak, “Empirical optimization of DFT  +  U and HSE for the band structure of ZnO”, *Journal of Physics: Condensed Matter*, vol. 30, no. 6. IOP Publishing, p. 065501, Jan. 12, 2018. doi: 10.1088/1361-648x/aaa441.  
  
G. B. Bhandari, “Thickness-Controlled Synthesis of Colloidal PbS Nanosheets and Their Thickness-Dependent Energy Gaps”, *Chemistry of Materials*, vol. 26, no. 19. American Chemical Society (ACS), pp. 5433–5436, Sep. 17, 2014. doi: 10.1021/cm502524z.  
  
F. W. Hilty, A. K. Kuhlman, F. Paulyand A. T. Zayak, “Raman Scattering from a Molecule–Semiconductor Interface Tuned by an Electric Field: Density Functional Theory Approach”, *The Journal of Physical Chemistry C*, vol. 119, no. 40. American Chemical Society (ACS), pp. 23113–23118, Sep. 29, 2015. doi: 10.1021/acs.jpcc.5b08089.  
  
A. K. Kuhlman and A. T. Zayak, “Revealing Interaction of Organic Adsorbates with Semiconductor Surfaces Using Chemically Enhanced Raman”, *The Journal of Physical Chemistry Letters*, vol. 5, no. 6. American Chemical Society (ACS), pp. 964–968, Mar. 03, 2014. doi: 10.1021/jz500024x.  
  
D. Yang, “Glucose Sensing Using Surface-Enhanced Raman-Mode Constraining”, *Analytical Chemistry*, vol. 90, no. 24. American Chemical Society (ACS), pp. 14269–14278, Oct. 29, 2018. doi: 10.1021/acs.analchem.8b03420.  
  
Y. Alaskar, “Theoretical and experimental study of highly textured GaAs on silicon using a graphene buffer layer”, *Journal of Crystal Growth*, vol. 425. Elsevier BV, pp. 268–273, Sep. 2015. doi: 10.1016/j.jcrysgro.2015.02.003.  
  
Y. Alaskar, “Towards van der Waals Epitaxial Growth of GaAs on Si using a Graphene Buffer Layer”, *Advanced Functional Materials*, vol. 24, no. 42. Wiley, pp. 6629–6638, Aug. 26, 2014. doi: 10.1002/adfm.201400960.  
  
E. Aytan, “Spin-phonon coupling in antiferromagnetic nickel oxide”, *Applied Physics Letters*, vol. 111, no. 25. AIP Publishing, p. 252402, Dec. 18, 2017. doi: 10.1063/1.5009598.  
  
F. Barati, M. Grossnickle, S. Su, R. K. Lake, V. Ajiand N. M. Gabor, “Hot carrier-enhanced interlayer electron–hole pair multiplication in 2D semiconductor heterostructure photocells”, *Nature Nanotechnology*, vol. 12, no. 12. Springer Science and Business Media LLC, pp. 1134–1139, Oct. 09, 2017. doi: 10.1038/nnano.2017.203.  
  
Y. Chai, S. Su, D. Yan, M. Ozkan, R. Lakeand C. S. Ozkan, “Strain Gated Bilayer Molybdenum Disulfide Field Effect Transistor with Edge Contacts”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Feb. 10, 2017. doi: 10.1038/srep41593.  
  
B. Debnath, Y. Barlas, D. Wickramaratne, M. R. Neupaneand R. K. Lake, “Exciton condensate in bilayer transition metal dichalcogenides: Strong coupling regime”, *Physical Review B*, vol. 96, no. 17. American Physical Society (APS), Nov. 08, 2017. doi: 10.1103/physrevb.96.174504.  
  
R. Dhall, “Direct Bandgap Transition in Many-Layer MoS2by Plasma-Induced Layer Decoupling”, *Advanced Materials*, vol. 27, no. 9. Wiley, pp. 1573–1578, Jan. 14, 2015. doi: 10.1002/adma.201405259.  
  
R. Dhall, “Strong Circularly Polarized Photoluminescence from Multilayer MoS2 Through Plasma Driven Direct-Gap Transition”, *ACS Photonics*, vol. 3, no. 3. American Chemical Society (ACS), pp. 310–314, Feb. 23, 2016. doi: 10.1021/acsphotonics.5b00593.  
  
S. Ge, “Interlayer transport through a graphene/rotated boron nitride/graphene heterostructure”, *Physical Review B*, vol. 95, no. 4. American Physical Society (APS), Jan. 06, 2017. doi: 10.1103/physrevb.95.045303.  
  
N. Gillgren, “Gate tunable quantum oscillations in air-stable and high mobility few-layer phosphorene heterostructures”, *2D Materials*, vol. 2, no. 1. IOP Publishing, p. 011001, Dec. 19, 2014. doi: 10.1088/2053-1583/2/1/011001.  
  
Y. Huang, “Tin Disulfide—An Emerging Layered Metal Dichalcogenide Semiconductor: Materials Properties and Device Characteristics”, *ACS Nano*, vol. 8, no. 10. American Chemical Society (ACS), pp. 10743–10755, Sep. 29, 2014. doi: 10.1021/nn504481r.  
  
F. Kargar, “Phonon and Thermal Properties of Quasi-Two-Dimensional FePS3and MnPS3Antiferromagnetic Semiconductors”, *ACS Nano*, vol. 14, no. 2. American Chemical Society (ACS), pp. 2424–2435, Jan. 17, 2020. doi: 10.1021/acsnano.9b09839.  
  
C. Li, “Commensurate lattice constant dependent thermal conductivity of misoriented bilayer graphene”, *Carbon*, vol. 138. Elsevier BV, pp. 451–457, Nov. 2018. doi: 10.1016/j.carbon.2018.07.071.  
  
Z. Mutlu, “Chemical vapor deposition and phase stability of pyrite on SiO2”, *Journal of Materials Chemistry C*, vol. 6, no. 17. Royal Society of Chemistry (RSC), pp. 4753–4759, 2018. doi: 10.1039/c8tc00584b.  
  
Z. Mutlu, “Synthesis, characterization, and electronic structure of few-layer MoSe2 granular films”, *physica status solidi (a)*, vol. 211, no. 12. Wiley, pp. 2671–2676, Jul. 14, 2014. doi: 10.1002/pssa.201431131.  
  
Z. Mutlu, “Two-Dimensional Layered Semiconductor Tungsten Disulfide and Molybdenum-Tungsten Disulfide: Synthesis, Materials Properties and Electronic Structure”, *Journal of Nanoscience and Nanotechnology*, vol. 16, no. 8. American Scientific Publishers, pp. 8419–8423, Aug. 01, 2016. doi: 10.1166/jnn.2016.12346.  
  
J. Renteria, “All-metallic electrically gated 2H-TaSe2 thin-film switches and logic circuits”, *Journal of Applied Physics*, vol. 115, no. 3. AIP Publishing, p. 034305, Jan. 21, 2014. doi: 10.1063/1.4862336.  
  
R. Samnakay, D. Wickramaratne, T. R. Pope, R. K. Lake, T. T. Salgueroand A. A. Balandin, “Zone-Folded Phonons and the Commensurate–Incommensurate Charge-Density-Wave Transition in 1*T*-TaSe2 Thin Films”, *Nano Letters*, vol. 15, no. 5. American Chemical Society (ACS), pp. 2965–2973, May 04, 2015. doi: 10.1021/nl504811s.  
  
S. Su, Y. Barlas, J. Li, J. Shiand R. K. Lake, “Effect of intervalley interaction on band topology of commensurate graphene/EuO heterostructures”, *Physical Review B*, vol. 95, no. 7. American Physical Society (APS), Feb. 15, 2017. doi: 10.1103/physrevb.95.075418.  
  
S. Su, P. Das, S. Geand R. K. Lake, “Graphene contacts to a HfSe2/SnS2 heterostructure”, *The Journal of Chemical Physics*, vol. 146, no. 6. AIP Publishing, p. 064701, Feb. 14, 2017. doi: 10.1063/1.4975178.  
  
X. Wen, Y. Liu, D. Xu, Y. Zhao, R. K. Lakeand J. Guo, “Room-Temperature Electrodeposition of Aluminum via Manipulating Coordination Structure in AlCl3 Solutions”, *The Journal of Physical Chemistry Letters*, vol. 11, no. 4. American Chemical Society (ACS), pp. 1589–1593, Feb. 10, 2020. doi: 10.1021/acs.jpclett.0c00256.  
  
D. Wickramaratne, F. Zahidand R. K. Lake, “Electronic and thermoelectric properties of few-layer transition metal dichalcogenides”, *The Journal of Chemical Physics*, vol. 140, no. 12. AIP Publishing, p. 124710, Mar. 28, 2014. doi: 10.1063/1.4869142.  
  
D. Wickramaratne, F. Zahidand R. K. Lake, “Electronic and thermoelectric properties of van der Waals materials with ring-shaped valence bands”, *Journal of Applied Physics*, vol. 118, no. 7. AIP Publishing, p. 075101, Aug. 21, 2015. doi: 10.1063/1.4928559.  
  
K. Zhou, D. Wickramaratne, S. Ge, S. Su, A. Deand R. K. Lake, “Interlayer resistance of misoriented MoS2”, *Physical Chemistry Chemical Physics*, vol. 19, no. 16. Royal Society of Chemistry (RSC), pp. 10406–10412, 2017. doi: 10.1039/c6cp08927e.  
  
S. P. Paradiso, K. T. Delaney, C. J. García-Cervera, H. D. Cenicerosand G. H. Fredrickson, “Block Copolymer Self Assembly during Rapid Solvent Evaporation: Insights into Cylinder Growth and Stability”, *ACS Macro Letters*, vol. 3, no. 1. American Chemical Society (ACS), pp. 16–20, Dec. 12, 2013. doi: 10.1021/mz400572r.  
  
N. Artrith and A. M. Kolpak, “Understanding the Composition and Activity of Electrocatalytic Nanoalloys in Aqueous Solvents: A Combination of DFT and Accurate Neural Network Potentials”, *Nano Letters*, vol. 14, no. 5. American Chemical Society (ACS), pp. 2670–2676, May 01, 2014. doi: 10.1021/nl5005674.  
  
T. Duguet, “Self-assembly of metal nanostructures on binary alloy surfaces”, *Proceedings of the National Academy of Sciences*, vol. 108, no. 3. Proceedings of the National Academy of Sciences, pp. 989–994, Nov. 19, 2010. doi: 10.1073/pnas.1008157107.  
  
A. K. Engstfeld, “Directed assembly of Ru nanoclusters on Ru(0001)-supported graphene: STM studies and atomistic modeling”, *Physical Review B*, vol. 86, no. 8. American Physical Society (APS), Aug. 22, 2012. doi: 10.1103/physrevb.86.085442.  
  
Y. Han, A. K. Engstfeld, R. J. Behmand J. W. Evans, “Atomistic modeling of the directed-assembly of bimetallic Pt-Ru nanoclusters on Ru(0001)-supported monolayer graphene”, *The Journal of Chemical Physics*, vol. 138, no. 13. AIP Publishing, p. 134703, Apr. 07, 2013. doi: 10.1063/1.4798348.  
  
Y. Han, A. K. Engstfeld, C.-Z. Wang, L. D. Roelofs, R. J. Behmand J. W. Evans, “Atomistic modeling of Ru nanocluster formation on graphene/Ru(0001): Thermodynamically versus kinetically directed-assembly”, *MRS Proceedings*, vol. 1498. Springer Science and Business Media LLC, pp. 249–254, 2013. doi: 10.1557/opl.2013.106.  
  
Y. Han and J. W. Evans, “Atomistic modeling of alloy self-growth by vapor deposition: Ni and Al on NiAl(110)”, *MRS Proceedings*, vol. 1411. Springer Science and Business Media LLC, 2012. doi: 10.1557/opl.2012.761.  
  
Y. Han, D. Jing, B. Ünal, P. A. Thieland J. W. Evans, “Far-from-equilibrium film growth on alloy surfaces: Ni and Al on NiAl(110)”, *Physical Review B*, vol. 84, no. 11. American Physical Society (APS), Sep. 27, 2011. doi: 10.1103/physrevb.84.113414.  
  
Y. Han, “Anisotropic coarsening: One-dimensional decay of Ag islands on Ag(110)”, *Physical Review B*, vol. 87, no. 15. American Physical Society (APS), Apr. 17, 2013. doi: 10.1103/physrevb.87.155420.  
  
Y. Han, B. Ünaland J. W. Evans, “Formation of a Novel OrderedSurface Structure by Codeposition on NiAl(110)”, *Physical Review Letters*, vol. 108, no. 21. American Physical Society (APS), May 23, 2012. doi: 10.1103/physrevlett.108.216102.  
  
Y. Han, B. Ünal, D. Jing, P. A. Thieland J. W. Evans, “Temperature-dependent growth shapes of Ni nanoclusters on NiAl(110)”, *The Journal of Chemical Physics*, vol. 135, no. 8. AIP Publishing, p. 084706, Aug. 28, 2011. doi: 10.1063/1.3626581.  
  
D. Jing, Y. Han, B. Ünal, J. W. Evansand P. A. Thiel, “Formation of Irregular Al Islands by Room-Temperature Deposition on NiAl(110)”, *MRS Proceedings*, vol. 1318. Springer Science and Business Media LLC, 2011. doi: 10.1557/opl.2011.484.  
  
M. Liu, Y. Han, L. Tang, J.-F. Jia, Q.-K. Xueand F. Liu, “Interplay between quantum size effect and strain effect on growth of nanoscale metal thin films”, *Physical Review B*, vol. 86, no. 12. American Physical Society (APS), Sep. 17, 2012. doi: 10.1103/physrevb.86.125427.  
  
C.-J. Wang, Y. Han, H. Walen, S. M. Russell, P. A. Thieland J. W. Evans, “Analytic formulations for one-dimensional decay of rectangular homoepitaxial islands during coarsening on anisotropic fcc (110) surfaces”, *Physical Review B*, vol. 88, no. 15. American Physical Society (APS), Oct. 24, 2013. doi: 10.1103/physrevb.88.155434.  
  
E. Asadi, M. Asle Zaeemand M. I. Baskes, “Phase-Field Crystal Model for Fe Connected to MEAM Molecular Dynamics Simulations”, *JOM*, vol. 66, no. 3. Springer Science and Business Media LLC, pp. 429–436, Jan. 01, 2014. doi: 10.1007/s11837-013-0845-3.  
  
E. Asadi, M. Asle Zaeem, S. Nouranianand M. I. Baskes, “Two-phase solid–liquid coexistence of Ni, Cu, and Al by molecular dynamics simulations using the modified embedded-atom method”, *Acta Materialia*, vol. 86. Elsevier BV, pp. 169–181, Mar. 2015. doi: 10.1016/j.actamat.2014.12.010.  
  
E. Asadi and M. Asle Zaeem, “A Review of Quantitative Phase-Field Crystal Modeling of Solid–Liquid Structures”, *JOM*, vol. 67, no. 1. Springer Science and Business Media LLC, pp. 186–201, Dec. 02, 2014. doi: 10.1007/s11837-014-1232-4.  
  
E. Asadi and M. Asle Zaeem, “A modified two-mode phase-field crystal model applied to face-centered cubic and body-centered cubic orderings”, *Computational Materials Science*, vol. 105. Elsevier BV, pp. 110–113, Jul. 2015. doi: 10.1016/j.commatsci.2015.04.004.  
  
H. Ding and M. J. Demkowicz, “Hydrogen reverses the clustering tendency of carbon in amorphous silicon oxycarbide”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, Aug. 13, 2015. doi: 10.1038/srep13051.  
  
Q. Fang and F. Sansoz, “Influence of intrinsic kink-like defects on screw dislocation – coherent twin boundary interactions in copper”, *Acta Materialia*, vol. 123. Elsevier BV, pp. 383–393, Jan. 2017. doi: 10.1016/j.actamat.2016.10.032.  
  
X. Ke and F. Sansoz, “Segregation-affected yielding and stability in nanotwinned silver by microalloying”, *Physical Review Materials*, vol. 1, no. 6. American Physical Society (APS), Nov. 30, 2017. doi: 10.1103/physrevmaterials.1.063604.  
  
X. Ke, “Ideal maximum strengths and defect-induced softening in nanocrystalline-nanotwinned metals”, *Nature Materials*, vol. 18, no. 11. Springer Science and Business Media LLC, pp. 1207–1214, Sep. 23, 2019. doi: 10.1038/s41563-019-0484-3.  
  
J. Wang, G. Cao, Z. Zhangand F. Sansoz, “Size-dependent dislocation–twin interactions”, *Nanoscale*, vol. 11, no. 26. Royal Society of Chemistry (RSC), pp. 12672–12679, 2019. doi: 10.1039/c9nr03637g.  
  
L. Zhong, F. Sansoz, Y. He, C. Wang, Z. Zhangand S. X. Mao, “Slip-activated surface creep with room-temperature super-elongation in metallic nanocrystals”, *Nature Materials*, vol. 16, no. 4. Springer Science and Business Media LLC, pp. 439–445, Nov. 28, 2016. doi: 10.1038/nmat4813.  
  
X. Shen, Y. S. Puzyrevand S. T. Pantelides, “Vacancy breathing by grain boundaries—a mechanism of memristive switching in polycrystalline oxides”, *MRS Communications*, vol. 3, no. 3. Springer Science and Business Media LLC, pp. 167–170, Sep. 2013. doi: 10.1557/mrc.2013.32.  
  
X. Shen, Y. S. Puzyrevand S. T. Pantelides, “Vacancy breathing by grain boundaries—a mechanism of memristive switching in polycrystalline oxides”, *MRS Communications*, vol. 3, no. 3. Springer Science and Business Media LLC, pp. 167–170, Sep. 2013. doi: 10.1557/mrc.2013.32.  
  
X. Shen, “2D Nanovaristors at Grain Boundaries Account for Memristive Switching in Polycrystalline BiFeO3”, *Advanced Electronic Materials*, vol. 1, no. 5. Wiley, p. 1500019, Mar. 20, 2015. doi: 10.1002/aelm.201500019.  
  
T. Wei, T. Huang, B. Qiao, M. Zhang, H. Maand L. Zhang, “Structures, Dynamics, and Water Permeation Free Energy across Bilayers of Lipid A and Its Analog Studied with Molecular Dynamics Simulation”, *The Journal of Physical Chemistry B*, vol. 118, no. 46. American Chemical Society (ACS), pp. 13202–13209, Nov. 07, 2014. doi: 10.1021/jp508549m.  
  
C. M. Nakano, H. S. Byun, H. Ma, T. Weiand M. Y. El-Naggar, “A framework for stochastic simulations and visualization of biological electron-transfer dynamics”, *Computer Physics Communications*, vol. 193. Elsevier BV, pp. 1–9, Aug. 2015. doi: 10.1016/j.cpc.2015.03.009.  
  
P. Choudhury, L. Ravavarapu, R. Dekleand S. Chowdhury, “Modulating Electronic and Optical Properties of Monolayer MoS2 Using Nonbonded Phthalocyanine Molecules”, *The Journal of Physical Chemistry C*, vol. 121, no. 5. American Chemical Society (ACS), pp. 2959–2967, Jan. 30, 2017. doi: 10.1021/acs.jpcc.6b11239.  
  
S. Mussell and P. Choudhury, “Density Functional Theory Study of Iron Phthalocyanine Porous Layer Deposited on Graphene Substrate: A Pt-Free Electrocatalyst for Hydrogen Fuel Cells”, *The Journal of Physical Chemistry C*, vol. 120, no. 10. American Chemical Society (ACS), pp. 5384–5391, Mar. 08, 2016. doi: 10.1021/acs.jpcc.5b10327.  
  
J. A. Anderson, J. Antonaglia, J. A. Millan, M. Engeland S. C. Glotzer, “Shape and Symmetry Determine Two-Dimensional Melting Transitions of Hard Regular Polygons”, *Physical Review X*, vol. 7, no. 2. American Physical Society (APS), Apr. 05, 2017. doi: 10.1103/physrevx.7.021001.  
  
X. Ye, “Quasicrystalline nanocrystal superlattice with partial matching rules”, *Nature Materials*, vol. 16, no. 2. Springer Science and Business Media LLC, pp. 214–219, Sep. 26, 2016. doi: 10.1038/nmat4759.  
  
M. P. Howard, J. A. Anderson, A. Nikoubashman, S. C. Glotzerand A. Z. Panagiotopoulos, “Efficient neighbor list calculation for molecular simulation of colloidal systems using graphics processing units”, *Computer Physics Communications*, vol. 203. Elsevier BV, pp. 45–52, Jun. 2016. doi: 10.1016/j.cpc.2016.02.003.  
  
Y. Mo, S. P. Ongand G. Ceder, “Insights into Diffusion Mechanisms in P2 Layered Oxide Materials by First-Principles Calculations”, *Chemistry of Materials*, vol. 26, no. 18. American Chemical Society (ACS), pp. 5208–5214, Sep. 10, 2014. doi: 10.1021/cm501563f.  
  
Z. Feng, J. Qi, Y. Hanand T. Lu, “Deformation restraint of tape-casted transparent alumina ceramic wafers from optimized lamination”, *Ceramics International*, vol. 44, no. 1. Elsevier BV, pp. 1059–1065, Jan. 2018. doi: 10.1016/j.ceramint.2017.10.048.  
  
Y. Han, “Analysis of magic lengths in growth of supported metallic nanowires”, *Materials Research Express*, vol. 1, no. 4. IOP Publishing, p. 045030, Nov. 12, 2014. doi: 10.1088/2053-1591/1/4/045030.  
  
Y. Han and J. W. Evans, “Directing Anisotropic Assembly of Metallic Nanoclusters by Exploiting Linear Trio Interactions and Quantum Size Effects: Au Chains on Ag(100) Thin Films”, *The Journal of Physical Chemistry Letters*, vol. 6, no. 12. American Chemical Society (ACS), pp. 2194–2199, May 29, 2015. doi: 10.1021/acs.jpclett.5b00636.  
  
Y. Han and J. W. Evans, “Adsorption and diffusion of Ru adatoms on Ru(0001)-supported graphene: Large-scale first-principles calculations”, *The Journal of Chemical Physics*, vol. 143, no. 16. AIP Publishing, p. 164706, Oct. 28, 2015. doi: 10.1063/1.4934349.  
  
Y. Han, É. Gaudry, T. J. Oliveiraand J. W. Evans, “Point island models for nucleation and growth of supported nanoclusters during surface deposition”, *The Journal of Chemical Physics*, vol. 145, no. 21. AIP Publishing, p. 211904, Dec. 07, 2016. doi: 10.1063/1.4954410.  
  
Y. Han, “Nucleation and growth kinetics for intercalated islands during deposition on layered materials with isolated pointlike surface defects”, *Physical Review Materials*, vol. 1, no. 5. American Physical Society (APS), Oct. 13, 2017. doi: 10.1103/physrevmaterials.1.053403.  
  
Y. Han, M. Liand J. W. Evans, “Capture zone area distributions for nucleation and growth of islands during submonolayer deposition”, *The Journal of Chemical Physics*, vol. 145, no. 21. AIP Publishing, p. 211911, Dec. 07, 2016. doi: 10.1063/1.4961264.  
  
Y. Han, D.-J. Liuand J. W. Evans, “Real-Time Ab Initio KMC Simulation of the Self-Assembly and Sintering of Bimetallic Epitaxial Nanoclusters: Au + Ag on Ag(100)”, *Nano Letters*, vol. 14, no. 8. American Chemical Society (ACS), pp. 4646–4652, Jun. 30, 2014. doi: 10.1021/nl5017128.  
  
Y. Han, C. R. Stoldt, P. A. Thieland J. W. Evans, “Ab Initio Thermodynamics and Kinetics for Coalescence of Two-Dimensional Nanoislands and Nanopits on Metal (100) Surfaces”, *The Journal of Physical Chemistry C*, vol. 120, no. 38. American Chemical Society (ACS), pp. 21617–21630, Sep. 19, 2016. doi: 10.1021/acs.jpcc.6b07328.  
  
W.-K. Huang, “Tailoring Kinetics on a Topological Insulator Surface by Defect-Induced Strain: Pb Mobility on Bi2Te3”, *Nano Letters*, vol. 16, no. 7. American Chemical Society (ACS), pp. 4454–4461, Jun. 20, 2016. doi: 10.1021/acs.nanolett.6b01604.  
  
A. Lii-Rosales, “Formation of Multilayer Cu Islands Embedded beneath the Surface of Graphite: Characterization and Fundamental Insights”, *The Journal of Physical Chemistry C*, vol. 122, no. 8. American Chemical Society (ACS), pp. 4454–4469, Feb. 15, 2018. doi: 10.1021/acs.jpcc.7b12533.  
  
X. Liu, “Growth morphology and properties of metals on graphene”, *Progress in Surface Science*, vol. 90, no. 4. Elsevier BV, pp. 397–443, Dec. 2015. doi: 10.1016/j.progsurf.2015.07.001.  
  
W. Li, L. Huang, J. W. Evansand Y. Han, “Submonolayer Ag films on Fe(100): A first-principles analysis of energetics controlling adlayer thermodynamics and kinetics”, *Physical Review B*, vol. 93, no. 15. American Physical Society (APS), Apr. 11, 2016. doi: 10.1103/physrevb.93.155416.  
  
W. Li, “Thickness-dependent energetics for Pb adatoms on low-index Pb nanofilm surfaces: First-principles calculations”, *Physical Review B*, vol. 96, no. 20. American Physical Society (APS), Nov. 06, 2017. doi: 10.1103/physrevb.96.205409.  
  
N. Artrith, Z. Linand J. G. Chen, “Predicting the Activity and Selectivity of Bimetallic Metal Catalysts for Ethanol Reforming using Machine Learning”, *ACS Catalysis*, vol. 10, no. 16. American Chemical Society (ACS), pp. 9438–9444, Aug. 03, 2020. doi: 10.1021/acscatal.0c02089.  
  
N. Artrith and A. Urban, “An implementation of artificial neural-network potentials for atomistic materials simulations: Performance for TiO2”, *Computational Materials Science*, vol. 114. Elsevier BV, pp. 135–150, Mar. 2016. doi: 10.1016/j.commatsci.2015.11.047.  
  
N. Artrith, A. Urbanand G. Ceder, “Efficient and accurate machine-learning interpolation of atomic energies in compositions with many species”, *Physical Review B*, vol. 96, no. 1. American Physical Society (APS), Jul. 21, 2017. doi: 10.1103/physrevb.96.014112.  
  
N. Artrith, A. Urbanand G. Ceder, “Constructing first-principles phase diagrams of amorphous Li*x*Si using machine-learning-assisted sampling with an evolutionary algorithm”, *The Journal of Chemical Physics*, vol. 148, no. 24. AIP Publishing, p. 241711, Jun. 28, 2018. doi: 10.1063/1.5017661.  
  
A. M. Cooper, J. Kästner, A. Urbanand N. Artrith, “Efficient training of ANN potentials by including atomic forces via Taylor expansion and application to water and a transition-metal oxide”, *npj Computational Materials*, vol. 6, no. 1. Springer Science and Business Media LLC, May 13, 2020. doi: 10.1038/s41524-020-0323-8.  
  
E. Asadi, M. A. Zaeem, A. Moitraand M. A. Tschopp, “Effect of vacancy defects on generalized stacking fault energy of fcc metals”, *Journal of Physics: Condensed Matter*, vol. 26, no. 11. IOP Publishing, p. 115404, Mar. 03, 2014. doi: 10.1088/0953-8984/26/11/115404.  
  
E. Asadi and M. Asle Zaeem, “Quantitative phase-field crystal modeling of solid-liquid interfaces for FCC metals”, *Computational Materials Science*, vol. 127. Elsevier BV, pp. 236–243, Feb. 2017. doi: 10.1016/j.commatsci.2016.11.005.  
  
M. Asle Zaeem, N. Zhangand M. Mamivand, “A review of computational modeling techniques in study and design of shape memory ceramics”, *Computational Materials Science*, vol. 160. Elsevier BV, pp. 120–136, Apr. 2019. doi: 10.1016/j.commatsci.2018.12.062.  
  
M. Beyramali Kivy and M. Asle Zaeem, “Generalized stacking fault energies, ductilities, and twinnabilities of CoCrFeNi-based face-centered cubic high entropy alloys”, *Scripta Materialia*, vol. 139. Elsevier BV, pp. 83–86, Oct. 2017. doi: 10.1016/j.scriptamat.2017.06.014.  
  
M. Beyramali Kivy, M. Asle Zaeemand S. Lekakh, “Investigating phase formations in cast AlFeCoNiCu high entropy alloys by combination of computational modeling and experiments”, *Materials & Design*, vol. 127. Elsevier BV, pp. 224–232, Aug. 2017. doi: 10.1016/j.matdes.2017.04.086.  
  
Y. Hong, M. Beyramali Kivyand M. Asle Zaeem, “Competition between formation of Al2O3 and Cr2O3 in oxidation of Al0.3CoCrCuFeNi high entropy alloy: A first-principles study”, *Scripta Materialia*, vol. 168. Elsevier BV, pp. 139–143, Jul. 2019. doi: 10.1016/j.scriptamat.2019.04.041.  
  
Y. Hong, N. Zhangand M. A. Zaeem, “Metastable phase transformation and deformation twinning induced hardening-stiffening mechanism in compression of silicon nanoparticles”, *Acta Materialia*, vol. 145. Elsevier BV, pp. 8–18, Feb. 2018. doi: 10.1016/j.actamat.2017.11.034.  
  
S. Kavousi, B. R. Novak, M. I. Baskes, M. A. Zaeemand D. Moldovan, “Modified embedded-atom method potential for high-temperature crystal-melt properties of Ti–Ni alloys and its application to phase field simulation of solidification”, *Modelling and Simulation in Materials Science and Engineering*, vol. 28, no. 1. IOP Publishing, p. 015006, Dec. 02, 2019. doi: 10.1088/1361-651x/ab580c.  
  
A. Mahata and M. Asle Zaeem, “Evolution of solidification defects in deformation of nano-polycrystalline aluminum”, *Computational Materials Science*, vol. 163. Elsevier BV, pp. 176–185, Jun. 2019. doi: 10.1016/j.commatsci.2019.03.034.  
  
A. Mahata and M. Asle Zaeem, “Size effect in molecular dynamics simulation of nucleation process during solidification of pure metals: investigating modified embedded atom method interatomic potentials”, *Modelling and Simulation in Materials Science and Engineering*, vol. 27, no. 8. IOP Publishing, p. 085015, Oct. 01, 2019. doi: 10.1088/1361-651x/ab4b36.  
  
A. Mahata and M. Asle Zaeem, “Effects of solidification defects on nanoscale mechanical properties of rapid directionally solidified Al-Cu Alloy: A large scale molecular dynamics study”, *Journal of Crystal Growth*, vol. 527. Elsevier BV, p. 125255, Dec. 2019. doi: 10.1016/j.jcrysgro.2019.125255.  
  
A. Mahata, M. A. Zaeemand M. I. Baskes, “Understanding homogeneous nucleation in solidification of aluminum by molecular dynamics simulations”, *Modelling and Simulation in Materials Science and Engineering*, vol. 26, no. 2. IOP Publishing, p. 025007, Jan. 09, 2018. doi: 10.1088/1361-651x/aa9f36.  
  
S. Thomas and M. Asle Zaeem, “A new planar BCN lateral heterostructure with outstanding strength and defect-mediated superior semiconducting to metallic properties”, *Physical Chemistry Chemical Physics*, vol. 22, no. 38. Royal Society of Chemistry (RSC), pp. 22066–22077, 2020. doi: 10.1039/d0cp02973d.  
  
S. Thomas, O. Hildrethand M. A. Zaeem, “Unveiling the role of atomic defects on the electronic, mechanical and elemental diffusion properties in CuS”, *Scripta Materialia*, vol. 192. Elsevier BV, pp. 94–99, Feb. 2021. doi: 10.1016/j.scriptamat.2020.10.012.  
  
S. Thomas, V. Kumar, D. R. Royand M. A. Zaeem, “Two-Dimensional Boron–Phosphorus Monolayer for Reversible NO2 Gas Sensing”, *ACS Applied Nano Materials*, vol. 3, no. 10. American Chemical Society (ACS), pp. 10073–10081, Sep. 16, 2020. doi: 10.1021/acsanm.0c02072.  
  
S. Thomas, A. K. Madamand M. A. Zaeem, “Stone–Wales Defect Induced Performance Improvement of BC3 Monolayer for High Capacity Lithium-Ion Rechargeable Battery Anode Applications”, *The Journal of Physical Chemistry C*, vol. 124, no. 11. American Chemical Society (ACS), pp. 5910–5919, Feb. 26, 2020. doi: 10.1021/acs.jpcc.9b11441.  
  
S. Thomas, M. S. Manju, K. M. Ajith, S. U. Leeand M. Asle Zaeem, “Strain-induced work function in h-BN and BCN monolayers”, *Physica E: Low-dimensional Systems and Nanostructures*, vol. 123. Elsevier BV, p. 114180, Sep. 2020. doi: 10.1016/j.physe.2020.114180.  
  
N. Zhang and M. Asle Zaeem, “Effects of specimen size and yttria concentration on mechanical properties of single crystalline yttria-stabilized tetragonal zirconia nanopillars”, *Journal of Applied Physics*, vol. 122, no. 1. AIP Publishing, p. 014302, Jul. 06, 2017. doi: 10.1063/1.4991339.  
  
N. Zhang and M. Asle Zaeem, “Role of grain boundaries in determining strength and plastic deformation of yttria-stabilized tetragonal zirconia bicrystals”, *Journal of Materials Science*, vol. 53, no. 8. Springer Science and Business Media LLC, pp. 5706–5718, Sep. 25, 2017. doi: 10.1007/s10853-017-1595-3.  
  
N. Zhang and M. Asle Zaeem, “Effects of Crystal Orientation and Pre-existing Defects on Nanoscale Mechanical Properties of Yttria-Stabilized Tetragonal Zirconia Thin Films”, *JOM*, vol. 71, no. 11. Springer Science and Business Media LLC, pp. 3869–3875, Aug. 13, 2019. doi: 10.1007/s11837-019-03725-z.  
  
N. Zhang and M. Asle Zaeem, “Nanoscale self-healing mechanisms in shape memory ceramics”, *npj Computational Materials*, vol. 5, no. 1. Springer Science and Business Media LLC, May 01, 2019. doi: 10.1038/s41524-019-0194-z.  
  
N. Zhang and M. Asle Zaeem, “Understanding specimen- and grain-size effects on nanoscale plastic deformation mechanisms and mechanical properties of polycrystalline yttria-stabilized tetragonal zirconia nanopillars”, *European Journal of Mechanics - A/Solids*, vol. 76. Elsevier BV, pp. 80–90, Jul. 2019. doi: 10.1016/j.euromechsol.2019.03.015.  
  
N. Zhang and M. Asle Zaeem, “Nanoscale flaw tolerance behaviour of polycrystalline tetragonal zirconia nanopillars”, *International Journal of Mechanical Sciences*, vol. 173. Elsevier BV, p. 105405, May 2020. doi: 10.1016/j.ijmecsci.2019.105405.  
  
N. Zhang and M. Asle Zaeem, “Effects of grain orientations and pre-existing defects on mechanical properties and deformation mechanisms of polycrystalline yttria-stabilized tetragonal zirconia”, *Materialia*, vol. 9. Elsevier BV, p. 100553, Mar. 2020. doi: 10.1016/j.mtla.2019.100553.  
  
N. Zhang and M. Asle Zaeem, “Effects of twin boundaries and pre-existing defects on mechanical properties and deformation mechanisms of yttria-stabilized tetragonal zirconia”, *Journal of the European Ceramic Society*, vol. 40, no. 1. Elsevier BV, pp. 108–114, Jan. 2020. doi: 10.1016/j.jeurceramsoc.2019.09.017.  
  
N. Zhang, Y. Hong, S. Yazdanparastand M. Asle Zaeem, “Superior structural, elastic and electronic properties of 2D titanium nitride MXenes over carbide MXenes: a comprehensive first principles study”, *2D Materials*, vol. 5, no. 4. IOP Publishing, p. 045004, Jul. 13, 2018. doi: 10.1088/2053-1583/aacfb3.  
  
E. Asadi and M. Asle Zaeem, “Quantifying a two-mode phase-field crystal model for BCC metals at melting point”, *Computational Materials Science*, vol. 105. Elsevier BV, pp. 101–109, Jul. 2015. doi: 10.1016/j.commatsci.2015.03.051.  
  
E. Asadi and M. Asle Zaeem, “A modified two-mode phase-field crystal model applied to face-centered cubic and body-centered cubic orderings”, *Computational Materials Science*, vol. 105. Elsevier BV, pp. 110–113, Jul. 2015. doi: 10.1016/j.commatsci.2015.04.004.  
  
E. Asadi and M. Asle Zaeem, “The anisotropy of hexagonal close-packed and liquid interface free energy using molecular dynamics simulations based on modified embedded-atom method”, *Acta Materialia*, vol. 107. Elsevier BV, pp. 337–344, Apr. 2016. doi: 10.1016/j.actamat.2016.01.043.  
  
A. Emdadi, M. Asle Zaeemand E. Asadi, “Revisiting phase diagrams of two-mode phase-field crystal models”, *Computational Materials Science*, vol. 123. Elsevier BV, pp. 139–147, Oct. 2016. doi: 10.1016/j.commatsci.2016.06.018.  
  
N. Zhang and M. Asle Zaeem, “Competing mechanisms between dislocation and phase transformation in plastic deformation of single crystalline yttria-stabilized tetragonal zirconia nanopillars”, *Acta Materialia*, vol. 120. Elsevier BV, pp. 337–347, Nov. 2016. doi: 10.1016/j.actamat.2016.08.075.  
  
A. Sambasivam, A. V. Sangwaiand R. Sureshkumar, “Dynamics and Scission of Rodlike Cationic Surfactant Micelles in Shear Flow”, *Physical Review Letters*, vol. 114, no. 15. American Physical Society (APS), Apr. 17, 2015. doi: 10.1103/physrevlett.114.158302.  
  
X. Zhang, Q. Liu, J.-W. Luo, A. J. Freemanand A. Zunger, “Hidden spin polarization in inversion-symmetric bulk crystals”, *Nature Physics*, vol. 10, no. 5. Springer Science and Business Media LLC, pp. 387–393, Apr. 13, 2014. doi: 10.1038/nphys2933.  
  
B. Jelinek, M. Eshraghi, S. Felicelliand J. F. Peters, “Large-scale parallel lattice Boltzmann–cellular automaton model of two-dimensional dendritic growth”, *Computer Physics Communications*, vol. 185, no. 3. Elsevier BV, pp. 939–947, Mar. 2014. doi: 10.1016/j.cpc.2013.09.013.  
  
A. Roy, “Estimates of the thermal conductivity and the thermoelectric properties offrom first principles”, *Physical Review B*, vol. 93, no. 10. American Physical Society (APS), Mar. 09, 2016. doi: 10.1103/physrevb.93.100101.  
  
A. Roy, Y.-T. Chengand M. L. Falk, “Amorphous ZnO-Based Compounds as Thermoelectrics”, *The Journal of Physical Chemistry C*, vol. 120, no. 5. American Chemical Society (ACS), pp. 2529–2535, Jan. 28, 2016. doi: 10.1021/acs.jpcc.5b11618.  
  
S. Adhikari, “Charge Transfer to LaAlO3/SrTiO3Interfaces Controlled by Surface Water Adsorption and Proton Hopping”, *Advanced Functional Materials*, vol. 26, no. 30. Wiley, pp. 5453–5459, May 23, 2016. doi: 10.1002/adfm.201600820.  
  
G. Avendaño-Franco and A. H. Romero, “Firefly Algorithm for Structural Search”, *Journal of Chemical Theory and Computation*, vol. 12, no. 7. American Chemical Society (ACS), pp. 3416–3428, Jun. 29, 2016. doi: 10.1021/acs.jctc.5b01157.  
  
M. Aziziha, “Phonon Dynamics in Anisotropic Dilute CuAl1–*x*Fe*x*O2 Delafossite Alloys by a Weighted Dynamical Matrix Approach”, *The Journal of Physical Chemistry C*, vol. 123, no. 50. American Chemical Society (ACS), pp. 30604–30612, Nov. 19, 2019. doi: 10.1021/acs.jpcc.9b09402.  
  
P. Bach, I. Valencia-Jaime, U. Rütt, O. Gutowski, A. H. Romeroand F. U. Renner, “Electrochemical Lithiation Cycles of Gold Anodes Observed by In Situ High-Energy X-ray Diffraction”, *Chemistry of Materials*, vol. 28, no. 9. American Chemical Society (ACS), pp. 2941–2948, Apr. 25, 2016. doi: 10.1021/acs.chemmater.5b04719.  
  
S. E. Baltazar, A. H. Romeroand M. Salgado, “Adsorption of As(III) and As(V) compounds on Fe3O4(0 0 1) surfaces: A first principle study”, *Computational Materials Science*, vol. 127. Elsevier BV, pp. 110–120, Feb. 2017. doi: 10.1016/j.commatsci.2016.10.029.  
  
P. Borisov, “Multiferroic BaCoF4 in Thin Film Form: Ferroelectricity, Magnetic Ordering, and Strain”, *ACS Applied Materials & Interfaces*, vol. 8, no. 4. American Chemical Society (ACS), pp. 2694–2703, Jan. 20, 2016. doi: 10.1021/acsami.5b10814.  
  
W. Dai, “Tailoring LaAlO3/SrTiO3 Interface Metallicity by Oxygen Surface Adsorbates”, *Nano Letters*, vol. 16, no. 4. American Chemical Society (ACS), pp. 2739–2743, Mar. 07, 2016. doi: 10.1021/acs.nanolett.6b00421.  
  
P. Dey, “Biexciton formation and exciton coherent coupling in layered GaSe”, *The Journal of Chemical Physics*, vol. 142, no. 21. AIP Publishing, p. 212422, Apr. 14, 2015. doi: 10.1063/1.4917169.  
  
P. Dey, “Optical Coherence in Atomic-Monolayer Transition-Metal Dichalcogenides Limited by Electron-Phonon Interactions”, *Physical Review Letters*, vol. 116, no. 12. American Physical Society (APS), Mar. 25, 2016. doi: 10.1103/physrevlett.116.127402.  
  
A. C. Garcia-Castro, A. H. Romeroand E. Bousquet, “Noncollinear magnetism in post-perovskites from first principles: Comparison between CaRhO3and NaNiF3”, *physica status solidi (b)*, vol. 252, no. 4. Wiley, pp. 689–694, Feb. 16, 2015. doi: 10.1002/pssb.201451400.  
  
A. C. Garcia-Castro, A. H. Romeroand E. Bousquet, “Strain-Engineered Multiferroicity inFluoroperovskite”, *Physical Review Letters*, vol. 116, no. 11. American Physical Society (APS), Mar. 14, 2016. doi: 10.1103/physrevlett.116.117202.  
  
A. C. Garcia-Castro, M. G. Vergniory, E. Bousquetand A. H. Romero, “Spin texture induced by oxygen vacancies in strontium perovskite (001) surfaces: A theoretical comparison betweenand”, *Physical Review B*, vol. 93, no. 4. American Physical Society (APS), Jan. 07, 2016. doi: 10.1103/physrevb.93.045405.  
  
X. Gonze, “The Abinitproject: Impact, environment and recent developments”, *Computer Physics Communications*, vol. 248. Elsevier BV, p. 107042, Mar. 2020. doi: 10.1016/j.cpc.2019.107042.  
  
X. Gonze, “The Abinitproject: Impact, environment and recent developments”, *Computer Physics Communications*, vol. 248. Elsevier BV, p. 107042, Mar. 2020. doi: 10.1016/j.cpc.2019.107042.  
  
X. Gonze, “The Abinitproject: Impact, environment and recent developments”, *Computer Physics Communications*, vol. 248. Elsevier BV, p. 107042, Mar. 2020. doi: 10.1016/j.cpc.2019.107042.  
  
X. Gonze, “The Abinitproject: Impact, environment and recent developments”, *Computer Physics Communications*, vol. 248. Elsevier BV, p. 107042, Mar. 2020. doi: 10.1016/j.cpc.2019.107042.  
  
U. Herath, “PyProcar: A Python library for electronic structure pre/post-processing”, *Computer Physics Communications*, vol. 251. Elsevier BV, p. 107080, Jun. 2020. doi: 10.1016/j.cpc.2019.107080.  
  
U. Herath, “PyProcar: A Python library for electronic structure pre/post-processing”, *Computer Physics Communications*, vol. 251. Elsevier BV, p. 107080, Jun. 2020. doi: 10.1016/j.cpc.2019.107080.  
  
U. Herath, “PyProcar: A Python library for electronic structure pre/post-processing”, *Computer Physics Communications*, vol. 251. Elsevier BV, p. 107080, Jun. 2020. doi: 10.1016/j.cpc.2019.107080.  
  
U. Herath, “PyProcar: A Python library for electronic structure pre/post-processing”, *Computer Physics Communications*, vol. 251. Elsevier BV, p. 107080, Jun. 2020. doi: 10.1016/j.cpc.2019.107080.  
  
S. López-Moreno and A. H. Romero, “Atomic and molecular oxygen adsorbed on (111) transition metal surfaces: Cu and Ni”, *The Journal of Chemical Physics*, vol. 142, no. 15. AIP Publishing, p. 154702, Apr. 21, 2015. doi: 10.1063/1.4917259.  
  
S. López-Moreno, A. H. Romero, J. Mejía-Lópezand A. Muñoz, “First-principles study of pressure-induced structural phase transitions in MnF2”, *Physical Chemistry Chemical Physics*, vol. 18, no. 48. Royal Society of Chemistry (RSC), pp. 33250–33263, 2016. doi: 10.1039/c6cp05467f.  
  
F. Munoz, A. H. Romero, J. Mejía-López, I. V. Roshchin, R. I. Gonzálezand M. Kiwi, “Surface states of FeF2 (110) and its uncompensated magnetization”, *Journal of Magnetism and Magnetic Materials*, vol. 393. Elsevier BV, pp. 226–232, Nov. 2015. doi: 10.1016/j.jmmm.2015.05.064.  
  
F. Munoz, “Topological Crystalline Insulator in a New Bi Semiconducting Phase”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Feb. 24, 2016. doi: 10.1038/srep21790.  
  
C. N. M. Ouma, S. Singh, K. O. Obodo, G. O. Amoloand A. H. Romero, “Controlling the magnetic and optical responses of a MoS2 monolayer by lanthanide substitutional doping: a first-principles study”, *Physical Chemistry Chemical Physics*, vol. 19, no. 37. Royal Society of Chemistry (RSC), pp. 25555–25563, 2017. doi: 10.1039/c7cp03160b.  
  
O. Pavlic, “Design of Mg alloys: The effects of Li concentration on the structure and elastic properties in the Mg-Li binary system by first principles calculations”, *Journal of Alloys and Compounds*, vol. 691. Elsevier BV, pp. 15–25, Jan. 2017. doi: 10.1016/j.jallcom.2016.08.217.  
  
A. Payne, G. Avedaño-Franco, X. He, E. Bousquetand A. H. Romero, “Optimizing the orbital occupation in the multiple minima problem of magnetic materials from the metaheuristic firefly algorithm”, *Physical Chemistry Chemical Physics*, vol. 21, no. 39. Royal Society of Chemistry (RSC), pp. 21932–21941, 2019. doi: 10.1039/c9cp03618k.  
  
A. H. Romero, “ABINIT: Overview and focus on selected capabilities”, *The Journal of Chemical Physics*, vol. 152, no. 12. AIP Publishing, p. 124102, Mar. 31, 2020. doi: 10.1063/1.5144261.  
  
A. H. Romero, “ABINIT: Overview and focus on selected capabilities”, *The Journal of Chemical Physics*, vol. 152, no. 12. AIP Publishing, p. 124102, Mar. 31, 2020. doi: 10.1063/1.5144261.  
  
A. H. Romero, “ABINIT: Overview and focus on selected capabilities”, *The Journal of Chemical Physics*, vol. 152, no. 12. AIP Publishing, p. 124102, Mar. 31, 2020. doi: 10.1063/1.5144261.  
  
A. H. Romero, “ABINIT: Overview and focus on selected capabilities”, *The Journal of Chemical Physics*, vol. 152, no. 12. AIP Publishing, p. 124102, Mar. 31, 2020. doi: 10.1063/1.5144261.  
  
R. Sarmiento-Pérez, “Novel phases of lithium-aluminum binaries from first-principles structural search”, *The Journal of Chemical Physics*, vol. 142, no. 2. AIP Publishing, p. 024710, Jan. 14, 2015. doi: 10.1063/1.4905141.  
  
S. Singh, A. C. Garcia-Castro, I. Valencia-Jaime, F. Muñozand A. H. Romero, “Prediction and control of spin polarization in a Weyl semimetallic phase of BiSb”, *Physical Review B*, vol. 94, no. 16. American Physical Society (APS), Oct. 18, 2016. doi: 10.1103/physrevb.94.161116.  
  
S. Singh, W. Ibarra-Hernández, I. Valencia-Jaime, G. Avendaño-Francoand A. H. Romero, “Investigation of novel crystal structures of Bi–Sb binaries predicted using the minima hopping method”, *Physical Chemistry Chemical Physics*, vol. 18, no. 43. Royal Society of Chemistry (RSC), pp. 29771–29785, 2016. doi: 10.1039/c6cp05401c.  
  
S. Singh, “Low-Energy Phases of Bi Monolayer Predicted by Structure Search in Two Dimensions”, *The Journal of Physical Chemistry Letters*, vol. 10, no. 23. American Chemical Society (ACS), pp. 7324–7332, Nov. 04, 2019. doi: 10.1021/acs.jpclett.9b03043.  
  
A. Talapatra, R. Arróyave, P. Entel, I. Valencia-Jaimeand A. H. Romero, “Stability analysis of the martensitic phase transformation inHeusler alloy”, *Physical Review B*, vol. 92, no. 5. American Physical Society (APS), Aug. 13, 2015. doi: 10.1103/physrevb.92.054107.  
  
E. Tangarife, A. H. Romeroand J. Mejía-López, “A charge optimized many-body potential for iron/iron-fluoride systems”, *Physical Chemistry Chemical Physics*, vol. 21, no. 36. Royal Society of Chemistry (RSC), pp. 20118–20131, 2019. doi: 10.1039/c9cp01927h.  
  
I. Valencia-Jaime, “Novel crystal structures for lithium–silicon alloy predicted by minima hopping method”, *Journal of Alloys and Compounds*, vol. 655. Elsevier BV, pp. 147–154, Jan. 2016. doi: 10.1016/j.jallcom.2015.09.101.  
  
M. Yang, “Room temperature ferroelectricity in fluoroperovskite thin films”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Aug. 03, 2017. doi: 10.1038/s41598-017-07834-0.  
  
J. A. H. Zeledon, A. H. Romero, P. Ren, X. Wen, Y. Liand J. P. Lewis, “The structural information filtered features (SIFF) potential: Maximizing information stored in machine-learning descriptors for materials prediction”, *Journal of Applied Physics*, vol. 127, no. 21. AIP Publishing, p. 215108, Jun. 07, 2020. doi: 10.1063/5.0002252.  
  
J. A. H. Zeledon, A. H. Romero, P. Ren, X. Wen, Y. Liand J. P. Lewis, “The structural information filtered features (SIFF) potential: Maximizing information stored in machine-learning descriptors for materials prediction”, *Journal of Applied Physics*, vol. 127, no. 21. AIP Publishing, p. 215108, Jun. 07, 2020. doi: 10.1063/5.0002252.  
  
J. A. H. Zeledon, A. H. Romero, P. Ren, X. Wen, Y. Liand J. P. Lewis, “The structural information filtered features (SIFF) potential: Maximizing information stored in machine-learning descriptors for materials prediction”, *Journal of Applied Physics*, vol. 127, no. 21. AIP Publishing, p. 215108, Jun. 07, 2020. doi: 10.1063/5.0002252.  
  
J. A. H. Zeledon, A. H. Romero, P. Ren, X. Wen, Y. Liand J. P. Lewis, “The structural information filtered features (SIFF) potential: Maximizing information stored in machine-learning descriptors for materials prediction”, *Journal of Applied Physics*, vol. 127, no. 21. AIP Publishing, p. 215108, Jun. 07, 2020. doi: 10.1063/5.0002252.  
  
W. Y. Wang, “Impact of W on structural evolution and diffusivity of Ni–W melts: an ab initio molecular dynamics study”, *Journal of Materials Science*, vol. 50, no. 3. Springer Science and Business Media LLC, pp. 1071–1081, Oct. 17, 2014. doi: 10.1007/s10853-014-8664-7.  
  
P. Zhang, J. J. Maldonis, M. F. Besser, M. J. Kramerand P. M. Voyles, “Medium-range structure and glass forming ability in Zr–Cu–Al bulk metallic glasses”, *Acta Materialia*, vol. 109. Elsevier BV, pp. 103–114, May 2016. doi: 10.1016/j.actamat.2016.02.006.  
  
F. Xue, X. Wang, I. socolenco, Y. Gu, L.-Q. Chenand S.-W. Cheong, “Evolution of the statistical distribution in a topological defect network”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, Nov. 20, 2015. doi: 10.1038/srep17057.  
  
I. Basaran, M. Emami Khansari, A. Pramanik, B. M. Wongand M. A. Hossain, “Binding and selectivity of dihydrogen phosphate by H-bond donors and acceptors in a tripodal-based thiourea receptor”, *Tetrahedron Letters*, vol. 56, no. 1. Elsevier BV, pp. 115–118, Jan. 2015. doi: 10.1016/j.tetlet.2014.11.025.  
  
M. M. Rhaman, A. Alamgir, B. M. Wong, D. R. Powelland M. A. Hossain, “A highly efficient dinuclear Cu(ii) chemosensor for colorimetric and fluorescent detection of cyanide in water”, *RSC Adv.*, vol. 4, no. 97. Royal Society of Chemistry (RSC), pp. 54263–54267, Oct. 17, 2014. doi: 10.1039/c4ra10813b.  
  
M. M. Rhaman, A. Alamgir, B. M. Wong, D. R. Powelland M. A. Hossain, “A highly efficient dinuclear Cu(ii) chemosensor for colorimetric and fluorescent detection of cyanide in water”, *RSC Adv.*, vol. 4, no. 97. Royal Society of Chemistry (RSC), pp. 54263–54267, Oct. 17, 2014. doi: 10.1039/c4ra10813b.  
  
D. K. Ward, X. Zhou, B. M. Wongand F. P. Doty, “A refined parameterization of the analytical Cd–Zn–Te bond-order potential”, *Journal of Molecular Modeling*, vol. 19, no. 12. Springer Science and Business Media LLC, pp. 5469–5477, Nov. 13, 2013. doi: 10.1007/s00894-013-2004-8.  
  
S. Chakraborty, R. Dutta, B. M. Wongand P. Ghosh, “Anion directed conformational diversities of an arene based hexa-amide receptor and recognition of the [F4(H2O)6]4− cluster”, *RSC Adv.*, vol. 4, no. 107. Royal Society of Chemistry (RSC), pp. 62689–62693, 2014. doi: 10.1039/c4ra10795k.  
  
L. Ruiz, A. Benjamin, M. Sullivanand S. Keten, “Regulating Ion Transport in Peptide Nanotubes by Tailoring the Nanotube Lumen Chemistry”, *The Journal of Physical Chemistry Letters*, vol. 6, no. 9. American Chemical Society (ACS), pp. 1514–1520, Apr. 09, 2015. doi: 10.1021/acs.jpclett.5b00252.  
  
J. D’Emidio and R. K. Kaul, “New Easy-Plane Fixed Points”, *Physical Review Letters*, vol. 118, no. 18. American Physical Society (APS), May 03, 2017. doi: 10.1103/physrevlett.118.187202.  
  
R. K. Kaul, “Spin Nematics, Valence-Bond Solids, and Spin Liquids inQuantum Spin Models on the Triangular Lattice”, *Physical Review Letters*, vol. 115, no. 15. American Physical Society (APS), Oct. 07, 2015. doi: 10.1103/physrevlett.115.157202.  
  
R. K. Kaul, “Marshall-positivequantum spin systems and classical loop models: A practical strategy to design sign-problem-free spin Hamiltonians”, *Physical Review B*, vol. 91, no. 5. American Physical Society (APS), Feb. 19, 2015. doi: 10.1103/physrevb.91.054413.  
  
X. Chong, “Understanding the Intrinsic P-Type Behavior and Phase Stability of Thermoelectric α-Mg3Sb2”, *ACS Applied Energy Materials*, vol. 1, no. 11. American Chemical Society (ACS), pp. 6600–6608, Oct. 08, 2018. doi: 10.1021/acsaem.8b01520.  
  
C. Z. Hargather, S.-L. Shangand Z.-K. Liu, “Data set for diffusion coefficients and relative creep rate ratios of 26 dilute Ni-X alloy systems from first-principles calculations”, *Data in Brief*, vol. 20. Elsevier BV, pp. 1537–1551, Oct. 2018. doi: 10.1016/j.dib.2018.08.144.  
  
C. Z. Hargather, S.-L. Shangand Z.-K. Liu, “A comprehensive first-principles study of solute elements in dilute Ni alloys: Diffusion coefficients and their implications to tailor creep rate”, *Acta Materialia*, vol. 157. Elsevier BV, pp. 126–141, Sep. 2018. doi: 10.1016/j.actamat.2018.07.020.  
  
Y.-J. Hu, “Thermodynamic modeling of the La-Te system aided by first-principles calculations”, *Calphad*, vol. 61. Elsevier BV, pp. 227–236, Jun. 2018. doi: 10.1016/j.calphad.2018.03.003.  
  
Y.-J. Hu, “Effects of alloying elements and temperature on the elastic properties of W-based alloys by first-principles calculations”, *Journal of Alloys and Compounds*, vol. 671. Elsevier BV, pp. 267–275, Jun. 2016. doi: 10.1016/j.jallcom.2016.02.018.  
  
H. Kim, A. J. Ross, S.-L. Shang, Y. Wang, L. J. Kecskesand Z.-K. Liu, “First-principles calculations and thermodynamic modelling of long periodic stacking ordered (LPSO) phases in Mg-Al-Gd”, *Materialia*, vol. 4. Elsevier BV, pp. 192–202, Dec. 2018. doi: 10.1016/j.mtla.2018.09.013.  
  
H. Kim, W. Y. Wang, S.-L. Shang, L. J. Kecskes, K. A. Darlingand Z.-K. Liu, “Elastic properties of long periodic stacking ordered phases in Mg-Gd-Al alloys: A first-principles study”, *Intermetallics*, vol. 98. Elsevier BV, pp. 18–27, Jul. 2018. doi: 10.1016/j.intermet.2018.04.009.  
  
A. Leineweber, “From random stacking faults to polytypes: A 12-layer NiSn4 polytype”, *Journal of Alloys and Compounds*, vol. 774. Elsevier BV, pp. 265–273, Feb. 2019. doi: 10.1016/j.jallcom.2018.09.341.  
  
J. Liu, “Thermodynamic properties and phase stability of the Ba-Bi system: A combined computational and experimental study”, *Journal of Alloys and Compounds*, vol. 771. Elsevier BV, pp. 281–289, Jan. 2019. doi: 10.1016/j.jallcom.2018.08.324.  
  
X. L. Liu, S.-L. Shang, Y.-J. Hu, Y. Wang, Y. Duand Z.-K. Liu, “Insight into γ-Ni/γ′-Ni3Al interfacial energy affected by alloying elements”, *Materials & Design*, vol. 133. Elsevier BV, pp. 39–46, Nov. 2017. doi: 10.1016/j.matdes.2017.07.028.  
  
Z.-K. Liu, “Ocean of Data: Integrating First-Principles Calculations and CALPHAD Modeling with Machine Learning”, *Journal of Phase Equilibria and Diffusion*, vol. 39, no. 5. Springer Science and Business Media LLC, pp. 635–649, Jul. 02, 2018. doi: 10.1007/s11669-018-0654-z.  
  
Z. Liu, “Epitaxial Growth of Intermetallic MnPt Films on Oxides and Large Exchange Bias”, *Advanced Materials*, vol. 28, no. 1. Wiley, pp. 118–123, Nov. 05, 2015. doi: 10.1002/adma.201502606.  
  
Z. Li, S.-L. Shang, J. Shen, P.-H. Liao, Z.-K. Liuand T. J. Anderson, “Thermodynamic Assessment of the Ag-Se System Aided by First-Principles Calculations”, *Journal of Phase Equilibria and Diffusion*, vol. 39, no. 6. Springer Science and Business Media LLC, pp. 870–881, Sep. 28, 2018. doi: 10.1007/s11669-018-0683-7.  
  
C. Marker, S.-L. Shang, J.-C. Zhaoand Z.-K. Liu, “Thermodynamic description of the Ti-Mo-Nb-Ta-Zr system and its implications for phase stability of Ti bio-implant materials”, *Calphad*, vol. 61. Elsevier BV, pp. 72–84, Jun. 2018. doi: 10.1016/j.calphad.2018.02.004.  
  
C. Marker, S.-L. Shang, J.-C. Zhaoand Z.-K. Liu, “Effects of alloying elements on the elastic properties of bcc Ti-X alloys from first-principles calculations”, *Computational Materials Science*, vol. 142. Elsevier BV, pp. 215–226, Feb. 2018. doi: 10.1016/j.commatsci.2017.10.016.  
  
A. J. Ross, “A first-principles based description of the Hf-Ni system supported by high-temperature synchrotron experiments”, *Thermochimica Acta*, vol. 668. Elsevier BV, pp. 142–151, Oct. 2018. doi: 10.1016/j.tca.2018.08.011.  
  
S.-L. Shang, Y. Wang, B. Gleesonand Z.-K. Liu, “Understanding slow-growing alumina scale mediated by reactive elements: Perspective via local metal-oxygen bonding strength”, *Scripta Materialia*, vol. 150. Elsevier BV, pp. 139–142, Jun. 2018. doi: 10.1016/j.scriptamat.2018.03.002.  
  
S.-L. Shang, “A comprehensive first-principles study of pure elements: Vacancy formation and migration energies and self-diffusion coefficients”, *Acta Materialia*, vol. 109. Elsevier BV, pp. 128–141, May 2016. doi: 10.1016/j.actamat.2016.02.031.  
  
W. Y. Wang, “Lattice distortion induced anomalous ferromagnetism and electronic structure in FCC Fe and Fe-TM (TM = Cr, Ni, Ta and Zr) alloys”, *Materials Chemistry and Physics*, vol. 162. Elsevier BV, pp. 748–756, Jul. 2015. doi: 10.1016/j.matchemphys.2015.06.051.  
  
W. Y. Wang, “Atomic and electronic basis for solutes strengthened (010) anti-phase boundary of L12 Co3(Al, TM): A comprehensive first-principles study”, *Acta Materialia*, vol. 145. Elsevier BV, pp. 30–40, Feb. 2018. doi: 10.1016/j.actamat.2017.10.041.  
  
Y. Wang, “First-principles thermodynamic theory of Seebeck coefficients”, *Physical Review B*, vol. 98, no. 22. American Physical Society (APS), Dec. 03, 2018. doi: 10.1103/physrevb.98.224101.  
  
Y. Wang, “Quasiharmonic calculations of thermodynamic properties for La3−xTe4 system”, *Computational Materials Science*, vol. 142. Elsevier BV, pp. 417–426, Feb. 2018. doi: 10.1016/j.commatsci.2017.10.036.  
  
Y. Wang, “First-principles calculations of lattice dynamics and thermodynamic properties for Yb14MnSb11”, *Journal of Applied Physics*, vol. 123, no. 4. AIP Publishing, p. 045102, Jan. 28, 2018. doi: 10.1063/1.5013601.  
  
Y. Wang, “Computation of entropies and phase equilibria in refractory V-Nb-Mo-Ta-W high-entropy alloys”, *Acta Materialia*, vol. 143. Elsevier BV, pp. 88–101, Jan. 2018. doi: 10.1016/j.actamat.2017.10.017.  
  
W. W. Xu, “A first-principles study of the diffusion coefficients of alloying elements in dilute α-Ti alloys”, *Physical Chemistry Chemical Physics*, vol. 18, no. 25. Royal Society of Chemistry (RSC), pp. 16870–16881, 2016. doi: 10.1039/c6cp01899h.  
  
Z. Yu, “A quaternary sodium superionic conductor - Na10.8Sn1.9PS11.8”, *Nano Energy*, vol. 47. Elsevier BV, pp. 325–330, May 2018. doi: 10.1016/j.nanoen.2018.01.046.  
  
B.-C. Zhou, S.-L. Shang, Y. Wangand Z.-K. Liu, “Data set for diffusion coefficients of alloying elements in dilute Mg alloys from first-principles”, *Data in Brief*, vol. 5. Elsevier BV, pp. 900–912, Dec. 2015. doi: 10.1016/j.dib.2015.10.024.  
  
B.-C. Zhou, S.-L. Shang, Y. Wangand Z.-K. Liu, “Diffusion coefficients of alloying elements in dilute Mg alloys: A comprehensive first-principles study”, *Acta Materialia*, vol. 103. Elsevier BV, pp. 573–586, Jan. 2016. doi: 10.1016/j.actamat.2015.10.010.  
  
H. Fang, Y. Wang, S. Shangand Z.-K. Liu, “Nature of ferroelectric-paraelectric phase transition and origin of negative thermal expansion in”, *Physical Review B*, vol. 91, no. 2. American Physical Society (APS), Jan. 09, 2015. doi: 10.1103/physrevb.91.024104.  
  
X. L. Liu, T. Gheno, B. B. Lindahl, G. Lindwall, B. Gleesonand Z.-K. Liu, “First-Principles Calculations, Experimental Study, and Thermodynamic Modeling of the Al-Co-Cr System”, *PLOS ONE*, vol. 10, no. 4. Public Library of Science (PLoS), p. e0121386, Apr. 13, 2015. doi: 10.1371/journal.pone.0121386.  
  
Z.-K. Liu, Y. Wangand S. Shang, “Thermal Expansion Anomaly Regulated by Entropy”, *Scientific Reports*, vol. 4, no. 1. Springer Science and Business Media LLC, Nov. 13, 2014. doi: 10.1038/srep07043.  
  
S. Shang, “Insight into structural, elastic, phonon, and thermodynamic properties of α-sulfur and energy-related sulfides: a comprehensive first-principles study”, *Journal of Materials Chemistry A*, vol. 3, no. 15. Royal Society of Chemistry (RSC), pp. 8002–8014, 2015. doi: 10.1039/c4ta07062c.  
  
S. Shang, Y. Wang, G. Lindwall, N. R. Kelly, T. J. Andersonand Z.-K. Liu, “Cation Disorder Regulation by Microstate Configurational Entropy in Photovoltaic Absorber Materials Cu2ZnSn(S,Se)4”, *The Journal of Physical Chemistry C*, vol. 118, no. 43. American Chemical Society (ACS), pp. 24884–24889, Oct. 17, 2014. doi: 10.1021/jp508840s.  
  
W. Y. Wang, “Anomalous structural dynamics in liquid Al80Cu20: An ab initio molecular dynamics study”, *Acta Materialia*, vol. 97. Elsevier BV, pp. 75–85, Sep. 2015. doi: 10.1016/j.actamat.2015.07.001.  
  
A. Sambasivam, A. V. Sangwaiand R. Sureshkumar, “Self-Assembly of Nanoparticle–Surfactant Complexes with Rodlike Micelles: A Molecular Dynamics Study”, *Langmuir*, vol. 32, no. 5. American Chemical Society (ACS), pp. 1214–1219, Jan. 28, 2016. doi: 10.1021/acs.langmuir.5b03689.  
  
L. Fan, H. L. Zhuang, L. Gao, Y. Luand L. A. Archer, “Regulating Li deposition at artificial solid electrolyte interphases”, *Journal of Materials Chemistry A*, vol. 5, no. 7. Royal Society of Chemistry (RSC), pp. 3483–3492, 2017. doi: 10.1039/c6ta10204b.  
  
H. L. Zhuang and R. G. Hennig, “Stability and magnetism of strongly correlated single-layer”, *Physical Review B*, vol. 93, no. 5. American Physical Society (APS), Feb. 26, 2016. doi: 10.1103/physrevb.93.054429.  
  
H. L. Zhuang, P. R. C. Kentand R. G. Hennig, “Strong anisotropy and magnetostriction in the two-dimensional Stoner ferromagnet”, *Physical Review B*, vol. 93, no. 13. American Physical Society (APS), Apr. 06, 2016. doi: 10.1103/physrevb.93.134407.  
  
H. L. Zhuang, Y. Xie, P. R. C. Kentand P. Ganesh, “Computational discovery of ferromagnetic semiconducting single-layer”, *Physical Review B*, vol. 92, no. 3. American Physical Society (APS), Jul. 06, 2015. doi: 10.1103/physrevb.92.035407.  
  
H. L. Zhuang and J. Zhou, “Density functional theory study of bulk and single-layer magnetic semiconductor ”, *Physical Review B*, vol. 94, no. 19. American Physical Society (APS), Nov. 16, 2016. doi: 10.1103/physrevb.94.195307.  
  
L. Cao and T. Mueller, “Rational Design of Pt3Ni Surface Structures for the Oxygen Reduction Reaction”, *The Journal of Physical Chemistry C*, vol. 119, no. 31. American Chemical Society (ACS), pp. 17735–17747, Jul. 23, 2015. doi: 10.1021/acs.jpcc.5b04951.  
  
L. Cao and T. Mueller, “Theoretical Insights into the Effects of Oxidation and Mo-Doping on the Structure and Stability of Pt–Ni Nanoparticles”, *Nano Letters*, vol. 16, no. 12. American Chemical Society (ACS), pp. 7748–7754, Nov. 07, 2016. doi: 10.1021/acs.nanolett.6b03867.  
  
L. Cao, L. Niuand T. Mueller, “Computationally generated maps of surface structures and catalytic activities for alloy phase diagrams”, *Proceedings of the National Academy of Sciences*, vol. 116, no. 44. Proceedings of the National Academy of Sciences, pp. 22044–22051, Oct. 14, 2019. doi: 10.1073/pnas.1910724116.  
  
L. Cao, “Mechanistic Insights for Low-Overpotential Electroreduction of CO2 to CO on Copper Nanowires”, *ACS Catalysis*, vol. 7, no. 12. American Chemical Society (ACS), pp. 8578–8587, Nov. 17, 2017. doi: 10.1021/acscatal.7b03107.  
  
L. Cao, “Differential Surface Elemental Distribution Leads to Significantly Enhanced Stability of PtNi-Based ORR Catalysts”, *Matter*, vol. 1, no. 6. Elsevier BV, pp. 1567–1580, Dec. 2019. doi: 10.1016/j.matt.2019.07.015.  
  
X. Huang, “High-performance transition metal–doped Pt 3 Ni octahedra for oxygen reduction reaction”, *Science*, vol. 348, no. 6240. American Association for the Advancement of Science (AAAS), pp. 1230–1234, Jun. 12, 2015. doi: 10.1126/science.aaa8765.  
  
D. Raciti, “Low-Overpotential Electroreduction of Carbon Monoxide Using Copper Nanowires”, *ACS Catalysis*, vol. 7, no. 7. American Chemical Society (ACS), pp. 4467–4472, Jun. 05, 2017. doi: 10.1021/acscatal.7b01124.  
  
Y. Wang, “Ensemble Effect in Bimetallic Electrocatalysts for CO2 Reduction”, *Journal of the American Chemical Society*, vol. 141, no. 42. American Chemical Society (ACS), pp. 16635–16642, Sep. 11, 2019. doi: 10.1021/jacs.9b05766.  
  
S. Nazir, M. Behtashand K. Yang, “Enhancing interfacial conductivity and spatial charge confinement of LaAlO3/SrTiO3 heterostructures via strain engineering”, *Applied Physics Letters*, vol. 105, no. 14. AIP Publishing, p. 141602, Oct. 06, 2014. doi: 10.1063/1.4897626.  
  
S. Nazir, M. Behtashand K. Yang, “Towards enhancing two-dimensional electron gas quantum confinement effects in perovskite oxide heterostructures”, *Journal of Applied Physics*, vol. 117, no. 11. AIP Publishing, p. 115305, Mar. 21, 2015. doi: 10.1063/1.4915950.  
  
Y. Wang, W. Tang, J. Cheng, M. Behtashand K. Yang, “Creating Two-Dimensional Electron Gas in Polar/Polar Perovskite Oxide Heterostructures: First-Principles Characterization of LaAlO3/A+B5+O3”, *ACS Applied Materials & Interfaces*, vol. 8, no. 21. American Chemical Society (ACS), pp. 13659–13668, May 17, 2016. doi: 10.1021/acsami.6b02399.  
  
Y. Wang, W. Tang, J. Cheng, S. Nazirand K. Yang, “High-mobility two-dimensional electron gas in SrGeO3- and BaSnO3-based perovskite oxide heterostructures: an ab initio study”, *Physical Chemistry Chemical Physics*, vol. 18, no. 46. Royal Society of Chemistry (RSC), pp. 31924–31929, 2016. doi: 10.1039/c6cp05572a.  
  
K. Yang, S. Nazir, M. Behtashand J. Cheng, “High-Throughput Design of Two-Dimensional Electron Gas Systems Based on Polar/Nonpolar Perovskite Oxide Heterostructures”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Oct. 06, 2016. doi: 10.1038/srep34667.  
  
C. A. Stephenson, “Band structure of germanium carbides for direct bandgap silicon photonics”, *Journal of Applied Physics*, vol. 120, no. 5. AIP Publishing, p. 053102, Aug. 07, 2016. doi: 10.1063/1.4959255.  
  
Y. Chen, “A robust and active hybrid catalyst for facile oxygen reduction in solid oxide fuel cells”, *Energy & Environmental Science*, vol. 10, no. 4. Royal Society of Chemistry (RSC), pp. 964–971, 2017. doi: 10.1039/c6ee03656b.  
  
T. Wei, L. A. Zhang, Y. Chen, P. Yangand M. Liu, “Promising Proton Conductor for Intermediate-Temperature Fuel Cells: Li13.9Sr0.1Zn(GeO4)4”, *Chemistry of Materials*, vol. 29, no. 4. American Chemical Society (ACS), pp. 1490–1495, Feb. 10, 2017. doi: 10.1021/acs.chemmater.6b03471.  
  
B. Zhao, “A tailored double perovskite nanofiber catalyst enables ultrafast oxygen evolution”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Feb. 27, 2017. doi: 10.1038/ncomms14586.  
  
M. Dutt, O. Kuksenok, M. J. Nayhouse, S. R. Littleand A. C. Balazs, “Modeling the Self-Assembly of Lipids and Nanotubes in Solution: Forming Vesicles and Bicelles with Transmembrane Nanotube Channels”, *ACS Nano*, vol. 5, no. 6. American Chemical Society (ACS), pp. 4769–4782, May 31, 2011. doi: 10.1021/nn201260r.  
  
P. L. J. Conway, A. L. Shaw, L. Bassman, M. Ferryand K. J. Laws, “Stabilisation of Disordered bcc Phases in Magnesium-Rare Earth Alloys”, *The Minerals, Metals & Materials Series*. Springer International Publishing, pp. 497–503, 2017. doi: 10.1007/978-3-319-52392-7\_68.  
  
K. J. Laws, “High entropy brasses and bronzes – Microstructure, phase evolution and properties”, *Journal of Alloys and Compounds*, vol. 650. Elsevier BV, pp. 949–961, Nov. 2015. doi: 10.1016/j.jallcom.2015.07.285.  
  
S. Aron-Dine, G. S. Pomrehn, A. Pribram-Jones, K. J. Lawsand L. Bassman, “First-principles investigation of structural and magnetic disorder in CuNiMnAl and CuNiMnSn Heusler alloys”, *Physical Review B*, vol. 95, no. 2. American Physical Society (APS), Jan. 10, 2017. doi: 10.1103/physrevb.95.024108.  
  
A. K. Omar, “Aggregation Behavior of Rod–Coil–Rod Triblock Copolymers in a Coil-Selective Solvent”, *The Journal of Physical Chemistry B*, vol. 119, no. 1. American Chemical Society (ACS), pp. 330–337, Dec. 16, 2014. doi: 10.1021/jp509016c.  
  
L. Simine and P. J. Rossky, “Relating Chromophoric and Structural Disorder in Conjugated Polymers”, *The Journal of Physical Chemistry Letters*, vol. 8, no. 8. American Chemical Society (ACS), pp. 1752–1756, Apr. 06, 2017. doi: 10.1021/acs.jpclett.7b00290.  
  
M. M. Henry, “Simplified Models for Accelerated Structural Prediction of Conjugated Semiconducting Polymers”, *The Journal of Physical Chemistry C*, vol. 121, no. 47. American Chemical Society (ACS), pp. 26528–26538, Nov. 20, 2017. doi: 10.1021/acs.jpcc.7b09701.  
  
M. L. Jones and E. Jankowski, “Computationally connecting organic photovoltaic performance to atomistic arrangements and bulk morphology”, *Molecular Simulation*, vol. 43, no. 10–11. Informa UK Limited, pp. 756–773, Mar. 09, 2017. doi: 10.1080/08927022.2017.1296958.  
  
E. Miller, M. Jones, M. Henry, P. Chery, K. Millerand E. Jankowski, “Optimization and Validation of Efficient Models for Predicting Polythiophene Self-Assembly”, *Polymers*, vol. 10, no. 12. MDPI AG, p. 1305, Nov. 26, 2018. doi: 10.3390/polym10121305.  
  
E. D. Miller, M. L. Jonesand E. Jankowski, “Enhanced Computational Sampling of Perylene and Perylothiophene Packing with Rigid-Body Models”, *ACS Omega*, vol. 2, no. 1. American Chemical Society (ACS), pp. 353–362, Jan. 31, 2017. doi: 10.1021/acsomega.6b00371.  
  
E. Miller, M. Jonesand E. Jankowski, “Tying Together Multiscale Calculations for Charge Transport in P3HT: Structural Descriptors, Morphology, and Tie-Chains”, *Polymers*, vol. 10, no. 12. MDPI AG, p. 1358, Dec. 07, 2018. doi: 10.3390/polym10121358.  
  
X. Hu, Z. Zhongand G. A. Fiete, “First Principles Prediction of Topological Phases in Thin Films of Pyrochlore Iridates”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, Jun. 16, 2015. doi: 10.1038/srep11072.  
  
F. Aydin, “Self-Assembly and Critical Aggregation Concentration Measurements of ABA Triblock Copolymers with Varying B Block Types: Model Development, Prediction, and Validation”, *The Journal of Physical Chemistry B*, vol. 120, no. 15. American Chemical Society (ACS), pp. 3666–3676, Apr. 12, 2016. doi: 10.1021/acs.jpcb.5b12594.  
  
F. Aydin and M. Dutt, “Bioinspired Vesicles Encompassing Two-Tail Phospholipids: Self-Assembly and Phase Segregation via Implicit Solvent Coarse-Grained Molecular Dynamics”, *The Journal of Physical Chemistry B*, vol. 118, no. 29. American Chemical Society (ACS), pp. 8614–8623, Jul. 10, 2014. doi: 10.1021/jp503376r.  
  
F. Aydin and M. Dutt, “Surface Reconfiguration of Binary Lipid Vesicles via Electrostatically Induced Nanoparticle Adsorption”, *The Journal of Physical Chemistry B*, vol. 120, no. 27. American Chemical Society (ACS), pp. 6646–6656, Jul. 05, 2016. doi: 10.1021/acs.jpcb.6b02334.  
  
F. Aydin, G. Uppaladadiumand M. Dutt, “Harnessing Nanoscale Confinement to Design Sterically Stable Vesicles of Specific Shapes via Self-Assembly”, *The Journal of Physical Chemistry B*, vol. 119, no. 32. American Chemical Society (ACS), pp. 10207–10215, Jul. 31, 2015. doi: 10.1021/acs.jpcb.5b02239.  
  
F. Aydin, G. Uppaladadiumand M. Dutt, “The design of shape-tunable hairy vesicles”, *Colloids and Surfaces B: Biointerfaces*, vol. 128. Elsevier BV, pp. 268–275, Apr. 2015. doi: 10.1016/j.colsurfb.2015.01.049.  
  
F. Aydin, G. Uppaladadiumand M. Dutt, “Harnessing steric hindrance to control interfacial adsorption of patchy nanoparticles onto hairy vesicles”, *Colloids and Surfaces B: Biointerfaces*, vol. 141. Elsevier BV, pp. 458–466, May 2016. doi: 10.1016/j.colsurfb.2016.01.061.  
  
L. Chong, F. Aydinand M. Dutt, “Implicit solvent coarse-grained model of polyamidoamine dendrimers: Role of generation and pH”, *Journal of Computational Chemistry*, vol. 37, no. 10. Wiley, pp. 920–926, Dec. 17, 2015. doi: 10.1002/jcc.24277.  
  
L. Chong and M. Dutt, “Design of PAMAM-COO dendron-grafted surfaces to promote Pb(ii) ion adsorption”, *Physical Chemistry Chemical Physics*, vol. 17, no. 16. Royal Society of Chemistry (RSC), pp. 10615–10623, 2015. doi: 10.1039/c5cp00309a.  
  
X. Chu, F. Aydinand M. Dutt, “Modeling Interactions between Multicomponent Vesicles and Antimicrobial Peptide-Inspired Nanoparticles”, *ACS Nano*, vol. 10, no. 8. American Chemical Society (ACS), pp. 7351–7361, Jul. 21, 2016. doi: 10.1021/acsnano.5b08133.  
  
X. Chu, X. Yu, J. Greenstein, F. Aydin, G. Uppaladadiumand M. Dutt, “Flow-Induced Shape Reconfiguration, Phase Separation, and Rupture of Bio-Inspired Vesicles”, *ACS Nano*, vol. 11, no. 7. American Chemical Society (ACS), pp. 6661–6671, Jun. 12, 2017. doi: 10.1021/acsnano.7b00753.  
  
M. Dutt, L. Chong, S. Libringand V. Karra, “Self-assembly of virus capsids decorated with block copolymers: a simulation study”, *Journal of Materials Research*, vol. 32, no. 1. Springer Science and Business Media LLC, pp. 143–152, Dec. 05, 2016. doi: 10.1557/jmr.2016.427.  
  
J. Li, K. Jin, S. C. Mushnooriand M. Dutt, “Mechanisms underlying interactions between PAMAM dendron-grafted surfaces with DPPC membranes”, *RSC Advances*, vol. 8, no. 44. Royal Society of Chemistry (RSC), pp. 24982–24992, 2018. doi: 10.1039/c8ra03742f.  
  
A. Moretti, B. Zhang, B. Lee, M. Duttand K. E. Uhrich, “Degree of Unsaturation and Backbone Orientation of Amphiphilic Macromolecules Influence Local Lipid Properties in Large Unilamellar Vesicles”, *Langmuir*, vol. 33, no. 51. American Chemical Society (ACS), pp. 14663–14673, Dec. 13, 2017. doi: 10.1021/acs.langmuir.7b03043.  
  
S. Mushnoori, K. Schmidt, V. Nandaand M. Dutt, “Designing phenylalanine-based hybrid biological materials: controlling morphology *via* molecular composition”, *Organic & Biomolecular Chemistry*, vol. 16, no. 14. Royal Society of Chemistry (RSC), pp. 2499–2507, 2018. doi: 10.1039/c8ob00130h.  
  
V. C. Muthukumar, L. Chongand M. Dutt, “Designing soft nanomaterials via the self assembly of functionalized icosahedral viral capsid nanoparticles”, *Journal of Materials Research*, vol. 30, no. 1. Springer Science and Business Media LLC, pp. 141–150, Dec. 02, 2014. doi: 10.1557/jmr.2014.346.  
  
X. Yu and M. Dutt, “A multiscale approach to study molecular and interfacial characteristics of vesicles”, *Molecular Systems Design & Engineering*, vol. 3, no. 6. Royal Society of Chemistry (RSC), pp. 883–895, 2018. doi: 10.1039/c8me00029h.  
  
C. S. Adorf, J. Antonaglia, J. Dshemuchadseand S. C. Glotzer, “Inverse design of simple pair potentials for the self-assembly of complex structures”, *The Journal of Chemical Physics*, vol. 149, no. 20. AIP Publishing, p. 204102, Nov. 28, 2018. doi: 10.1063/1.5063802.  
  
J. A. Anderson, M. Eric Irrgangand S. C. Glotzer, “Scalable Metropolis Monte Carlo for simulation of hard shapes”, *Computer Physics Communications*, vol. 204. Elsevier BV, pp. 21–30, Jul. 2016. doi: 10.1016/j.cpc.2016.02.024.  
  
J. A. Anderson, J. Glaserand S. C. Glotzer, “HOOMD-blue: A Python package for high-performance molecular dynamics and hard particle Monte Carlo simulations”, *Computational Materials Science*, vol. 173. Elsevier BV, p. 109363, Feb. 2020. doi: 10.1016/j.commatsci.2019.109363.  
  
A. T. Cadotte, J. Dshemuchadse, P. F. Damasceno, R. S. Newmanand S. C. Glotzer, “Self-assembly of a space-tessellating structure in the binary system of hard tetrahedra and octahedra”, *Soft Matter*, vol. 12, no. 34. Royal Society of Chemistry (RSC), pp. 7073–7078, 2016. doi: 10.1039/c6sm01180b.  
  
R. K. Cersonsky, G. van Anders, P. M. Doddand S. C. Glotzer, “Relevance of packing to colloidal self-assembly”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 7. Proceedings of the National Academy of Sciences, pp. 1439–1444, Jan. 30, 2018. doi: 10.1073/pnas.1720139115.  
  
B. Dice, V. Ramasubramani, E. Harper, M. Spellings, J. Andersonand S. Glotzer, “Analyzing Particle Systems for Machine Learning and Data Visualization with freud”, *Proceedings of the 18th Python in Science Conference*. SciPy, 2019. doi: 10.25080/majora-7ddc1dd1-004.  
  
P. M. Dodd, P. F. Damascenoand S. C. Glotzer, “Universal folding pathways of polyhedron nets”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 29. Proceedings of the National Academy of Sciences, Jul. 03, 2018. doi: 10.1073/pnas.1722681115.  
  
C. X. Du, G. van Anders, R. S. Newmanand S. C. Glotzer, “Shape-driven solid–solid transitions in colloids”, *Proceedings of the National Academy of Sciences*, vol. 114, no. 20. Proceedings of the National Academy of Sciences, May 2017. doi: 10.1073/pnas.1621348114.  
  
K. C. Elbert, “Dendrimer Ligand Directed Nanoplate Assembly”, *ACS Nano*, vol. 13, no. 12. American Chemical Society (ACS), pp. 14241–14251, Nov. 22, 2019. doi: 10.1021/acsnano.9b07348.  
  
J. Glaser, A. S. Karasand S. C. Glotzer, “A parallel algorithm for implicit depletant simulations”, *The Journal of Chemical Physics*, vol. 143, no. 18. AIP Publishing, p. 184110, Nov. 14, 2015. doi: 10.1063/1.4935175.  
  
E. S. Harper, R. L. Marson, J. A. Anderson, G. van Andersand S. C. Glotzer, “Shape allophiles improve entropic assembly”, *Soft Matter*, vol. 11, no. 37. Royal Society of Chemistry (RSC), pp. 7250–7256, 2015. doi: 10.1039/c5sm01351h.  
  
E. S. Harper, G. van Andersand S. C. Glotzer, “The entropic bond in colloidal crystals”, *Proceedings of the National Academy of Sciences*, vol. 116, no. 34. Proceedings of the National Academy of Sciences, pp. 16703–16710, Aug. 02, 2019. doi: 10.1073/pnas.1822092116.  
  
E. S. Harper, B. Watersand S. C. Glotzer, “Hierarchical self-assembly of hard cube derivatives”, *Soft Matter*, vol. 15, no. 18. Royal Society of Chemistry (RSC), pp. 3733–3739, 2019. doi: 10.1039/c8sm02619j.  
  
L. C. Hsiao, “Metastable orientational order of colloidal discoids”, *Nature Communications*, vol. 6, no. 1. Springer Science and Business Media LLC, Oct. 07, 2015. doi: 10.1038/ncomms9507.  
  
A. S. Karas, J. Dshemuchadse, G. van Andersand S. C. Glotzer, “Phase behavior and design rules for plastic colloidal crystals of hard polyhedra *via* consideration of directional entropic forces”, *Soft Matter*, vol. 15, no. 27. Royal Society of Chemistry (RSC), pp. 5380–5389, 2019. doi: 10.1039/c8sm02643b.  
  
A. S. Karas, J. Glaserand S. C. Glotzer, “Using depletion to control colloidal crystal assemblies of hard cuboctahedra”, *Soft Matter*, vol. 12, no. 23. Royal Society of Chemistry (RSC), pp. 5199–5204, 2016. doi: 10.1039/c6sm00620e.  
  
S. Lee, E. G. Teich, M. Engeland S. C. Glotzer, “Entropic colloidal crystallization pathways via fluid–fluid transitions and multidimensional prenucleation motifs”, *Proceedings of the National Academy of Sciences*, vol. 116, no. 30. Proceedings of the National Academy of Sciences, pp. 14843–14851, Jul. 08, 2019. doi: 10.1073/pnas.1905929116.  
  
R. S. Newman, S. Nola, J. Dshemuchadseand S. C. Glotzer, “Shape-controlled crystallisation pathways in dense fluids of *ccp*-forming hard polyhedra”, *Molecular Physics*, vol. 117, no. 23–24. Informa UK Limited, pp. 3819–3826, Sep. 24, 2019. doi: 10.1080/00268976.2019.1668574.  
  
J. S. Oh, S. Lee, S. C. Glotzer, G.-R. Yiand D. J. Pine, “Colloidal fibers and rings by cooperative assembly”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Sep. 02, 2019. doi: 10.1038/s41467-019-11915-1.  
  
E. G. Teich, G. van Anders, D. Klotsa, J. Dshemuchadseand S. C. Glotzer, “Clusters of polyhedra in spherical confinement”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 6. Proceedings of the National Academy of Sciences, Jan. 25, 2016. doi: 10.1073/pnas.1524875113.  
  
B. VanSaders and S. C. Glotzer, “Designing active particles for colloidal microstructure manipulation *via* strain field alchemy”, *Soft Matter*, vol. 15, no. 30. Royal Society of Chemistry (RSC), pp. 6086–6096, 2019. doi: 10.1039/c9sm00896a.  
  
B. VanSaders and S. C. Glotzer, “Pinning dislocations in colloidal crystals with active particles that seek stacking faults”, *Soft Matter*, vol. 16, no. 17. Royal Society of Chemistry (RSC), pp. 4182–4191, 2020. doi: 10.1039/c9sm02514f.  
  
D. Filonowich, M. Luna, T. Quinnand P. Choudhury, “Electronic Descriptor of Single Metal-Oxo Species on Phthalocyanine- and Porphyrin-Functionalized Graphene toward Methane Activation Process”, *The Journal of Physical Chemistry C*, vol. 124, no. 8. American Chemical Society (ACS), pp. 4502–4510, Jan. 29, 2020. doi: 10.1021/acs.jpcc.9b08697.  
  
J. H. Park, “*In Situ* Observation of Initial Stage in Dielectric Growth and Deposition of Ultrahigh Nucleation Density Dielectric on Two-Dimensional Surfaces”, *Nano Letters*, vol. 15, no. 10. American Chemical Society (ACS), pp. 6626–6633, Sep. 28, 2015. doi: 10.1021/acs.nanolett.5b02429.  
  
T. Quinn and P. Choudhury, “Direct oxidation of methane to methanol on single-site copper-oxo species of copper porphyrin functionalized graphene: A DFT study”, *Molecular Catalysis*, vol. 431. Elsevier BV, pp. 9–14, Apr. 2017. doi: 10.1016/j.mcat.2017.01.018.  
  
C. Stephenson, M. Gillett-Kunnath, W. O’Brien, R. Kudrawiecand M. Wistey, “Gas Source Techniques for Molecular Beam Epitaxy of Highly Mismatched Ge Alloys”, *Crystals*, vol. 6, no. 12. MDPI AG, p. 159, Dec. 02, 2016. doi: 10.3390/cryst6120159.  
  
C. A. Stephenson, W. A. O’brien, M. Qi, M. Penninger, W. F. Schneiderand M. A. Wistey, “Band Anticrossing in Dilute Germanium Carbides Using Hybrid Density Functionals”, *Journal of Electronic Materials*, vol. 45, no. 4. Springer Science and Business Media LLC, pp. 2121–2126, Dec. 30, 2015. doi: 10.1007/s11664-015-4300-9.  
  
B. Ozdemir and V. Barone, “Structural and electronic properties of crystalline graphite-like BC3”, *Computational Materials Science*, vol. 109. Elsevier BV, pp. 248–252, Nov. 2015. doi: 10.1016/j.commatsci.2015.07.009.  
  
X. Ren, “Atom Probe Tomography Analysis of Ag Doping in 2D Layered Material (PbSe)5(Bi2Se3)3”, *Nano Letters*, vol. 16, no. 10. American Chemical Society (ACS), pp. 6064–6069, Sep. 09, 2016. doi: 10.1021/acs.nanolett.6b02104.  
  
Z. Li, K. A. Fichthornand S. T. Milner, “Surfactant Binding to Polymer–Water Interfaces in Atomistic Simulations”, *Langmuir*, vol. 32, no. 30. American Chemical Society (ACS), pp. 7519–7529, Jul. 22, 2016. doi: 10.1021/acs.langmuir.6b01393.  
  
A. Shavit and R. A. Riggleman, “The dynamics of unentangled polymers during capillary rise infiltration into a nanoparticle packing”, *Soft Matter*, vol. 11, no. 42. Royal Society of Chemistry (RSC), pp. 8285–8295, 2015. doi: 10.1039/c5sm01866h.  
  
R. Beams, “Characterization of Few-Layer 1T′ MoTe2 by Polarization-Resolved Second Harmonic Generation and Raman Scattering”, *ACS Nano*, vol. 10, no. 10. American Chemical Society (ACS), pp. 9626–9636, Oct. 13, 2016. doi: 10.1021/acsnano.6b05127.  
  
M. R. Hasan, “An Antimony Selenide Molecular Ink for Flexible Broadband Photodetectors”, *Advanced Electronic Materials*, vol. 2, no. 9. Wiley, p. 1600182, Aug. 03, 2016. doi: 10.1002/aelm.201600182.  
  
K. Mathew, “MPInterfaces: A Materials Project based Python tool for high-throughput computational screening of interfacial systems”, *Computational Materials Science*, vol. 122. Elsevier BV, pp. 183–190, Sep. 2016. doi: 10.1016/j.commatsci.2016.05.020.  
  
S. M. Oliver, “The structural phases and vibrational properties of Mo 1−x W x Te 2 alloys”, *2D Materials*, vol. 4, no. 4. IOP Publishing, p. 045008, Aug. 31, 2017. doi: 10.1088/2053-1583/aa7a32.  
  
A. Shinde, “Discovery of Manganese-Based Solar Fuel Photoanodes via Integration of Electronic Structure Calculations, Pourbaix Stability Modeling, and High-Throughput Experiments”, *ACS Energy Letters*, vol. 2, no. 10. American Chemical Society (ACS), pp. 2307–2312, Sep. 12, 2017. doi: 10.1021/acsenergylett.7b00607.  
  
A. K. Singh, J. H. Montoya, J. M. Gregoireand K. A. Persson, “Robust and synthesizable photocatalysts for CO2 reduction: a data-driven materials discovery”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Jan. 25, 2019. doi: 10.1038/s41467-019-08356-1.  
  
A. K. Singh, “Electrochemical Stability of Metastable Materials”, *Chemistry of Materials*, vol. 29, no. 23. American Chemical Society (ACS), pp. 10159–10167, Nov. 17, 2017. doi: 10.1021/acs.chemmater.7b03980.  
  
G. Ceder, G. Hautier, A. Jainand S. P. Ong, “Recharging lithium battery research with first-principles methods”, *MRS Bulletin*, vol. 36, no. 3. Springer Science and Business Media LLC, pp. 185–191, Mar. 2011. doi: 10.1557/mrs.2011.31.  
  
C. Chen, Z. Deng, R. Tran, H. Tang, I.-H. Chuand S. P. Ong, “Accurate force field for molybdenum by machine learning large materials data”, *Physical Review Materials*, vol. 1, no. 4. American Physical Society (APS), Sep. 15, 2017. doi: 10.1103/physrevmaterials.1.043603.  
  
C. Chen, W. Ye, Y. Zuo, C. Zhengand S. P. Ong, “Graph Networks as a Universal Machine Learning Framework for Molecules and Crystals”, *Chemistry of Materials*, vol. 31, no. 9. American Chemical Society (ACS), pp. 3564–3572, Apr. 10, 2019. doi: 10.1021/acs.chemmater.9b01294.  
  
L. Cheng, “Accelerating Electrolyte Discovery for Energy Storage with High-Throughput Screening”, *The Journal of Physical Chemistry Letters*, vol. 6, no. 2. American Chemical Society (ACS), pp. 283–291, Jan. 06, 2015. doi: 10.1021/jz502319n.  
  
V. L. Chevrier, G. Hautier, S. P. Ong, R. E. Doeand G. Ceder, “First-principles study of iron oxyfluorides and lithiation of FeOF”, *Physical Review B*, vol. 87, no. 9. American Physical Society (APS), Mar. 29, 2013. doi: 10.1103/physrevb.87.094118.  
  
V. L. Chevrier, S. P. Ong, R. Armiento, M. K. Y. Chanand G. Ceder, “Hybrid density functional calculations of redox potentials and formation energies of transition metal compounds”, *Physical Review B*, vol. 82, no. 7. American Physical Society (APS), Aug. 12, 2010. doi: 10.1103/physrevb.82.075122.  
  
I.-H. Chu, “Room-Temperature All-solid-state Rechargeable Sodium-ion Batteries with a Cl-doped Na3PS4 Superionic Conductor”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Sep. 20, 2016. doi: 10.1038/srep33733.  
  
I.-H. Chu, “Insights into the Performance Limits of the Li7P3S11Superionic Conductor: A Combined First-Principles and Experimental Study”, *ACS Applied Materials & Interfaces*, vol. 8, no. 12. American Chemical Society (ACS), pp. 7843–7853, Mar. 17, 2016. doi: 10.1021/acsami.6b00833.  
  
I.-H. Chu, M. Zhang, S. P. Ongand Y. S. Meng, “Battery Electrodes, Electrolytes, and Their Interfaces”, *Handbook of Materials Modeling*. Springer International Publishing, pp. 1–24, 2018. doi: 10.1007/978-3-319-50257-1\_96-1.  
  
Z. Deng, C. Chen, X.-G. Liand S. P. Ong, “An electrostatic spectral neighbor analysis potential for lithium nitride”, *npj Computational Materials*, vol. 5, no. 1. Springer Science and Business Media LLC, Jul. 16, 2019. doi: 10.1038/s41524-019-0212-1.  
  
Z. Deng, Y. Moand S. P. Ong, “Computational studies of solid-state alkali conduction in rechargeable alkali-ion batteries”, *NPG Asia Materials*, vol. 8, no. 3. Springer Science and Business Media LLC, pp. e254–e254, Mar. 2016. doi: 10.1038/am.2016.7.  
  
Z. Deng, B. Radhakrishnanand S. P. Ong, “Rational Composition Optimization of the Lithium-Rich Li3OCl1–*x*Br*x* Anti-Perovskite Superionic Conductors”, *Chemistry of Materials*, vol. 27, no. 10. American Chemical Society (ACS), pp. 3749–3755, May 08, 2015. doi: 10.1021/acs.chemmater.5b00988.  
  
Z. Deng, Z. Wang, I.-H. Chu, J. Luoand S. P. Ong, “Elastic Properties of Alkali Superionic Conductor Electrolytes from First Principles Calculations”, *Journal of The Electrochemical Society*, vol. 163, no. 2. The Electrochemical Society, pp. A67–A74, Nov. 05, 2015. doi: 10.1149/2.0061602jes.  
  
Z. Deng, Z. Zhu, I.-H. Chuand S. P. Ong, “Data-Driven First-Principles Methods for the Study and Design of Alkali Superionic Conductors”, *Chemistry of Materials*, vol. 29, no. 1. American Chemical Society (ACS), pp. 281–288, Sep. 13, 2016. doi: 10.1021/acs.chemmater.6b02648.  
  
J. Ding, “KVOPO 4 : A New High Capacity Multielectron Na‐Ion Battery Cathode”, *Advanced Energy Materials*, vol. 8, no. 21. Wiley, p. 1800221, May 09, 2018. doi: 10.1002/aenm.201800221.  
  
M. T. Dunstan, “Large scale computational screening and experimental discovery of novel materials for high temperature CO2 capture”, *Energy & Environmental Science*, vol. 9, no. 4. Royal Society of Chemistry (RSC), pp. 1346–1360, 2016. doi: 10.1039/c5ee03253a.  
  
X. Feng, “Studies of Functional Defects for Fast Na‐Ion Conduction in Na 3− *y* PS 4− *x* Cl *x* with a Combined Experimental and Computational Approach”, *Advanced Functional Materials*, vol. 29, no. 9. Wiley, p. 1807951, Jan. 18, 2019. doi: 10.1002/adfm.201807951.  
  
J. M. Florez, “First-principles insights on the magnetism of cubic SrTi1−*x*Co*x*O3−*δ*”, *Applied Physics Letters*, vol. 100, no. 25. AIP Publishing, p. 252904, Jun. 18, 2012. doi: 10.1063/1.4729830.  
  
D. Gunter, “Community Accessible Datastore of High-Throughput Calculations: Experiences from the Materials Project”, *2012 SC Companion: High Performance Computing, Networking Storage and Analysis*. IEEE, Nov. 2012. doi: 10.1109/sc.companion.2012.150.  
  
X. Guo, “Water Contributes to Higher Energy Density and Cycling Stability of Prussian Blue Analogue Cathodes for Aqueous Sodium-Ion Batteries”, *Chemistry of Materials*, vol. 31, no. 15. American Chemical Society (ACS), pp. 5933–5942, Jul. 18, 2019. doi: 10.1021/acs.chemmater.9b02269.  
  
J. Ha, “Color tunable single-phase Eu2+and Ce3+co-activated Sr2LiAlO4phosphors”, *Journal of Materials Chemistry C*, vol. 7, no. 25. Royal Society of Chemistry (RSC), pp. 7734–7744, 2019. doi: 10.1039/c8tc05777j.  
  
J. Ha, “An integrated first principles and experimental investigation of the relationship between structural rigidity and quantum efficiency in phosphors for solid state lighting”, *Journal of Luminescence*, vol. 179. Elsevier BV, pp. 297–305, Nov. 2016. doi: 10.1016/j.jlumin.2016.07.006.  
  
G. Hautier, A. Jain, H. Chen, C. Moore, S. P. Ongand G. Ceder, “Novel mixed polyanions lithium-ion battery cathode materials predicted by high-throughput ab initio computations”, *Journal of Materials Chemistry*, vol. 21, no. 43. Royal Society of Chemistry (RSC), p. 17147, 2011. doi: 10.1039/c1jm12216a.  
  
G. Hautier, A. Jainand S. P. Ong, “From the computer to the laboratory: materials discovery and design using first-principles calculations”, *Journal of Materials Science*, vol. 47, no. 21. Springer Science and Business Media LLC, pp. 7317–7340, May 10, 2012. doi: 10.1007/s10853-012-6424-0.  
  
G. Hautier, “Phosphates as Lithium-Ion Battery Cathodes: An Evaluation Based on High-Throughput *ab Initio* Calculations”, *Chemistry of Materials*, vol. 23, no. 15. American Chemical Society (ACS), pp. 3495–3508, Jul. 13, 2011. doi: 10.1021/cm200949v.  
  
G. Hautier, S. P. Ong, A. Jain, C. J. Mooreand G. Ceder, “Accuracy of density functional theory in predicting formation energies of ternary oxides from binary oxides and its implication on phase stability”, *Physical Review B*, vol. 85, no. 15. American Physical Society (APS), Apr. 30, 2012. doi: 10.1103/physrevb.85.155208.  
  
M. F. V. Hidalgo, “Rational synthesis and electrochemical performance of LiVOPO4 polymorphs”, *Journal of Materials Chemistry A*, vol. 7, no. 14. Royal Society of Chemistry (RSC), pp. 8423–8432, 2019. doi: 10.1039/c8ta12531g.  
  
Y. Huang, “Thermal Stability and Reactivity of Cathode Materials for Li-Ion Batteries”, *ACS Applied Materials & Interfaces*, vol. 8, no. 11. American Chemical Society (ACS), pp. 7013–7021, Mar. 11, 2016. doi: 10.1021/acsami.5b12081.  
  
A. Jain, G. Hautier, S. P. Ong, S. Dacekand G. Ceder, “Relating voltage and thermal safety in Li-ion battery cathodes: a high-throughput computational study”, *Physical Chemistry Chemical Physics*, vol. 17, no. 8. Royal Society of Chemistry (RSC), pp. 5942–5953, 2015. doi: 10.1039/c5cp00250h.  
  
A. Jain, “Formation enthalpies by mixing GGA and GGAcalculations”, *Physical Review B*, vol. 84, no. 4. American Physical Society (APS), Jul. 12, 2011. doi: 10.1103/physrevb.84.045115.  
  
A. Jain, G. Hautier, S. P. Ongand K. Persson, “New opportunities for materials informatics: Resources and data mining techniques for uncovering hidden relationships”, *Journal of Materials Research*, vol. 31, no. 8. Springer Science and Business Media LLC, pp. 977–994, Apr. 01, 2016. doi: 10.1557/jmr.2016.80.  
  
A. Jain, “The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools”, *Handbook of Materials Modeling*. Springer International Publishing, pp. 1–34, 2018. doi: 10.1007/978-3-319-42913-7\_60-1.  
  
A. Jain, “FireWorks: a dynamic workflow system designed for high‐throughput applications”, *Concurrency and Computation: Practice and Experience*, vol. 27, no. 17. Wiley, pp. 5037–5059, May 18, 2015. doi: 10.1002/cpe.3505.  
  
A. Jain, “Commentary: The Materials Project: A materials genome approach to accelerating materials innovation”, *APL Materials*, vol. 1, no. 1. AIP Publishing, p. 011002, Jul. 2013. doi: 10.1063/1.4812323.  
  
H. Li, “Understanding the Electrochemical Mechanisms Induced by Gradient Mg2+ Distribution of Na-Rich Na3+*x*V2–*x*Mg*x*(PO4)3/C for Sodium Ion Batteries”, *Chemistry of Materials*, vol. 30, no. 8. American Chemical Society (ACS), pp. 2498–2505, Apr. 03, 2018. doi: 10.1021/acs.chemmater.7b03903.  
  
Y.-C. Lin, “Thermodynamics, Kinetics and Structural Evolution of ε-LiVOPO4 over Multiple Lithium Intercalation”, *Chemistry of Materials*, vol. 28, no. 6. American Chemical Society (ACS), pp. 1794–1805, Mar. 10, 2016. doi: 10.1021/acs.chemmater.5b04880.  
  
S. Li, “Data-Driven Discovery of Full-Visible-Spectrum Phosphor”, *Chemistry of Materials*, vol. 31, no. 16. American Chemical Society (ACS), pp. 6286–6294, Aug. 02, 2019. doi: 10.1021/acs.chemmater.9b02505.  
  
H. Liu, “Elucidating the Limit of Li Insertion into the Spinel Li4Ti5O12”, *ACS Materials Letters*, vol. 1, no. 1. American Chemical Society (ACS), pp. 96–102, May 24, 2019. doi: 10.1021/acsmaterialslett.9b00099.  
  
X. Li, “Direct visualization of the Jahn–Teller effect coupled to Na ordering in Na5/8MnO2”, *Nature Materials*, vol. 13, no. 6. Springer Science and Business Media LLC, pp. 586–592, May 18, 2014. doi: 10.1038/nmat3964.  
  
K. Mathew, “High-throughput computational X-ray absorption spectroscopy”, *Scientific Data*, vol. 5, no. 1. Springer Science and Business Media LLC, Jul. 31, 2018. doi: 10.1038/sdata.2018.151.  
  
L. J. Miara, “Effect of Rb and Ta Doping on the Ionic Conductivity and Stability of the Garnet Li7+2*x*–*y*(La3–*x*Rb*x*)(Zr2–*y*Ta*y*)O12 (0 ≤ *x* ≤ 0.375, 0 ≤ *y* ≤ 1) Superionic Conductor: A First Principles Investigation”, *Chemistry of Materials*, vol. 25, no. 15. American Chemical Society (ACS), pp. 3048–3055, Jul. 16, 2013. doi: 10.1021/cm401232r.  
  
Y. Mo, S. P. Ongand G. Ceder, “First Principles Study of the Li10GeP2S12 Lithium Super Ionic Conductor Material”, *Chemistry of Materials*, vol. 24, no. 1. American Chemical Society (ACS), pp. 15–17, Dec. 21, 2011. doi: 10.1021/cm203303y.  
  
Y. Mo, S. P. Ongand G. Ceder, “First-principles study of the oxygen evolution reaction of lithium peroxide in the lithium-air battery”, *Physical Review B*, vol. 84, no. 20. American Physical Society (APS), Nov. 21, 2011. doi: 10.1103/physrevb.84.205446.  
  
H. Nguyen, “Experimental and Computational Evaluation of a Sodium-Rich Anti-Perovskite for Solid State Electrolytes”, *Journal of The Electrochemical Society*, vol. 163, no. 10. The Electrochemical Society, pp. A2165–A2171, 2016. doi: 10.1149/2.0091610jes.  
  
S. P. Ong, “Accelerating materials science with high-throughput computations and machine learning”, *Computational Materials Science*, vol. 161. Elsevier BV, pp. 143–150, Apr. 2019. doi: 10.1016/j.commatsci.2019.01.013.  
  
S. P. Ong, O. Andreussi, Y. Wu, N. Marzariand G. Ceder, “Electrochemical Windows of Room-Temperature Ionic Liquids from Molecular Dynamics and Density Functional Theory Calculations”, *Chemistry of Materials*, vol. 23, no. 11. American Chemical Society (ACS), pp. 2979–2986, May 10, 2011. doi: 10.1021/cm200679y.  
  
S. P. Ong and G. Ceder, “Investigation of the Effect of Functional Group Substitutions on the Gas-Phase Electron Affinities and Ionization Energies of Room-Temperature Ionic Liquids Ions using Density Functional Theory”, *Electrochimica Acta*, vol. 55, no. 11. Elsevier BV, pp. 3804–3811, Apr. 2010. doi: 10.1016/j.electacta.2010.01.091.  
  
S. P. Ong, V. L. Chevrierand G. Ceder, “Comparison of small polaron migration and phase separation in olivine LiMnPOand LiFePOusing hybrid density functional theory”, *Physical Review B*, vol. 83, no. 7. American Physical Society (APS), Feb. 16, 2011. doi: 10.1103/physrevb.83.075112.  
  
S. P. Ong, “Voltage, stability and diffusion barrier differences between sodium-ion and lithium-ion intercalation materials”, *Energy & Environmental Science*, vol. 4, no. 9. Royal Society of Chemistry (RSC), p. 3680, 2011. doi: 10.1039/c1ee01782a.  
  
S. P. Ong, “The Materials Application Programming Interface (API): A simple, flexible and efficient API for materials data based on REpresentational State Transfer (REST) principles”, *Computational Materials Science*, vol. 97. Elsevier BV, pp. 209–215, Feb. 2015. doi: 10.1016/j.commatsci.2014.10.037.  
  
S. P. Ong, A. Jain, G. Hautier, B. Kangand G. Ceder, “Thermal stabilities of delithiated olivine MPO4 (M=Fe, Mn) cathodes investigated using first principles calculations”, *Electrochemistry Communications*, vol. 12, no. 3. Elsevier BV, pp. 427–430, Mar. 2010. doi: 10.1016/j.elecom.2010.01.010.  
  
S. P. Ong, Y. Moand G. Ceder, “Low hole polaron migration barrier in lithium peroxide”, *Physical Review B*, vol. 85, no. 8. American Physical Society (APS), Feb. 17, 2012. doi: 10.1103/physrevb.85.081105.  
  
S. P. Ong, “Python Materials Genomics (pymatgen): A robust, open-source python library for materials analysis”, *Computational Materials Science*, vol. 68. Elsevier BV, pp. 314–319, Feb. 2013. doi: 10.1016/j.commatsci.2012.10.028.  
  
P. Patel and S. P. Ong, “Artificial intelligence is aiding the search for energy materials”, *MRS Bulletin*, vol. 44, no. 3. Springer Science and Business Media LLC, pp. 162–163, Mar. 2019. doi: 10.1557/mrs.2019.51.  
  
J. Qiao, “Engineering of K3YSi2O7 To Tune Photoluminescence with Selected Activators and Site Occupancy”, *Chemistry of Materials*, vol. 31, no. 18. American Chemical Society (ACS), pp. 7770–7778, Aug. 13, 2019. doi: 10.1021/acs.chemmater.9b02990.  
  
N. F. Quackenbush, “Interfacial Effects in ε-Li*x*VOPO4 and Evolution of the Electronic Structure”, *Chemistry of Materials*, vol. 27, no. 24. American Chemical Society (ACS), pp. 8211–8219, Dec. 09, 2015. doi: 10.1021/acs.chemmater.5b02145.  
  
X. Qu, “The Electrolyte Genome project: A big data approach in battery materials discovery”, *Computational Materials Science*, vol. 103. Elsevier BV, pp. 56–67, Jun. 2015. doi: 10.1016/j.commatsci.2015.02.050.  
  
B. Radhakrishnan and S. P. Ong, “Aqueous Stability of Alkali Superionic Conductors from First-Principles Calculations”, *Frontiers in Energy Research*, vol. 4. Frontiers Media SA, Apr. 21, 2016. doi: 10.3389/fenrg.2016.00016.  
  
M. Samiee, “Divalent-doped Na3Zr2Si2PO12 natrium superionic conductor: Improving the ionic conductivity via simultaneously optimizing the phase and chemistry of the primary and secondary phases”, *Journal of Power Sources*, vol. 347. Elsevier BV, pp. 229–237, Apr. 2017. doi: 10.1016/j.jpowsour.2017.02.042.  
  
Y. Shi, “Understanding the Electrochemical Properties of Naphthalene Diimide: Implication for Stable and High-Rate Lithium-Ion Battery Electrodes”, *Chemistry of Materials*, vol. 30, no. 10. American Chemical Society (ACS), pp. 3508–3517, Apr. 27, 2018. doi: 10.1021/acs.chemmater.8b01304.  
  
D. H. S. Tan, “Enabling Thin and Flexible Solid-State Composite Electrolytes by the Scalable Solution Process”, *ACS Applied Energy Materials*, vol. 2, no. 9. American Chemical Society (ACS), pp. 6542–6550, Aug. 09, 2019. doi: 10.1021/acsaem.9b01111.  
  
H. Tang, “Probing Solid–Solid Interfacial Reactions in All-Solid-State Sodium-Ion Batteries with First-Principles Calculations”, *Chemistry of Materials*, vol. 30, no. 1. American Chemical Society (ACS), pp. 163–173, Dec. 28, 2017. doi: 10.1021/acs.chemmater.7b04096.  
  
A. J. Toumar, S. P. Ong, W. D. Richards, S. Dacekand G. Ceder, “Vacancy Ordering in -Type Layered Metal Oxide Sodium-Ion Battery Cathodes”, *Physical Review Applied*, vol. 4, no. 6. American Physical Society (APS), Dec. 11, 2015. doi: 10.1103/physrevapplied.4.064002.  
  
R. Tran, X.-G. Li, J. H. Montoya, D. Winston, K. A. Perssonand S. P. Ong, “Anisotropic work function of elemental crystals”, *Surface Science*, vol. 687. Elsevier BV, pp. 48–55, Sep. 2019. doi: 10.1016/j.susc.2019.05.002.  
  
R. Tran, “Surface energies of elemental crystals”, *Scientific Data*, vol. 3, no. 1. Springer Science and Business Media LLC, Sep. 13, 2016. doi: 10.1038/sdata.2016.80.  
  
R. Tran, Z. Xu, N. Zhou, B. Radhakrishnan, J. Luoand S. P. Ong, “Computational study of metallic dopant segregation and embrittlement at molybdenum grain boundaries”, *Acta Materialia*, vol. 117. Elsevier BV, pp. 91–99, Sep. 2016. doi: 10.1016/j.actamat.2016.07.005.  
  
L. W. Wangoh, “Uniform second Li ion intercalation in solid state ϵ-LiVOPO4”, *Applied Physics Letters*, vol. 109, no. 5. AIP Publishing, p. 053904, Aug. 01, 2016. doi: 10.1063/1.4960452.  
  
W. Wang, “Chlorine-Doped Perovskite Oxide: A Platinum-Free Cathode for Dye-Sensitized Solar Cells”, *ACS Applied Materials & Interfaces*, vol. 11, no. 39. American Chemical Society (ACS), pp. 35641–35652, Sep. 05, 2019. doi: 10.1021/acsami.9b07966.  
  
X. Wang, “Structural Changes in a High-Energy Density VO2F Cathode upon Heating and Li Cycling”, *ACS Applied Energy Materials*, vol. 1, no. 9. American Chemical Society (ACS), pp. 4514–4521, Aug. 28, 2018. doi: 10.1021/acsaem.8b00473.  
  
Z. Wang, I.-H. Chu, F. Zhouand S. P. Ong, “Electronic Structure Descriptor for the Discovery of Narrow-Band Red-Emitting Phosphors”, *Chemistry of Materials*, vol. 28, no. 11. American Chemical Society (ACS), pp. 4024–4031, May 16, 2016. doi: 10.1021/acs.chemmater.6b01496.  
  
Z. Wang, J. Ha, Y. H. Kim, W. B. Im, J. McKittrickand S. P. Ong, “Mining Unexplored Chemistries for Phosphors for High-Color-Quality White-Light-Emitting Diodes”, *Joule*, vol. 2, no. 5. Elsevier BV, pp. 914–926, May 2018. doi: 10.1016/j.joule.2018.01.015.  
  
Z. Wang, W. Ye, I.-H. Chuand S. P. Ong, “Elucidating Structure–Composition–Property Relationships of the β-SiAlON:Eu2+ Phosphor”, *Chemistry of Materials*, vol. 28, no. 23. American Chemical Society (ACS), pp. 8622–8630, Nov. 30, 2016. doi: 10.1021/acs.chemmater.6b03555.  
  
B. Wen, “Molybdenum Substituted Vanadyl Phosphate ε-VOPO4 with Enhanced Two-Electron Transfer Reversibility and Kinetics for Lithium-Ion Batteries”, *Chemistry of Materials*, vol. 28, no. 9. American Chemical Society (ACS), pp. 3159–3170, Apr. 19, 2016. doi: 10.1021/acs.chemmater.6b00891.  
  
E. A. Wu, “New Insights into the Interphase between the Na Metal Anode and Sulfide Solid-State Electrolytes: A Joint Experimental and Computational Study”, *ACS Applied Materials & Interfaces*, vol. 10, no. 12. American Chemical Society (ACS), pp. 10076–10086, Mar. 12, 2018. doi: 10.1021/acsami.7b19037.  
  
S. Yang, N. Zhou, H. Zheng, S. P. Ongand J. Luo, “First-Order Interfacial Transformations with a Critical Point: Breaking the Symmetry at a Symmetric Tilt Grain Boundary”, *Physical Review Letters*, vol. 120, no. 8. American Physical Society (APS), Feb. 22, 2018. doi: 10.1103/physrevlett.120.085702.  
  
W. Ye, C. Chen, S. Dwaraknath, A. Jain, S. P. Ongand K. A. Persson, “Harnessing the Materials Project for machine-learning and accelerated discovery”, *MRS Bulletin*, vol. 43, no. 9. Springer Science and Business Media LLC, pp. 664–669, Sep. 2018. doi: 10.1557/mrs.2018.202.  
  
W. Ye, C. Chen, Z. Wang, I.-H. Chuand S. P. Ong, “Deep neural networks for accurate predictions of crystal stability”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Sep. 18, 2018. doi: 10.1038/s41467-018-06322-x.  
  
C. Zheng, “Automated generation and ensemble-learned matching of X-ray absorption spectra”, *npj Computational Materials*, vol. 4, no. 1. Springer Science and Business Media LLC, Mar. 20, 2018. doi: 10.1038/s41524-018-0067-x.  
  
C. Zheng, B. Radhakrishnan, I.-H. Chu, Z. Wangand S. P. Ong, “Effects of Transition-Metal Mixing on Na Ordering and Kinetics in Layered Oxides”, *Physical Review Applied*, vol. 7, no. 6. American Physical Society (APS), Jun. 06, 2017. doi: 10.1103/physrevapplied.7.064003.  
  
H. Zheng, “Grain boundary properties of elemental metals”, *Acta Materialia*, vol. 186. Elsevier BV, pp. 40–49, Mar. 2020. doi: 10.1016/j.actamat.2019.12.030.  
  
H. Zheng, R. Tran, X.-G. Li, B. Radhakrishnanand S. P. Ong, “Role of Zr in strengthening MoSi2 from density functional theory calculations”, *Acta Materialia*, vol. 145. Elsevier BV, pp. 470–476, Feb. 2018. doi: 10.1016/j.actamat.2017.12.017.  
  
J. Zhou, “2DMatPedia, an open computational database of two-dimensional materials from top-down and bottom-up approaches”, *Scientific Data*, vol. 6, no. 1. Springer Science and Business Media LLC, Jun. 12, 2019. doi: 10.1038/s41597-019-0097-3.  
  
Z. Zhu, I.-H. Chu, Z. Dengand S. P. Ong, “Role of Na+ Interstitials and Dopants in Enhancing the Na+ Conductivity of the Cubic Na3PS4 Superionic Conductor”, *Chemistry of Materials*, vol. 27, no. 24. American Chemical Society (ACS), pp. 8318–8325, Dec. 11, 2015. doi: 10.1021/acs.chemmater.5b03656.  
  
Z. Zhu, I.-H. Chuand S. P. Ong, “Li3Y(PS4)2 and Li5PS4Cl2: New Lithium Superionic Conductors Predicted from Silver Thiophosphates using Efficiently Tiered Ab Initio Molecular Dynamics Simulations”, *Chemistry of Materials*, vol. 29, no. 6. American Chemical Society (ACS), pp. 2474–2484, Jan. 03, 2017. doi: 10.1021/acs.chemmater.6b04049.  
  
Z. Zhu, Z. Deng, I.-H. Chu, B. Radhakrishnanand S. Ping Ong, “Ab Initio Molecular Dynamics Studies of Fast Ion Conductors”, *Computational Materials System Design*. Springer International Publishing, pp. 147–168, Nov. 11, 2017. doi: 10.1007/978-3-319-68280-8\_7.  
  
K. Mathew, “Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows”, *Computational Materials Science*, vol. 139. Elsevier BV, pp. 140–152, Nov. 2017. doi: 10.1016/j.commatsci.2017.07.030.  
  
D. K. Lewis, M. Matsubara, E. Bellottiand S. Sharifzadeh, “Quasiparticle and hybrid density functional methods in defect studies: An application to the nitrogen vacancy in GaN”, *Physical Review B*, vol. 96, no. 23. American Physical Society (APS), Dec. 18, 2017. doi: 10.1103/physrevb.96.235203.  
  
B. J. Nordell, “The influence of hydrogen on the chemical, mechanical, optical/electronic, and electrical transport properties of amorphous hydrogenated boron carbide”, *Journal of Applied Physics*, vol. 118, no. 3. AIP Publishing, p. 035703, Jul. 21, 2015. doi: 10.1063/1.4927037.  
  
S. A. Etesami and E. Asadi, “Molecular dynamics for near melting temperatures simulations of metals using modified embedded-atom method”, *Journal of Physics and Chemistry of Solids*, vol. 112. Elsevier BV, pp. 61–72, Jan. 2018. doi: 10.1016/j.jpcs.2017.09.001.  
  
S. L. Thomas, A. H. Kingand D. J. Srolovitz, “When twins collide: Twin junctions in nanocrystalline nickel”, *Acta Materialia*, vol. 113. Elsevier BV, pp. 301–310, Jul. 2016. doi: 10.1016/j.actamat.2016.04.030.  
  
H. Chao, B. J. Lindsayand R. A. Riggleman, “Field-Theoretic Simulations of the Distribution of Nanorods in Diblock Copolymer Thin Films”, *The Journal of Physical Chemistry B*, vol. 121, no. 49. American Chemical Society (ACS), pp. 11198–11209, Nov. 30, 2017. doi: 10.1021/acs.jpcb.7b07862.  
  
H. Chao and R. A. Riggleman, “Inverse design of grafted nanoparticles for targeted self-assembly”, *Molecular Systems Design & Engineering*, vol. 3, no. 1. Royal Society of Chemistry (RSC), pp. 214–222, 2018. doi: 10.1039/c7me00081b.  
  
R. J. S. Ivancic and R. A. Riggleman, “Identifying structural signatures of shear banding in model polymer nanopillars”, *Soft Matter*, vol. 15, no. 22. Royal Society of Chemistry (RSC), pp. 4548–4561, 2019. doi: 10.1039/c8sm02423e.  
  
R. J. S. Ivancic and R. A. Riggleman, “Dynamic phase transitions in freestanding polymer thin films”, *Proceedings of the National Academy of Sciences*, vol. 117, no. 41. Proceedings of the National Academy of Sciences, pp. 25407–25413, Oct. 02, 2020. doi: 10.1073/pnas.2006703117.  
  
J. Koski, B. Hagbergand R. A. Riggleman, “Attraction of Nanoparticles to Tilt Grain Boundaries in Block Copolymers”, *Macromolecular Chemistry and Physics*, vol. 217, no. 3. Wiley, pp. 509–518, Jan. 05, 2016. doi: 10.1002/macp.201500299.  
  
J. P. Koski and R. A. Riggleman, “Field-theoretic simulations of block copolymer nanocomposites in a constant interfacial tension ensemble”, *The Journal of Chemical Physics*, vol. 146, no. 16. AIP Publishing, p. 164903, Apr. 28, 2017. doi: 10.1063/1.4981912.  
  
N. M. Krook, “Experiments and Simulations Probing Local Domain Bulge and String Assembly of Aligned Nanoplates in a Lamellar Diblock Copolymer”, *Macromolecules*, vol. 52, no. 22. American Chemical Society (ACS), pp. 8989–8999, Nov. 13, 2019. doi: 10.1021/acs.macromol.9b01324.  
  
C.-C. Lin, “Nanorod Mobility Influences Polymer Diffusion in Polymer Nanocomposites”, *ACS Macro Letters*, vol. 6, no. 8. American Chemical Society (ACS), pp. 869–874, Aug. 01, 2017. doi: 10.1021/acsmacrolett.7b00533.  
  
C.-C. Lin, “Grafted polymer chains suppress nanoparticle diffusion in athermal polymer melts”, *The Journal of Chemical Physics*, vol. 146, no. 20. AIP Publishing, p. 203332, May 28, 2017. doi: 10.1063/1.4982216.  
  
B. J. Lindsay, R. J. Compostoand R. A. Riggleman, “Equilibrium Field Theoretic Study of Nanoparticle Interactions in Diblock Copolymer Melts”, *The Journal of Physical Chemistry B*, vol. 123, no. 44. American Chemical Society (ACS), pp. 9466–9480, Oct. 07, 2019. doi: 10.1021/acs.jpcb.9b05771.  
  
E. Y. Lin, A. L. Frischknechtand R. A. Riggleman, “Origin of Mechanical Enhancement in Polymer Nanoparticle (NP) Composites with Ultrahigh NP Loading”, *Macromolecules*, vol. 53, no. 8. American Chemical Society (ACS), pp. 2976–2982, Apr. 06, 2020. doi: 10.1021/acs.macromol.9b02733.  
  
E. Y. Lin and R. A. Riggleman, “Distinguishing failure modes in oligomeric polymer nanopillars”, *Soft Matter*, vol. 15, no. 32. Royal Society of Chemistry (RSC), pp. 6589–6595, 2019. doi: 10.1039/c9sm00699k.  
  
A. R. Moore, G. Huang, S. Wolf, P. J. Walsh, Z. Fakhraaiand R. A. Riggleman, “Effects of microstructure formation on the stability of vapor-deposited glasses”, *Proceedings of the National Academy of Sciences*, vol. 116, no. 13. Proceedings of the National Academy of Sciences, pp. 5937–5942, Mar. 13, 2019. doi: 10.1073/pnas.1821761116.  
  
J. F. Pressly, R. A. Rigglemanand K. I. Winey, “Polymer Diffusion Is Fastest at Intermediate Levels of Cylindrical Confinement”, *Macromolecules*, vol. 51, no. 23. American Chemical Society (ACS), pp. 9789–9797, Nov. 27, 2018. doi: 10.1021/acs.macromol.8b01728.  
  
J. F. Pressly, R. A. Rigglemanand K. I. Winey, “Increased Polymer Diffusivity in Thin-Film Confinement”, *Macromolecules*, vol. 52, no. 16. American Chemical Society (ACS), pp. 6116–6125, Aug. 07, 2019. doi: 10.1021/acs.macromol.9b01001.  
  
D. J. Ring, R. A. Rigglemanand D. Lee, “Critical Contact Angle to Induce Capillary Rise of Polymers in Nanopores Does Not Depend on Chain Length”, *ACS Macro Letters*, vol. 8, no. 1. American Chemical Society (ACS), pp. 31–35, Dec. 18, 2018. doi: 10.1021/acsmacrolett.8b00953.  
  
S. Sharick, J. Koski, R. A. Rigglemanand K. I. Winey, “Isolating the Effect of Molecular Weight on Ion Transport of Non-Ionic Diblock Copolymer/Ionic Liquid Mixtures”, *Macromolecules*, vol. 49, no. 6. American Chemical Society (ACS), pp. 2245–2256, Mar. 07, 2016. doi: 10.1021/acs.macromol.5b02445.  
  
R. B. Venkatesh, T. Zhang, N. Manohar, K. J. Stebe, R. A. Rigglemanand D. Lee, “Effect of polymer–nanoparticle interactions on solvent-driven infiltration of polymer (SIP) into nanoparticle packings: a molecular dynamics study”, *Molecular Systems Design & Engineering*, vol. 5, no. 3. Royal Society of Chemistry (RSC), pp. 666–674, 2020. doi: 10.1039/c9me00148d.  
  
E. Yang, R. J. S. Ivancic, E. Y. Linand R. A. Riggleman, “Effect of polymer–nanoparticle interaction on strain localization in polymer nanopillars”, *Soft Matter*, vol. 16, no. 37. Royal Society of Chemistry (RSC), pp. 8639–8646, 2020. doi: 10.1039/d0sm00991a.  
  
Z. Ye and R. A. Riggleman, “Molecular View of Cavitation in Model-Solvated Polymer Networks”, *Macromolecules*, vol. 53, no. 18. American Chemical Society (ACS), pp. 7825–7834, Sep. 02, 2020. doi: 10.1021/acs.macromol.0c00994.  
  
T. Zhang, K. I. Wineyand R. A. Riggleman, “Polymer Conformations and Dynamics under Confinement with Two Length Scales”, *Macromolecules*, vol. 52, no. 1. American Chemical Society (ACS), pp. 217–226, Dec. 19, 2018. doi: 10.1021/acs.macromol.8b01779.  
  
Y. Zhang, C. N. Woods, M. Alvarez, Y. Jin, R. A. Rigglemanand Z. Fakhraai, “Effect of substrate interactions on the glass transition and length-scale of correlated dynamics in ultra-thin molecular glass films”, *The Journal of Chemical Physics*, vol. 149, no. 18. AIP Publishing, p. 184902, Nov. 14, 2018. doi: 10.1063/1.5038174.  
  
M. Iyer, V. Gaviniand T. M. Pollock, “Energetics and nucleation of point defects in aluminum under extreme tensile hydrostatic stresses”, *Physical Review B*, vol. 89, no. 1. American Physical Society (APS), Jan. 28, 2014. doi: 10.1103/physrevb.89.014108.  
  
M. Iyer, B. Radhakrishnanand V. Gavini, “Electronic-structure study of an edge dislocation in Aluminum and the role of macroscopic deformations on its energetics”, *Journal of the Mechanics and Physics of Solids*, vol. 76. Elsevier BV, pp. 260–275, Mar. 2015. doi: 10.1016/j.jmps.2014.12.009.  
  
B. Kanungo and V. Gavini, “Large-scale all-electron density functional theory calculations using an enriched finite-element basis”, *Physical Review B*, vol. 95, no. 3. American Physical Society (APS), Jan. 05, 2017. doi: 10.1103/physrevb.95.035112.  
  
P. Motamarri, V. Gavini, K. Bhattacharyaand M. Ortiz, “Spectrum-splitting approach for Fermi-operator expansion in all-electron Kohn-Sham DFT calculations”, *Physical Review B*, vol. 95, no. 3. American Physical Society (APS), Jan. 05, 2017. doi: 10.1103/physrevb.95.035111.  
  
J. D’Emidio and R. K. Kaul, “First-order superfluid to valence-bond solid phase transitions in easy-planemagnets for small”, *Physical Review B*, vol. 93, no. 5. American Physical Society (APS), Feb. 03, 2016. doi: 10.1103/physrevb.93.054406.  
  
S. Pujari, T. C. Lang, G. Murthyand R. K. Kaul, “Interaction-Induced Dirac Fermions from Quadratic Band Touching in Bilayer Graphene”, *Physical Review Letters*, vol. 117, no. 8. American Physical Society (APS), Aug. 19, 2016. doi: 10.1103/physrevlett.117.086404.  
  
Q. Bai, X. He, Y. Zhuand Y. Mo, “First-Principles Study of Oxyhydride H– Ion Conductors: Toward Facile Anion Conduction in Oxide-Based Materials”, *ACS Applied Energy Materials*, vol. 1, no. 4. American Chemical Society (ACS), pp. 1626–1634, Mar. 26, 2018. doi: 10.1021/acsaem.8b00077.  
  
Q. Bai, Y. Zhu, X. He, E. Wachsmanand Y. Mo, “First principles hybrid functional study of small polarons in doped SrCeO3 perovskite: towards computation design of materials with tailored polaron”, *Ionics*, vol. 24, no. 4. Springer Science and Business Media LLC, pp. 1139–1151, Sep. 18, 2017. doi: 10.1007/s11581-017-2268-6.  
  
F. Han, Y. Zhu, X. He, Y. Moand C. Wang, “Electrochemical Stability of Li10 GeP2 S12 and Li7 La3 Zr2 O12 Solid Electrolytes”, *Advanced Energy Materials*, vol. 6, no. 8. Wiley, p. 1501590, Jan. 21, 2016. doi: 10.1002/aenm.201501590.  
  
X. Han, “Negating interfacial impedance in garnet-based solid-state Li metal batteries”, *Nature Materials*, vol. 16, no. 5. Springer Science and Business Media LLC, pp. 572–579, Dec. 19, 2016. doi: 10.1038/nmat4821.  
  
K. He, “Sodiation Kinetics of Metal Oxide Conversion Electrodes: A Comparative Study with Lithiation”, *Nano Letters*, vol. 15, no. 9. American Chemical Society (ACS), pp. 5755–5763, Aug. 25, 2015. doi: 10.1021/acs.nanolett.5b01709.  
  
K. He, “Visualizing non-equilibrium lithiation of spinel oxide via in situ transmission electron microscopy”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, May 09, 2016. doi: 10.1038/ncomms11441.  
  
X. He and Y. Mo, “Accelerated materials design of Na0.5Bi0.5TiO3 oxygen ionic conductors based on first principles calculations”, *Physical Chemistry Chemical Physics*, vol. 17, no. 27. Royal Society of Chemistry (RSC), pp. 18035–18044, 2015. doi: 10.1039/c5cp02181b.  
  
X. He, Y. Zhu, A. Epsteinand Y. Mo, “Statistical variances of diffusional properties from ab initio molecular dynamics simulations”, *npj Computational Materials*, vol. 4, no. 1. Springer Science and Business Media LLC, Apr. 03, 2018. doi: 10.1038/s41524-018-0074-y.  
  
X. He, Y. Zhuand Y. Mo, “Origin of fast ion diffusion in super-ionic conductors”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Jun. 21, 2017. doi: 10.1038/ncomms15893.  
  
W. Luo, “Transition from Superlithiophobicity to Superlithiophilicity of Garnet Solid-State Electrolyte”, *Journal of the American Chemical Society*, vol. 138, no. 37. American Chemical Society (ACS), pp. 12258–12262, Sep. 08, 2016. doi: 10.1021/jacs.6b06777.  
  
S. Xiong, “Computation‐Guided Design of LiTaSiO 5 , a New Lithium Ionic Conductor with Sphene Structure”, *Advanced Energy Materials*, vol. 9, no. 22. Wiley, p. 1803821, Apr. 24, 2019. doi: 10.1002/aenm.201803821.  
  
Y. Zhu, X. Heand Y. Mo, “Origin of Outstanding Stability in the Lithium Solid Electrolyte Materials: Insights from Thermodynamic Analyses Based on First-Principles Calculations”, *ACS Applied Materials & Interfaces*, vol. 7, no. 42. American Chemical Society (ACS), pp. 23685–23693, Oct. 15, 2015. doi: 10.1021/acsami.5b07517.  
  
Y. Zhu, X. Heand Y. Mo, “First principles study on electrochemical and chemical stability of solid electrolyte–electrode interfaces in all-solid-state Li-ion batteries”, *Journal of Materials Chemistry A*, vol. 4, no. 9. Royal Society of Chemistry (RSC), pp. 3253–3266, 2016. doi: 10.1039/c5ta08574h.  
  
Y. Zhu, X. Heand Y. Mo, “Strategies Based on Nitride Materials Chemistry to Stabilize Li Metal Anode”, *Advanced Science*, vol. 4, no. 8. Wiley, p. 1600517, Mar. 03, 2017. doi: 10.1002/advs.201600517.  
  
A. Govind Rajan, M. S. Stranoand D. Blankschtein, “Ab Initio Molecular Dynamics and Lattice Dynamics-Based Force Field for Modeling Hexagonal Boron Nitride in Mechanical and Interfacial Applications”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 7. American Chemical Society (ACS), pp. 1584–1591, Mar. 12, 2018. doi: 10.1021/acs.jpclett.7b03443.  
  
R. P. Misra and D. Blankschtein, “Insights on the Role of Many-Body Polarization Effects in the Wetting of Graphitic Surfaces by Water”, *The Journal of Physical Chemistry C*, vol. 121, no. 50. American Chemical Society (ACS), pp. 28166–28179, Dec. 12, 2017. doi: 10.1021/acs.jpcc.7b08891.  
  
V. Sresht, A. Govind Rajan, E. Bordes, M. S. Strano, A. A. H. Páduaand D. Blankschtein, “Quantitative Modeling of MoS2–Solvent Interfaces: Predicting Contact Angles and Exfoliation Performance using Molecular Dynamics”, *The Journal of Physical Chemistry C*, vol. 121, no. 16. American Chemical Society (ACS), pp. 9022–9031, Mar. 22, 2017. doi: 10.1021/acs.jpcc.7b00484.  
  
V. Sresht, A. A. H. Páduaand D. Blankschtein, “Liquid-Phase Exfoliation of Phosphorene: Design Rules from Molecular Dynamics Simulations”, *ACS Nano*, vol. 9, no. 8. American Chemical Society (ACS), pp. 8255–8268, Jul. 24, 2015. doi: 10.1021/acsnano.5b02683.  
  
Z. Yuan, “Mechanism and Prediction of Gas Permeation through Sub-Nanometer Graphene Pores: Comparison of Theory and Simulation”, *ACS Nano*, vol. 11, no. 8. American Chemical Society (ACS), pp. 7974–7987, Jul. 19, 2017. doi: 10.1021/acsnano.7b02523.  
  
A. Kinaci, “Electronic transport in VO2—Experimentally calibrated Boltzmann transport modeling”, *Applied Physics Letters*, vol. 107, no. 26. AIP Publishing, p. 262108, Dec. 28, 2015. doi: 10.1063/1.4938555.  
  
A. Kinaci, “Unraveling the Planar-Globular Transition in Gold Nanoclusters through Evolutionary Search”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Nov. 28, 2016. doi: 10.1038/srep34974.  
  
B. Narayanan, “Development of a Modified Embedded Atom Force Field for Zirconium Nitride Using Multi-Objective Evolutionary Optimization”, *The Journal of Physical Chemistry C*, vol. 120, no. 31. American Chemical Society (ACS), pp. 17475–17483, Jul. 28, 2016. doi: 10.1021/acs.jpcc.6b05296.  
  
F. G. Sen, “Towards accurate prediction of catalytic activity in IrO2 nanoclusters via first principles-based variable charge force field”, *Journal of Materials Chemistry A*, vol. 3, no. 37. Royal Society of Chemistry (RSC), pp. 18970–18982, 2015. doi: 10.1039/c5ta04678e.  
  
C. Sun, “Atomic and electronic structure of Lomer dislocations at CdTe bicrystal interface”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Jun. 03, 2016. doi: 10.1038/srep27009.  
  
Y. A. Wu, “Visualizing Redox Dynamics of a Single Ag/AgCl Heterogeneous Nanocatalyst at Atomic Resolution”, *ACS Nano*, vol. 10, no. 3. American Chemical Society (ACS), pp. 3738–3746, Mar. 07, 2016. doi: 10.1021/acsnano.6b00355.  
  
V. Sharma, “Effects of moisture on (La, A)MnO3 (A = Ca, Sr, and Ba) solid oxide fuel cell cathodes: a first-principles and experimental study”, *Journal of Materials Chemistry A*, vol. 4, no. 15. Royal Society of Chemistry (RSC), pp. 5605–5615, 2016. doi: 10.1039/c6ta00603e.  
  
J. Wang, B. Lukose, M. O. Thompsonand P. Clancy, “*Ab initio* modeling of vacancies, antisites, and Si dopants in ordered InGaAs”, *Journal of Applied Physics*, vol. 121, no. 4. AIP Publishing, p. 045106, Jan. 28, 2017. doi: 10.1063/1.4974949.  
  
S. D. Pinge, D. Baskaranand Y. L. Joo, “Evaluation of line-edge/line-width roughness of directed self-assembled PS-b-PMMA patterns using coarse-grained molecular dynamics simulation”, *Novel Patterning Technologies 2018*. SPIE, Mar. 19, 2018. doi: 10.1117/12.2297485.  
  
S. Pinge, G. Lin, D. Baskaran, M. Padmanabanand Y. L. Joo, “Designing an ordered template of cylindrical arrays based on a simple flat plate confinement of block copolymers: a coarse-grained molecular dynamics study”, *Soft Matter*, vol. 14, no. 4. Royal Society of Chemistry (RSC), pp. 597–613, 2018. doi: 10.1039/c7sm02015e.  
  
S. Pinge, Y. Qiu, V. Monreal, D. Baskaran, A. Ravirajanand Y. L. Joo, “Three-dimensional line edge roughness in pre- and post-dry etch line and space patterns of block copolymer lithography”, *Physical Chemistry Chemical Physics*, vol. 22, no. 2. Royal Society of Chemistry (RSC), pp. 478–488, 2020. doi: 10.1039/c9cp05398k.  
  
D. Rodriquez, “Comparison of Methods for Determining the Mechanical Properties of Semiconducting Polymer Films for Stretchable Electronics”, *ACS Applied Materials & Interfaces*, vol. 9, no. 10. American Chemical Society (ACS), pp. 8855–8862, Mar. 02, 2017. doi: 10.1021/acsami.6b16115.  
  
S. E. Root, M. A. Alkhadra, D. Rodriquez, A. D. Printzand D. J. Lipomi, “Measuring the Glass Transition Temperature of Conjugated Polymer Films with Ultraviolet–Visible Spectroscopy”, *Chemistry of Materials*, vol. 29, no. 7. American Chemical Society (ACS), pp. 2646–2654, Mar. 24, 2017. doi: 10.1021/acs.chemmater.7b00242.  
  
S. E. Root, N. E. Jackson, S. Savagatrup, G. Aryaand D. J. Lipomi, “Modelling the morphology and thermomechanical behaviour of low-bandgap conjugated polymers and bulk heterojunction films”, *Energy & Environmental Science*, vol. 10, no. 2. Royal Society of Chemistry (RSC), pp. 558–569, 2017. doi: 10.1039/c6ee03456j.  
  
S. E. Root, S. Savagatrup, C. J. Pais, G. Aryaand D. J. Lipomi, “Predicting the Mechanical Properties of Organic Semiconductors Using Coarse-Grained Molecular Dynamics Simulations”, *Macromolecules*, vol. 49, no. 7. American Chemical Society (ACS), pp. 2886–2894, Mar. 31, 2016. doi: 10.1021/acs.macromol.6b00204.  
  
M. A. Alkhadra, S. E. Root, K. M. Hilby, D. Rodriquez, F. Sugiyamaand D. J. Lipomi, “Quantifying the Fracture Behavior of Brittle and Ductile Thin Films of Semiconducting Polymers”, *Chemistry of Materials*, vol. 29, no. 23. American Chemical Society (ACS), pp. 10139–10149, Nov. 30, 2017. doi: 10.1021/acs.chemmater.7b03922.  
  
B. C. Marin, J. Ramírez, S. E. Root, E. Aklileand D. J. Lipomi, “Metallic nanoislands on graphene: a metamaterial for chemical, mechanical, optical, and biological applications”, *Nanoscale Horiz.*, vol. 2, no. 6. Royal Society of Chemistry (RSC), pp. 311–318, 2017. doi: 10.1039/c7nh00095b.  
  
A. V. Zaretski, “Metallic Nanoislands on Graphene as Highly Sensitive Transducers of Mechanical, Biological, and Optical Signals”, *Nano Letters*, vol. 16, no. 2. American Chemical Society (ACS), pp. 1375–1380, Jan. 14, 2016. doi: 10.1021/acs.nanolett.5b04821.  
  
S. Dey, “Experimental and theoretical investigation of a mesoporous KxWO3material having superior mechanical strength”, *Nanoscale*, vol. 8, no. 5. Royal Society of Chemistry (RSC), pp. 2937–2943, 2016. doi: 10.1039/c5nr07941a.  
  
M. D. Hossain, S. Dey, R. A. Mayanovicand M. Benamara, “Structural and Magnetic Properties of Well-Ordered Inverted Core-Shell α-Cr2O3/ α-MxCr2-xO3 (M=Co, Ni, Mn, Fe) Nanoparticles”, *MRS Advances*, vol. 1, no. 34. Springer Science and Business Media LLC, pp. 2387–2392, May 12, 2016. doi: 10.1557/adv.2016.324.  
  
M. D. Hossain, R. A. Mayanovic, R. Sakidjaand M. Benamara, “An experimental and theoretical study of the optical, electronic, and magnetic properties of novel inverted α-Cr2O3@α-Mn<sub>0.35Cr1.65O2.94core shell nanoparticles”, *Journal of Materials Research*, vol. 32, no. 2. Springer Science and Business Media LLC, pp. 269–278, Jan. 05, 2017. doi: 10.1557/jmr.2016.504.  
  
D. G. Kizzire, “Investigations of the Mechanical and Hydrothermal Stabilities of SBA-15 and Al-SBA-15 Mesoporous Materials”, *MRS Advances*, vol. 1, no. 35. Springer Science and Business Media LLC, pp. 2453–2458, Jul. 2016. doi: 10.1557/adv.2016.499.  
  
T.-Y. Tang and G. Arya, “Anisotropic Three-Particle Interactions between Spherical Polymer-Grafted Nanoparticles in a Polymer Matrix”, *Macromolecules*, vol. 50, no. 3. American Chemical Society (ACS), pp. 1167–1183, Jan. 20, 2017. doi: 10.1021/acs.macromol.6b01936.  
  
Y. Zhuang and P. Charbonneau, “Communication: Microphase equilibrium and assembly dynamics”, *The Journal of Chemical Physics*, vol. 147, no. 9. AIP Publishing, p. 091102, Sep. 07, 2017. doi: 10.1063/1.4996904.  
  
K. Co, F.-C. Sun, S. P. Alpayand S. K. Nayak, “Polarization rotation in by isovalent doping at the fluorite sublattice”, *Physical Review B*, vol. 99, no. 1. American Physical Society (APS), Jan. 02, 2019. doi: 10.1103/physrevb.99.014101.  
  
Z. Gui and A. Janotti, “Carrier-Density-Induced Ferromagnetism in Bulk and Heterostructures”, *Physical Review Letters*, vol. 123, no. 12. American Physical Society (APS), Sep. 17, 2019. doi: 10.1103/physrevlett.123.127201.  
  
S. D. Harrington, “Growth, electrical, structural, and magnetic properties of half-Heusler ”, *Physical Review Materials*, vol. 2, no. 1. American Physical Society (APS), Jan. 12, 2018. doi: 10.1103/physrevmaterials.2.014406.  
  
S. D. Harrington, “Valence-band offsets of CoTiSb/In0.53Ga0.47As and CoTiSb/In0.52Al0.48As heterojunctions”, *Applied Physics Letters*, vol. 111, no. 6. AIP Publishing, p. 061605, Aug. 07, 2017. doi: 10.1063/1.4985200.  
  
A. J. Hauser, E. Mikheev, A. P. Kajdosand A. Janotti, “Small polaron-related recombination in BaxSr1−xTiO3 thin films by cathodoluminescence spectroscopy”, *Applied Physics Letters*, vol. 108, no. 10. AIP Publishing, p. 102901, Mar. 07, 2016. doi: 10.1063/1.4943191.  
  
B. Himmetoglu and A. Janotti, “Transport properties of KTaO3from first-principles”, *Journal of Physics: Condensed Matter*, vol. 28, no. 6. IOP Publishing, p. 065502, Jan. 21, 2016. doi: 10.1088/0953-8984/28/6/065502.  
  
J. K. Kawasaki, “A simple electron counting model for half-Heusler surfaces”, *Science Advances*, vol. 4, no. 6. American Association for the Advancement of Science (AAAS), Jun. 2018. doi: 10.1126/sciadv.aar5832.  
  
J. A. Logan, “Observation of a topologically non-trivial surface state in half-Heusler PtLuSb (001) thin films”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Jun. 27, 2016. doi: 10.1038/ncomms11993.  
  
J. E. Padilha, A. Janotti, A. Fazzioand A. J. R. da Silva, “Substrate-supported large-band-gap quantum spin Hall insulator based on III-V bismuth layers”, *Physical Review B*, vol. 94, no. 19. American Physical Society (APS), Nov. 16, 2016. doi: 10.1103/physrevb.94.195424.  
  
A. Sharan, Z. Guiand A. Janotti, “Hybrid-Functional Calculations of the Copper Impurity in Silicon”, *Physical Review Applied*, vol. 8, no. 2. American Physical Society (APS), Aug. 25, 2017. doi: 10.1103/physrevapplied.8.024023.  
  
L. Sun, X. Huang, L. Wangand A. Janotti, “Disentangling the role of small polarons and oxygen vacancies in ”, *Physical Review B*, vol. 95, no. 24. American Physical Society (APS), Jun. 01, 2017. doi: 10.1103/physrevb.95.245101.  
  
N. Umezawa and A. Janotti, “Controlling the Electronic Structures of Perovskite Oxynitrides and their Solid Solutions for Photocatalysis”, *ChemSusChem*, vol. 9, no. 9. Wiley, pp. 1027–1031, Apr. 13, 2016. doi: 10.1002/cssc.201600040.  
  
T. Wang, Z. Gui, A. Janotti, C. Niand P. Karandikar, “Strong effect of electron-phonon interaction on the lattice thermal conductivity in 3C-SiC”, *Physical Review Materials*, vol. 1, no. 3. American Physical Society (APS), Aug. 03, 2017. doi: 10.1103/physrevmaterials.1.034601.  
  
T. Wang, W. Li, C. Niand A. Janotti, “Band Gap and Band Offset of and Alloys”, *Physical Review Applied*, vol. 10, no. 1. American Physical Society (APS), Jul. 31, 2018. doi: 10.1103/physrevapplied.10.011003.  
  
N. Ye, “Thermal transport across metal silicide-silicon interfaces: An experimental comparison between epitaxial and nonepitaxial interfaces”, *Physical Review B*, vol. 95, no. 8. American Physical Society (APS), Feb. 22, 2017. doi: 10.1103/physrevb.95.085430.  
  
J. Zhang, Y. Wang, S. Khalid, A. Janotti, G. Haugstadand J. M. O. Zide, “Strong band gap reduction in highly mismatched alloy InAlBiAs grown by molecular beam epitaxy”, *Journal of Applied Physics*, vol. 126, no. 9. AIP Publishing, p. 095704, Sep. 07, 2019. doi: 10.1063/1.5097846.  
  
A. E. Maughan, A. M. Ganose, M. M. Bordelon, E. M. Miller, D. O. Scanlonand J. R. Neilson, “Defect Tolerance to Intolerance in the Vacancy-Ordered Double Perovskite Semiconductors Cs2SnI6 and Cs2TeI6”, *Journal of the American Chemical Society*, vol. 138, no. 27. American Chemical Society (ACS), pp. 8453–8464, Jul. 05, 2016. doi: 10.1021/jacs.6b03207.  
  
I. Altan and P. Charbonneau, “Obtaining Soft Matter Models of Proteins and their Phase Behavior”, *Methods in Molecular Biology*. Springer New York, pp. 209–228, 2019. doi: 10.1007/978-1-4939-9678-0\_15.  
  
I. Altan, D. Fusco, P. V. Afonineand P. Charbonneau, “Learning about Biomolecular Solvation from Water in Protein Crystals”, *The Journal of Physical Chemistry B*, vol. 122, no. 9. American Chemical Society (ACS), pp. 2475–2486, Feb. 04, 2018. doi: 10.1021/acs.jpcb.7b09898.  
  
I. Altan, A. R. Khan, S. James, M. K. Quinn, J. J. McManusand P. Charbonneau, “Using Schematic Models to Understand the Microscopic Basis for Inverted Solubility in γD-Crystallin”, *The Journal of Physical Chemistry B*, vol. 123, no. 47. American Chemical Society (ACS), pp. 10061–10072, Sep. 26, 2019. doi: 10.1021/acs.jpcb.9b07774.  
  
L. Berthier, P. Charbonneauand J. Kundu, “Bypassing sluggishness: SWAP algorithm and glassiness in high dimensions”, *Physical Review E*, vol. 99, no. 3. American Physical Society (APS), Mar. 04, 2019. doi: 10.1103/physreve.99.031301.  
  
A. R. Khan, S. James, M. K. Quinn, I. Altan, P. Charbonneauand J. J. McManus, “Temperature-Dependent Interactions Explain Normal and Inverted Solubility in a γD-Crystallin Mutant”, *Biophysical Journal*, vol. 117, no. 5. Elsevier BV, pp. 930–937, Sep. 2019. doi: 10.1016/j.bpj.2019.07.019.  
  
Y. Zhuang and P. Charbonneau, “Equilibrium Phase Behavior of the Square-Well Linear Microphase-Forming Model”, *The Journal of Physical Chemistry B*, vol. 120, no. 26. American Chemical Society (ACS), pp. 6178–6188, May 18, 2016. doi: 10.1021/acs.jpcb.6b02167.  
  
R. Aguirre, J. J. Chavez, X. W. Zhou, S. F. Almeidaand D. Zubia, “Molecular dynamics simulations of ZnTe/Cu back contacts for CdTe solar cells”, *2016 IEEE 43rd Photovoltaic Specialists Conference (PVSC)*. IEEE, Jun. 2016. doi: 10.1109/pvsc.2016.7749845.  
  
S. Almeida, J. J. Chavez, X. W. Zhouand D. Zubia, “Effect of substrate orientation on CdS homoepitaxy by molecular dynamics”, *Journal of Crystal Growth*, vol. 441. Elsevier BV, pp. 89–94, May 2016. doi: 10.1016/j.jcrysgro.2016.02.006.  
  
M. Motta and S. Zhang, “Computation of Ground-State Properties in Molecular Systems: Back-Propagation with Auxiliary-Field Quantum Monte Carlo”, *Journal of Chemical Theory and Computation*, vol. 13, no. 11. American Chemical Society (ACS), pp. 5367–5378, Nov. 02, 2017. doi: 10.1021/acs.jctc.7b00730.  
  
M. Motta and S. Zhang, “Communication: Calculation of interatomic forces and optimization of molecular geometry with auxiliary-field quantum Monte Carlo”, *The Journal of Chemical Physics*, vol. 148, no. 18. AIP Publishing, p. 181101, May 14, 2018. doi: 10.1063/1.5029508.  
  
M. Motta and S. Zhang, “Ab initio computations of molecular systems by the auxiliary‐field quantum Monte Carlo method”, *WIREs Computational Molecular Science*, vol. 8, no. 5. Wiley, May 25, 2018. doi: 10.1002/wcms.1364.  
  
M. Qin, H. Shiand S. Zhang, “Benchmark study of the two-dimensional Hubbard model with auxiliary-field quantum Monte Carlo method”, *Physical Review B*, vol. 94, no. 8. American Physical Society (APS), Aug. 04, 2016. doi: 10.1103/physrevb.94.085103.  
  
M. Qin, H. Shiand S. Zhang, “Numerical results on the short-range spin correlation functions in the ground state of the two-dimensional Hubbard model”, *Physical Review B*, vol. 96, no. 7. American Physical Society (APS), Aug. 25, 2017. doi: 10.1103/physrevb.96.075156.  
  
P. Rosenberg, H. Shiand S. Zhang, “Ultracold Atoms in a Square Lattice with Spin-Orbit Coupling: Charge Order, Superfluidity, and Topological Signatures”, *Physical Review Letters*, vol. 119, no. 26. American Physical Society (APS), Dec. 28, 2017. doi: 10.1103/physrevlett.119.265301.  
  
P. Rosenberg, H. Shiand S. Zhang, “Accurate computations of Rashba spin-orbit coupling in interacting systems: From the Fermi gas to real materials”, *Journal of Physics and Chemistry of Solids*, vol. 128. Elsevier BV, pp. 161–168, May 2019. doi: 10.1016/j.jpcs.2017.12.026.  
  
H. Shi and S. Zhang, “Many-body computations by stochastic sampling in Hartree-Fock-Bogoliubov space”, *Physical Review B*, vol. 95, no. 4. American Physical Society (APS), Jan. 27, 2017. doi: 10.1103/physrevb.95.045144.  
  
E. Vitali and J. Gonzalez, “Dynamical BCS Theory of a Two-Dimensional Attractive Fermi Gas: Effective Interactions from Quantum Monte Carlo Calculations”, *Journal of Low Temperature Physics*, vol. 197, no. 5–6. Springer Science and Business Media LLC, pp. 389–401, Aug. 20, 2019. doi: 10.1007/s10909-019-02226-2.  
  
E. Vitali, P. Rosenbergand S. Zhang, “Calculating ground-state properties of correlated fermionic systems with BCS trial wave functions in Slater determinant path-integral approaches”, *Physical Review A*, vol. 100, no. 2. American Physical Society (APS), Aug. 23, 2019. doi: 10.1103/physreva.100.023621.  
  
E. Vitali, H. Shi, M. Qinand S. Zhang, “Computation of dynamical correlation functions for many-fermion systems with auxiliary-field quantum Monte Carlo”, *Physical Review B*, vol. 94, no. 8. American Physical Society (APS), Aug. 23, 2016. doi: 10.1103/physrevb.94.085140.  
  
E. Vitali, H. Shi, M. Qinand S. Zhang, “Response Functions for the Two-Dimensional Ultracold Fermi Gas: Dynamical BCS Theory and Beyond”, *Journal of Low Temperature Physics*, vol. 189, no. 5–6. Springer Science and Business Media LLC, pp. 312–327, Aug. 07, 2017. doi: 10.1007/s10909-017-1805-z.  
  
E. Vitali, H. Shi, M. Qinand S. Zhang, “Visualizing the BEC-BCS crossover in a two-dimensional Fermi gas: Pairing gaps and dynamical response functions from *ab initio* computations”, *Physical Review A*, vol. 96, no. 6. American Physical Society (APS), Dec. 04, 2017. doi: 10.1103/physreva.96.061601.  
  
B.-X. Zheng, “Stripe order in the underdoped region of the two-dimensional Hubbard model”, *Science*, vol. 358, no. 6367. American Association for the Advancement of Science (AAAS), pp. 1155–1160, Dec. 2017. doi: 10.1126/science.aam7127.  
  
M. C. Heiber, “Ising\_Opv: Ising\_Opv V3.0”. Zenodo, Aug. 18, 2016. doi: 10.5281/ZENODO.60505.  
  
M. C. Heiber and A. Dhinojwala, “Erratum: Efficient Generation of Model Bulk Heterojunction Morphologies for Organic Photovoltaic Device Modeling [Phys. Rev. Applied **2** , 014008 (2014)]”, *Physical Review Applied*, vol. 8, no. 1. American Physical Society (APS), Jul. 20, 2017. doi: 10.1103/physrevapplied.8.019902.  
  
M. C. Heiber, K. Kister, A. Baumann, V. Dyakonov, C. Deibeland T.-Q. Nguyen, “Impact of Tortuosity on Charge-Carrier Transport in Organic Bulk Heterojunction Blends”, *Physical Review Applied*, vol. 8, no. 5. American Physical Society (APS), Nov. 22, 2017. doi: 10.1103/physrevapplied.8.054043.  
  
Y. Liu, H. Xiaoand W. A. Goddard III, “Two-Dimensional Halide Perovskites: Tuning Electronic Activities of Defects”, *Nano Letters*, vol. 16, no. 5. American Chemical Society (ACS), pp. 3335–3340, Apr. 25, 2016. doi: 10.1021/acs.nanolett.6b00964.  
  
N. Sivadas, H. Dixit, V. R. Cooperand D. Xiao, “Thickness-dependent carrier density at the surface of(111) slabs”, *Physical Review B*, vol. 89, no. 7. American Physical Society (APS), Feb. 05, 2014. doi: 10.1103/physrevb.89.075303.  
  
A. M. Scheer, J. D. Strotherand C. Z. Hargather, “First-Principles Calculations of Stacking Fault Energies in Quinary High-Entropy Alloy Systems”, *The Minerals, Metals & Materials Series*. Springer International Publishing, pp. 661–667, 2018. doi: 10.1007/978-3-319-72526-0\_62.  
  
X. Chen, “Atmospheric pressure chemical vapor deposition of methylammonium bismuth iodide thin films”, *Journal of Materials Chemistry A*, vol. 5, no. 47. Royal Society of Chemistry (RSC), pp. 24728–24739, 2017. doi: 10.1039/c7ta06578g.  
  
S. B. Cho, J. Gazquez, X. Huang, Y. Myung, P. Banerjeeand R. Mishra, “Intrinsic point defects and intergrowths in layered bismuth triiodide”, *Physical Review Materials*, vol. 2, no. 6. American Physical Society (APS), Jun. 07, 2018. doi: 10.1103/physrevmaterials.2.064602.  
  
S. B. Cho and R. Mishra, “Epitaxial engineering of polar *ε*-Ga2O3 for tunable two-dimensional electron gas at the heterointerface”, *Applied Physics Letters*, vol. 112, no. 16. AIP Publishing, p. 162101, Apr. 16, 2018. doi: 10.1063/1.5019721.  
  
Z. Gao, “Doping Mechanism in Transparent, Conducting Tantalum Doped ZnO Films Deposited Using Atomic Layer Deposition”, *Advanced Materials Interfaces*, vol. 3, no. 21. Wiley, p. 1600496, Sep. 29, 2016. doi: 10.1002/admi.201600496.  
  
S. T. Hartman, S. B. Choand R. Mishra, “Multiferroism in Iron-Based Oxyfluoride Perovskites”, *Inorganic Chemistry*, vol. 57, no. 17. American Chemical Society (ACS), pp. 10616–10624, Aug. 14, 2018. doi: 10.1021/acs.inorgchem.8b01253.  
  
S. T. Hartman, “Direct observation of apical oxygen vacancies in the high-temperature superconductor ”, *Physical Review Materials*, vol. 3, no. 11. American Physical Society (APS), Nov. 22, 2019. doi: 10.1103/physrevmaterials.3.114806.  
  
Z. Hemmat, “Quasi‐Binary Transition Metal Dichalcogenide Alloys: Thermodynamic Stability Prediction, Scalable Synthesis, and Application”, *Advanced Materials*, vol. 32, no. 26. Wiley, p. 1907041, May 25, 2020. doi: 10.1002/adma.201907041.  
  
X. Huang, S. Huang, P. Biswasand R. Mishra, “Band Gap Insensitivity to Large Chemical Pressures in Ternary Bismuth Iodides for Photovoltaic Applications”, *The Journal of Physical Chemistry C*, vol. 120, no. 51. American Chemical Society (ACS), pp. 28924–28932, Dec. 15, 2016. doi: 10.1021/acs.jpcc.6b09567.  
  
X. Hu, “Controlling Nanoscale Thermal Expansion of Monolayer Transition Metal Dichalcogenides by Alloy Engineering”, *Small*, vol. 16, no. 3. Wiley, p. 1905892, Dec. 12, 2019. doi: 10.1002/smll.201905892.  
  
D. H. Kim, “Flexible Crossbar‐Structured Phase Change Memory Array via Mo‐Based Interfacial Physical Lift‐Off”, *Advanced Functional Materials*, vol. 29, no. 6. Wiley, p. 1806338, Dec. 20, 2018. doi: 10.1002/adfm.201806338.  
  
G. Luo, X. Wang, M. R. Zachariahand R. Mishra, “Ignition Threshold of Perovskite-Based Oxides for Solid Fuel Oxidation from First-Principles Calculations”, *The Journal of Physical Chemistry C*, vol. 123, no. 29. American Chemical Society (ACS), pp. 17644–17649, Jun. 26, 2019. doi: 10.1021/acs.jpcc.9b01609.  
  
L. Majidi, “New Class of Electrocatalysts Based on 2D Transition Metal Dichalcogenides in Ionic Liquid”, *Advanced Materials*, vol. 31, no. 4. Wiley, p. 1804453, Nov. 30, 2018. doi: 10.1002/adma.201804453.  
  
T. Mazaheri, “Stochastic replica voting machine prediction of stable cubic and double perovskite materials and binary alloys”, *Physical Review Materials*, vol. 3, no. 6. American Physical Society (APS), Jun. 19, 2019. doi: 10.1103/physrevmaterials.3.063802.  
  
R. Mishra, “Towards spin-polarized two-dimensional electron gas at a surface of an antiferromagnetic insulating oxide”, *Physical Review B*, vol. 94, no. 4. American Physical Society (APS), Jul. 18, 2016. doi: 10.1103/physrevb.94.045123.  
  
M. V. Morrell, “Significantly Enhanced Emission Stability of CsPbBr3 Nanocrystals via Chemically Induced Fusion Growth for Optoelectronic Devices”, *ACS Applied Nano Materials*, vol. 1, no. 11. American Chemical Society (ACS), pp. 6091–6098, Oct. 16, 2018. doi: 10.1021/acsanm.8b01298.  
  
B. Mundet, “An Atomic-Scale Perspective of the Challenging Microstructure of YBa2Cu3O7−x Thin Films”, *Superconductivity*. Springer International Publishing, pp. 189–212, Aug. 22, 2019. doi: 10.1007/978-3-030-23303-7\_7.  
  
B. Mundet, “Local strain-driven migration of oxygen vacancies to apical sites in YBa2Cu3O7−x”, *Nanoscale*, vol. 12, no. 10. Royal Society of Chemistry (RSC), pp. 5922–5931, 2020. doi: 10.1039/d0nr00666a.  
  
P. Ranga, S. B. Cho, R. Mishraand S. Krishnamoorthy, “Highly tunable, polarization-engineered two-dimensional electron gas in *ε*-AlGaO3/*ε*-Ga2O3 heterostructures”, *Applied Physics Express*, vol. 13, no. 6. IOP Publishing, p. 061009, May 26, 2020. doi: 10.35848/1882-0786/ab9168.  
  
J. A. Santana, “Quantum Many-Body Effects in Defective Transition-Metal-Oxide Superlattices”, *Journal of Chemical Theory and Computation*, vol. 13, no. 11. American Chemical Society (ACS), pp. 5604–5609, Oct. 06, 2017. doi: 10.1021/acs.jctc.7b00483.  
  
M. Shen, “Nanoscale Colocalization of Fluorogenic Probes Reveals the Role of Oxygen Vacancies in the Photocatalytic Activity of Tungsten Oxide Nanowires”, *ACS Catalysis*, vol. 10, no. 3. American Chemical Society (ACS), pp. 2088–2099, Jan. 08, 2020. doi: 10.1021/acscatal.9b04481.  
  
A. S. Thind, X. Huang, J. Sunand R. Mishra, “First-Principles Prediction of a Stable Hexagonal Phase of CH3NH3PbI3”, *Chemistry of Materials*, vol. 29, no. 14. American Chemical Society (ACS), pp. 6003–6011, Jun. 15, 2017. doi: 10.1021/acs.chemmater.7b01781.  
  
A. S. Thind, “KBaTeBiO6: A Lead-Free, Inorganic Double-Perovskite Semiconductor for Photovoltaic Applications”, *Chemistry of Materials*, vol. 31, no. 13. American Chemical Society (ACS), pp. 4769–4778, Jun. 11, 2019. doi: 10.1021/acs.chemmater.9b01025.  
  
A. S. Thind, “Atomic Structure and Electrical Activity of Grain Boundaries and Ruddlesden–Popper Faults in Cesium Lead Bromide Perovskite”, *Advanced Materials*, vol. 31, no. 4. Wiley, p. 1805047, Dec. 03, 2018. doi: 10.1002/adma.201805047.  
  
S. Wang, “Phase‐Dependent Band Gap Engineering in Alloys of Metal‐Semiconductor Transition Metal Dichalcogenides”, *Advanced Functional Materials*, vol. 30, no. 51. Wiley, p. 2004912, Sep. 22, 2020. doi: 10.1002/adfm.202004912.  
  
B. Yin, X. Huang, R. Mishraand B. Sadtler, “Compositionally Induced Twin Defects Control the Shape of Ternary Silver Halide Nanocrystals”, *Chemistry of Materials*, vol. 29, no. 3. American Chemical Society (ACS), pp. 1014–1021, Jan. 27, 2017. doi: 10.1021/acs.chemmater.6b03660.  
  
Z. Zhang, M. Li, K. Floresand R. Mishra, “Machine learning formation enthalpies of intermetallics”, *Journal of Applied Physics*, vol. 128, no. 10. AIP Publishing, p. 105103, Sep. 14, 2020. doi: 10.1063/5.0012323.  
  
J. Zhou, “Synthesis of Co‐Doped MoS 2 Monolayers with Enhanced Valley Splitting”, *Advanced Materials*, vol. 32, no. 11. Wiley, p. 1906536, Feb. 06, 2020. doi: 10.1002/adma.201906536.  
  
L. Adamska, S. Sadasivam, J. J. Foley IV, P. Darancetand S. Sharifzadeh, “First-Principles Investigation of Borophene as a Monolayer Transparent Conductor”, *The Journal of Physical Chemistry C*, vol. 122, no. 7. American Chemical Society (ACS), pp. 4037–4045, Feb. 13, 2018. doi: 10.1021/acs.jpcc.7b10197.  
  
L. Adamska and S. Sharifzadeh, “Fine-Tuning the Optoelectronic Properties of Freestanding Borophene by Strain”, *ACS Omega*, vol. 2, no. 11. American Chemical Society (ACS), pp. 8290–8299, Nov. 21, 2017. doi: 10.1021/acsomega.7b01232.  
  
T. Huang, D. K. Lewisand S. Sharifzadeh, “Assessing the Role of Inter-Molecular Interactions in a Perylene-Based Nanowire Using First-Principles Many-Body Perturbation Theory”, *[]*. American Chemical Society (ACS), Apr. 05, 2019. doi: 10.26434/chemrxiv.7956248.v1.  
  
A. Roy and H. K. Pal, “Tetrahedral bonding in twisted bilayer graphene by carbon intercalation”, *The European Physical Journal B*, vol. 90, no. 8. Springer Science and Business Media LLC, Aug. 2017. doi: 10.1140/epjb/e2017-80141-5.  
  
C. E. Ekuma, V. Dobrosavljevićand D. Gunlycke, “First-Principles-Based Method for Electron Localization: Application to Monolayer Hexagonal Boron Nitride”, *Physical Review Letters*, vol. 118, no. 10. American Physical Society (APS), Mar. 10, 2017. doi: 10.1103/physrevlett.118.106404.  
  
S.-F. Liou, Z.-X. Huand K. Yang, “Topological quantum phase transition from a fermionic integer quantum Hall phase to a bosonic fractional quantum Hall phase through a -wave Feshbach resonance”, *Physical Review B*, vol. 95, no. 24. American Physical Society (APS), Jun. 08, 2017. doi: 10.1103/physrevb.95.241106.  
  
A. Vishnyakov, T. Liand A. V. Neimark, “Adhesion of Phospholipid Bilayers to Hydroxylated Silica: Existence of Nanometer-Thick Water Interlayers”, *Langmuir*, vol. 33, no. 45. American Chemical Society (ACS), pp. 13148–13156, Oct. 31, 2017. doi: 10.1021/acs.langmuir.7b03582.  
  
M. Amsler and C. Wolverton, “Dense superconducting phases of copper-bismuth at high pressure”, *Physical Review Materials*, vol. 1, no. 3. American Physical Society (APS), Aug. 28, 2017. doi: 10.1103/physrevmaterials.1.031801.  
  
M. Amsler, Z. Yaoand C. Wolverton, “Cubine, a Quasi Two-Dimensional Copper–Bismuth Nanosheet”, *Chemistry of Materials*, vol. 29, no. 22. American Chemical Society (ACS), pp. 9819–9828, Nov. 10, 2017. doi: 10.1021/acs.chemmater.7b03997.  
  
J. He, S. S. Naghavi, V. I. Hegde, M. Amslerand C. Wolverton, “Designing and Discovering a New Family of Semiconducting Quaternary Heusler Compounds Based on the 18-Electron Rule”, *Chemistry of Materials*, vol. 30, no. 15. American Chemical Society (ACS), pp. 4978–4985, Jun. 13, 2018. doi: 10.1021/acs.chemmater.8b01096.  
  
S. Kim, “First-Principles Study of Lithium Cobalt Spinel Oxides: Correlating Structure and Electrochemistry”, *ACS Applied Materials & Interfaces*, vol. 10, no. 16. American Chemical Society (ACS), pp. 13479–13490, Apr. 04, 2018. doi: 10.1021/acsami.8b00394.  
  
S. Mohr, M. Eixarch, M. Amsler, M. J. Mantsinenand L. Genovese, “Linear scaling DFT calculations for large tungsten systems using an optimized local basis”, *Nuclear Materials and Energy*, vol. 15. Elsevier BV, pp. 64–70, May 2018. doi: 10.1016/j.nme.2018.01.002.  
  
K. M. Powderly, “High-pressure discovery of β-NiBi”, *Chem. Commun.*, vol. 53, no. 81. Royal Society of Chemistry (RSC), pp. 11241–11244, 2017. doi: 10.1039/c7cc06471c.  
  
M. Behtash, Y. Wang, J. Luoand K. Yang, “Oxygen vacancy formation in the SrTiO 3 Σ5 [001] twist grain boundary from first‐principles”, *Journal of the American Ceramic Society*, vol. 101, no. 7. Wiley, pp. 3118–3129, Feb. 2018. doi: 10.1111/jace.15454.  
  
J. Cheng, J. Luoand K. Yang, “Comparison Studies of Interfacial Electronic and Energetic Properties of LaAlO3/TiO2 and TiO2/LaAlO3 Heterostructures from First-Principles Calculations”, *ACS Applied Materials & Interfaces*, vol. 9, no. 8. American Chemical Society (ACS), pp. 7682–7690, Feb. 13, 2017. doi: 10.1021/acsami.6b12254.  
  
J. Cheng, J. Luoand K. Yang, “Aimsgb: An algorithm and open-source python library to generate periodic grain boundary structures”, *Computational Materials Science*, vol. 155. Elsevier BV, pp. 92–103, Dec. 2018. doi: 10.1016/j.commatsci.2018.08.029.  
  
J. Cheng, S. Nazirand K. Yang, “First-Principles Prediction of Two-Dimensional Electron Gas Driven by Polarization Discontinuity in Nonpolar/Nonpolar AHfO3/SrTiO3 (A = Ca, Sr, and Ba) Heterostructures”, *ACS Applied Materials & Interfaces*, vol. 8, no. 46. American Chemical Society (ACS), pp. 31959–31967, Nov. 10, 2016. doi: 10.1021/acsami.6b06907.  
  
J. Cheng, Y. Wang, J. Luoand K. Yang, “δ‐Doping Effects on Electronic and Energetic Properties of LaAlO 3 /SrTiO 3 Heterostructure: First‐Principles Analysis of 23 Transition‐Metal Dopants”, *Advanced Materials Interfaces*, vol. 4, no. 21. Wiley, p. 1700579, Aug. 25, 2017. doi: 10.1002/admi.201700579.  
  
J. Cheng and K. Yang, “Design of two-dimensional electron gas systems *via* polarization discontinuity from large-scale first-principles calculations”, *Journal of Materials Chemistry C*, vol. 6, no. 25. Royal Society of Chemistry (RSC), pp. 6680–6690, 2018. doi: 10.1039/c8tc01893f.  
  
P. H. Joo, J. Chengand K. Yang, “Size effects and odd–even effects in MoS2 nanosheets: first-principles studies”, *Physical Chemistry Chemical Physics*, vol. 19, no. 44. Royal Society of Chemistry (RSC), pp. 29927–29933, 2017. doi: 10.1039/c7cp05402e.  
  
P. H. Joo and K. Yang, “Descriptors of transition metal promoters on MoS2 nanocatalysts for hydrodesulfurization: binding energy of metal sulfides from first principles”, *Molecular Systems Design & Engineering*, vol. 4, no. 4. Royal Society of Chemistry (RSC), pp. 974–982, 2019. doi: 10.1039/c9me00044e.  
  
L. Li, “Self-assembled two-dimensional layered oxide supercells with modulated layer stacking and tunable physical properties”, *Materials Today Nano*, vol. 6. Elsevier BV, p. 100037, Jun. 2019. doi: 10.1016/j.mtnano.2019.100037.  
  
Y. Li, M. Behtash, J. Wongand K. Yang, “Enhancing Ferroelectric Dipole Ordering in Organic–Inorganic Hybrid Perovskite CH3NH3PbI3: Strain and Doping Engineering”, *The Journal of Physical Chemistry C*, vol. 122, no. 1. American Chemical Society (ACS), pp. 177–184, Dec. 28, 2017. doi: 10.1021/acs.jpcc.7b10413.  
  
Y. Li and K. Yang, “High-throughput computational design of organic–inorganic hybrid halide semiconductors beyond perovskites for optoelectronics”, *Energy & Environmental Science*, vol. 12, no. 7. Royal Society of Chemistry (RSC), pp. 2233–2243, 2019. doi: 10.1039/c9ee01371g.  
  
S. Nazir, S. Jiang, J. Chengand K. Yang, “Enhanced interfacial perpendicular magnetic anisotropy in Fe/MgO heterostructure via interfacial engineering”, *Applied Physics Letters*, vol. 114, no. 7. AIP Publishing, p. 072407, Feb. 18, 2019. doi: 10.1063/1.5081834.  
  
Y. Wang, J. Cheng, M. Behtash, W. Tang, J. Luoand K. Yang, “First-principles studies of polar perovskite KTaO3 surfaces: structural reconstruction, charge compensation, and stability diagram”, *Physical Chemistry Chemical Physics*, vol. 20, no. 27. Royal Society of Chemistry (RSC), pp. 18515–18527, 2018. doi: 10.1039/c8cp02540a.  
  
L. Wu, P. Lu, Y. Li, Y. Sun, J. Wongand K. Yang, “First-principles characterization of two-dimensional (CH3(CH2)3NH3)2(CH3NH3)n−1GenI3n+1 perovskite”, *Journal of Materials Chemistry A*, vol. 6, no. 47. Royal Society of Chemistry (RSC), pp. 24389–24396, 2018. doi: 10.1039/c8ta10055a.  
  
G. Khalsa and N. A. Benedek, “Ultrafast optically induced ferromagnetic/anti-ferromagnetic phase transition in GdTiO3 from first principles”, *npj Quantum Materials*, vol. 3, no. 1. Springer Science and Business Media LLC, Mar. 12, 2018. doi: 10.1038/s41535-018-0086-3.  
  
T. Zhu, “Theory and Neutrons Combine To Reveal a Family of Layered Perovskites without Inversion Symmetry”, *Chemistry of Materials*, vol. 29, no. 21. American Chemical Society (ACS), pp. 9489–9497, Oct. 17, 2017. doi: 10.1021/acs.chemmater.7b03604.  
  
D. delToro, “Functional Dissection of a Viral DNA Packaging Machine’s Walker B Motif”, *Journal of Molecular Biology*, vol. 431, no. 22. Elsevier BV, pp. 4455–4474, Nov. 2019. doi: 10.1016/j.jmb.2019.08.012.  
  
B. H.-. jong . Lee and G. Arya, “Orientational phase behavior of polymer-grafted nanocubes”, *Nanoscale*, vol. 11, no. 34. Royal Society of Chemistry (RSC), pp. 15939–15957, 2019. doi: 10.1039/c9nr04859f.  
  
D. Ortiz, “Evidence that a catalytic glutamate and an ‘Arginine Toggle’ act in concert to mediate ATP hydrolysis and mechanochemical coupling in a viral DNA packaging motor”, *Nucleic Acids Research*, vol. 47, no. 3. Oxford University Press (OUP), pp. 1404–1415, Dec. 12, 2018. doi: 10.1093/nar/gky1217.  
  
Z. Shi and G. Arya, “Free energy landscape of salt-actuated reconfigurable DNA nanodevices”, *Nucleic Acids Research*, vol. 48, no. 2. Oxford University Press (OUP), pp. 548–560, Dec. 04, 2019. doi: 10.1093/nar/gkz1137.  
  
Z. Shi, C. E. Castroand G. Arya, “Conformational Dynamics of Mechanically Compliant DNA Nanostructures from Coarse-Grained Molecular Dynamics Simulations”, *ACS Nano*, vol. 11, no. 5. American Chemical Society (ACS), pp. 4617–4630, Apr. 24, 2017. doi: 10.1021/acsnano.7b00242.  
  
J.-J. Song, “One-Dimensional Anomalous Diffusion of Gold Nanoparticles in a Polymer Melt”, *Physical Review Letters*, vol. 122, no. 10. American Physical Society (APS), Mar. 15, 2019. doi: 10.1103/physrevlett.122.107802.  
  
T.-Y. Tang, Y. Zhouand G. Arya, “Interfacial Assembly of Tunable Anisotropic Nanoparticle Architectures”, *ACS Nano*, vol. 13, no. 4. American Chemical Society (ACS), pp. 4111–4123, Mar. 18, 2019. doi: 10.1021/acsnano.8b08733.  
  
S. Feng, “Mapping a stable solvent structure landscape for aprotic Li–air battery organic electrolytes”, *Journal of Materials Chemistry A*, vol. 5, no. 45. Royal Society of Chemistry (RSC), pp. 23987–23998, 2017. doi: 10.1039/c7ta08321a.  
  
M. Gauthier, “Probing Surface Chemistry Changes Using LiCoO2-only Electrodes in Li-Ion Batteries”, *Journal of The Electrochemical Society*, vol. 165, no. 7. The Electrochemical Society, pp. A1377–A1387, 2018. doi: 10.1149/2.0431807jes.  
  
B. Han, “Iron-Based Perovskites for Catalyzing Oxygen Evolution Reaction”, *The Journal of Physical Chemistry C*, vol. 122, no. 15. American Chemical Society (ACS), pp. 8445–8454, Mar. 29, 2018. doi: 10.1021/acs.jpcc.8b01397.  
  
B. Huang, “Non-covalent interactions in electrochemical reactions and implications in clean energy applications”, *Physical Chemistry Chemical Physics*, vol. 20, no. 23. Royal Society of Chemistry (RSC), pp. 15680–15686, 2018. doi: 10.1039/c8cp02512f.  
  
M. Huang, “Fluorinated Aryl Sulfonimide Tagged (FAST) salts: modular synthesis and structure–property relationships for battery applications”, *Energy & Environmental Science*, vol. 11, no. 5. Royal Society of Chemistry (RSC), pp. 1326–1334, 2018. doi: 10.1039/c7ee03509h.  
  
Y. Katayama, “Surface (Electro)chemistry of CO2 on Pt Surface: An *in Situ* Surface-Enhanced Infrared Absorption Spectroscopy Study”, *The Journal of Physical Chemistry C*, vol. 122, no. 23. American Chemical Society (ACS), pp. 12341–12349, May 23, 2018. doi: 10.1021/acs.jpcc.8b03556.  
  
T. Krauskopf, “Comparing the Descriptors for Investigating the Influence of Lattice Dynamics on Ionic Transport Using the Superionic Conductor Na3PS4–*x*Se*x*”, *Journal of the American Chemical Society*, vol. 140, no. 43. American Chemical Society (ACS), pp. 14464–14473, Oct. 04, 2018. doi: 10.1021/jacs.8b09340.  
  
S. Muy, “Lithium Conductivity and Meyer-Neldel Rule in Li3PO4–Li3VO4–Li4GeO4 Lithium Superionic Conductors”, *Chemistry of Materials*, vol. 30, no. 16. American Chemical Society (ACS), pp. 5573–5582, Jul. 26, 2018. doi: 10.1021/acs.chemmater.8b01504.  
  
S. Muy, “Tuning mobility and stability of lithium ion conductors based on lattice dynamics”, *Energy & Environmental Science*, vol. 11, no. 4. Royal Society of Chemistry (RSC), pp. 850–859, 2018. doi: 10.1039/c7ee03364h.  
  
R. R. Rao, “Surface Orientation Dependent Water Dissociation on Rutile Ruthenium Dioxide”, *The Journal of Physical Chemistry C*, vol. 122, no. 31. American Chemical Society (ACS), pp. 17802–17811, Jul. 12, 2018. doi: 10.1021/acs.jpcc.8b04284.  
  
R. Tatara, “Tuning NaO2 Cube Sizes by Controlling Na+ and Solvent Activity in Na–O2 Batteries”, *The Journal of Physical Chemistry C*, vol. 122, no. 32. American Chemical Society (ACS), pp. 18316–18328, Jul. 23, 2018. doi: 10.1021/acs.jpcc.8b05418.  
  
M. T. McDonnell, D. A. Greeley, K. M. Kitand D. J. Keffer, “Molecular Dynamics Simulations of Hydration Effects on Solvation, Diffusivity, and Permeability in Chitosan/Chitin Films”, *The Journal of Physical Chemistry B*, vol. 120, no. 34. American Chemical Society (ACS), pp. 8997–9010, Aug. 18, 2016. doi: 10.1021/acs.jpcb.6b05999.  
  
M. T. McDonnell, H. Xuand D. J. Keffer, “Ab Initio Molecular Dynamics Simulations of an Excess Proton in a Triethylene Glycol–Water Solution: Solvation Structure, Mechanism, and Kinetics”, *The Journal of Physical Chemistry B*, vol. 120, no. 23. American Chemical Society (ACS), pp. 5223–5242, Jun. 03, 2016. doi: 10.1021/acs.jpcb.6b02445.  
  
D. Choudhuri, R. Banerjeeand S. G. Srinivasan, “Interfacial structures and energetics of the strengthening precipitate phase in creep-resistant Mg-Nd-based alloys”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Jan. 17, 2017. doi: 10.1038/srep40540.  
  
D. Choudhuri, S. G. Srinivasan, M. A. Gibsonand R. Banerjee, “Bonding Environments in a Creep–Resistant Mg–RE–Zn Alloy”, *The Minerals, Metals & Materials Series*. Springer International Publishing, pp. 471–475, 2017. doi: 10.1007/978-3-319-52392-7\_64.  
  
R. Salloom, R. Banerjeeand S. G. Srinivasan, “Effect of β-stabilizer elements on stacking faults energies and ductility of α-titanium using first-principles calculations”, *Journal of Applied Physics*, vol. 120, no. 17. AIP Publishing, p. 175105, Nov. 07, 2016. doi: 10.1063/1.4966939.  
  
D. E. Schipper, J.-H. Chenand K. H. Whitmire, “Iron carbonyl clusters with ECl2 units (E = P, As)”, *Journal of Organometallic Chemistry*, vol. 849–850. Elsevier BV, pp. 279–285, Nov. 2017. doi: 10.1016/j.jorganchem.2017.03.008.  
  
D. Doratotaj, J. R. Simpsonand J.-A. Yan, “Probing the uniaxial strains inusing polarized Raman spectroscopy: A first-principles study”, *Physical Review B*, vol. 93, no. 7. American Physical Society (APS), Feb. 01, 2016. doi: 10.1103/physrevb.93.075401.  
  
R. He, “Interlayer breathing and shear modes in NbSe 2 atomic layers”, *2D Materials*, vol. 3, no. 3. IOP Publishing, p. 031008, Aug. 26, 2016. doi: 10.1088/2053-1583/3/3/031008.  
  
R. He, “Coupling and Stacking Order of ReS2 Atomic Layers Revealed by Ultralow-Frequency Raman Spectroscopy”, *Nano Letters*, vol. 16, no. 2. American Chemical Society (ACS), pp. 1404–1409, Jan. 14, 2016. doi: 10.1021/acs.nanolett.5b04925.  
  
W. C. Yap, Z. Yang, M. Mehboudi, J.-A. Yan, S. Barraza-Lopezand W. Zhu, “Layered material GeSe and vertical GeSe/MoS2 p-n heterojunctions”, *Nano Research*, vol. 11, no. 1. Springer Science and Business Media LLC, pp. 420–430, Aug. 03, 2017. doi: 10.1007/s12274-017-1646-8.  
  
Z. Zhu, Q.-R. Wang, D. N. Shengand Z.-Y. Weng, “Exact sign structure of the t – J chain and the single hole ground state”, *Nuclear Physics B*, vol. 903. Elsevier BV, pp. 51–77, Feb. 2016. doi: 10.1016/j.nuclphysb.2015.12.004.  
  
Z. Zhu and Z.-Y. Weng, “Quasiparticle collapsing in an anisotropicladder”, *Physical Review B*, vol. 92, no. 23. American Physical Society (APS), Dec. 31, 2015. doi: 10.1103/physrevb.92.235156.  
  
S. Zuluaga, P. Manchanda, Y.-Y. Zhangand S. T. Pantelides, “Design of Optimally Stable Molecular Coatings for Fe-Based Nanoparticles in Aqueous Environments”, *ACS Omega*, vol. 2, no. 8. American Chemical Society (ACS), pp. 4480–4487, Aug. 11, 2017. doi: 10.1021/acsomega.7b00762.  
  
S. Gazit, M. Randeriaand A. Vishwanath, “Emergent Dirac fermions and broken symmetries in confined and deconfined phases of Z2 gauge theories”, *Nature Physics*, vol. 13, no. 5. Springer Science and Business Media LLC, pp. 484–490, Feb. 06, 2017. doi: 10.1038/nphys4028.  
  
Q. Pang, H. DorMohammadi, O. B. Isgorand L. Árnadóttir, “Density functional theory study on the effect of OH and Cl adsorption on the surface structure of α-Fe2O3”, *Computational and Theoretical Chemistry*, vol. 1100. Elsevier BV, pp. 91–101, Jan. 2017. doi: 10.1016/j.comptc.2016.12.009.  
  
H. DorMohammadi, Q. Pang, P. Murkute, L. Árnadóttirand O. Burkan Isgor, “Investigation of iron passivity in highly alkaline media using reactive-force field molecular dynamics”, *Corrosion Science*, vol. 157. Elsevier BV, pp. 31–40, Aug. 2019. doi: 10.1016/j.corsci.2019.05.016.  
  
H. DorMohammadi, Q. Pang, P. Murkute, L. Árnadóttirand O. B. Isgor, “Investigation of chloride-induced depassivation of iron in alkaline media by reactive force field molecular dynamics”, *npj Materials Degradation*, vol. 3, no. 1. Springer Science and Business Media LLC, Apr. 23, 2019. doi: 10.1038/s41529-019-0081-6.  
  
Q. Pang, H. DorMohammadi, O. B. Isgorand L. Árnadóttir, “The effect of surface vacancies on the interactions of Cl with a α-Fe2O3 (0001) surface and the role of Cl in depassivation”, *Corrosion Science*, vol. 154. Elsevier BV, pp. 61–69, Jul. 2019. doi: 10.1016/j.corsci.2019.03.052.  
  
L. H. Sprowl, B. M. Adam, J. D. Tuckerand L. Árnadóttir, “First-principles study of the products of CO2 dissociation on nickel-based alloys: Trends in energetics with alloying element”, *Surface Science*, vol. 677. Elsevier BV, pp. 219–231, Nov. 2018. doi: 10.1016/j.susc.2018.06.011.  
  
Z. Zhu, L. Fuand D. N. Sheng, “Numerical Study of Quantum Hall Bilayers at Total Filling : A New Phase at Intermediate Layer Distances”, *Physical Review Letters*, vol. 119, no. 17. American Physical Society (APS), Oct. 23, 2017. doi: 10.1103/physrevlett.119.177601.  
  
Z. Zhu, I. Sodemann, D. N. Shengand L. Fu, “Anisotropy-driven transition from the Moore-Read state to quantum Hall stripes”, *Physical Review B*, vol. 95, no. 20. American Physical Society (APS), May 30, 2017. doi: 10.1103/physrevb.95.201116.  
  
J. A. Barr, F.-Y. Lin, M. Ashton, R. G. Hennigand S. B. Sinnott, “High-throughput density functional calculations to optimize properties and interfacial chemistry of piezoelectric materials”, *Physical Review Materials*, vol. 2, no. 2. American Physical Society (APS), Feb. 28, 2018. doi: 10.1103/physrevmaterials.2.025002.  
  
T. Kou, “Theoretical and Experimental Insight into the Effect of Nitrogen Doping on Hydrogen Evolution Activity of Ni 3 S 2 in Alkaline Medium”, *Advanced Energy Materials*, vol. 8, no. 19. Wiley, p. 1703538, Mar. 15, 2018. doi: 10.1002/aenm.201703538.  
  
B. Lu, “Nitrogen and Iron-Codoped Carbon Hollow Nanotubules as High-Performance Catalysts toward Oxygen Reduction Reaction: A Combined Experimental and Theoretical Study”, *Chemistry of Materials*, vol. 29, no. 13. American Chemical Society (ACS), pp. 5617–5628, Jun. 21, 2017. doi: 10.1021/acs.chemmater.7b01265.  
  
Y. Peng, “Hydrogen evolution reaction catalyzed by ruthenium ion-complexed graphitic carbon nitride nanosheets”, *Journal of Materials Chemistry A*, vol. 5, no. 34. Royal Society of Chemistry (RSC), pp. 18261–18269, 2017. doi: 10.1039/c7ta03826g.  
  
Y. Peng, “Point of Anchor: Impacts on Interfacial Charge Transfer of Metal Oxide Nanoparticles”, *Journal of the American Chemical Society*, vol. 140, no. 45. American Chemical Society (ACS), pp. 15290–15299, Oct. 22, 2018. doi: 10.1021/jacs.8b08035.  
  
T. J. Smart, A. C. Cardiel, F. Wu, K.-S. Choiand Y. Ping, “Mechanistic insights of enhanced spin polaron conduction in CuO through atomic doping”, *npj Computational Materials*, vol. 4, no. 1. Springer Science and Business Media LLC, Nov. 19, 2018. doi: 10.1038/s41524-018-0118-3.  
  
T. J. Smart and Y. Ping, “Effect of defects on the small polaron formation and transport properties of hematite from first-principles calculations”, *Journal of Physics: Condensed Matter*, vol. 29, no. 39. IOP Publishing, p. 394006, Aug. 23, 2017. doi: 10.1088/1361-648x/aa7e3d.  
  
T. J. Smart, F. Wu, M. Govoniand Y. Ping, “Fundamental principles for calculating charged defect ionization energies in ultrathin two-dimensional materials”, *Physical Review Materials*, vol. 2, no. 12. American Physical Society (APS), Dec. 20, 2018. doi: 10.1103/physrevmaterials.2.124002.  
  
R. Sundararaman and Y. Ping, “First-principles electrostatic potentials for reliable alignment at interfaces and defects”, *The Journal of Chemical Physics*, vol. 146, no. 10. AIP Publishing, p. 104109, Mar. 14, 2017. doi: 10.1063/1.4978238.  
  
F. Wu, A. Galatas, R. Sundararaman, D. Roccaand Y. Ping, “First-principles engineering of charged defects for two-dimensional quantum technologies”, *Physical Review Materials*, vol. 1, no. 7. American Physical Society (APS), Dec. 06, 2017. doi: 10.1103/physrevmaterials.1.071001.  
  
W. Zhang, “Unconventional Relation between Charge Transport and Photocurrent via Boosting Small Polaron Hopping for Photoelectrochemical Water Splitting”, *ACS Energy Letters*, vol. 3, no. 9. American Chemical Society (ACS), pp. 2232–2239, Aug. 27, 2018. doi: 10.1021/acsenergylett.8b01445.  
  
F. Wu and Y. Ping, “Combining Landau–Zener theory and kinetic Monte Carlo sampling for small polaron mobility of doped BiVO4 from first-principles”, *Journal of Materials Chemistry A*, vol. 6, no. 41. Royal Society of Chemistry (RSC), pp. 20025–20036, 2018. doi: 10.1039/c8ta07437b.  
  
K. R. Hinkle and F. R. Phelan Jr., “Solvation of Carbon Nanoparticles in Water/Alcohol Mixtures: Using Molecular Simulation To Probe Energetics, Structure, and Dynamics”, *The Journal of Physical Chemistry C*, vol. 121, no. 41. American Chemical Society (ACS), pp. 22926–22938, Oct. 06, 2017. doi: 10.1021/acs.jpcc.7b07769.  
  
K. R. Hinkle and F. R. Phelan Jr., “Solvation Free Energy of Self-Assembled Complexes: Using Molecular Dynamics to Understand the Separation of ssDNA-Wrapped Single-Walled Carbon Nanotubes”, *The Journal of Physical Chemistry C*, vol. 124, no. 24. American Chemical Society (ACS), pp. 13127–13140, May 20, 2020. doi: 10.1021/acs.jpcc.0c00983.  
  
M. Amsler, S. S. Naghaviand C. Wolverton, “Prediction of superconducting iron–bismuth intermetallic compounds at high pressure”, *Chemical Science*, vol. 8, no. 3. Royal Society of Chemistry (RSC), pp. 2226–2234, 2017. doi: 10.1039/c6sc04683e.  
  
E. B. Isaacs, G. M. Luand C. Wolverton, “Inverse Design of Ultralow Lattice Thermal Conductivity Materials via Materials Database Screening of Lone Pair Cation Coordination Environment”, *The Journal of Physical Chemistry Letters*, vol. 11, no. 14. American Chemical Society (ACS), pp. 5577–5583, Jun. 23, 2020. doi: 10.1021/acs.jpclett.0c01077.  
  
E. B. Isaacs and C. Wolverton, “Electronic Structure and Phase Stability of Yb-Filled CoSb3 Skutterudite Thermoelectrics from First-Principles”, *Chemistry of Materials*, vol. 31, no. 16. American Chemical Society (ACS), pp. 6154–6162, Aug. 05, 2019. doi: 10.1021/acs.chemmater.9b01630.  
  
S. M. Clarke, “Creating Binary Cu–Bi Compounds via High-Pressure Synthesis: A Combined Experimental and Theoretical Study”, *Chemistry of Materials*, vol. 29, no. 12. American Chemical Society (ACS), pp. 5276–5285, Jun. 19, 2017. doi: 10.1021/acs.chemmater.7b01418.  
  
H. A. Eivari, “Two-Dimensional Hexagonal Sheet of TiO2”, *Chemistry of Materials*, vol. 29, no. 20. American Chemical Society (ACS), pp. 8594–8603, Aug. 17, 2017. doi: 10.1021/acs.chemmater.7b02031.  
  
S. Ohno, “Achieving zT > 1 in Inexpensive Zintl Phase Ca 9 Zn 4+ *x* Sb 9 by Phase Boundary Mapping”, *Advanced Functional Materials*, vol. 27, no. 20. Wiley, p. 1606361, Mar. 29, 2017. doi: 10.1002/adfm.201606361.  
  
T. Cheng, A. Fortunelliand W. A. Goddard III, “Reaction intermediates during operando electrocatalysis identified from full solvent quantum mechanics molecular dynamics”, *Proceedings of the National Academy of Sciences*, vol. 116, no. 16. Proceedings of the National Academy of Sciences, pp. 7718–7722, Mar. 13, 2019. doi: 10.1073/pnas.1821709116.  
  
T. Cheng, Y. Huang, H. Xiaoand W. A. Goddard III, “Predicted Structures of the Active Sites Responsible for the Improved Reduction of Carbon Dioxide by Gold Nanoparticles”, *The Journal of Physical Chemistry Letters*, vol. 8, no. 14. American Chemical Society (ACS), pp. 3317–3320, Jul. 07, 2017. doi: 10.1021/acs.jpclett.7b01335.  
  
T. Cheng, A. Jaramillo-Botero, Q. An, D. V. Ilyin, S. Naserifarand W. A. Goddard III, “First principles-based multiscale atomistic methods for input into first principles nonequilibrium transport across interfaces”, *Proceedings of the National Academy of Sciences*, vol. 116, no. 37. Proceedings of the National Academy of Sciences, pp. 18193–18201, Aug. 03, 2018. doi: 10.1073/pnas.1800035115.  
  
T. Cheng, L. Wang, B. V. Merinovand W. A. Goddard III, “Explanation of Dramatic pH-Dependence of Hydrogen Binding on Noble Metal Electrode: Greatly Weakened Water Adsorption at High pH”, *Journal of the American Chemical Society*, vol. 140, no. 25. American Chemical Society (ACS), pp. 7787–7790, May 24, 2018. doi: 10.1021/jacs.8b04006.  
  
T. Cheng, H. Xiaoand W. A. Goddard III, “Full atomistic reaction mechanism with kinetics for CO reduction on Cu(100) from ab initio molecular dynamics free-energy calculations at 298 K”, *Proceedings of the National Academy of Sciences*, vol. 114, no. 8. Proceedings of the National Academy of Sciences, pp. 1795–1800, Feb. 06, 2017. doi: 10.1073/pnas.1612106114.  
  
J. Chen, R. J. Nielsen, W. A. Goddard III, B. A. McKeown, D. A. Dickieand T. B. Gunnoe, “Catalytic Synthesis of Superlinear Alkenyl Arenes Using a Rh(I) Catalyst Supported by a “Capping Arene” Ligand: Access to Aerobic Catalysis”, *Journal of the American Chemical Society*, vol. 140, no. 49. American Chemical Society (ACS), pp. 17007–17018, Nov. 29, 2018. doi: 10.1021/jacs.8b07728.  
  
C. Choi, “A Highly Active Star Decahedron Cu Nanocatalyst for Hydrocarbon Production at Low Overpotentials”, *Advanced Materials*, vol. 31, no. 6. Wiley, p. 1805405, Dec. 14, 2018. doi: 10.1002/adma.201805405.  
  
D. V. Ilyin, W. A. Goddard III, J. J. Oppenheimand T. Cheng, “First-principles–based reaction kinetics from reactive molecular dynamics simulations: Application to hydrogen peroxide decomposition”, *Proceedings of the National Academy of Sciences*, vol. 116, no. 37. Proceedings of the National Academy of Sciences, pp. 18202–18208, Sep. 21, 2018. doi: 10.1073/pnas.1701383115.  
  
S. Kwon, S. Naserifar, H. M. Leeand W. A. Goddard III, “Polarizable Charge Equilibration Model for Transition-Metal Elements”, *The Journal of Physical Chemistry A*, vol. 122, no. 48. American Chemical Society (ACS), pp. 9350–9358, Nov. 09, 2018. doi: 10.1021/acs.jpca.8b07290.  
  
C. Ladewig, “Ordered three-fold symmetric graphene oxide/buckled graphene/graphene heterostructures on MgO(111) by carbon molecular beam epitaxy”, *Journal of Materials Chemistry C*, vol. 6, no. 15. Royal Society of Chemistry (RSC), pp. 4225–4233, 2018. doi: 10.1039/c8tc00178b.  
  
M. Li, “Single-atom tailoring of platinum nanocatalysts for high-performance multifunctional electrocatalysis”, *Nature Catalysis*, vol. 2, no. 6. Springer Science and Business Media LLC, pp. 495–503, May 20, 2019. doi: 10.1038/s41929-019-0279-6.  
  
D. Lionetti, “Effects of Lewis Acidic Metal Ions (M) on Oxygen-Atom Transfer Reactivity of Heterometallic Mn3MO4 Cubane and Fe3MO(OH) and Mn3MO(OH) Clusters”, *Inorganic Chemistry*, vol. 58, no. 4. American Chemical Society (ACS), pp. 2336–2345, Feb. 07, 2019. doi: 10.1021/acs.inorgchem.8b02701.  
  
Y. Lum, T. Cheng, W. A. Goddard IIIand J. W. Ager, “Electrochemical CO Reduction Builds Solvent Water into Oxygenate Products”, *Journal of the American Chemical Society*, vol. 140, no. 30. American Chemical Society (ACS), pp. 9337–9340, Jul. 16, 2018. doi: 10.1021/jacs.8b03986.  
  
S. Naserifar and W. A. Goddard III, “Anomalies in Supercooled Water at ∼230 K Arise from a 1D Polymer to 2D Network Topological Transformation”, *The Journal of Physical Chemistry Letters*, vol. 10, no. 20. American Chemical Society (ACS), pp. 6267–6273, Sep. 27, 2019. doi: 10.1021/acs.jpclett.9b02443.  
  
S. Naserifar and W. A. Goddard III, “The quantum mechanics-based polarizable force field for water simulations”, *The Journal of Chemical Physics*, vol. 149, no. 17. AIP Publishing, p. 174502, Nov. 07, 2018. doi: 10.1063/1.5042658.  
  
S. Naserifar and W. A. Goddard III, “Liquid water is a dynamic polydisperse branched polymer”, *Proceedings of the National Academy of Sciences*, vol. 116, no. 6. Proceedings of the National Academy of Sciences, pp. 1998–2003, Jan. 24, 2019. doi: 10.1073/pnas.1817383116.  
  
S. Naserifar and W. A. Goddard III, “Liquid water is a dynamic polydisperse branched polymer”, *Proceedings of the National Academy of Sciences*, vol. 116, no. 6. Proceedings of the National Academy of Sciences, pp. 1998–2003, Jan. 24, 2019. doi: 10.1073/pnas.1817383116.  
  
J. Qian, A. Fortunelliand W. A. Goddard III, “Effect of Co doping on mechanism and kinetics of ammonia synthesis on Fe(1 1 1) surface”, *Journal of Catalysis*, vol. 370. Elsevier BV, pp. 364–371, Feb. 2019. doi: 10.1016/j.jcat.2019.01.001.  
  
J. Qian, A. Fortunelliand W. A. Goddard III, “Effect of Co doping on mechanism and kinetics of ammonia synthesis on Fe(1 1 1) surface”, *Journal of Catalysis*, vol. 370. Elsevier BV, pp. 364–371, Feb. 2019. doi: 10.1016/j.jcat.2019.01.001.  
  
J. Qian, Y. Ye, H. Yang, J. Yano, E. J. Crumlinand W. A. Goddard III, “Initial Steps in Forming the Electrode–Electrolyte Interface: H2O Adsorption and Complex Formation on the Ag(111) Surface from Combining Quantum Mechanics Calculations and Ambient Pressure X-ray Photoelectron Spectroscopy”, *Journal of the American Chemical Society*, vol. 141, no. 17. American Chemical Society (ACS), pp. 6946–6954, Apr. 04, 2019. doi: 10.1021/jacs.8b13672.  
  
J. Qian, Y. Ye, H. Yang, J. Yano, E. J. Crumlinand W. A. Goddard III, “Initial Steps in Forming the Electrode–Electrolyte Interface: H2O Adsorption and Complex Formation on the Ag(111) Surface from Combining Quantum Mechanics Calculations and Ambient Pressure X-ray Photoelectron Spectroscopy”, *Journal of the American Chemical Society*, vol. 141, no. 17. American Chemical Society (ACS), pp. 6946–6954, Apr. 04, 2019. doi: 10.1021/jacs.8b13672.  
  
Y. Wang, “Neighboring Component Effect in a Tri-stable [2]Rotaxane”, *Journal of the American Chemical Society*, vol. 140, no. 42. American Chemical Society (ACS), pp. 13827–13834, Sep. 25, 2018. doi: 10.1021/jacs.8b08519.  
  
Z. Wang, “Surface Ligand Promotion of Carbon Dioxide Reduction through Stabilizing Chemisorbed Reactive Intermediates”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 11. American Chemical Society (ACS), pp. 3057–3061, May 22, 2018. doi: 10.1021/acs.jpclett.8b00959.  
  
H. Yang, T. Cheng, W. A. Goddard IIIand X.-M. Ren, “Design of a One-Dimensional Stacked Spin Peierls System with Room-Temperature Switching from Quantum Mechanical Predictions”, *The Journal of Physical Chemistry Letters*, vol. 10, no. 21. American Chemical Society (ACS), pp. 6432–6437, Oct. 03, 2019. doi: 10.1021/acs.jpclett.9b02219.  
  
Y. Ye, “Dramatic differences in carbon dioxide adsorption and initial steps of reduction between silver and copper”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Apr. 23, 2019. doi: 10.1038/s41467-019-09846-y.  
  
T. Cheng, H. Xiaoand W. A. Goddard, “Nature of the Active Sites for CO Reduction on Copper Nanoparticles; Suggestions for Optimizing Performance”, *Journal of the American Chemical Society*, vol. 139, no. 34. American Chemical Society (ACS), pp. 11642–11645, Aug. 18, 2017. doi: 10.1021/jacs.7b03300.  
  
K. Sun, “Ultrahigh Mass Activity for Carbon Dioxide Reduction Enabled by Gold–Iron Core–Shell Nanoparticles”, *Journal of the American Chemical Society*, vol. 139, no. 44. American Chemical Society (ACS), pp. 15608–15611, Oct. 11, 2017. doi: 10.1021/jacs.7b09251.  
  
K. P. Santo, A. Vishnyakov, Y. Brunand A. V. Neimark, “Adhesion and Separation of Nanoparticles on Polymer-Grafted Porous Substrates”, *Langmuir*, vol. 34, no. 4. American Chemical Society (ACS), pp. 1481–1496, Oct. 03, 2017. doi: 10.1021/acs.langmuir.7b02914.  
  
A. Vishnyakov, R. Mao, M.-T. Leeand A. V. Neimark, “Coarse-grained model of nanoscale segregation, water diffusion, and proton transport in Nafion membranes”, *The Journal of Chemical Physics*, vol. 148, no. 2. AIP Publishing, p. 024108, Jan. 14, 2018. doi: 10.1063/1.4997401.  
  
C. M. Andolina, M. T. Curnan, Q. Zhu, W. A. Saidiand J. C. Yang, “Constructing a Predictive Model of Copper Oxidation from Experiment and Theory”, *Microscopy and Microanalysis*, vol. 23, no. S1. Oxford University Press (OUP), pp. 920–921, Jul. 2017. doi: 10.1017/s1431927617005268.  
  
H. Chi, “Dependence of H2 and CO2 selectivity on Cu oxidation state during partial oxidation of methanol on Cu/ZnO”, *Applied Catalysis A: General*, vol. 556. Elsevier BV, pp. 64–72, Apr. 2018. doi: 10.1016/j.apcata.2018.02.028.  
  
B. J. Foley, “Controlling nucleation, growth, and orientation of metal halide perovskite thin films with rationally selected additives”, *Journal of Materials Chemistry A*, vol. 5, no. 1. Royal Society of Chemistry (RSC), pp. 113–123, 2017. doi: 10.1039/c6ta07671h.  
  
Y. Guo, Q. Wangand W. A. Saidi, “Structural Stabilities and Electronic Properties of High-Angle Grain Boundaries in Perovskite Cesium Lead Halides”, *The Journal of Physical Chemistry C*, vol. 121, no. 3. American Chemical Society (ACS), pp. 1715–1722, Jan. 13, 2017. doi: 10.1021/acs.jpcc.6b11434.  
  
T. T. Yang and W. A. Saidi, “Tuning the hydrogen evolution activity of β-Mo2C nanoparticles via control of their growth conditions”, *Nanoscale*, vol. 9, no. 9. Royal Society of Chemistry (RSC), pp. 3252–3260, 2017. doi: 10.1039/c6nr09893b.  
  
Q. Zhu, W. A. Saidiand J. C. Yang, “Enhanced Mass Transfer in the Step Edge Induced Oxidation on Cu(100) Surface”, *The Journal of Physical Chemistry C*, vol. 121, no. 21. American Chemical Society (ACS), pp. 11251–11260, May 22, 2017. doi: 10.1021/acs.jpcc.6b13055.  
  
A. Alkabsh, H. Samassekouand D. Mazumdar, “A simple approach to analyze layer-dependent optical properties of few-layer transition metal dichalcogenide thin films”, *Nanotechnology*, vol. 30, no. 3. IOP Publishing, pp. 03LT02, Nov. 12, 2018. doi: 10.1088/1361-6528/aaeaff.  
  
H. Samassekou, A. Alkabsh, K. Stiwinter, A. Khatriand D. Mazumdar, “Atomic-level insights through spectroscopic and transport measurements into the large-area synthesis of MoS2 thin films”, *MRS Communications*, vol. 8, no. 3. Springer Science and Business Media LLC, pp. 1328–1334, Aug. 15, 2018. doi: 10.1557/mrc.2018.167.  
  
Z. J. Morgan and Y. M. Jin, “Phase field modeling of pore electromigration in anisotropic conducting polycrystals”, *Computational Materials Science*, vol. 172. Elsevier BV, p. 109362, Feb. 2020. doi: 10.1016/j.commatsci.2019.109362.  
  
S. E. Weitzner and I. Dabo, “Voltage-dependent cluster expansion for electrified solid-liquid interfaces: Application to the electrochemical deposition of transition metals”, *Physical Review B*, vol. 96, no. 20. American Physical Society (APS), Nov. 17, 2017. doi: 10.1103/physrevb.96.205134.  
  
R. Chavez III, L. Diodati, D. L. Wheeler, J. Shaw, A. L. Tomlinsonand M. Jeffries-EL, “Evaluating the Impact of Fluorination on the Electro-optical Properties of Cross-Conjugated Benzobisoxazoles”, *The Journal of Physical Chemistry A*, vol. 123, no. 7. American Chemical Society (ACS), pp. 1343–1352, Jan. 25, 2019. doi: 10.1021/acs.jpca.8b07778.  
  
D. T. Christiansen, S. Ohtani, Y. Chujo, A. L. Tomlinsonand J. R. Reynolds, “All Donor Electrochromic Polymers Tunable across the Visible Spectrum via Random Copolymerization”, *Chemistry of Materials*, vol. 31, no. 17. American Chemical Society (ACS), pp. 6841–6849, Jun. 14, 2019. doi: 10.1021/acs.chemmater.9b01293.  
  
D. T. Christiansen, A. L. Tomlinsonand J. R. Reynolds, “New Design Paradigm for Color Control in Anodically Coloring Electrochromic Molecules”, *Journal of the American Chemical Society*, vol. 141, no. 9. American Chemical Society (ACS), pp. 3859–3862, Feb. 22, 2019. doi: 10.1021/jacs.9b01507.  
  
D. T. Christiansen, D. L. Wheeler, A. L. Tomlinsonand J. R. Reynolds, “Electrochromism of alkylene-linked discrete chromophore polymers with broad radical cation light absorption”, *Polymer Chemistry*, vol. 9, no. 22. Royal Society of Chemistry (RSC), pp. 3055–3066, 2018. doi: 10.1039/c8py00385h.  
  
D. L. Wheeler, L. E. Rainwater, A. R. Greenand A. L. Tomlinson, “Modeling electrochromic poly-dioxythiophene-containing materials through TDDFT”, *Physical Chemistry Chemical Physics*, vol. 19, no. 30. Royal Society of Chemistry (RSC), pp. 20251–20258, 2017. doi: 10.1039/c7cp04130f.  
  
B. Feng and M. Widom, “Elastic stability and lattice distortion of refractory high entropy alloys”, *Materials Chemistry and Physics*, vol. 210. Elsevier BV, pp. 309–314, May 2018. doi: 10.1016/j.matchemphys.2017.06.038.  
  
R. Feng, P. K. Liaw, M. C. Gaoand M. Widom, “First-principles prediction of high-entropy-alloy stability”, *npj Computational Materials*, vol. 3, no. 1. Springer Science and Business Media LLC, Nov. 21, 2017. doi: 10.1038/s41524-017-0049-4.  
  
M. Heine, O. Hellmanand D. Broido, “Effect of thermal lattice and magnetic disorder on phonons in bcc Fe: A first-principles study”, *Physical Review B*, vol. 100, no. 10. American Physical Society (APS), Sep. 12, 2019. doi: 10.1103/physrevb.100.104304.  
  
S. Burgess, A. Vishnyakov, C. Tsovkoand A. V. Neimark, “Nanoparticle-Engendered Rupture of Lipid Membranes”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 17. American Chemical Society (ACS), pp. 4872–4877, Aug. 07, 2018. doi: 10.1021/acs.jpclett.8b01696.  
  
N. Charles, Y. Yu, L. Giordano, R. Jung, F. Magliaand Y. Shao-Horn, “Toward Establishing Electronic and Phononic Signatures of Reversible Lattice Oxygen Oxidation in Lithium Transition Metal Oxides For Li-Ion Batteries”, *Chemistry of Materials*, vol. 32, no. 13. American Chemical Society (ACS), pp. 5502–5514, May 26, 2020. doi: 10.1021/acs.chemmater.0c00245.  
  
S. Feng, “Molecular Design of Stable Sulfamide- and Sulfonamide-Based Electrolytes for Aprotic Li-O2 Batteries”, *Chem*, vol. 5, no. 10. Elsevier BV, pp. 2630–2641, Oct. 2019. doi: 10.1016/j.chempr.2019.07.003.  
  
L. Giordano, “Chemical Reactivity Descriptor for the Oxide-Electrolyte Interface in Li-Ion Batteries”, *The Journal of Physical Chemistry Letters*, vol. 8, no. 16. American Chemical Society (ACS), pp. 3881–3887, Aug. 07, 2017. doi: 10.1021/acs.jpclett.7b01655.  
  
L. Giordano, “Ligand-Dependent Energetics for Dehydrogenation: Implications in Li-Ion Battery Electrolyte Stability and Selective Oxidation Catalysis of Hydrogen-Containing Molecules”, *Chemistry of Materials*, vol. 31, no. 15. American Chemical Society (ACS), pp. 5464–5474, Jul. 03, 2019. doi: 10.1021/acs.chemmater.9b00767.  
  
J. Hwang, K. Akkiraju, J. Corchado-Garcíaand Y. Shao-Horn, “A Perovskite Electronic Structure Descriptor for Electrochemical CO2 Reduction and the Competing H2 Evolution Reaction”, *The Journal of Physical Chemistry C*, vol. 123, no. 40. American Chemical Society (ACS), pp. 24469–24476, Sep. 03, 2019. doi: 10.1021/acs.jpcc.9b04120.  
  
P. Karayaylali, “The Role of Diphenyl Carbonate Additive on the Interfacial Reactivity of Positive Electrodes in Li-ion Batteries”, *Journal of The Electrochemical Society*, vol. 167, no. 4. The Electrochemical Society, p. 040522, Mar. 04, 2020. doi: 10.1149/1945-7111/ab78fe.  
  
Y. Katayama, “An *In Situ* Surface-Enhanced Infrared Absorption Spectroscopy Study of Electrochemical CO2 Reduction: Selectivity Dependence on Surface C-Bound and O-Bound Reaction Intermediates”, *The Journal of Physical Chemistry C*, vol. 123, no. 10. American Chemical Society (ACS), pp. 5951–5963, Dec. 19, 2018. doi: 10.1021/acs.jpcc.8b09598.  
  
D. A. Kuznetsov, J. Peng, L. Giordano, Y. Román-Leshkovand Y. Shao-Horn, “Bismuth Substituted Strontium Cobalt Perovskites for Catalyzing Oxygen Evolution”, *The Journal of Physical Chemistry C*, vol. 124, no. 12. American Chemical Society (ACS), pp. 6562–6570, Feb. 28, 2020. doi: 10.1021/acs.jpcc.0c01401.  
  
R. R. Rao, “Operando identification of site-dependent water oxidation activity on ruthenium dioxide single-crystal surfaces”, *Nature Catalysis*, vol. 3, no. 6. Springer Science and Business Media LLC, pp. 516–525, May 11, 2020. doi: 10.1038/s41929-020-0457-6.  
  
K. A. Stoerzinger, “Orientation-Dependent Oxygen Evolution on RuO2 without Lattice Exchange”, *ACS Energy Letters*, vol. 2, no. 4. American Chemical Society (ACS), pp. 876–881, Mar. 20, 2017. doi: 10.1021/acsenergylett.7b00135.  
  
R. Tatara, “Enhanced Cycling Performance of Ni-Rich Positive Electrodes (NMC) in Li-Ion Batteries by Reducing Electrolyte Free-Solvent Activity”, *ACS Applied Materials & Interfaces*, vol. 11, no. 38. American Chemical Society (ACS), pp. 34973–34988, Aug. 21, 2019. doi: 10.1021/acsami.9b11942.  
  
Y. Yu, “Revealing Electronic Signatures of Lattice Oxygen Redox in Lithium Ruthenates and Implications for High-Energy Li-Ion Battery Material Designs”, *Chemistry of Materials*, vol. 31, no. 19. American Chemical Society (ACS), pp. 7864–7876, Sep. 11, 2019. doi: 10.1021/acs.chemmater.9b01821.  
  
D. Daggag, T. Dorlusand T. Dinadayalane, “Binding of histidine and proline with graphene: DFT study”, *Chemical Physics Letters*, vol. 730. Elsevier BV, pp. 147–152, Sep. 2019. doi: 10.1016/j.cplett.2019.05.043.  
  
D. Daggag, J. Lazareand T. Dinadayalane, “Data related to conformation dependence of tyrosine binding on the surface of graphene: Bent prefers over parallel orientation”, *Data in Brief*, vol. 26. Elsevier BV, p. 104420, Oct. 2019. doi: 10.1016/j.dib.2019.104420.  
  
D. Daggag, J. Lazareand T. Dinadayalane, “Conformation dependence of tyrosine binding on the surface of graphene: Bent prefers over parallel orientation”, *Applied Surface Science*, vol. 483. Elsevier BV, pp. 178–186, Jul. 2019. doi: 10.1016/j.apsusc.2019.03.181.  
  
T. Dinadayalane and N. J. Bowen, “Computational Chemistry and Biology Courses for Undergraduates at an HBCU: Cultivating a Diverse Computational Science Community”, *Growing Diverse STEM Communities: Methodology, Impact, and Evidence*. American Chemical Society, pp. 67–81, Jan. 2019. doi: 10.1021/bk-2019-1328.ch005.  
  
D. Herath and T. Dinadayalane, “Computational investigation of double nitrogen doping on graphene”, *Journal of Molecular Modeling*, vol. 24, no. 1. Springer Science and Business Media LLC, Dec. 22, 2017. doi: 10.1007/s00894-017-3560-0.  
  
A. Mirchi, N. Sizochenko, T. Dinadayalaneand J. Leszczynski, “Binding of Alkali Metal Ions with 1,3,5-Tri(phenyl)benzene and 1,3,5-Tri(naphthyl)benzene: The Effect of Phenyl and Naphthyl Ring Substitution on Cation−π Interactions Revealed by DFT Study”, *The Journal of Physical Chemistry A*, vol. 121, no. 46. American Chemical Society (ACS), pp. 8927–8938, Nov. 08, 2017. doi: 10.1021/acs.jpca.7b08725.  
  
S. Hasan, R. A. Mayanovicand M. Benamara, “Synthesis and Characterization of Novel Inverted NiO@NixMn1-xO Core-Shell Nanoparticles”, *MRS Advances*, vol. 2, no. 56. Springer Science and Business Media LLC, pp. 3465–3470, Nov. 2017. doi: 10.1557/adv.2017.445.  
  
M. D. Hossain, R. A. Mayanovic, S. Dey, R. Sakidjaand M. Benamara, “Room-temperature ferromagnetism in Ni(ii)-chromia based core–shell nanoparticles: experiment and first principles calculations”, *Physical Chemistry Chemical Physics*, vol. 20, no. 15. Royal Society of Chemistry (RSC), pp. 10396–10406, 2018. doi: 10.1039/c7cp08597d.  
  
M. D. Hossain, R. A. Mayanovic, R. Sakidja, M. Benamaraand R. Wirth, “Magnetic properties of core–shell nanoparticles possessing a novel Fe(ii)-chromia phase: an experimental and theoretical approach”, *Nanoscale*, vol. 10, no. 4. Royal Society of Chemistry (RSC), pp. 2138–2147, 2018. doi: 10.1039/c7nr04770c.  
  
D. G. Kizzire, “Studies of the mechanical and extreme hydrothermal properties of periodic mesoporous silica and aluminosilica materials”, *Microporous and Mesoporous Materials*, vol. 252. Elsevier BV, pp. 69–78, Nov. 2017. doi: 10.1016/j.micromeso.2017.06.016.  
  
A. M. Steiner, “Macroscopic Strain-Induced Transition from Quasi-infinite Gold Nanoparticle Chains to Defined Plasmonic Oligomers”, *ACS Nano*, vol. 11, no. 9. American Chemical Society (ACS), pp. 8871–8880, Aug. 29, 2017. doi: 10.1021/acsnano.7b03087.  
  
S. Nikolov, A. Fernandez-Nievesand A. Alexeev, “Mesoscale modeling of microgel mechanics and kinetics through the swelling transition”, *Applied Mathematics and Mechanics*, vol. 39, no. 1. Springer Science and Business Media LLC, pp. 47–62, Dec. 30, 2017. doi: 10.1007/s10483-018-2259-6.  
  
D. Choudhuri, R. Banerjeeand S. G. Srinivasan, “Uniaxial deformation of face-centered-cubic(Ni)-ordered B2(NiAl) bicrystals: atomistic mechanisms near a Kurdjumov–Sachs interface”, *Journal of Materials Science*, vol. 53, no. 8. Springer Science and Business Media LLC, pp. 5684–5695, Dec. 28, 2017. doi: 10.1007/s10853-017-1937-1.  
  
D. Choudhuri, “Exceptional increase in the creep life of magnesium rare-earth alloys due to localized bond stiffening”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Dec. 08, 2017. doi: 10.1038/s41467-017-02112-z.  
  
D. Choudhuri, “Coupled experimental and computational investigation of omega phase evolution in a high misfit titanium-vanadium alloy”, *Acta Materialia*, vol. 130. Elsevier BV, pp. 215–228, May 2017. doi: 10.1016/j.actamat.2017.03.047.  
  
R. Salloom, D. Reith, R. Banerjeeand S. G. Srinivasan, “First principles calculations on the effect of interstitial oxygen on phase stability and β–α″ martensitic transformation in Ti–Nb alloys”, *Journal of Materials Science*, vol. 53, no. 16. Springer Science and Business Media LLC, pp. 11473–11487, May 09, 2018. doi: 10.1007/s10853-018-2381-6.  
  
S. Das, “Enhanced flexoelectricity at reduced dimensions revealed by mechanically tunable quantum tunnelling”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Feb. 01, 2019. doi: 10.1038/s41467-019-08462-0.  
  
K. Momeni, Y. Ji, K. Zhang, J. A. Robinsonand L.-Q. Chen, “Multiscale framework for simulation-guided growth of 2D materials”, *npj 2D Materials and Applications*, vol. 2, no. 1. Springer Science and Business Media LLC, Sep. 14, 2018. doi: 10.1038/s41699-018-0072-4.  
  
S. M. Park, “Selective control of multiple ferroelectric switching pathways using a trailing flexoelectric field”, *Nature Nanotechnology*, vol. 13, no. 5. Springer Science and Business Media LLC, pp. 366–370, Mar. 12, 2018. doi: 10.1038/s41565-018-0083-5.  
  
R.-C. Peng, “Switching the chirality of a magnetic vortex deterministically with an electric field”, *Materials Research Letters*, vol. 6, no. 12. Informa UK Limited, pp. 669–675, Oct. 26, 2018. doi: 10.1080/21663831.2018.1538022.  
  
B. Wang, H.-N. Chen, J.-J. Wangand L.-Q. Chen, “Ferroelectric domain structures and temperature-misfit strain phase diagrams of K1-xNaxNbO3 thin films: A phase-field study”, *Applied Physics Letters*, vol. 115, no. 9. AIP Publishing, p. 092902, Aug. 26, 2019. doi: 10.1063/1.5116910.  
  
J.-J. Wang, “Strain anisotropy and magnetic domain structures in multiferroic heterostructures: High-throughput finite-element and phase-field studies”, *Acta Materialia*, vol. 176. Elsevier BV, pp. 73–83, Sep. 2019. doi: 10.1016/j.actamat.2019.06.043.  
  
F. Xue, X. Wang, Y. Shi, S.-W. Cheongand L.-Q. Chen, “Strain-induced incommensurate phases in hexagonal manganites”, *Physical Review B*, vol. 96, no. 10. American Physical Society (APS), Sep. 20, 2017. doi: 10.1103/physrevb.96.104109.  
  
K. Beach, M. C. Luckingand H. Terrones, “Strain dependence of second harmonic generation in transition metal dichalcogenide monolayers and the fine structure of the exciton”, *Physical Review B*, vol. 101, no. 15. American Physical Society (APS), Apr. 29, 2020. doi: 10.1103/physrevb.101.155431.  
  
I. Bilgin, “Resonant Raman and Exciton Coupling in High-Quality Single Crystals of Atomically Thin Molybdenum Diselenide Grown by Vapor-Phase Chalcogenization”, *ACS Nano*, vol. 12, no. 1. American Chemical Society (ACS), pp. 740–750, Jan. 02, 2018. doi: 10.1021/acsnano.7b07933.  
  
E. Kahn, “Selective Synthesis of Bi2Te3/WS2 Heterostructures with Strong Interlayer Coupling”, *ACS Applied Materials & Interfaces*. American Chemical Society (ACS), Jun. 19, 2020. doi: 10.1021/acsami.0c03656.  
  
M. C. Lucking, K. Beachand H. Terrones, “Large second harmonic generation in alloyed TMDs and boron nitride nanostructures”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, Jul. 04, 2018. doi: 10.1038/s41598-018-27702-9.  
  
Y. Meng, “Excitonic Complexes and Emerging Interlayer Electron–Phonon Coupling in BN Encapsulated Monolayer Semiconductor Alloy: WS0.6Se1.4”, *Nano Letters*, vol. 19, no. 1. American Chemical Society (ACS), pp. 299–307, Dec. 17, 2018. doi: 10.1021/acs.nanolett.8b03918.  
  
N. R. Pradhan, “Raman and electrical transport properties of few-layered arsenic-doped black phosphorus”, *Nanoscale*, vol. 11, no. 39. Royal Society of Chemistry (RSC), pp. 18449–18463, 2019. doi: 10.1039/c9nr04598h.  
  
T. Zhang, “Universal *In Situ* Substitutional Doping of Transition Metal Dichalcogenides by Liquid-Phase Precursor-Assisted Synthesis”, *ACS Nano*, vol. 14, no. 4. American Chemical Society (ACS), pp. 4326–4335, Mar. 25, 2020. doi: 10.1021/acsnano.9b09857.  
  
K. Sagiyama and K. Garikipati, “Unconditionally stable, second-order schemes for gradient-regularized, non-convex, finite-strain elasticity modeling martensitic phase transformations”, *Computer Methods in Applied Mechanics and Engineering*, vol. 338. Elsevier BV, pp. 597–617, Aug. 2018. doi: 10.1016/j.cma.2018.04.036.  
  
X. Liu, Y. Wang, M. Eisenbachand G. M. Stocks, “Fully-relativistic full-potential multiple scattering theory: A pathology-free scheme”, *Computer Physics Communications*, vol. 224. Elsevier BV, pp. 265–272, Mar. 2018. doi: 10.1016/j.cpc.2017.10.011.  
  
V. S. Proshchenko, P. P. Dholabhai, T. C. Sterlingand S. Neogi, “Heat and charge transport in bulk semiconductors with interstitial defects”, *Physical Review B*, vol. 99, no. 1. American Physical Society (APS), Jan. 22, 2019. doi: 10.1103/physrevb.99.014207.  
  
S. S. Galley, “Uncovering the Origin of Divergence in the CsM(CrO4)2 (M = La, Pr, Nd, Sm, Eu; Am) Family through Examination of the Chemical Bonding in a Molecular Cluster and by Band Structure Analysis”, *Journal of the American Chemical Society*, vol. 140, no. 5. American Chemical Society (ACS), pp. 1674–1685, Jan. 10, 2018. doi: 10.1021/jacs.7b09474.  
  
Z. Wang and C. D. Batista, “Dynamics and Instabilities of the Shastry-Sutherland Model”, *Physical Review Letters*, vol. 120, no. 24. American Physical Society (APS), Jun. 12, 2018. doi: 10.1103/physrevlett.120.247201.  
  
R. Kashfi-Sadabad, S. Yazdani, T. D. Huan, Z. Caiand M. T. Pettes, “Role of Oxygen Vacancy Defects in the Electrocatalytic Activity of Substoichiometric Molybdenum Oxide”, *The Journal of Physical Chemistry C*, vol. 122, no. 32. American Chemical Society (ACS), pp. 18212–18222, Jul. 23, 2018. doi: 10.1021/acs.jpcc.8b03536.  
  
T. D. Huan, “Pressure-stabilized binary compounds of magnesium and silicon”, *Physical Review Materials*, vol. 2, no. 2. American Physical Society (APS), Feb. 21, 2018. doi: 10.1103/physrevmaterials.2.023803.  
  
V. N. Tuoc and T. D. Huan, “Predicted Binary Compounds of Tin and Sulfur”, *The Journal of Physical Chemistry C*, vol. 122, no. 30. American Chemical Society (ACS), pp. 17067–17072, Jul. 19, 2018. doi: 10.1021/acs.jpcc.8b04328.  
  
V. N. Tuoc and T. D. Huan, “Lead-free hybrid organic-inorganic perovskites for solar cell applications”, *The Journal of Chemical Physics*, vol. 152, no. 1. AIP Publishing, p. 014104, Jan. 07, 2020. doi: 10.1063/1.5128603.  
  
S. Yazdani, “Highly charged interface trap states in PbS1−*x* govern electro-thermal transport”, *APL Materials*, vol. 7, no. 7. AIP Publishing, p. 071105, Jul. 01, 2019. doi: 10.1063/1.5096786.  
  
S. Yazdani, “Thermal transport in phase-stabilized lithium zirconate phosphates”, *Applied Physics Letters*, vol. 117, no. 1. AIP Publishing, p. 011903, Jul. 06, 2020. doi: 10.1063/5.0013716.  
  
S. Yazdani, R. Kashfi-Sadabad, T. D. Huan, M. D. Morales-Acostaand M. T. Pettes, “Polyelectrolyte-Assisted Oxygen Vacancies: A New Route to Defect Engineering in Molybdenum Oxide”, *Langmuir*, vol. 34, no. 21. American Chemical Society (ACS), pp. 6296–6306, May 04, 2018. doi: 10.1021/acs.langmuir.8b00539.  
  
W. Ding, R. Žitko, P. Mai, E. Perepelitskyand B. S. Shastry, “Strange metal from Gutzwiller correlations in infinite dimensions”, *Physical Review B*, vol. 96, no. 5. American Physical Society (APS), Aug. 18, 2017. doi: 10.1103/physrevb.96.054114.  
  
W. Ding, R. Žitkoand B. S. Shastry, “Strange metal from Gutzwiller correlations in infinite dimensions: Transverse transport, optical response, and rise of two relaxation rates”, *Physical Review B*, vol. 96, no. 11. American Physical Society (APS), Sep. 25, 2017. doi: 10.1103/physrevb.96.115153.  
  
P. Mai, S. R. Whiteand B. S. Shastry, “ model in one dimension using extremely correlated Fermi-liquid theory and time-dependent density matrix renormalization group”, *Physical Review B*, vol. 98, no. 3. American Physical Society (APS), Jul. 06, 2018. doi: 10.1103/physrevb.98.035108.  
  
B. S. Shastry and P. Mai, “Extremely correlated Fermi liquid theory of the*t-J*model in 2 dimensions: low energy properties”, *New Journal of Physics*, vol. 20, no. 1. IOP Publishing, p. 013027, Jan. 22, 2018. doi: 10.1088/1367-2630/aa9b74.  
  
R. Rao, “Dynamics of cleaning, passivating and doping monolayer MoS 2 by controlled laser irradiation”, *2D Materials*, vol. 6, no. 4. IOP Publishing, p. 045031, Aug. 16, 2019. doi: 10.1088/2053-1583/ab33ab.  
  
Y. Wang, B. R. Carvalhoand V. H. Crespi, “Strong exciton regulation of Raman scattering in monolayer ”, *Physical Review B*, vol. 98, no. 16. American Physical Society (APS), Oct. 17, 2018. doi: 10.1103/physrevb.98.161405.  
  
Y. Xuan, “Multi-scale modeling of gas-phase reactions in metal-organic chemical vapor deposition growth of WSe2”, *Journal of Crystal Growth*, vol. 527. Elsevier BV, p. 125247, Dec. 2019. doi: 10.1016/j.jcrysgro.2019.125247.  
  
F. Zhang, “Full orientation control of epitaxial on hBN assisted by substrate defects”, *Physical Review B*, vol. 99, no. 15. American Physical Society (APS), Apr. 29, 2019. doi: 10.1103/physrevb.99.155430.  
  
K. Zhang, “Probing the origin of lateral heterogeneities in synthetic monolayer molybdenum disulfide”, *2D Materials*, vol. 6, no. 2. IOP Publishing, p. 025008, Feb. 01, 2019. doi: 10.1088/2053-1583/aafd9a.  
  
X. Zhang, “Defect-Controlled Nucleation and Orientation of WSe2 on hBN: A Route to Single-Crystal Epitaxial Monolayers”, *ACS Nano*, vol. 13, no. 3. American Chemical Society (ACS), pp. 3341–3352, Feb. 13, 2019. doi: 10.1021/acsnano.8b09230.  
  
T.-C. Lu and T. Grover, “Singularity in entanglement negativity across finite-temperature phase transitions”, *Physical Review B*, vol. 99, no. 7. American Physical Society (APS), Feb. 26, 2019. doi: 10.1103/physrevb.99.075157.  
  
T.-C. Lu and T. Grover, “Renyi entropy of chaotic eigenstates”, *Physical Review E*, vol. 99, no. 3. American Physical Society (APS), Mar. 08, 2019. doi: 10.1103/physreve.99.032111.  
  
L. Li, E. Lee, J. W. Freeland, T. T. Fister, M. M. Thackerayand M. K. Y. Chan, “Identifying the Chemical Origin of Oxygen Redox Activity in Li-Rich Anti-Fluorite Lithium Iron Oxide by Experimental and Theoretical X-ray Absorption Spectroscopy”, *The Journal of Physical Chemistry Letters*, vol. 10, no. 4. American Chemical Society (ACS), pp. 806–812, Jan. 07, 2019. doi: 10.1021/acs.jpclett.8b03271.  
  
L. Li, “Imaging Catalytic Activation of CO2 on Cu2O (110): A First-Principles Study”, *Chemistry of Materials*, vol. 30, no. 6. American Chemical Society (ACS), pp. 1912–1923, Mar. 05, 2018. doi: 10.1021/acs.chemmater.7b04803.  
  
S. Basu, “Utilizing van der Waals Slippery Interfaces to Enhance the Electrochemical Stability of Silicon Film Anodes in Lithium-Ion Batteries”, *ACS Applied Materials & Interfaces*, vol. 10, no. 16. American Chemical Society (ACS), pp. 13442–13451, Apr. 05, 2018. doi: 10.1021/acsami.8b00258.  
  
A. Agarwal, “Anomalous isoelectronic chalcogen rejection in 2D anisotropic vdW TiS3(1−x)Se3x trichalcogenides”, *Nanoscale*, vol. 10, no. 33. Royal Society of Chemistry (RSC), pp. 15654–15660, 2018. doi: 10.1039/c8nr04274h.  
  
L. Fan, “Enabling Stable Lithium Metal Anode via 3D Inorganic Skeleton with Superlithiophilic Interphase”, *Advanced Energy Materials*, vol. 8, no. 33. Wiley, p. 1802350, Oct. 07, 2018. doi: 10.1002/aenm.201802350.  
  
L. Fan, H. L. Zhuang, W. Zhang, Y. Fu, Z. Liaoand Y. Lu, “Stable Lithium Electrodeposition at Ultra-High Current Densities Enabled by 3D PMF/Li Composite Anode”, *Advanced Energy Materials*, vol. 8, no. 15. Wiley, p. 1703360, Feb. 13, 2018. doi: 10.1002/aenm.201703360.  
  
W. Huang, P. Martinand H. L. Zhuang, “Machine-learning phase prediction of high-entropy alloys”, *Acta Materialia*, vol. 169. Elsevier BV, pp. 225–236, May 2019. doi: 10.1016/j.actamat.2019.03.012.  
  
N. Islam, W. Huangand H. L. Zhuang, “Machine learning for phase selection in multi-principal element alloys”, *Computational Materials Science*, vol. 150. Elsevier BV, pp. 230–235, Jul. 2018. doi: 10.1016/j.commatsci.2018.04.003.  
  
G. T. Lin, “Magnetoelectric and Raman spectroscopic studies of monocrystalline ”, *Physical Review B*, vol. 97, no. 6. American Physical Society (APS), Feb. 12, 2018. doi: 10.1103/physrevb.97.064405.  
  
L. Liu, I. Kankamand H. L. Zhuang, “Can an element form a two-dimensional nanosheet of type 15 pentagons?”, *Computational Materials Science*, vol. 154. Elsevier BV, pp. 37–40, Nov. 2018. doi: 10.1016/j.commatsci.2018.07.031.  
  
L. Liu, I. Kankamand H. L. Zhuang, “*Ab initio* playing of pentagonal puzzles”, *Electronic Structure*, vol. 1, no. 1. IOP Publishing, p. 015004, Nov. 20, 2018. doi: 10.1088/2516-1075/aae303.  
  
L. Liu, D. Wang, S. Lakamsani, W. Huang, C. Priceand H. L. Zhuang, “Dimension engineering of single-layer PtN 2 with the Cairo tessellation”, *Journal of Applied Physics*, vol. 125, no. 20. AIP Publishing, p. 204302, May 28, 2019. doi: 10.1063/1.5095239.  
  
L. Liu and H. L. Zhuang, “ : An example of exploring the hidden Cairo tessellation in the pyrite structure for discovering novel two-dimensional materials”, *Physical Review Materials*, vol. 2, no. 11. American Physical Society (APS), Nov. 06, 2018. doi: 10.1103/physrevmaterials.2.114003.  
  
L. Liu and H. L. Zhuang, “High-throughput functionalization of single-layer electride Ca2N”, *Materials Research Express*, vol. 5, no. 7. IOP Publishing, p. 076306, Jul. 11, 2018. doi: 10.1088/2053-1591/aad024.  
  
L. Liu and H. L. Zhuang, “Tunable phase transition in single-layer TiSe2 via electric field”, *Journal of Solid State Chemistry*, vol. 262. Elsevier BV, pp. 309–312, Jun. 2018. doi: 10.1016/j.jssc.2018.03.034.  
  
L. Liu and H. L. Zhuang, “Computational prediction and characterization of two-dimensional pentagonal arsenopyrite FeAsS”, *Computational Materials Science*, vol. 166. Elsevier BV, pp. 105–110, Aug. 2019. doi: 10.1016/j.commatsci.2019.04.040.  
  
J. Qian, “Electrochemical surface passivation of LiCoO2 particles at ultrahigh voltage and its applications in lithium-based batteries”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Nov. 21, 2018. doi: 10.1038/s41467-018-07296-6.  
  
Y. Shen, “Ultimate Control over Hydrogen Bond Formation and Reaction Rates for Scalable Synthesis of Highly Crystalline vdW MOF Nanosheets with Large Aspect Ratio”, *Advanced Materials*, vol. 30, no. 52. Wiley, p. 1802497, Nov. 02, 2018. doi: 10.1002/adma.201802497.  
  
M. H. Tran, “Synthesis of a Smart Hybrid MXene with Switchable Conductivity for Temperature Sensing”, *ACS Applied Nano Materials*, vol. 3, no. 5. American Chemical Society (ACS), pp. 4069–4076, Mar. 24, 2020. doi: 10.1021/acsanm.0c00118.  
  
D. Wang, “Scalable and controlled creation of nanoholes in graphene by microwave-assisted chemical etching for improved electrochemical properties”, *Carbon*, vol. 161. Elsevier BV, pp. 880–891, May 2020. doi: 10.1016/j.carbon.2020.01.076.  
  
D. Wang, L. Liu, W. Huangand H. L. Zhuang, “Semiconducting SiGeSn high-entropy alloy: A density functional theory study”, *Journal of Applied Physics*, vol. 126, no. 22. AIP Publishing, p. 225703, Dec. 14, 2019. doi: 10.1063/1.5135324.  
  
D. Wang, L. Liuand H. L. Zhuang, “Toward obtaining 2D and 3D and 1D PtPN with pentagonal pattern”, *Journal of Materials Science*, vol. 54, no. 22. Springer Science and Business Media LLC, pp. 14029–14037, Aug. 01, 2019. doi: 10.1007/s10853-019-03886-x.  
  
X. Wang, “Ionic liquid-reinforced carbon nanofiber matrix enabled lean-electrolyte Li-S batteries via electrostatic attraction”, *Energy Storage Materials*, vol. 26. Elsevier BV, pp. 378–384, Apr. 2020. doi: 10.1016/j.ensm.2019.11.008.  
  
K. Wu, “Phase Transition across Anisotropic NbS 3 and Direct Gap Semiconductor TiS 3 at Nominal Titanium Alloying Limit”, *Advanced Materials*, vol. 32, no. 17. Wiley, p. 2000018, Mar. 13, 2020. doi: 10.1002/adma.202000018.  
  
C. Xu, “Synthesis and Fundamental Studies of Si-Compatible (Si)GeSn and GeSn Mid-IR Systems with Ultrahigh Sn Contents”, *Chemistry of Materials*, vol. 31, no. 23. American Chemical Society (ACS), pp. 9831–9842, Nov. 07, 2019. doi: 10.1021/acs.chemmater.9b03909.  
  
S. Yang, “Highly crystalline synthesis of tellurene sheets on two-dimensional surfaces: Control over helical chain direction of tellurene”, *Physical Review Materials*, vol. 2, no. 10. American Physical Society (APS), Oct. 11, 2018. doi: 10.1103/physrevmaterials.2.104002.  
  
W. Zhang, H. L. Zhuang, L. Fan, L. Gaoand Y. Lu, “A “cation-anion regulation” synergistic anode host for dendrite-free lithium metal batteries”, *Science Advances*, vol. 4, no. 2. American Association for the Advancement of Science (AAAS), Feb. 02, 2018. doi: 10.1126/sciadv.aar4410.  
  
J. Zhou, H. L. Zhuangand H. Wang, “Layered tetragonal zinc chalcogenides for energy-related applications: from photocatalysts for water splitting to cathode materials for Li-ion batteries”, *Nanoscale*, vol. 9, no. 44. Royal Society of Chemistry (RSC), pp. 17303–17311, 2017. doi: 10.1039/c7nr04289b.  
  
H. L. Zhuang, “From pentagonal geometries to two-dimensional materials”, *Computational Materials Science*, vol. 159. Elsevier BV, pp. 448–453, Mar. 2019. doi: 10.1016/j.commatsci.2018.12.041.  
  
N. K. Ravichandran and D. Broido, “Unified first-principles theory of thermal properties of insulators”, *Physical Review B*, vol. 98, no. 8. American Physical Society (APS), Aug. 13, 2018. doi: 10.1103/physrevb.98.085205.  
  
N. K. Ravichandran and D. Broido, “Non-monotonic pressure dependence of the thermal conductivity of boron arsenide”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Feb. 19, 2019. doi: 10.1038/s41467-019-08713-0.  
  
J. Spalding, S.-W. Tsaiand D. K. Campbell, “Critical entanglement for the half-filled extended Hubbard model”, *Physical Review B*, vol. 99, no. 19. American Physical Society (APS), May 24, 2019. doi: 10.1103/physrevb.99.195445.  
  
V. Kocevski, D. A. Lopes, A. J. Claisseand T. M. Besmann, “Understanding the interface interaction between U3Si2 fuel and SiC cladding”, *Nature Communications*, vol. 11, no. 1. Springer Science and Business Media LLC, May 26, 2020. doi: 10.1038/s41467-020-16435-x.  
  
T. Chen and C. Zhou, “Effect of the grain size and distribution of nanograins on the deformation of nanodomained heterogeneous nickel”, *Materials Letters*, vol. 236. Elsevier BV, pp. 661–664, Feb. 2019. doi: 10.1016/j.matlet.2018.11.045.  
  
S. Huang and C. Zhou, “Fracture resistance of Cu/Nb metallic nanolayered composite”, *Journal of Materials Research*, vol. 34, no. 9. Springer Science and Business Media LLC, pp. 1533–1541, May 14, 2019. doi: 10.1557/jmr.2019.115.  
  
S. Huang, J. Wang, N. Li, J. Zhangand C. Zhou, “Atomistic simulations of plasticity in heterogeneous nanocrystalline Ni lamella”, *Computational Materials Science*, vol. 141. Elsevier BV, pp. 229–234, Jan. 2018. doi: 10.1016/j.commatsci.2017.09.035.  
  
S. Huang, J. Wangand C. Zhou, “Deformation of Heterogeneous Nanocrystalline Lamella with a Preexisting Crack”, *JOM*, vol. 70, no. 1. Springer Science and Business Media LLC, pp. 60–65, Oct. 24, 2017. doi: 10.1007/s11837-017-2626-x.  
  
J. Liu and S. T. Pantelides, “Anisotropic thermal expansion of group-IV monochalcogenide monolayers”, *Applied Physics Express*, vol. 11, no. 10. IOP Publishing, p. 101301, Aug. 28, 2018. doi: 10.7567/apex.11.101301.  
  
J. Liu and S. T. Pantelides, “Mechanisms of Pyroelectricity in Three- and Two-Dimensional Materials”, *Physical Review Letters*, vol. 120, no. 20. American Physical Society (APS), May 17, 2018. doi: 10.1103/physrevlett.120.207602.  
  
V. Martelli, “Sequential localization of a complex electron fluid”, *Proceedings of the National Academy of Sciences*, vol. 116, no. 36. Proceedings of the National Academy of Sciences, pp. 17701–17706, Aug. 20, 2019. doi: 10.1073/pnas.1908101116.  
  
Y. X. Ye, “Evaluating elastic properties of a body-centered cubic NbHfZrTi high-entropy alloy – A direct comparison between experiments and ab initio calculations”, *Intermetallics*, vol. 109. Elsevier BV, pp. 167–173, Jun. 2019. doi: 10.1016/j.intermet.2019.04.003.  
  
J. N. Cross, “Origins of the odd optical observables in plutonium and americium tungstates”, *Chemical Science*, vol. 10, no. 26. Royal Society of Chemistry (RSC), pp. 6508–6518, 2019. doi: 10.1039/c9sc01174a.  
  
T.-H. Lee, T. Ayral, Y.-X. Yao, N. Lanataand G. Kotliar, “Rotationally invariant slave-boson and density matrix embedding theory: Unified framework and comparative study on the one-dimensional and two-dimensional Hubbard model”, *Physical Review B*, vol. 99, no. 11. American Physical Society (APS), Mar. 20, 2019. doi: 10.1103/physrevb.99.115129.  
  
N. Deshpande, A. Parulkar, R. Joshi, B. Diep, A. Kulkarniand N. A. Brunelli, “Epoxide ring opening with alcohols using heterogeneous Lewis acid catalysts: Regioselectivity and mechanism”, *Journal of Catalysis*, vol. 370. Elsevier BV, pp. 46–54, Feb. 2019. doi: 10.1016/j.jcat.2018.11.038.  
  
J. Young, P. M. Kulick, T. R. Juranand M. Smeu, “Comparative Study of Ethylene Carbonate-Based Electrolyte Decomposition at Li, Ca, and Al Anode Interfaces”, *ACS Applied Energy Materials*, vol. 2, no. 3. American Chemical Society (ACS), pp. 1676–1684, Feb. 19, 2019. doi: 10.1021/acsaem.8b01707.  
  
J. Young and M. Smeu, “Ethylene Carbonate-Based Electrolyte Decomposition and Solid–Electrolyte Interphase Formation on Ca Metal Anodes”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 12. American Chemical Society (ACS), pp. 3295–3300, Jun. 01, 2018. doi: 10.1021/acs.jpclett.8b01261.  
  
H.-J. Chang, “Electronic Nature of Neutral and Charged Two-Photon Absorbing Squaraines for Fluorescence Bioimaging Application”, *ACS Omega*, vol. 4, no. 12. American Chemical Society (ACS), pp. 14669–14679, Sep. 04, 2019. doi: 10.1021/acsomega.9b00718.  
  
S. K. Ignatov, A. G. Razuvaev, A. S. Loginovaand A. E. Masunov, “Global Structure Optimization of Pt Clusters Based on the Modified Empirical Potentials, Calibrated using Density Functional Theory”, *The Journal of Physical Chemistry C*, vol. 123, no. 47. American Chemical Society (ACS), pp. 29024–29036, Oct. 29, 2019. doi: 10.1021/acs.jpcc.9b08691.  
  
A. E. Masunov, “First principles crystal engineering of nonlinear optical materials. I. Prototypical case of urea”, *The Journal of Chemical Physics*, vol. 146, no. 24. AIP Publishing, p. 244104, Jun. 28, 2017. doi: 10.1063/1.4986793.  
  
A. E. Masunov, K. Torres, A. A. Dyakov, I. D. Yushinaand E. V. Bartashevich, “First-Principles Crystal Engineering of Nonlinear Optical Materials. II. Effect of Halogen Bonds on the Structure and Properties of Triiodobenzenes”, *The Journal of Physical Chemistry C*, vol. 122, no. 39. American Chemical Society (ACS), pp. 22622–22631, Sep. 10, 2018. doi: 10.1021/acs.jpcc.8b04932.  
  
A. E. Masunov, M. Wiratmo, A. A. Dyakov, Y. V. Matveychukand E. V. Bartashevich, “Virtual Tensile Test for Brittle, Plastic, and Elastic Polymorphs of 4-Bromophenyl 4-Bromobenzoate”, *Crystal Growth & Design*, vol. 20, no. 9. American Chemical Society (ACS), pp. 6093–6100, Aug. 04, 2020. doi: 10.1021/acs.cgd.0c00798.  
  
H. J. Rivera-Jacquez and A. E. Masunov, “Theoretical study of chromophores for biological sensing: Understanding the mechanism of rhodol based multi-chromophoric systems”, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 198. Elsevier BV, pp. 123–135, Jun. 2018. doi: 10.1016/j.saa.2018.02.047.  
  
L. A. Varlamova, S. K. Ignatov, D. G. Fukina, A. A. Konakov, A. E. Masunovand E. V. Suleymanov, “Nonlinear Optical Properties of Mixed Oxide Crystals CsNbMoO6 and CsTaMoO6: A Periodic CPHF/KS Study”, *The Journal of Physical Chemistry C*, vol. 122, no. 43. American Chemical Society (ACS), pp. 24907–24916, Sep. 29, 2018. doi: 10.1021/acs.jpcc.8b07117.  
  
M. Xu, C.-H. Wang, A. C. Terracciano, A. E. Masunovand S. S. Vasu, “High accuracy machine learning identification of fentanyl-relevant molecular compound classification via constituent functional group analysis”, *Scientific Reports*, vol. 10, no. 1. Springer Science and Business Media LLC, Aug. 11, 2020. doi: 10.1038/s41598-020-70471-7.  
  
I. D. Yushina, A. E. Masunov, D. Lopez, A. A. Dyakovand E. V. Bartashevich, “Toward First-Principles Design of Organic Nonlinear Optical Materials: Crystal Structure Prediction and Halogen Bonding Impact on Hyperpolarizabilities of 2-Iodo-3-hydroxypyridine”, *Crystal Growth & Design*, vol. 18, no. 9. American Chemical Society (ACS), pp. 5069–5079, Aug. 01, 2018. doi: 10.1021/acs.cgd.8b00529.  
  
M. Woodcox, J. Youngand M. Smeu, “*Ab initio* investigation of the temperature-dependent elastic properties of Bi, Te and Cu”, *Journal of Physics: Condensed Matter*, vol. 32, no. 48. IOP Publishing, p. 485902, Sep. 09, 2020. doi: 10.1088/1361-648x/ababdf.  
  
P. Yasini, S. Shepard, T. Albrecht, M. Smeuand E. Borguet, “Combined Impact of Denticity and Orientation on Molecular-Scale Charge Transport”, *The Journal of Physical Chemistry C*, vol. 124, no. 17. American Chemical Society (ACS), pp. 9460–9469, Apr. 17, 2020. doi: 10.1021/acs.jpcc.9b10566.  
  
K. Ghatak, S. Basu, T. Das, V. Sharma, H. Kumarand D. Datta, “Effect of cobalt content on the electrochemical properties and structural stability of NCA type cathode materials”, *Physical Chemistry Chemical Physics*, vol. 20, no. 35. Royal Society of Chemistry (RSC), pp. 22805–22817, 2018. doi: 10.1039/c8cp03237h.  
  
K. Ghatak, K. N. Kang, E.-H. Yangand D. Datta, “Controlled edge dependent stacking of WS2-WS2 Homo- and WS2-WSe2 Hetero-structures: A Computational Study”, *Scientific Reports*, vol. 10, no. 1. Springer Science and Business Media LLC, Feb. 03, 2020. doi: 10.1038/s41598-020-58149-6.  
  
J. Kashyap, E.-H. Yangand D. Datta, “Computational study of the water-driven graphene wrinkle life-cycle towards applications in flexible electronics”, *Scientific Reports*, vol. 10, no. 1. Springer Science and Business Media LLC, Jul. 09, 2020. doi: 10.1038/s41598-020-68080-5.  
  
V. Sharma, K. Ghatakand D. Datta, “Amorphous germanium as a promising anode material for sodium ion batteries: a first principle study”, *Journal of Materials Science*, vol. 53, no. 20. Springer Science and Business Media LLC, pp. 14423–14434, Jul. 09, 2018. doi: 10.1007/s10853-018-2661-1.  
  
V. Sharma, K. Ghatakand D. Datta, “Two-dimensional materials and its heterostructures for energy storage”, *Synthesis, Modeling, and Characterization of 2D Materials, and Their Heterostructures*. Elsevier, pp. 385–401, 2020. doi: 10.1016/b978-0-12-818475-2.00017-9.  
  
P. Solanky, V. Sharma, K. Ghatak, J. Kashyapand D. Datta, “The inherent behavior of graphene flakes in water: A molecular dynamics study”, *Computational Materials Science*, vol. 162. Elsevier BV, pp. 140–147, May 2019. doi: 10.1016/j.commatsci.2019.02.021.  
  
C. N. Singh and W.-C. Lee, “Importance of orbital fluctuations for the magnetic dynamics in the heavy-fermion compound ”, *Physical Review B*, vol. 97, no. 24. American Physical Society (APS), Jun. 14, 2018. doi: 10.1103/physrevb.97.241107.  
  
Z. Cheng, “Tunable Thermal Energy Transport across Diamond Membranes and Diamond–Si Interfaces by Nanoscale Graphoepitaxy”, *ACS Applied Materials & Interfaces*, vol. 11, no. 20. American Chemical Society (ACS), pp. 18517–18527, May 01, 2019. doi: 10.1021/acsami.9b02234.  
  
Z. Cheng, “Diffuson-driven ultralow thermal conductivity in amorphous thin films”, *Physical Review Materials*, vol. 3, no. 2. American Physical Society (APS), Feb. 21, 2019. doi: 10.1103/physrevmaterials.3.025002.  
  
M. Jin, “Super Large Sn1–*x*Se Single Crystals with Excellent Thermoelectric Performance”, *ACS Applied Materials & Interfaces*, vol. 11, no. 8. American Chemical Society (ACS), pp. 8051–8059, Feb. 05, 2019. doi: 10.1021/acsami.8b21699.  
  
A. D. Oyedele, “Defect-Mediated Phase Transformation in Anisotropic Two-Dimensional PdSe2 Crystals for Seamless Electrical Contacts”, *Journal of the American Chemical Society*, vol. 141, no. 22. American Chemical Society (ACS), pp. 8928–8936, May 15, 2019. doi: 10.1021/jacs.9b02593.  
  
M. Saghayezhian, “Atomic-scale determination of spontaneous magnetic reversal in oxide heterostructures”, *Proceedings of the National Academy of Sciences*, vol. 116, no. 21. Proceedings of the National Academy of Sciences, pp. 10309–10316, May 08, 2019. doi: 10.1073/pnas.1819570116.  
  
X. Shi, “High Thermoelectric Performance in p‐type Polycrystalline Cd‐doped SnSe Achieved by a Combination of Cation Vacancies and Localized Lattice Engineering”, *Advanced Energy Materials*, vol. 9, no. 11. Wiley, p. 1803242, Jan. 29, 2019. doi: 10.1002/aenm.201803242.  
  
J. Zhu, “Record-Low and Anisotropic Thermal Conductivity of a Quasi-One-Dimensional Bulk ZrTe5 Single Crystal”, *ACS Applied Materials & Interfaces*, vol. 10, no. 47. American Chemical Society (ACS), pp. 40740–40747, Nov. 02, 2018. doi: 10.1021/acsami.8b12504.  
  
Y.-W. Chang, “Extreme thermodynamics with polymer gel tori: Harnessing thermodynamic instabilities to induce large-scale deformations”, *Physical Review E*, vol. 98, no. 2. American Physical Society (APS), Aug. 01, 2018. doi: 10.1103/physreve.98.020501.  
  
S. Nikolov, A. Fernandez-Nievesand A. Alexeev, “Phagocyte-Inspired Smart Microcapsules”, *ACS Macro Letters*, vol. 8, no. 4. American Chemical Society (ACS), pp. 421–426, Mar. 26, 2019. doi: 10.1021/acsmacrolett.8b00992.  
  
A. R. Oganov, C. J. Pickard, Q. Zhuand R. J. Needs, “Structure prediction drives materials discovery”, *Nature Reviews Materials*, vol. 4, no. 5. Springer Science and Business Media LLC, pp. 331–348, Apr. 04, 2019. doi: 10.1038/s41578-019-0101-8.  
  
J. Qu, S. Zhu, W. Zhangand Q. Zhu, “Electrides with Dinitrogen Ligands”, *ACS Applied Materials & Interfaces*, vol. 11, no. 5. American Chemical Society (ACS), pp. 5256–5263, Jan. 15, 2019. doi: 10.1021/acsami.8b18676.  
  
Q. Zhu, T. Frolovand K. Choudhary, “Computational Discovery of Inorganic Electrides from an Automated Screening”, *Matter*, vol. 1, no. 5. Elsevier BV, pp. 1293–1303, Nov. 2019. doi: 10.1016/j.matt.2019.06.017.  
  
S.-. cai . Zhu, “Structure-Controlled Oxygen Concentration in Fe2O3 and FeO2”, *Inorganic Chemistry*, vol. 58, no. 9. American Chemical Society (ACS), pp. 5476–5482, Dec. 17, 2018. doi: 10.1021/acs.inorgchem.8b02764.  
  
S.-C. Zhu, “Computational design of flexible electrides with nontrivial band topology”, *Physical Review Materials*, vol. 3, no. 2. American Physical Society (APS), Feb. 25, 2019. doi: 10.1103/physrevmaterials.3.024205.  
  
S.-. cai . Zhu, X.-. zhi . Yan, J. Liu, A. R. Oganovand Q. Zhu, “A Revisited Mechanism of the Graphite-to-Diamond Transition at High Temperature”, *Matter*, vol. 3, no. 3. Elsevier BV, pp. 864–878, Sep. 2020. doi: 10.1016/j.matt.2020.05.013.  
  
J. Wang, Q. Zhu, Z. Wangand H. Hosono, “Ternary inorganic electrides with mixed bonding”, *Physical Review B*, vol. 99, no. 6. American Physical Society (APS), Feb. 08, 2019. doi: 10.1103/physrevb.99.064104.  
  
J. S. Kang, M. Li, H. Wu, H. Nguyenand Y. Hu, “Experimental observation of high thermal conductivity in boron arsenide”, *Science*, vol. 361, no. 6402. American Association for the Advancement of Science (AAAS), pp. 575–578, Aug. 10, 2018. doi: 10.1126/science.aat5522.  
  
H. T. Chorsi, “Widely Tunable Optical and Thermal Properties of Dirac Semimetal Cd 3 As 2”, *Advanced Optical Materials*, vol. 8, no. 8. Wiley, p. 1901192, Feb. 20, 2020. doi: 10.1002/adom.201901192.  
  
U. Choudhry, S. Yueand B. Liao, “Origins of significant reduction of lattice thermal conductivity in graphene allotropes”, *Physical Review B*, vol. 100, no. 16. American Physical Society (APS), Oct. 01, 2019. doi: 10.1103/physrevb.100.165401.  
  
T. Hou, “Nitrogen-Doped graphene coated FeS2 microsphere composite as high-performance anode materials for sodium-ion batteries enhanced by the chemical and structural synergistic effect”, *Applied Surface Science*, vol. 505. Elsevier BV, p. 144633, Mar. 2020. doi: 10.1016/j.apsusc.2019.144633.  
  
A. Vega-Flick, D. Jung, S. Yue, J. E. Bowersand B. Liao, “Reduced thermal conductivity of epitaxial GaAs on Si due to symmetry-breaking biaxial strain”, *Physical Review Materials*, vol. 3, no. 3. American Physical Society (APS), Mar. 11, 2019. doi: 10.1103/physrevmaterials.3.034603.  
  
S. Yue, “Soft phonons and ultralow lattice thermal conductivity in the Dirac semimetal ”, *Physical Review Research*, vol. 1, no. 3. American Physical Society (APS), Nov. 14, 2019. doi: 10.1103/physrevresearch.1.033101.  
  
S.-Y. Yue, T. Xuand B. Liao, “Ultralow thermal conductivity in a two-dimensional material due to surface-enhanced resonant bonding”, *Materials Today Physics*, vol. 7. Elsevier BV, pp. 89–95, Dec. 2018. doi: 10.1016/j.mtphys.2018.11.005.  
  
S.-Y. Yue, R. Yangand B. Liao, “Controlling thermal conductivity of two-dimensional materials via externally induced phonon-electron interaction”, *Physical Review B*, vol. 100, no. 11. American Physical Society (APS), Sep. 06, 2019. doi: 10.1103/physrevb.100.115408.  
  
H. Paudyal, S. Poncé, F. Giustinoand E. R. Margine, “Superconducting properties of from *ab initio* anisotropic Migdal-Eliashberg theory”, *Physical Review B*, vol. 101, no. 21. American Physical Society (APS), Jun. 11, 2020. doi: 10.1103/physrevb.101.214515.  
  
R. Liu, R. Schaller, C. Q. Chenand C. Bayram, “High Internal Quantum Efficiency Ultraviolet Emission from Phase-Transition Cubic GaN Integrated on Nanopatterned Si(100)”, *ACS Photonics*, vol. 5, no. 3. American Chemical Society (ACS), pp. 955–963, Jan. 08, 2018. doi: 10.1021/acsphotonics.7b01231.  
  
Y.-C. Tsai and C. Bayram, “Structural and Electronic Properties of Hexagonal and Cubic Phase AlGaInN Alloys Investigated Using First Principles Calculations”, *Scientific Reports*, vol. 9, no. 1. Springer Science and Business Media LLC, Apr. 29, 2019. doi: 10.1038/s41598-019-43113-w.  
  
A. Ramasubramanian, V. Yurkiv, T. Foroozan, M. Ragone, R. Shahbazian-Yassarand F. Mashayek, “Lithium Diffusion Mechanism through Solid–Electrolyte Interphase in Rechargeable Lithium Batteries”, *The Journal of Physical Chemistry C*, vol. 123, no. 16. American Chemical Society (ACS), pp. 10237–10245, Mar. 29, 2019. doi: 10.1021/acs.jpcc.9b00436.  
  
M. Asadikiya, V. Drozd, S. Yangand Y. Zhong, “Enthalpies and elastic properties of Ni-Co binary system by ab initio calculations and an energy comparison with the CALPHAD approach”, *Materials Today Communications*, vol. 23. Elsevier BV, p. 100905, Jun. 2020. doi: 10.1016/j.mtcomm.2020.100905.  
  
J. Herran, “Structural and magnetic properties of bulk Mn2PtSn”, *Journal of Physics: Condensed Matter*, vol. 30, no. 47. IOP Publishing, p. 475801, Oct. 31, 2018. doi: 10.1088/1361-648x/aae652.  
  
S. Prophet, R. Dalal, P. R. Khareland P. V. Lukashev, “Half-metallic surfaces in thin-film Ti2MnAl0.5Sn0.5”, *Journal of Physics: Condensed Matter*, vol. 31, no. 5. IOP Publishing, p. 055801, Dec. 19, 2018. doi: 10.1088/1361-648x/aaf343.  
  
J. Herran, R. Carlile, P. Khareland P. V. Lukashev, “Half-metallicity in CrAl-terminated Co2CrAl thin film”, *Journal of Physics: Condensed Matter*, vol. 31, no. 49. IOP Publishing, p. 495801, Sep. 09, 2019. doi: 10.1088/1361-648x/ab3d6c.  
  
A. B. Pun, L. M. Camposand D. N. Congreve, “Tunable Emission from Triplet Fusion Upconversion in Diketopyrrolopyrroles”, *Journal of the American Chemical Society*, vol. 141, no. 9. American Chemical Society (ACS), pp. 3777–3781, Feb. 22, 2019. doi: 10.1021/jacs.8b11796.  
  
A. B. Pun, S. N. Sanders, M. Y. Sfeir, L. M. Camposand D. N. Congreve, “Annihilator dimers enhance triplet fusion upconversion”, *Chemical Science*, vol. 10, no. 14. Royal Society of Chemistry (RSC), pp. 3969–3975, 2019. doi: 10.1039/c8sc03725f.  
  
A. Anikin, R. D. Schaller, G. P. Wiederrecht, E. R. Margine, I. I. Mazinand G. Karapetrov, “Ultrafast dynamics in the high-symmetry and in the charge density wave phase of ”, *Physical Review B*, vol. 102, no. 20. American Physical Society (APS), Nov. 30, 2020. doi: 10.1103/physrevb.102.205139.  
  
G. P. Kafle, C. Heil, H. Paudyaland E. R. Margine, “Electronic, vibrational, and electron–phonon coupling properties in SnSe2 and SnS2 under pressure”, *Journal of Materials Chemistry C*, vol. 8, no. 46. Royal Society of Chemistry (RSC), pp. 16404–16417, 2020. doi: 10.1039/d0tc04356g.  
  
R. Banerjee, K. Sagiyama, G. H. Teichertand K. Garikipati, “A graph theoretic framework for representation, exploration and analysis on computed states of physical systems”, *Computer Methods in Applied Mechanics and Engineering*, vol. 351. Elsevier BV, pp. 501–530, Jul. 2019. doi: 10.1016/j.cma.2019.03.053.  
  
G. H. Teichert, A. R. Natarajan, A. Van der Venand K. Garikipati, “Scale bridging materials physics: Active learning workflows and integrable deep neural networks for free energy function representations in alloys”, *Computer Methods in Applied Mechanics and Engineering*, vol. 371. Elsevier BV, p. 113281, Nov. 2020. doi: 10.1016/j.cma.2020.113281.  
  
Y.-C. Tsai and C. Bayram, “Band Alignments of Ternary Wurtzite and Zincblende III-Nitrides Investigated by Hybrid Density Functional Theory”, *ACS Omega*, vol. 5, no. 8. American Chemical Society (ACS), pp. 3917–3923, Jan. 30, 2020. doi: 10.1021/acsomega.9b03353.  
  
M. Dai and J.-M. Hu, “Field-free spin–orbit torque perpendicular magnetization switching in ultrathin nanostructures”, *npj Computational Materials*, vol. 6, no. 1. Springer Science and Business Media LLC, Jun. 12, 2020. doi: 10.1038/s41524-020-0347-0.  
  
S. Basak, K. A. Dahmenand E. W. Carlson, “Period multiplication cascade at the order-by-disorder transition in uniaxial random field XY magnets”, *Nature Communications*, vol. 11, no. 1. Springer Science and Business Media LLC, Sep. 16, 2020. doi: 10.1038/s41467-020-18270-6.  
  
T. Foroozan, V. Yurkiv, S. Sharifi-Asl, R. Rojaee, F. Mashayekand R. Shahbazian-Yassar, “Non-Dendritic Zn Electrodeposition Enabled by Zincophilic Graphene Substrates”, *ACS Applied Materials & Interfaces*, vol. 11, no. 47. American Chemical Society (ACS), pp. 44077–44089, Nov. 01, 2019. doi: 10.1021/acsami.9b13174.  
  
S. Sharifi-Asl, “Revealing Grain-Boundary-Induced Degradation Mechanisms in Li-Rich Cathode Materials”, *Nano Letters*, vol. 20, no. 2. American Chemical Society (ACS), pp. 1208–1217, Dec. 23, 2019. doi: 10.1021/acs.nanolett.9b04620.  
  
W. Yao, “Tuning Li2O2 Formation Routes by Facet Engineering of MnO2 Cathode Catalysts”, *Journal of the American Chemical Society*, vol. 141, no. 32. American Chemical Society (ACS), pp. 12832–12838, Jul. 23, 2019. doi: 10.1021/jacs.9b05992.  
  
H. Fan, H. Wu, L. Lindsayand Y. Hu, “*Ab initio* investigation of single-layer high thermal conductivity boron compounds”, *Physical Review B*, vol. 100, no. 8. American Physical Society (APS), Aug. 14, 2019. doi: 10.1103/physrevb.100.085420.  
  
J. S. Kang, M. Li, H. Wu, H. Nguyenand Y. Hu, “Basic physical properties of cubic boron arsenide”, *Applied Physics Letters*, vol. 115, no. 12. AIP Publishing, p. 122103, Sep. 16, 2019. doi: 10.1063/1.5116025.  
  
J. S. Kang, H. Wu, M. Liand Y. Hu, “Intrinsic Low Thermal Conductivity and Phonon Renormalization Due to Strong Anharmonicity of Single-Crystal Tin Selenide”, *Nano Letters*, vol. 19, no. 8. American Chemical Society (ACS), pp. 4941–4948, Jul. 02, 2019. doi: 10.1021/acs.nanolett.9b01056.  
  
M. Ke, H. D. Nguyen, H. Fan, M. Li, H. Wuand Y. Hu, “Complementary doping of van der Waals materials through controlled intercalation for monolithically integrated electronics”, *Nano Research*, vol. 13, no. 5. Springer Science and Business Media LLC, pp. 1369–1375, Mar. 11, 2020. doi: 10.1007/s12274-020-2634-y.  
  
M. Li, J. S. Kang, H. D. Nguyen, H. Wu, T. Aokiand Y. Hu, “Anisotropic Thermal Boundary Resistance across 2D Black Phosphorus: Experiment and Atomistic Modeling of Interfacial Energy Transport”, *Advanced Materials*, vol. 31, no. 33. Wiley, p. 1901021, Jun. 24, 2019. doi: 10.1002/adma.201901021.  
  
S. S. Ghosh, Y. Quanand W. E. Pickett, “Strong particle-hole asymmetry in a 200 Kelvin superconductor”, *Physical Review B*, vol. 100, no. 9. American Physical Society (APS), Sep. 16, 2019. doi: 10.1103/physrevb.100.094521.  
  
Y. Quan, S. S. Ghoshand W. E. Pickett, “Compressed hydrides as metallic hydrogen superconductors”, *Physical Review B*, vol. 100, no. 18. American Physical Society (APS), Nov. 05, 2019. doi: 10.1103/physrevb.100.184505.  
  
J. Chai, Z. Zheng, H. Pan, S. Zhang, K. V. Lakshmiand Y.-Y. Sun, “Significance of hydrogen bonding networks in the proton-coupled electron transfer reactions of photosystem II from a quantum-mechanics perspective”, *Physical Chemistry Chemical Physics*, vol. 21, no. 17. Royal Society of Chemistry (RSC), pp. 8721–8728, 2019. doi: 10.1039/c9cp00868c.  
  
K. Cheng, H. Wang, J. Bang, D. West, J. Zhaoand S. Zhang, “Carrier Dynamics and Transfer across the CdS/MoS2 Interface upon Optical Excitation”, *The Journal of Physical Chemistry Letters*, vol. 11, no. 16. American Chemical Society (ACS), pp. 6544–6550, Jul. 22, 2020. doi: 10.1021/acs.jpclett.0c01188.  
  
J. Ma, “Emergence of Nontrivial Low‐Energy Dirac Fermions in Antiferromagnetic EuCd 2 As 2”, *Advanced Materials*, vol. 32, no. 14. Wiley, p. 1907565, Feb. 24, 2020. doi: 10.1002/adma.201907565.  
  
X. Ko, J. D. Olivo, B. Brown, S. Nešićand S. Sharma, “Experiments and Molecular Simulations to Study the Role of Coadsorption of Oil in Corrosion Inhibitor Films in Improving Corrosion Mitigation”, *Corrosion*, vol. 76, no. 11. NACE International, Jul. 29, 2020. doi: 10.5006/3606.  
  
S. Sharma, H. Singhand X. Ko, “A Quantitatively Accurate Theory To Predict Adsorbed Configurations of Linear Surfactants on Polar Surfaces”, *The Journal of Physical Chemistry B*, vol. 123, no. 34. American Chemical Society (ACS), pp. 7464–7470, Aug. 06, 2019. doi: 10.1021/acs.jpcb.9b05861.  
  
H. Singh and S. Sharma, “Disintegration of Surfactant Micelles at Metal–Water Interfaces Promotes Their Strong Adsorption”, *The Journal of Physical Chemistry B*, vol. 124, no. 11. American Chemical Society (ACS), pp. 2262–2267, Feb. 24, 2020. doi: 10.1021/acs.jpcb.9b10780.  
  
S. Kadkhodaei and A. Davariashtiyani, “Phonon-assisted diffusion in bcc phase of titanium and zirconium from first principles”, *Physical Review Materials*, vol. 4, no. 4. American Physical Society (APS), Apr. 13, 2020. doi: 10.1103/physrevmaterials.4.043802.  
  
A. Scheie, “Multiphase magnetism in Yb 2 Ti 2 O 7”, *Proceedings of the National Academy of Sciences*, vol. 117, no. 44. Proceedings of the National Academy of Sciences, pp. 27245–27254, Oct. 23, 2020. doi: 10.1073/pnas.2008791117.  
  
A. Jain, M. B. Sadanand A. Ramasubramaniam, “Promoting Active Sites for Hydrogen Evolution in MoSe2 via Transition-Metal Doping”, *The Journal of Physical Chemistry C*, vol. 124, no. 23. American Chemical Society (ACS), pp. 12324–12336, May 13, 2020. doi: 10.1021/acs.jpcc.0c00013.  
  
V. Kuraganti, A. Jain, R. Bar-Ziv, A. Ramasubramaniamand M. Bar-Sadan, “Manganese Doping of MoSe2 Promotes Active Defect Sites for Hydrogen Evolution”, *ACS Applied Materials & Interfaces*, vol. 11, no. 28. American Chemical Society (ACS), pp. 25155–25162, Jun. 25, 2019. doi: 10.1021/acsami.9b05670.  
  
Y.-J. Hu, “Local electronic descriptors for solute-defect interactions in bcc refractory metals”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Oct. 02, 2019. doi: 10.1038/s41467-019-12452-7.  
  
Y.-J. Hu, “Predicting densities and elastic moduli of SiO2-based glasses by machine learning”, *npj Computational Materials*, vol. 6, no. 1. Springer Science and Business Media LLC, Mar. 20, 2020. doi: 10.1038/s41524-020-0291-z.  
  
C. Yang, M. Zhangand L. Qi, “Grain boundary structure search by using an evolutionary algorithm with effective mutation methods”, *Computational Materials Science*, vol. 184. Elsevier BV, p. 109812, Nov. 2020. doi: 10.1016/j.commatsci.2020.109812.  
  
R. T. Clay, N. Gomesand S. Mazumdar, “Theory of triangular lattice quasi-one-dimensional charge-transfer solids”, *Physical Review B*, vol. 100, no. 11. American Physical Society (APS), Sep. 27, 2019. doi: 10.1103/physrevb.100.115158.  
  
R. Rowsey, E. E. Taylor, S. Irle, N. P. Stadieand R. K. Szilagyi, “Methane Adsorption on Heteroatom-Modified *Maquettes* of Porous Carbon Surfaces”, *The Journal of Physical Chemistry A*, vol. 125, no. 28. American Chemical Society (ACS), pp. 6042–6058, Jul. 07, 2021. doi: 10.1021/acs.jpca.0c11284.  
  
B. Dahal, A. Al Maruf, S. Prophet, Y. Huh, P. V. Lukashevand P. Kharel, “Electronic, magnetic, and structural properties of Fe2MnSn Heusler alloy”, *AIP Advances*, vol. 10, no. 1. AIP Publishing, p. 015118, Jan. 01, 2020. doi: 10.1063/1.5127671.  
  
E. O’Leary, B. Dahal, P. Khareland P. Lukashev, “Various challenges in realizing spin-gapless semiconductivity in Ti2CoSi”, *Journal of Magnetism and Magnetic Materials*, vol. 514. Elsevier BV, p. 167188, Nov. 2020. doi: 10.1016/j.jmmm.2020.167188.  
  
R. T. Clay and D. Roy, “Superconductivity due to cooperation of electron-electron and electron-phonon interactions at quarter filling”, *Physical Review Research*, vol. 2, no. 2. American Physical Society (APS), Apr. 03, 2020. doi: 10.1103/physrevresearch.2.023006.  
  
R. Jayan and M. M. Islam, “Functionalized MXenes as effective polyselenide immobilizers for lithium–selenium batteries: a density functional theory (DFT) study”, *Nanoscale*, vol. 12, no. 26. Royal Society of Chemistry (RSC), pp. 14087–14095, 2020. doi: 10.1039/d0nr02296a.  
  
R. Jayan and M. M. Islam, “First-Principles Investigation of the Anchoring Behavior of Pristine and Defect-Engineered Tungsten Disulfide for Lithium–Sulfur Batteries”, *The Journal of Physical Chemistry C*, vol. 124, no. 50. American Chemical Society (ACS), pp. 27323–27332, Dec. 09, 2020. doi: 10.1021/acs.jpcc.0c08170.  
  
K. Choudhary, K. F. Garrity, J. Jiang, R. Pachterand F. Tavazza, “Computational search for magnetic and non-magnetic 2D topological materials using unified spin–orbit spillage screening”, *npj Computational Materials*, vol. 6, no. 1. Springer Science and Business Media LLC, May 07, 2020. doi: 10.1038/s41524-020-0319-4.  
  
K. Choudhary, K. F. Garrity, V. Sharma, A. J. Biacchi, A. R. Hight Walkerand F. Tavazza, “High-throughput density functional perturbation theory and machine learning predictions of infrared, piezoelectric, and dielectric responses”, *npj Computational Materials*, vol. 6, no. 1. Springer Science and Business Media LLC, May 27, 2020. doi: 10.1038/s41524-020-0337-2.  
  
A. Muralidharan, J. R. Schmidtand A. Yethiraj, “Solvation Induced Ring Puckering Effect in Fluorinated Prolines and Its Inclusion in Classical Force Fields”, *The Journal of Physical Chemistry B*, vol. 124, no. 28. American Chemical Society (ACS), pp. 5899–5906, Jun. 18, 2020. doi: 10.1021/acs.jpcb.0c04312.  
  
J. Holoubek, “An All-Fluorinated Ester Electrolyte for Stable High-Voltage Li Metal Batteries Capable of Ultra-Low-Temperature Operation”, *ACS Energy Letters*, vol. 5, no. 5. American Chemical Society (ACS), pp. 1438–1447, Apr. 09, 2020. doi: 10.1021/acsenergylett.0c00643.  
  
S. Seacat, J. L. Lyonsand H. Peelaers, “Orthorhombic alloys of Ga 2 O 3 and Al 2 O 3”, *Applied Physics Letters*, vol. 116, no. 23. AIP Publishing, p. 232102, Jun. 08, 2020. doi: 10.1063/5.0010354.  
  
R. C. Longo, A. Ranjanand P. L. G. Ventzek, “Density Functional Theory Study of Oxygen Adsorption on Polymer Surfaces for Atomic-Layer Etching: Implications for Semiconductor Device Fabrication”, *ACS Applied Nano Materials*, vol. 3, no. 6. American Chemical Society (ACS), pp. 5189–5202, May 04, 2020. doi: 10.1021/acsanm.0c00618.  
  
V. Sharma, P. Kumar, P. Devand G. Pilania, “Machine learning substitutional defect formation energies in ABO3 perovskites”, *Journal of Applied Physics*, vol. 128, no. 3. AIP Publishing, p. 034902, Jul. 21, 2020. doi: 10.1063/5.0015538.  
  
A. Abdellahi, A. Urban, S. Dacekand G. Ceder, “The Effect of Cation Disorder on the Average Li Intercalation Voltage of Transition-Metal Oxides”, *Chemistry of Materials*, vol. 28, no. 11. American Chemical Society (ACS), pp. 3659–3665, May 17, 2016. doi: 10.1021/acs.chemmater.6b00205.  
  
A. Abdellahi, A. Urban, S. Dacekand G. Ceder, “Understanding the Effect of Cation Disorder on the Voltage Profile of Lithium Transition-Metal Oxides”, *Chemistry of Materials*, vol. 28, no. 15. American Chemical Society (ACS), pp. 5373–5383, Jul. 28, 2016. doi: 10.1021/acs.chemmater.6b01438.  
  
M. Bianchini, P. Xiao, Y. Wangand G. Ceder, “Additional Sodium Insertion into Polyanionic Cathodes for Higher-Energy Na-Ion Batteries”, *Advanced Energy Materials*, vol. 7, no. 18. Wiley, p. 1700514, May 16, 2017. doi: 10.1002/aenm.201700514.  
  
S.-H. Bo, Y. Wangand G. Ceder, “Structural and Na-ion conduction characteristics of Na3PSxSe4−x”, *Journal of Materials Chemistry A*, vol. 4, no. 23. Royal Society of Chemistry (RSC), pp. 9044–9053, 2016. doi: 10.1039/c6ta03027k.  
  
S.-H. Bo, Y. Wang, J. C. Kim, W. D. Richardsand G. Ceder, “Computational and Experimental Investigations of Na-Ion Conduction in Cubic Na3PSe4”, *Chemistry of Materials*, vol. 28, no. 1. American Chemical Society (ACS), pp. 252–258, Dec. 18, 2015. doi: 10.1021/acs.chemmater.5b04013.  
  
H. Chen, “Carbonophosphates: A New Family of Cathode Materials for Li-Ion Batteries Identified Computationally”, *Chemistry of Materials*, vol. 24, no. 11. American Chemical Society (ACS), pp. 2009–2016, May 31, 2012. doi: 10.1021/cm203243x.  
  
T. Chen, G. Sai Gautam, W. Huangand G. Ceder, “First-Principles Study of the Voltage Profile and Mobility of Mg Intercalation in a Chromium Oxide Spinel”, *Chemistry of Materials*, vol. 30, no. 1. American Chemical Society (ACS), pp. 153–162, Dec. 21, 2017. doi: 10.1021/acs.chemmater.7b04038.  
  
S. T. Dacek, W. D. Richards, D. A. Kitchaevand G. Ceder, “Structure and Dynamics of Fluorophosphate Na-Ion Battery Cathodes”, *Chemistry of Materials*, vol. 28, no. 15. American Chemical Society (ACS), pp. 5450–5460, Jul. 26, 2016. doi: 10.1021/acs.chemmater.6b01989.  
  
J. E. S. Haggerty, “High-fraction brookite films from amorphous precursors”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Nov. 09, 2017. doi: 10.1038/s41598-017-15364-y.  
  
A. Jain, “A Computational Investigation of Li9M3(P2O7)3(PO4)2(M = V, Mo) as Cathodes for Li Ion Batteries”, *Journal of The Electrochemical Society*, vol. 159, no. 5. The Electrochemical Society, pp. A622–A633, 2012. doi: 10.1149/2.080205jes.  
  
S. Kang, Y. Mo, S. P. Ongand G. Ceder, “A Facile Mechanism for Recharging Li2O2 in Li–O2 Batteries”, *Chemistry of Materials*, vol. 25, no. 16. American Chemical Society (ACS), pp. 3328–3336, Aug. 09, 2013. doi: 10.1021/cm401720n.  
  
S. Kang, Y. Mo, S. P. Ongand G. Ceder, “Nanoscale Stabilization of Sodium Oxides: Implications for Na–O2 Batteries”, *Nano Letters*, vol. 14, no. 2. American Chemical Society (ACS), pp. 1016–1020, Jan. 14, 2014. doi: 10.1021/nl404557w.  
  
H. Kim, J. C. Kim, M. Bianchini, D. Seo, J. Rodriguez‐Garciaand G. Ceder, “Recent Progress and Perspective in Electrode Materials for K‐Ion Batteries”, *Advanced Energy Materials*, vol. 8, no. 9. Wiley, p. 1702384, Dec. 04, 2017. doi: 10.1002/aenm.201702384.  
  
H. Kim, “A New Strategy for High‐Voltage Cathodes for K‐Ion Batteries: Stoichiometric KVPO 4 F”, *Advanced Energy Materials*, vol. 8, no. 26. Wiley, p. 1801591, Jul. 18, 2018. doi: 10.1002/aenm.201801591.  
  
H. Kim, “Investigation of Potassium Storage in Layered P3‐Type K 0.5 MnO 2 Cathode”, *Advanced Materials*, vol. 29, no. 37. Wiley, p. 1702480, Aug. 07, 2017. doi: 10.1002/adma.201702480.  
  
H. Kim, “Stoichiometric Layered Potassium Transition Metal Oxide for Rechargeable Potassium Batteries”, *Chemistry of Materials*, vol. 30, no. 18. American Chemical Society (ACS), pp. 6532–6539, Aug. 29, 2018. doi: 10.1021/acs.chemmater.8b03228.  
  
J. C. Kim, “Analysis of Charged State Stability for Monoclinic LiMnBO3 Cathode”, *Chemistry of Materials*, vol. 26, no. 14. American Chemical Society (ACS), pp. 4200–4206, Jul. 07, 2014. doi: 10.1021/cm5014174.  
  
J. C. Kim, C. J. Moore, B. Kang, G. Hautier, A. Jainand G. Ceder, “Synthesis and Electrochemical Properties of Monoclinic LiMnBO[sub 3] as a Li Intercalation Material”, *Journal of The Electrochemical Society*, vol. 158, no. 3. The Electrochemical Society, p. A309, 2011. doi: 10.1149/1.3536532.  
  
J. C. Kim, D.-H. Seo, H. Chenand G. Ceder, “The Effect of Antisite Disorder and Particle Size on Li Intercalation Kinetics in Monoclinic LiMnBO3”, *Advanced Energy Materials*, vol. 5, no. 8. Wiley, p. 1401916, Jan. 21, 2015. doi: 10.1002/aenm.201401916.  
  
S. Kim, X. Ma, S. P. Ongand G. Ceder, “A comparison of destabilization mechanisms of the layered NaxMO2 and LixMO2 compounds upon alkali de-intercalation”, *Physical Chemistry Chemical Physics*, vol. 14, no. 44. Royal Society of Chemistry (RSC), p. 15571, 2012. doi: 10.1039/c2cp43377j.  
  
D. A. Kitchaev, “Design principles for high transition metal capacity in disordered rocksalt Li-ion cathodes”, *Energy & Environmental Science*, vol. 11, no. 8. Royal Society of Chemistry (RSC), pp. 2159–2171, 2018. doi: 10.1039/c8ee00816g.  
  
V. Lacivita, N. Artrithand G. Ceder, “Structural and Compositional Factors That Control the Li-Ion Conductivity in LiPON Electrolytes”, *Chemistry of Materials*, vol. 30, no. 20. American Chemical Society (ACS), pp. 7077–7090, Sep. 15, 2018. doi: 10.1021/acs.chemmater.8b02812.  
  
V. Lacivita, “Resolving the Amorphous Structure of Lithium Phosphorus Oxynitride (Lipon)”, *Journal of the American Chemical Society*, vol. 140, no. 35. American Chemical Society (ACS), pp. 11029–11038, Jul. 23, 2018. doi: 10.1021/jacs.8b05192.  
  
J. Lee, “Reversible Mn2+/Mn4+ double redox in lithium-excess cathode materials”, *Nature*, vol. 556, no. 7700. Springer Science and Business Media LLC, pp. 185–190, Apr. 2018. doi: 10.1038/s41586-018-0015-4.  
  
J. Lee, D.-H. Seo, M. Balasubramanian, N. Twu, X. Liand G. Ceder, “A new class of high capacity cation-disordered oxides for rechargeable lithium batteries: Li–Ni–Ti–Mo oxides”, *Energy & Environmental Science*, vol. 8, no. 11. Royal Society of Chemistry (RSC), pp. 3255–3265, 2015. doi: 10.1039/c5ee02329g.  
  
J. Lee, A. Urban, X. Li, D. Su, G. Hautierand G. Ceder, “Unlocking the Potential of Cation-Disordered Oxides for Rechargeable Lithium Batteries”, *Science*, vol. 343, no. 6170. American Association for the Advancement of Science (AAAS), pp. 519–522, Jan. 31, 2014. doi: 10.1126/science.1246432.  
  
L. J. Miara, N. Suzuki, W. D. Richards, Y. Wang, J. C. Kimand G. Ceder, “Li-ion conductivity in Li9S3N”, *Journal of Materials Chemistry A*, vol. 3, no. 40. Royal Society of Chemistry (RSC), pp. 20338–20344, 2015. doi: 10.1039/c5ta05432j.  
  
S. P. Ong, Y. Mo, W. D. Richards, L. Miara, H. S. Leeand G. Ceder, “Phase stability, electrochemical stability and ionic conductivity of the Li10±1MP2X12(M = Ge, Si, Sn, Al or P, and X = O, S or Se) family of superionic conductors”, *Energy Environ. Sci.*, vol. 6, no. 1. Royal Society of Chemistry (RSC), pp. 148–156, 2013. doi: 10.1039/c2ee23355j.  
  
W. D. Richards, S. T. Dacek, D. A. Kitchaevand G. Ceder, “Fluorination of Lithium‐Excess Transition Metal Oxide Cathode Materials”, *Advanced Energy Materials*, vol. 8, no. 5. Wiley, p. 1701533, Oct. 04, 2017. doi: 10.1002/aenm.201701533.  
  
W. D. Richards, L. J. Miara, Y. Wang, J. C. Kimand G. Ceder, “Interface Stability in Solid-State Batteries”, *Chemistry of Materials*, vol. 28, no. 1. American Chemical Society (ACS), pp. 266–273, Dec. 18, 2015. doi: 10.1021/acs.chemmater.5b04082.  
  
W. D. Richards, “Design and synthesis of the superionic conductor Na10SnP2S12”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Mar. 17, 2016. doi: 10.1038/ncomms11009.  
  
W. D. Richards, Y. Wang, L. J. Miara, J. C. Kimand G. Ceder, “Design of Li1+2xZn1−xPS4, a new lithium ion conductor”, *Energy & Environmental Science*, vol. 9, no. 10. Royal Society of Chemistry (RSC), pp. 3272–3278, 2016. doi: 10.1039/c6ee02094a.  
  
D.-H. Seo, J. Lee, A. Urban, R. Malik, S. Kangand G. Ceder, “The structural and chemical origin of the oxygen redox activity in layered and cation-disordered Li-excess cathode materials”, *Nature Chemistry*, vol. 8, no. 7. Springer Science and Business Media LLC, pp. 692–697, May 30, 2016. doi: 10.1038/nchem.2524.  
  
D.-H. Seo, A. Urbanand G. Ceder, “Calibrating transition-metal energy levels and oxygen bands in first-principles calculations: Accurate prediction of redox potentials and charge transfer in lithium transition-metal oxides”, *Physical Review B*, vol. 92, no. 11. American Physical Society (APS), Sep. 08, 2015. doi: 10.1103/physrevb.92.115118.  
  
R. Sun, M. K. Y. Chanand G. Ceder, “First-principles electronic structure and relative stability of pyrite and marcasite: Implications for photovoltaic performance”, *Physical Review B*, vol. 83, no. 23. American Physical Society (APS), Jun. 08, 2011. doi: 10.1103/physrevb.83.235311.  
  
R. Sun, M. K. Y. Chan, S. Kangand G. Ceder, “Intrinsic stoichiometry and oxygen-induced-type conductivity of pyrite FeS”, *Physical Review B*, vol. 84, no. 3. American Physical Society (APS), Jul. 29, 2011. doi: 10.1103/physrevb.84.035212.  
  
Y. Tian, “Compatibility issues between electrodes and electrolytes in solid-state batteries”, *Energy & Environmental Science*, vol. 10, no. 5. Royal Society of Chemistry (RSC), pp. 1150–1166, 2017. doi: 10.1039/c7ee00534b.  
  
N. Twu, X. Li, C. Mooreand G. Ceder, “Synthesis and Lithiation Mechanisms of Dirutile and Rutile LiMnF4: Two New Conversion Cathode Materials”, *Journal of The Electrochemical Society*, vol. 160, no. 11. The Electrochemical Society, pp. A1944–A1951, 2013. doi: 10.1149/2.022311jes.  
  
N. Twu, “Designing New Lithium-Excess Cathode Materials from Percolation Theory: Nanohighways in Li*x*Ni2–4*x*/3Sb*x*/3O2”, *Nano Letters*, vol. 15, no. 1. American Chemical Society (ACS), pp. 596–602, Dec. 22, 2014. doi: 10.1021/nl5040754.  
  
A. Urban, A. Abdellahi, S. Dacek, N. Artrithand G. Ceder, “Electronic-Structure Origin of Cation Disorder in Transition-Metal Oxides”, *Physical Review Letters*, vol. 119, no. 17. American Physical Society (APS), Oct. 25, 2017. doi: 10.1103/physrevlett.119.176402.  
  
A. Urban, J. Leeand G. Ceder, “The Configurational Space of Rocksalt-Type Oxides for High-Capacity Lithium Battery Electrodes”, *Advanced Energy Materials*, vol. 4, no. 13. Wiley, p. 1400478, May 11, 2014. doi: 10.1002/aenm.201400478.  
  
A. Urban, I. Matts, A. Abdellahiand G. Ceder, “Computational Design and Preparation of Cation‐Disordered Oxides for High‐Energy‐Density Li‐Ion Batteries”, *Advanced Energy Materials*, vol. 6, no. 15. Wiley, p. 1600488, May 31, 2016. doi: 10.1002/aenm.201600488.  
  
P. Vassilaras, “Electrochemical properties and structural evolution of O3-type layered sodium mixed transition metal oxides with trivalent nickel”, *Journal of Materials Chemistry A*, vol. 5, no. 9. Royal Society of Chemistry (RSC), pp. 4596–4606, 2017. doi: 10.1039/c6ta09220a.  
  
Y. Wang, W. D. Richards, S.-H. Bo, L. J. Miaraand G. Ceder, “Computational Prediction and Evaluation of Solid-State Sodium Superionic Conductors Na7P3X11 (X = O, S, Se)”, *Chemistry of Materials*, vol. 29, no. 17. American Chemical Society (ACS), pp. 7475–7482, Aug. 15, 2017. doi: 10.1021/acs.chemmater.7b02476.  
  
Y. Wang, “Design principles for solid-state lithium superionic conductors”, *Nature Materials*, vol. 14, no. 10. Springer Science and Business Media LLC, pp. 1026–1031, Aug. 17, 2015. doi: 10.1038/nmat4369.  
  
Y. Wu and G. Ceder, “First Principles Study on Ta3N5:Ti3O3N2 Solid Solution As a Water-Splitting Photocatalyst”, *The Journal of Physical Chemistry C*, vol. 117, no. 47. American Chemical Society (ACS), pp. 24710–24715, Nov. 18, 2013. doi: 10.1021/jp407911g.  
  
Y. Wu, M. K. Y. Chanand G. Ceder, “Prediction of semiconductor band edge positions in aqueous environments from first principles”, *Physical Review B*, vol. 83, no. 23. American Physical Society (APS), Jun. 01, 2011. doi: 10.1103/physrevb.83.235301.  
  
Y. Wu, P. Lazic, G. Hautier, K. Perssonand G. Ceder, “First principles high throughput screening of oxynitrides for water-splitting photocatalysts”, *Energy Environ. Sci.*, vol. 6, no. 1. Royal Society of Chemistry (RSC), pp. 157–168, 2013. doi: 10.1039/c2ee23482c.  
  
N. Boruah and P. Dimitrakopoulos, “Motion and deformation of a droplet in a microfluidic cross-junction”, *Journal of Colloid and Interface Science*, vol. 453. Elsevier BV, pp. 216–225, Sep. 2015. doi: 10.1016/j.jcis.2015.04.067.  
  
P. Dimitrakopoulos, “Effects of membrane hardness and scaling analysis for capsules in planar extensional flows”, *Journal of Fluid Mechanics*, vol. 745. Cambridge University Press (CUP), pp. 487–508, Mar. 24, 2014. doi: 10.1017/jfm.2014.66.  
  
P. Dimitrakopoulos, “Dumbbell formation for elastic capsules in nonlinear extensional Stokes flows”, *Physical Review Fluids*, vol. 2, no. 6. American Physical Society (APS), Jun. 27, 2017. doi: 10.1103/physrevfluids.2.063101.  
  
P. Dimitrakopoulos and S. Kuriakose, “Determining a membrane’s shear modulus, independent of its area-dilatation modulus, via capsule flow in a converging micro-capillary”, *Soft Matter*, vol. 11, no. 14. Royal Society of Chemistry (RSC), pp. 2782–2793, 2015. doi: 10.1039/c4sm02898h.  
  
W. R. Dodson III and P. Dimitrakopoulos, “Tank-Treading of Erythrocytes in Strong Shear Flows via a Nonstiff Cytoskeleton-Based Continuum Computational Modeling”, *Biophysical Journal*, vol. 99, no. 9. Elsevier BV, pp. 2906–2916, Nov. 2010. doi: 10.1016/j.bpj.2010.08.048.  
  
W. R. Dodson III and P. Dimitrakopoulos, “Properties of the spindle-to-cusp transition in extensional capsule dynamics”, *EPL (Europhysics Letters)*, vol. 106, no. 4. IOP Publishing, p. 48003, May 01, 2014. doi: 10.1209/0295-5075/106/48003.  
  
A. Koolivand and P. Dimitrakopoulos, “Deformation of an elastic capsule in a microfluidic T-junction: settling shape and moduli determination”, *Microfluidics and Nanofluidics*, vol. 21, no. 5. Springer Science and Business Media LLC, Apr. 26, 2017. doi: 10.1007/s10404-017-1923-6.  
  
S. Kuriakose and P. Dimitrakopoulos, “Deformation of an elastic capsule in a rectangular microfluidic channel”, *Soft Matter*, vol. 9, no. 16. Royal Society of Chemistry (RSC), p. 4284, 2013. doi: 10.1039/c3sm27683j.  
  
S.-Y. Park and P. Dimitrakopoulos, “Transient dynamics of an elastic capsule in a microfluidic constriction”, *Soft Matter*, vol. 9, no. 37. Royal Society of Chemistry (RSC), p. 8844, 2013. doi: 10.1039/c3sm51516h.  
  
Y. Wang and P. Dimitrakopoulos, “Low-Reynolds-number droplet motion in a square microfluidic channel”, *Theoretical and Computational Fluid Dynamics*, vol. 26, no. 1–4. Springer Science and Business Media LLC, pp. 361–379, Jul. 22, 2011. doi: 10.1007/s00162-011-0238-6.  
  
S. Brach, M. Z. Hossain, B. Bourdinand K. Bhattacharya, “Anisotropy of the effective toughness of layered media”, *Journal of the Mechanics and Physics of Solids*, vol. 131. Elsevier BV, pp. 96–111, Oct. 2019. doi: 10.1016/j.jmps.2019.06.021.  
  
S. Brach, E. Tanné, B. Bourdinand K. Bhattacharya, “Phase-field study of crack nucleation and propagation in elastic–perfectly plastic bodies”, *Computer Methods in Applied Mechanics and Engineering*, vol. 353. Elsevier BV, pp. 44–65, Aug. 2019. doi: 10.1016/j.cma.2019.04.027.  
  
C.-J. Hsueh, L. Avellar, B. Bourdin, G. Ravichandranand K. Bhattacharya, “Stress fluctuation, crack renucleation and toughening in layered materials”, *Journal of the Mechanics and Physics of Solids*, vol. 120. Elsevier BV, pp. 68–78, Nov. 2018. doi: 10.1016/j.jmps.2018.04.011.  
  
A. Mesgarnejad, B. Bourdinand M. M. Khonsari, “A variational approach to the fracture of brittle thin films subject to out-of-plane loading”, *Journal of the Mechanics and Physics of Solids*, vol. 61, no. 11. Elsevier BV, pp. 2360–2379, Nov. 2013. doi: 10.1016/j.jmps.2013.05.001.  
  
A. Mesgarnejad, B. Bourdinand M. M. Khonsari, “Validation simulations for the variational approach to fracture”, *Computer Methods in Applied Mechanics and Engineering*, vol. 290. Elsevier BV, pp. 420–437, Jun. 2015. doi: 10.1016/j.cma.2014.10.052.  
  
E. Tanné, T. Li, B. Bourdin, J.-J. Marigoand C. Maurini, “Crack nucleation in variational phase-field models of brittle fracture”, *Journal of the Mechanics and Physics of Solids*, vol. 110. Elsevier BV, pp. 80–99, Jan. 2018. doi: 10.1016/j.jmps.2017.09.006.  
  
K. Yoshioka and B. Bourdin, “A variational hydraulic fracturing model coupled to a reservoir simulator”, *International Journal of Rock Mechanics and Mining Sciences*, vol. 88. Elsevier BV, pp. 137–150, Oct. 2016. doi: 10.1016/j.ijrmms.2016.07.020.  
  
B. Bass, J. N. Irza, J. Proft, P. Bedientand C. Dawson, “Fidelity of the integrated kinetic energy factor as an indicator of storm surge impacts”, *Natural Hazards*, vol. 85, no. 1. Springer Science and Business Media LLC, pp. 575–595, Sep. 22, 2016. doi: 10.1007/s11069-016-2587-3.  
  
B. Bass, “Surge dynamics across a complex bay coastline, Galveston Bay, TX”, *Coastal Engineering*, vol. 138. Elsevier BV, pp. 165–183, Aug. 2018. doi: 10.1016/j.coastaleng.2018.04.019.  
  
M. Bremer, K. Kazhyken, H. Kaiser, C. Michoskiand C. Dawson, “Performance Comparison of HPX Versus Traditional Parallelization Strategies for the Discontinuous Galerkin Method”, *Journal of Scientific Computing*, vol. 80, no. 2. Springer Science and Business Media LLC, pp. 878–902, May 02, 2019. doi: 10.1007/s10915-019-00960-z.  
  
S. R. Brus, D. Wirasaet, J. J. Westerinkand C. Dawson, “Performance and Scalability Improvements for Discontinuous Galerkin Solutions to Conservation Laws on Unstructured Grids”, *Journal of Scientific Computing*, vol. 70, no. 1. Springer Science and Business Media LLC, pp. 210–242, Aug. 01, 2016. doi: 10.1007/s10915-016-0249-y.  
  
R. Cyriac, “Variability in Coastal Flooding predictions due to forecast errors during Hurricane Arthur”, *Coastal Engineering*, vol. 137. Elsevier BV, pp. 59–78, Jul. 2018. doi: 10.1016/j.coastaleng.2018.02.008.  
  
J. C. Dietrich, “Surface trajectories of oil transport along the Northern Coastline of the Gulf of Mexico”, *Continental Shelf Research*, vol. 41. Elsevier BV, pp. 17–47, Jun. 2012. doi: 10.1016/j.csr.2012.03.015.  
  
J. C. Dietrich, “Limiters for spectral propagation velocities in SWAN”, *Ocean Modelling*, vol. 70. Elsevier BV, pp. 85–102, Oct. 2013. doi: 10.1016/j.ocemod.2012.11.005.  
  
J. C. Dietrich, “Modeling hurricane waves and storm surge using integrally-coupled, scalable computations”, *Coastal Engineering*, vol. 58, no. 1. Elsevier BV, pp. 45–65, Jan. 2011. doi: 10.1016/j.coastaleng.2010.08.001.  
  
L. Graham, T. Butler, S. Walsh, C. Dawsonand J. J. Westerink, “A Measure-Theoretic Algorithm for Estimating Bottom Friction in a Coastal Inlet: Case Study of Bay St. Louis during Hurricane Gustav (2008)”, *Monthly Weather Review*, vol. 145, no. 3. American Meteorological Society, pp. 929–954, Mar. 2017. doi: 10.1175/mwr-d-16-0149.1.  
  
L. Graham, S. Mattis, S. Walsh, T. Butler, M. Pilosovand D. McDougall, “Bet: Butler, Estep, Tavener Method V2.0.0”. Zenodo, Aug. 10, 2016. doi: 10.5281/ZENODO.59964.  
  
J. He, S. A. Mattis, T. D. Butlerand C. N. Dawson, “Data-driven uncertainty quantification for predictive flow and transport modeling using support vector machines”, *Computational Geosciences*, vol. 23, no. 4. Springer Science and Business Media LLC, pp. 631–645, Aug. 02, 2018. doi: 10.1007/s10596-018-9762-4.  
  
S. A. Mattis, T. D. Butler, C. N. Dawson, D. Estepand V. V. Vesselinov, “Parameter estimation and prediction for groundwater contamination based on measure theory”, *Water Resources Research*, vol. 51, no. 9. American Geophysical Union (AGU), pp. 7608–7629, Sep. 2015. doi: 10.1002/2015wr017295.  
  
S. A. Mattis, C. E. Kees, M. V. Wei, A. Dimakopoulosand C. N. Dawson, “Computational Model for Wave Attenuation by Flexible Vegetation”, *Journal of Waterway, Port, Coastal, and Ocean Engineering*, vol. 145, no. 1. American Society of Civil Engineers (ASCE), Jan. 2019. doi: 10.1061/(asce)ww.1943-5460.0000487.  
  
C. Michoski, A. Alexanderian, C. Paillet, E. J. Kubatkoand C. Dawson, “Stability of Nonlinear Convection–Diffusion–Reaction Systems in Discontinuous Galerkin Methods”, *Journal of Scientific Computing*, vol. 70, no. 2. Springer Science and Business Media LLC, pp. 516–550, Aug. 10, 2016. doi: 10.1007/s10915-016-0256-z.  
  
A. Samii, K. Kazhyken, C. Michoskiand C. Dawson, “A Comparison of the Explicit and Implicit Hybridizable Discontinuous Galerkin Methods for Nonlinear Shallow Water Equations”, *Journal of Scientific Computing*, vol. 80, no. 3. Springer Science and Business Media LLC, pp. 1936–1956, Jul. 13, 2019. doi: 10.1007/s10915-019-01007-z.  
  
A. Samii, C. Michoskiand C. Dawson, “A parallel and adaptive hybridized discontinuous Galerkin method for anisotropic nonhomogeneous diffusion”, *Computer Methods in Applied Mechanics and Engineering*, vol. 304. Elsevier BV, pp. 118–139, Jun. 2016. doi: 10.1016/j.cma.2016.02.009.  
  
N. Sund, D. Bolster, S. Mattisand C. Dawson, “Pre-asymptotic Transport Upscaling in Inertial and Unsteady Flows Through Porous Media”, *Transport in Porous Media*, vol. 109, no. 2. Springer Science and Business Media LLC, pp. 411–432, Jun. 16, 2015. doi: 10.1007/s11242-015-0526-5.  
  
J. M. Torres, “Modeling the Hydrodynamic Performance of a Conceptual Storm Surge Barrier System for the Galveston Bay Region”, *Journal of Waterway, Port, Coastal, and Ocean Engineering*, vol. 143, no. 5. American Society of Civil Engineers (ASCE), Sep. 2017. doi: 10.1061/(asce)ww.1943-5460.0000389.  
  
J. M. Torres, “Characterizing the hydraulic interactions of hurricane storm surge and rainfall–runoff for the Houston–Galveston region”, *Coastal Engineering*, vol. 106. Elsevier BV, pp. 7–19, Dec. 2015. doi: 10.1016/j.coastaleng.2015.09.004.  
  
D. Wirasaet, S. R. Brus, C. E. Michoski, E. J. Kubatko, J. J. Westerinkand C. Dawson, “Artificial boundary layers in discontinuous Galerkin solutions to shallow water equations in channels”, *Journal of Computational Physics*, vol. 299. Elsevier BV, pp. 597–612, Oct. 2015. doi: 10.1016/j.jcp.2015.07.015.  
  
M. U. Altaf, “A Comparison of Ensemble Kalman Filters for Storm Surge Assimilation”, *Monthly Weather Review*, vol. 142, no. 8. American Meteorological Society, pp. 2899–2914, Aug. 01, 2014. doi: 10.1175/mwr-d-13-00266.1.  
  
D. W. Burleson, H. S. Rifai, J. K. Proft, C. N. Dawsonand P. B. Bedient, “Vulnerability of an industrial corridor in Texas to storm surge”, *Natural Hazards*, vol. 77, no. 2. Springer Science and Business Media LLC, pp. 1183–1203, Feb. 12, 2015. doi: 10.1007/s11069-015-1652-7.  
  
T. Butler, L. Graham, D. Estep, C. Dawsonand J. J. Westerink, “Definition and solution of a stochastic inverse problem for the Manning’s n parameter field in hydrodynamic models”, *Advances in Water Resources*, vol. 78. Elsevier BV, pp. 60–79, Apr. 2015. doi: 10.1016/j.advwatres.2015.01.011.  
  
Z. Kanar Seymen, H. Yüceland B. Karasözen, “Distributed optimal control of time-dependent diffusion–convection–reaction equations using space–time discretization”, *Journal of Computational and Applied Mathematics*, vol. 261. Elsevier BV, pp. 146–157, May 2014. doi: 10.1016/j.cam.2013.11.006.  
  
S. A. Mattis, C. N. Dawson, C. E. Keesand M. W. Farthing, “An immersed structure approach for fluid-vegetation interaction”, *Advances in Water Resources*, vol. 80. Elsevier BV, pp. 1–16, Jun. 2015. doi: 10.1016/j.advwatres.2015.02.014.  
  
A. Sebastian, J. Proft, J. C. Dietrich, W. Du, P. B. Bedientand C. N. Dawson, “Characterizing hurricane storm surge behavior in Galveston Bay using the SWAN+ADCIRC model”, *Coastal Engineering*, vol. 88. Elsevier BV, pp. 171–181, Jun. 2014. doi: 10.1016/j.coastaleng.2014.03.002.  
  
A. Sebastian, J. Proft, J. C. Dietrich, W. Du, P. B. Bedientand C. N. Dawson, “Characterizing hurricane storm surge behavior in Galveston Bay using the SWAN+ADCIRC model”, *Coastal Engineering*, vol. 88. Elsevier BV, pp. 171–181, Jun. 2014. doi: 10.1016/j.coastaleng.2014.03.002.  
  
A. Sebastian, J. Proft, J. C. Dietrich, W. Du, P. B. Bedientand C. N. Dawson, “Characterizing hurricane storm surge behavior in Galveston Bay using the SWAN+ADCIRC model”, *Coastal Engineering*, vol. 88. Elsevier BV, pp. 171–181, Jun. 2014. doi: 10.1016/j.coastaleng.2014.03.002.  
  
D. Wirasaet, E. J. Kubatko, C. E. Michoski, S. Tanaka, J. J. Westerinkand C. Dawson, “Discontinuous Galerkin methods with nodal and hybrid modal/nodal triangular, quadrilateral, and polygonal elements for nonlinear shallow water flow”, *Computer Methods in Applied Mechanics and Engineering*, vol. 270. Elsevier BV, pp. 113–149, Mar. 2014. doi: 10.1016/j.cma.2013.11.006.  
  
F. Q. Hu, “An efficient solution of time domain boundary integral equations for acoustic scattering and its acceleration by Graphics Processing Units”, *19th AIAA/CEAS Aeroacoustics Conference*. American Institute of Aeronautics and Astronautics, May 24, 2013. doi: 10.2514/6.2013-2018.  
  
F. Q. Hu, “Further development of a time domain boundary integral equation method for aeroacoustic scattering computations”, *20th AIAA/CEAS Aeroacoustics Conference*. American Institute of Aeronautics and Astronautics, Jun. 13, 2014. doi: 10.2514/6.2014-3194.  
  
F. Q. Hu and A. M. Fernando, “A study of accuracy on numerical methods for nonuniform meshes (Invited)”, *21st AIAA/CEAS Aeroacoustics Conference*. American Institute of Aeronautics and Astronautics, Jun. 18, 2015. doi: 10.2514/6.2015-3131.  
  
F. Hu, I. Kocaoguland X. Li, “On the adjoint problem in duct acoustics and its solution by the Time Domain Wave Packet method”, *18th AIAA/CEAS Aeroacoustics Conference (33rd AIAA Aeroacoustics Conference)*. American Institute of Aeronautics and Astronautics, Jun. 04, 2012. doi: 10.2514/6.2012-2247.  
  
F. Q. Hu, X. D. Li, X. Y. Liand M. Jiang, “Time Domain Wave Packet Method and Suppression of Instability Waves in Aeroacoustic Computations”, *Journal of Fluids Engineering*, vol. 136, no. 6. ASME International, Apr. 28, 2014. doi: 10.1115/1.4025866.  
  
F. Q. Hu and M. E. Pizzo, “On the assessment of acoustic scattering and shielding by time domain boundary integral equation solutions”, *22nd AIAA/CEAS Aeroacoustics Conference*. American Institute of Aeronautics and Astronautics, May 27, 2016. doi: 10.2514/6.2016-2779.  
  
F. Q. Hu, M. E. Pizzoand D. M. Nark, “A new formulation of time domain boundary integral equation for acoustic wave scattering in the presence of a uniform mean flow”, *23rd AIAA/CEAS Aeroacoustics Conference*. American Institute of Aeronautics and Astronautics, Jun. 02, 2017. doi: 10.2514/6.2017-3510.  
  
F. Q. Hu, M. E. Pizzoand D. M. Nark, “On a time domain boundary integral equation formulation for acoustic scattering by rigid bodies in uniform mean flow”, *The Journal of the Acoustical Society of America*, vol. 142, no. 6. Acoustical Society of America (ASA), pp. 3624–3636, Dec. 2017. doi: 10.1121/1.5017734.  
  
F. Q. Hu, M. E. Pizzoand D. M. Nark, “On the use of a Prandtl-Glauert-Lorentz transformation for acoustic scattering by rigid bodies with a uniform flow”, *Journal of Sound and Vibration*, vol. 443. Elsevier BV, pp. 198–211, Mar. 2019. doi: 10.1016/j.jsv.2018.11.043.  
  
M. E. Pizzo, F. Q. Huand D. M. Nark, “Simulation of Sound Absorption by Scattering Bodies Treated with Acoustic Liners Using a Time-Domain Boundary Element Method”, *2018 AIAA/CEAS Aeroacoustics Conference*. American Institute of Aeronautics and Astronautics, Jun. 24, 2018. doi: 10.2514/6.2018-3456.  
  
R. Calderer and A. Masud, “Residual-based variational multiscale turbulence models for unstructured tetrahedral meshes”, *Computer Methods in Applied Mechanics and Engineering*, vol. 254. Elsevier BV, pp. 238–253, Feb. 2013. doi: 10.1016/j.cma.2012.09.015.  
  
R. Calderer, L. Zhu, R. Gibsonand A. Masud, “Residual-based turbulence models and arbitrary Lagrangian–Eulerian framework for free surface flows”, *Mathematical Models and Methods in Applied Sciences*, vol. 25, no. 12. World Scientific Pub Co Pte Lt, pp. 2287–2317, Aug. 24, 2015. doi: 10.1142/s0218202515400096.  
  
A. Masud and R. Calderer, “A variational multiscale method for incompressible turbulent flows: Bubble functions and fine scale fields”, *Computer Methods in Applied Mechanics and Engineering*, vol. 200, no. 33–36. Elsevier BV, pp. 2577–2593, Aug. 2011. doi: 10.1016/j.cma.2011.04.010.  
  
A. Masud and R. Calderer, “Residual-based turbulence models for moving boundary flows: hierarchical application of variational multiscale method and three-level scale separation”, *International Journal for Numerical Methods in Fluids*, vol. 73, no. 3. Wiley, pp. 284–305, May 03, 2013. doi: 10.1002/fld.3801.  
  
L. Zhu, S. A. Gorayaand A. Masud, “Interface-Capturing Method for Free-Surface Plunging and Breaking Waves”, *Journal of Engineering Mechanics*, vol. 145, no. 11. American Society of Civil Engineers (ASCE), Nov. 2019. doi: 10.1061/(asce)em.1943-7889.0001641.  
  
M. Safari, M. R. H. Sheikhi, M. Janbozorgiand H. Metghalchi, “Entropy Transport Equation in Large Eddy Simulation for Exergy Analysis of Turbulent Combustion Systems”, *Entropy*, vol. 12, no. 3. MDPI AG, pp. 434–444, Mar. 08, 2010. doi: 10.3390/e12030434.  
  
M. R. H. Sheikhi, M. Safariand H. Metghalchi, “Large Eddy Simulation for Local Entropy Generation Analysis of Turbulent Flows”, *Journal of Energy Resources Technology*, vol. 134, no. 4. ASME International, Oct. 19, 2012. doi: 10.1115/1.4007482.  
  
G. X. Hu, D. R. Kuipersand Y. Zeng, “Bayesian Inference via Filtering Equations for Ultrahigh Frequency Data (I): Model and Estimation”, *SIAM/ASA Journal on Uncertainty Quantification*, vol. 6, no. 1. Society for Industrial & Applied Mathematics (SIAM), pp. 34–60, Jan. 2018. doi: 10.1137/16m1094762.  
  
G. X. Hu, D. R. Kuipersand Y. Zeng, “Bayesian Inference via Filtering Equations for Ultrahigh Frequency Data (II): Model Selection”, *SIAM/ASA Journal on Uncertainty Quantification*, vol. 6, no. 1. Society for Industrial & Applied Mathematics (SIAM), pp. 61–86, Jan. 2018. doi: 10.1137/16m1094774.  
  
P. Motamarri and V. Gavini, “Subquadratic-scaling subspace projection method for large-scale Kohn-Sham density functional theory calculations using spectral finite-element discretization”, *Physical Review B*, vol. 90, no. 11. American Physical Society (APS), Sep. 15, 2014. doi: 10.1103/physrevb.90.115127.  
  
P. Motamarri, M. Iyer, J. Knapand V. Gavini, “Higher-order adaptive finite-element methods for orbital-free density functional theory”, *Journal of Computational Physics*, vol. 231, no. 20. Elsevier BV, pp. 6596–6621, Aug. 2012. doi: 10.1016/j.jcp.2012.04.036.  
  
P. Motamarri, M. R. Nowak, K. Leiter, J. Knapand V. Gavini, “Higher-order adaptive finite-element methods for Kohn–Sham density functional theory”, *Journal of Computational Physics*, vol. 253. Elsevier BV, pp. 308–343, Nov. 2013. doi: 10.1016/j.jcp.2013.06.042.  
  
M. Safari, F. Hadiand M. Sheikhi, “Progress in the Prediction of Entropy Generation in Turbulent Reacting Flows Using Large Eddy Simulation”, *Entropy*, vol. 16, no. 10. MDPI AG, pp. 5159–5177, Sep. 26, 2014. doi: 10.3390/e16105159.  
  
M. Safari and M. R. H. Sheikhi, “Large Eddy Simulation for Prediction of Entropy Generation in a Nonpremixed Turbulent Jet Flame”, *Journal of Energy Resources Technology*, vol. 136, no. 2. ASME International, Jan. 15, 2014. doi: 10.1115/1.4025974.  
  
M. R. H. Sheikhi, M. Safariand F. Hadi, “Entropy Filtered Density Function for Large Eddy Simulation of Turbulent Flows”, *AIAA Journal*, vol. 53, no. 9. American Institute of Aeronautics and Astronautics (AIAA), pp. 2571–2587, Sep. 2015. doi: 10.2514/1.j053679.  
  
J. M. Abowd and M. J. Schneider, “An Application of Differentially Private Linear Mixed Modeling”, *2011 IEEE 11th International Conference on Data Mining Workshops*. IEEE, Dec. 2011. doi: 10.1109/icdmw.2011.26.  
  
M. J. Schneider and J. M. Abowd, “A new method for protecting interrelated time series with Bayesian prior distributions and synthetic data”, *Journal of the Royal Statistical Society: Series A (Statistics in Society)*, vol. 178, no. 4. Oxford University Press (OUP), pp. 963–975, Jan. 27, 2015. doi: 10.1111/rssa.12100.  
  
M. J. Schneider, S. Jagpal, S. Gupta, S. Liand Y. Yu, “Protecting customer privacy when marketing with second-party data”, *International Journal of Research in Marketing*, vol. 34, no. 3. Elsevier BV, pp. 593–603, Sep. 2017. doi: 10.1016/j.ijresmar.2017.02.003.  
  
M. J. Schneider, S. Jagpal, S. Gupta, S. Liand Y. Yu, “A Flexible Method for Protecting Marketing Data: An Application to Point-of-Sale Data”, *Marketing Science*, vol. 37, no. 1. Institute for Operations Research and the Management Sciences (INFORMS), pp. 153–171, Jan. 2018. doi: 10.1287/mksc.2017.1064.  
  
M. Amara, S. Chaudhry, J. Diaz, R. Djellouliand S. L. Fiedler, “A local wave tracking strategy for efficiently solving mid- and high-frequency Helmholtz problems”, *Computer Methods in Applied Mechanics and Engineering*, vol. 276. Elsevier BV, pp. 473–508, Jul. 2014. doi: 10.1016/j.cma.2014.03.012.  
  
L. Xu and M. Nitsche, “Scaling behaviour in impulsively started viscous flow past a finite flat plate”, *Journal of Fluid Mechanics*, vol. 756. Cambridge University Press (CUP), pp. 689–715, Sep. 04, 2014. doi: 10.1017/jfm.2014.451.  
  
D. Colbry, “iCER Interns”, *Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment*. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616573.  
  
H.-Y. Chang, A. Yazdani, X. J. Li, K. A. A. Douglas, C. S. Mantzorosand G. E. Karniadakis, “Quantifying Platelet Margination in Diabetic Blood Flow”, *[]*. Cold Spring Harbor Laboratory, Jun. 12, 2018. doi: 10.1101/344655.  
  
X. Li, “Dissipative Particle Dynamics, Overview”, *Encyclopedia of Nanotechnology*. Springer Netherlands, pp. 1–8, 2015. doi: 10.1007/978-94-007-6178-0\_100954-1.  
  
N. Perakakis, A. Yazdani, G. E. Karniadakisand C. Mantzoros, “Omics, big data and machine learning as tools to propel understanding of biological mechanisms and to discover novel diagnostics and therapeutics”, *Metabolism*, vol. 87. Elsevier BV, pp. A1–A9, Oct. 2018. doi: 10.1016/j.metabol.2018.08.002.  
  
A. Witthoft, A. Yazdani, Z. Peng, C. Bellini, J. D. Humphreyand G. E. Karniadakis, “A discrete mesoscopic particle model of the mechanics of a multi-constituent arterial wall”, *Journal of The Royal Society Interface*, vol. 13, no. 114. The Royal Society, p. 20150964, Jan. 2016. doi: 10.1098/rsif.2015.0964.  
  
A. Yazdani, M. Deng, B. Caswelland G. E. Karniadakis, “Flow in complex domains simulated by Dissipative Particle Dynamics driven by geometry-specific body-forces”, *Journal of Computational Physics*, vol. 305. Elsevier BV, pp. 906–920, Jan. 2016. doi: 10.1016/j.jcp.2015.11.001.  
  
A. Yazdani and G. E. Karniadakis, “Sub-cellular modeling of platelet transport in blood flow through microchannels with constriction”, *Soft Matter*, vol. 12, no. 19. Royal Society of Chemistry (RSC), pp. 4339–4351, 2016. doi: 10.1039/c6sm00154h.  
  
A. Yazdani, “Data-driven Modeling of Hemodynamics and its Role on Thrombus Size and Shape in Aortic Dissections”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, Feb. 06, 2018. doi: 10.1038/s41598-018-20603-x.  
  
A. Yazdani, H. Li, J. D. Humphreyand G. E. Karniadakis, “A General Shear-Dependent Model for Thrombus Formation”, *PLOS Computational Biology*, vol. 13, no. 1. Public Library of Science (PLoS), p. e1005291, Jan. 17, 2017. doi: 10.1371/journal.pcbi.1005291.  
  
A. Yazdani, X. Liand G. E. Karniadakis, “Dynamic and rheological properties of soft biological cell suspensions”, *Rheologica Acta*, vol. 55, no. 6. Springer Science and Business Media LLC, pp. 433–449, Sep. 03, 2015. doi: 10.1007/s00397-015-0869-4.  
  
A. Yazdani, Z. Li, J. D. Humphreyand G. E. Karniadakis, “Seamless Multiscale Modeling of Coagulation Using Dissipative Particle Dynamics”, *[]*. Cold Spring Harbor Laboratory, Aug. 26, 2017. doi: 10.1101/181099.  
  
G. Falkovich and N. Vladimirova, “Cascades in nonlocal turbulence”, *Physical Review E*, vol. 91, no. 4. American Physical Society (APS), Apr. 29, 2015. doi: 10.1103/physreve.91.041201.  
  
P. M. Lushnikov and N. Vladimirova, “Nonlinear combining of laser beams”, *Optics Letters*, vol. 39, no. 12. The Optical Society, p. 3429, Jun. 04, 2014. doi: 10.1364/ol.39.003429.  
  
P. M. Lushnikov and N. Vladimirova, “Modeling of nonlinear combining of multiple laser beams in Kerr medium”, *Optics Express*, vol. 23, no. 24. The Optical Society, p. 31120, Nov. 20, 2015. doi: 10.1364/oe.23.031120.  
  
P. Miller, N. Vladimirovaand G. Falkovich, “Oscillations in a turbulence-condensate system”, *Physical Review E*, vol. 87, no. 6. American Physical Society (APS), Jun. 17, 2013. doi: 10.1103/physreve.87.065202.  
  
W. Deng, J. Xuand S. Zhao, “On developing stable finite element methods for pseudo-time simulation of biomolecular electrostatics”, *Journal of Computational and Applied Mathematics*, vol. 330. Elsevier BV, pp. 456–474, Mar. 2018. doi: 10.1016/j.cam.2017.09.004.  
  
H. Ji and Y. Li, “A breakdown-free block conjugate gradient method”, *BIT Numerical Mathematics*, vol. 57, no. 2. Springer Science and Business Media LLC, pp. 379–403, Oct. 05, 2016. doi: 10.1007/s10543-016-0631-z.  
  
D. E. Manosalvas, T. D. Economon, F. Palaciosand A. Jameson, “Techniques for the Design of Active Flow Control Systems in Heavy Vehicles”, *33rd AIAA Applied Aerodynamics Conference*. American Institute of Aeronautics and Astronautics, Jun. 19, 2015. doi: 10.2514/6.2015-3312.  
  
D. E. Manosalvas, T. D. Economon, C. Othmerand A. Jameson, “Computational Design of Drag Diminishing Active Flow Control Systems for Heavy Vehicles”, *8th AIAA Flow Control Conference*. American Institute of Aeronautics and Astronautics, Jun. 10, 2016. doi: 10.2514/6.2016-4082.  
  
C. E. Clancy, “Multiscale Modeling in the Clinic: Drug Design and Development”, *Annals of Biomedical Engineering*, vol. 44, no. 9. Springer Science and Business Media LLC, pp. 2591–2610, Feb. 17, 2016. doi: 10.1007/s10439-016-1563-0.  
  
Dongmin Guo, A. L. van de Venand Xiaobo Zhou, “Red Blood Cell Tracking Using Optical Flow Methods”, *IEEE Journal of Biomedical and Health Informatics*, vol. 18, no. 3. Institute of Electrical and Electronics Engineers (IEEE), pp. 991–998, May 2014. doi: 10.1109/jbhi.2013.2281915.  
  
D. Guo, K. C. Li, T. R. Peters, B. M. Snively, K. A. Poehlingand X. Zhou, “Multi-scale modeling for the transmission of influenza and the evaluation of interventions toward it”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, Mar. 11, 2015. doi: 10.1038/srep08980.  
  
B. Jiang, W. Dai, A. Khaliq, M. Carey, X. Zhouand L. Zhang, “Novel 3D GPU based numerical parallel diffusion algorithms in cylindrical coordinates for health care simulation”, *Mathematics and Computers in Simulation*, vol. 109. Elsevier BV, pp. 1–19, Mar. 2015. doi: 10.1016/j.matcom.2014.07.003.  
  
L. Liu, W. Zhaoand X. Zhou, “Modeling co-occupancy of transcription factors using chromatin features”, *Nucleic Acids Research*, vol. 44, no. 5. Oxford University Press (OUP), pp. e49–e49, Nov. 20, 2015. doi: 10.1093/nar/gkv1281.  
  
L. D. Miller, “Immunogenic Subtypes of Breast Cancer Delineated by Gene Classifiers of Immune Responsiveness”, *Cancer Immunology Research*, vol. 4, no. 7. American Association for Cancer Research (AACR), pp. 600–610, Jun. 30, 2016. doi: 10.1158/2326-6066.cir-15-0149.  
  
B. Pan, “Prediction of soft tissue deformations after CMF surgery with incremental kernel ridge regression”, *Computers in Biology and Medicine*, vol. 75. Elsevier BV, pp. 1–9, Aug. 2016. doi: 10.1016/j.compbiomed.2016.04.020.  
  
X. Qian, H. Tan, J. Zhang, W. Zhao, M. D. Chanand X. Zhou, “Stratification of pseudoprogression and true progression of glioblastoma multiform based on longitudinal diffusion tensor imaging without segmentation”, *Medical Physics*, vol. 43, no. 11. Wiley, pp. 5889–5902, Oct. 05, 2016. doi: 10.1118/1.4963812.  
  
X. Qian, “Objective classification system for sagittal craniosynostosis based on suture segmentation”, *Medical Physics*, vol. 42, no. 9. Wiley, pp. 5545–5558, Aug. 28, 2015. doi: 10.1118/1.4928708.  
  
X. Sun, Y. Kang, J. Bao, Y. Zhang, Y. Yangand X. Zhou, “Modeling vascularized bone regeneration within a porous biodegradable CaP scaffold loaded with growth factors”, *Biomaterials*, vol. 34, no. 21. Elsevier BV, pp. 4971–4981, Jul. 2013. doi: 10.1016/j.biomaterials.2013.03.015.  
  
V. Suresh, L. Liu, D. Adjerohand X. Zhou, “RPI-Pred: predicting ncRNA-protein interaction using sequence and structural information”, *Nucleic Acids Research*, vol. 43, no. 3. Oxford University Press (OUP), pp. 1370–1379, Jan. 21, 2015. doi: 10.1093/nar/gkv020.  
  
H. Tan, J. Baoand X. Zhou, “Genome-wide mutational spectra analysis reveals significant cancer-specific heterogeneity”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, Jul. 27, 2015. doi: 10.1038/srep12566.  
  
H. Tan, H. Yi, W. Zhao, J.-X. Ma, Y. Zhangand X. Zhou, “Intraglomerular crosstalk elaborately regulates podocyte injury and repair in diabetic patients: insights from a 3D multiscale modeling study”, *Oncotarget*, vol. 7, no. 45. Impact Journals, LLC, pp. 73130–73146, Sep. 24, 2016. doi: 10.18632/oncotarget.12233.  
  
F. Xing, “Activation of the c-Met Pathway Mobilizes an Inflammatory Network in the Brain Microenvironment to Promote Brain Metastasis of Breast Cancer”, *Cancer Research*, vol. 76, no. 17. American Association for Cancer Research (AACR), pp. 4970–4980, Aug. 31, 2016. doi: 10.1158/0008-5472.can-15-3541.  
  
T. E. Yankeelov, “Multi-scale Modeling in Clinical Oncology: Opportunities and Barriers to Success”, *Annals of Biomedical Engineering*, vol. 44, no. 9. Springer Science and Business Media LLC, pp. 2626–2641, Jul. 06, 2016. doi: 10.1007/s10439-016-1691-6.  
  
D. Zhang, G. Wei, P. Li, X. Zhouand Y. Zhang, “Urine-derived stem cells: A novel and versatile progenitor source for cell-based therapy and regenerative medicine”, *Genes & Diseases*, vol. 1, no. 1. Elsevier BV, pp. 8–17, Sep. 2014. doi: 10.1016/j.gendis.2014.07.001.  
  
G. Zhang, J. J. Xia, M. Liebschner, X. Zhang, D. Kimand X. Zhou, “Improved Rubin–Bodner model for the prediction of soft tissue deformations”, *Medical Engineering & Physics*, vol. 38, no. 11. Elsevier BV, pp. 1369–1375, Nov. 2016. doi: 10.1016/j.medengphy.2016.09.008.  
  
J. Zhang, “Pseudo progression identification of glioblastoma with dictionary learning”, *Computers in Biology and Medicine*, vol. 73. Elsevier BV, pp. 94–101, Jun. 2016. doi: 10.1016/j.compbiomed.2016.03.027.  
  
L. Zhang, “Investigation of mechanism of bone regeneration in a porous biodegradable calcium phosphate (CaP) scaffold by a combination of a multi-scale agent-based model and experimental optimization/validation”, *Nanoscale*, vol. 8, no. 31. Royal Society of Chemistry (RSC), pp. 14877–14887, 2016. doi: 10.1039/c6nr01637e.  
  
L. Zhang, “Investigation of mechanism of bone regeneration in a porous biodegradable calcium phosphate (CaP) scaffold by a combination of a multi-scale agent-based model and experimental optimization/validation”, *Nanoscale*, vol. 8, no. 31. Royal Society of Chemistry (RSC), pp. 14877–14887, 2016. doi: 10.1039/c6nr01637e.  
  
X. Zhang, “An eFace-Template Method for Efficiently Generating Patient-Specific Anatomically-Detailed Facial Soft Tissue FE Models for Craniomaxillofacial Surgery Simulation”, *Annals of Biomedical Engineering*, vol. 44, no. 5. Springer Science and Business Media LLC, pp. 1656–1671, Oct. 13, 2015. doi: 10.1007/s10439-015-1480-7.  
  
J. Kaderli, J. Zweck, A. Safinand S. E. Minkoff, “An analytic solution to the coupled pressure–temperature equations for modeling of photoacoustic trace gas sensors”, *Journal of Engineering Mathematics*, vol. 103, no. 1. Springer Science and Business Media LLC, pp. 173–193, Jul. 29, 2016. doi: 10.1007/s10665-016-9867-5.  
  
P. Huang, M. Caiand F. Wang, “A Newton type linearization based two grid method for coupling fluid flow with porous media flow”, *Applied Numerical Mathematics*, vol. 106. Elsevier BV, pp. 182–198, Aug. 2016. doi: 10.1016/j.apnum.2016.04.003.  
  
M. Cai, “Analysis of some projection method based preconditioners for models of incompressible flow”, *Applied Numerical Mathematics*, vol. 90. Elsevier BV, pp. 77–90, Apr. 2015. doi: 10.1016/j.apnum.2014.12.003.  
  
C. Ma, M. Shaoand C. Kingsford, “SQUID: transcriptomic structural variation detection from RNA-seq”, *Genome Biology*, vol. 19, no. 1. Springer Science and Business Media LLC, Apr. 12, 2018. doi: 10.1186/s13059-018-1421-5.  
  
M. Ruffalo and Z. Bar-Joseph, “Protein interaction disruption in cancer”, *BMC Cancer*, vol. 19, no. 1. Springer Science and Business Media LLC, Apr. 23, 2019. doi: 10.1186/s12885-019-5532-5.  
  
C. Zhou and R. C. Paffenroth, “Anomaly Detection with Robust Deep Autoencoders”, *Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. ACM, Aug. 04, 2017. doi: 10.1145/3097983.3098052.  
  
M. Huang, “SAVER: gene expression recovery for single-cell RNA sequencing”, *Nature Methods*, vol. 15, no. 7. Springer Science and Business Media LLC, pp. 539–542, Jun. 25, 2018. doi: 10.1038/s41592-018-0033-z.  
  
K. I. Aycock, R. L. Campbell, F. C. Lynch, K. B. Manningand B. A. Craven, “Computational predictions of the embolus-trapping performance of an IVC filter in patient-specific and idealized IVC geometries”, *Biomechanics and Modeling in Mechanobiology*, vol. 16, no. 6. Springer Science and Business Media LLC, pp. 1957–1969, Jun. 27, 2017. doi: 10.1007/s10237-017-0931-5.  
  
K. P. Mainali, “Statistical analysis of co-occurrence patterns in microbial presence-absence datasets”, *PLOS ONE*, vol. 12, no. 11. Public Library of Science (PLoS), p. e0187132, Nov. 16, 2017. doi: 10.1371/journal.pone.0187132.  
  
K. P. Mainali, “Projecting future expansion of invasive species: comparing and improving methodologies for species distribution modeling”, *Global Change Biology*, vol. 21, no. 12. Wiley, pp. 4464–4480, Nov. 06, 2015. doi: 10.1111/gcb.13038.  
  
K. Wang, “Efficient counting of degree sequences”, *Discrete Mathematics*, vol. 342, no. 3. Elsevier BV, pp. 888–897, Mar. 2019. doi: 10.1016/j.disc.2018.11.024.  
  
H. Sun, S. Zhou, L.-T. Chengand B. Li, “Numerical methods for solvent Stokes flow and solute-solvent interfacial dynamics of charged molecules”, *Journal of Computational Physics*, vol. 374. Elsevier BV, pp. 533–549, Dec. 2018. doi: 10.1016/j.jcp.2018.07.046.  
  
K. Gajamannage and R. Paffenroth, “Bounded manifold completion”, *Pattern Recognition*, vol. 111. Elsevier BV, p. 107661, Mar. 2021. doi: 10.1016/j.patcog.2020.107661.  
  
K. Gajamannage, R. Paffenrothand E. M. Bollt, “A nonlinear dimensionality reduction framework using smooth geodesics”, *Pattern Recognition*, vol. 87. Elsevier BV, pp. 226–236, Mar. 2019. doi: 10.1016/j.patcog.2018.10.020.  
  
C. Zheng and N. Wang, “Collaborative representation with k-nearest classes for classification”, *Pattern Recognition Letters*, vol. 117. Elsevier BV, pp. 30–36, Jan. 2019. doi: 10.1016/j.patrec.2018.11.005.  
  
D. Agarwal, J. Wangand N. R. Zhang, “Data Denoising and Post-Denoising Corrections in Single Cell RNA Sequencing”, *Statistical Science*, vol. 35, no. 1. Institute of Mathematical Statistics, Feb. 01, 2020. doi: 10.1214/19-sts7560.  
  
J. Wang, “Data denoising with transfer learning in single-cell transcriptomics”, *Nature Methods*, vol. 16, no. 9. Springer Science and Business Media LLC, pp. 875–878, Aug. 30, 2019. doi: 10.1038/s41592-019-0537-1.  
  
A. Alekseenko, A. Grandilliand A. Wood, “An ultra-sparse approximation of kinetic solutions to spatially homogeneous flows of non-continuum gas”, *Results in Applied Mathematics*, vol. 5. Elsevier BV, p. 100085, Feb. 2020. doi: 10.1016/j.rinam.2019.100085.  
  
H. Li, “Predictive modelling of thrombus formation in diabetic retinal microaneurysms”, *Royal Society Open Science*, vol. 7, no. 8. The Royal Society, p. 201102, Aug. 2020. doi: 10.1098/rsos.201102.  
  
X. Zheng, A. Yazdani, H. Li, J. D. Humphreyand G. E. Karniadakis, “A three-dimensional phase-field model for multiscale modeling of thrombus biomechanics in blood vessels”, *PLOS Computational Biology*, vol. 16, no. 4. Public Library of Science (PLoS), p. e1007709, Apr. 28, 2020. doi: 10.1371/journal.pcbi.1007709.  
  
V. Ramasubramanian and W. D. Beavis, “Factors Affecting Response to Recurrent Genomic Selection in Soybeans”, *[]*. Cold Spring Harbor Laboratory, Feb. 14, 2020. doi: 10.1101/2020.02.14.949008.  
  
I. Grooms, “Analog ensemble data assimilation and a method for constructing analogs with variational autoencoders”, *Quarterly Journal of the Royal Meteorological Society*, vol. 147, no. 734. Wiley, pp. 139–149, Oct. 13, 2020. doi: 10.1002/qj.3910.  
  
E. Molina, B. Y. Zhou, J. J. Alonso, M. Righiand R. G. Silva, “Flow and Noise Predictions Around Tandem Cylinders using DDES approach with SU2”, *AIAA Scitech 2019 Forum*. American Institute of Aeronautics and Astronautics, Jan. 06, 2019. doi: 10.2514/6.2019-0326.  
  
C. Burstedde, “Large-scale adaptive mantle convection simulation”, *Geophysical Journal International*, vol. 192, no. 3. Oxford University Press (OUP), pp. 889–906, Jan. 09, 2013. doi: 10.1093/gji/ggs070.  
  
I. D. Fernando, S. Jayasena, M. Fernandoand H. Sundar, “A Scalable Hierarchical Semi-Separable Library for Heterogeneous Clusters”, *2017 46th International Conference on Parallel Processing (ICPP)*. IEEE, Aug. 2017. doi: 10.1109/icpp.2017.60.  
  
T. Isaac, N. Petra, G. Stadlerand O. Ghattas, “Scalable and efficient algorithms for the propagation of uncertainty from data through inference to prediction for large-scale problems, with application to flow of the Antarctic ice sheet”, *Journal of Computational Physics*, vol. 296. Elsevier BV, pp. 348–368, Sep. 2015. doi: 10.1016/j.jcp.2015.04.047.  
  
L. Lu, M. J. Morse, A. Rahimian, G. Stadlerand D. Zorin, “Scalable simulation of realistic volume fraction red blood cell flows through vascular networks”, *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*. ACM, Nov. 17, 2019. doi: 10.1145/3295500.3356203.  
  
V. Ratnaswamy, G. Stadlerand M. Gurnis, “Adjoint-based estimation of plate coupling in a non-linear mantle flow model: theory and examples”, *Geophysical Journal International*, vol. 202, no. 2. Oxford University Press (OUP), pp. 768–786, May 29, 2015. doi: 10.1093/gji/ggv166.  
  
J. Rudi, G. Stadlerand O. Ghattas, “Weighted BFBT Preconditioner for Stokes Flow Problems with Highly Heterogeneous Viscosity”, *SIAM Journal on Scientific Computing*, vol. 39, no. 5. Society for Industrial & Applied Mathematics (SIAM), pp. S272–S297, Jan. 2017. doi: 10.1137/16m108450x.  
  
J. Worthen, G. Stadler, N. Petra, M. Gurnisand O. Ghattas, “Towards adjoint-based inversion for rheological parameters in nonlinear viscous mantle flow”, *Physics of the Earth and Planetary Interiors*, vol. 234. Elsevier BV, pp. 23–34, Sep. 2014. doi: 10.1016/j.pepi.2014.06.006.  
  
H. Zhu, S. Li, S. Fomel, G. Stadlerand O. Ghattas, “A Bayesian approach to estimate uncertainty for full-waveform inversion using a priori information from depth migration”, *GEOPHYSICS*, vol. 81, no. 5. Society of Exploration Geophysicists, pp. R307–R323, Sep. 2016. doi: 10.1190/geo2015-0641.1.  
  
G. Stadler, M. Gurnis, C. Burstedde, L. C. Wilcox, L. Alisicand O. Ghattas, “The Dynamics of Plate Tectonics and Mantle Flow: From Local to Global Scales”, *Science*, vol. 329, no. 5995. American Association for the Advancement of Science (AAAS), pp. 1033–1038, Aug. 27, 2010. doi: 10.1126/science.1191223.  
  
M. Fernando, D. Duplyakinand H. Sundar, “Machine and Application Aware Partitioning for Adaptive Mesh Refinement Applications”, *Proceedings of the 26th International Symposium on High-Performance Parallel and Distributed Computing*. ACM, Jun. 26, 2017. doi: 10.1145/3078597.3078610.  
  
M. Ishii, M. Fernando, K. Saurabh, B. Khara, B. Ganapathysubramanianand H. Sundar, “Solving PDEs in space-time”, *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*. ACM, Nov. 17, 2019. doi: 10.1145/3295500.3356198.  
  
D. Li, M. Gurnisand G. Stadler, “Towards adjoint-based inversion of time-dependent mantle convection with non-linear viscosity”, *Geophysical Journal International*. Oxford University Press (OUP), p. ggw493, Jan. 13, 2017. doi: 10.1093/gji/ggw493.  
  
A. J. Lloyd, “Seismic Structure of the Antarctic Upper Mantle Imaged with Adjoint Tomography”, *Journal of Geophysical Research: Solid Earth*, vol. 125, no. 3. American Geophysical Union (AGU), Mar. 2020. doi: 10.1029/2019jb017823.  
  
A. K. Liljedahl, “Pan-Arctic ice-wedge degradation in warming permafrost and its influence on tundra hydrology”, *Nature Geoscience*, vol. 9, no. 4. Springer Science and Business Media LLC, pp. 312–318, Mar. 14, 2016. doi: 10.1038/ngeo2674.  
  
I. Das, “Multidecadal Basal Melt Rates and Structure of the Ross Ice Shelf, Antarctica, Using Airborne Ice Penetrating Radar”, *Journal of Geophysical Research: Earth Surface*, vol. 125, no. 3. American Geophysical Union (AGU), Mar. 2020. doi: 10.1029/2019jf005241.  
  
E. Klein, “Annual cycle in flow of Ross Ice Shelf, Antarctica: contribution of variable basal melting”, *Journal of Glaciology*, vol. 66, no. 259. Cambridge University Press (CUP), pp. 861–875, Aug. 03, 2020. doi: 10.1017/jog.2020.61.  
  
C. Mosbeux, T. J. W. Wagner, M. K. Beckerand H. A. Fricker, “Viscous and elastic buoyancy stresses as drivers of ice-shelf calving”, *Journal of Glaciology*, vol. 66, no. 258. Cambridge University Press (CUP), pp. 643–657, Jun. 03, 2020. doi: 10.1017/jog.2020.35.  
  
Y. Wu, “Elucidating the Inhibitory Effect of Resveratrol and Its Structural Analogs on Selected Nucleotide-Related Enzymes”, *Biomolecules*, vol. 10, no. 9. MDPI AG, p. 1223, Aug. 22, 2020. doi: 10.3390/biom10091223.  
  
Y. Wu, L. Louand Z.-R. Xie, “A Pilot Study of All-Computational Drug Design Protocol–From Structure Prediction to Interaction Analysis”, *Frontiers in Chemistry*, vol. 8. Frontiers Media SA, Feb. 12, 2020. doi: 10.3389/fchem.2020.00081.  
  
C. M. Cooper, M. S. Millerand L. Moresi, “The structural evolution of the deep continental lithosphere”, *Tectonophysics*, vol. 695. Elsevier BV, pp. 100–121, Jan. 2017. doi: 10.1016/j.tecto.2016.12.004.  
  
J. R. Kasprzyk, P. M. Reedand D. M. Hadka, “Battling Arrow’s Paradox to Discover Robust Water Management Alternatives”, *Journal of Water Resources Planning and Management*, vol. 142, no. 2. American Society of Civil Engineers (ASCE), Feb. 2016. doi: 10.1061/(asce)wr.1943-5452.0000572.  
  
L. Zhao, W. Lee, C. X. Song, M. Huberand A. Goldner, “Bringing high performance climate modeling into the classroom”, *Proceedings of the 2010 TeraGrid Conference*. ACM, Aug. 02, 2010. doi: 10.1145/1838574.1838598.  
  
M. A. Jadamec and M. I. Billen, “Reconciling surface plate motions with rapid three-dimensional mantle flow around a slab edge”, *Nature*, vol. 465, no. 7296. Springer Science and Business Media LLC, pp. 338–341, May 2010. doi: 10.1038/nature09053.  
  
M. A. Jadamec, M. I. Billenand O. Kreylos, “Three-dimensional simulations of geometrically complex subduction with large viscosity variations”, *Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment: Bridging from the eXtreme to the campus and beyond*. ACM, Jul. 16, 2012. doi: 10.1145/2335755.2335827.  
  
B. Buffett and H. Matsui, “Equatorially trapped waves in Earth’s core”, *Geophysical Journal International*, vol. 218, no. 2. Oxford University Press (OUP), pp. 1210–1225, May 17, 2019. doi: 10.1093/gji/ggz233.  
  
J. Dannberg and R. Gassmöller, “Chemical trends in ocean islands explained by plume–slab interaction”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 17. Proceedings of the National Academy of Sciences, pp. 4351–4356, Apr. 09, 2018. doi: 10.1073/pnas.1714125115.  
  
J. Dannberg, R. Gassmöller, R. Groveand T. Heister, “A new formulation for coupled magma/mantle dynamics”, *Geophysical Journal International*. Oxford University Press (OUP), May 17, 2019. doi: 10.1093/gji/ggz190.  
  
R. Gassmöller, H. Lokavarapu, E. Heien, E. G. Puckettand W. Bangerth, “Flexible and Scalable Particle‐in‐Cell Methods With Adaptive Mesh Refinement for Geodynamic Computations”, *Geochemistry, Geophysics, Geosystems*, vol. 19, no. 9. American Geophysical Union (AGU), pp. 3596–3604, Sep. 2018. doi: 10.1029/2018gc007508.  
  
S. Noda, “The circulation pattern and day-night heat transport in the atmosphere of a synchronously rotating aquaplanet: Dependence on planetary rotation rate”, *Icarus*, vol. 282. Elsevier BV, pp. 1–18, Jan. 2017. doi: 10.1016/j.icarus.2016.09.004.  
  
S.-. ichi . Takehiro and Y. Sasaki, “Penetration of steady fluid motions into an outer stable layer excited by MHD thermal convection in rotating spherical shells”, *Physics of the Earth and Planetary Interiors*, vol. 276. Elsevier BV, pp. 258–264, Mar. 2018. doi: 10.1016/j.pepi.2017.03.001.  
  
H. Matsui, “Performance benchmarks for a next generation numerical dynamo model”, *Geochemistry, Geophysics, Geosystems*, vol. 17, no. 5. American Geophysical Union (AGU), pp. 1586–1607, May 2016. doi: 10.1002/2015gc006159.  
  
B. Buffett and H. Matsui, “The fluid dynamics of inner-core growth”, *Physics of the Earth and Planetary Interiors*, vol. 243. Elsevier BV, pp. 22–29, Jun. 2015. doi: 10.1016/j.pepi.2015.04.001.  
  
W. Herreman, C. Nore, L. Cappaneraand J.-L. Guermond, “Tayler instability in liquid metal columns and liquid metal batteries”, *Journal of Fluid Mechanics*, vol. 771. Cambridge University Press (CUP), pp. 79–114, Apr. 15, 2015. doi: 10.1017/jfm.2015.159.  
  
X. Liu and S. Zhong, “The long-wavelength geoid from three-dimensional spherical models of thermal and thermochemical mantle convection”, *Journal of Geophysical Research: Solid Earth*, vol. 120, no. 6. American Geophysical Union (AGU), pp. 4572–4596, Jun. 2015. doi: 10.1002/2015jb012016.  
  
H. Matsui, E. Kingand B. Buffett, “Multiscale convection in a geodynamo simulation with uniform heat flux along the outer boundary”, *Geochemistry, Geophysics, Geosystems*, vol. 15, no. 8. American Geophysical Union (AGU), pp. 3212–3225, Aug. 2014. doi: 10.1002/2014gc005432.  
  
C. Nore, D. Castanon Quiroz, J.-L. Guermond, J. Léoratand F. Luddens, “Numerical dynamo action in cylindrical containers”, *The European Physical Journal Applied Physics*, vol. 70, no. 3. EDP Sciences, p. 31101, Jun. 2015. doi: 10.1051/epjap/2015150049.  
  
C. Nore, J. Léorat, J.-L. Guermondand A. Giesecke, “Mean-field model of the von Kármán sodium dynamo experiment using soft iron impellers”, *Physical Review E*, vol. 91, no. 1. American Physical Society (APS), Jan. 14, 2015. doi: 10.1103/physreve.91.013008.  
  
A. Ribeiro, G. Fabre, J.-L. Guermondand J. Aurnou, “Canonical Models of Geophysical and Astrophysical Flows: Turbulent Convection Experiments in Liquid Metals”, *Metals*, vol. 5, no. 1. MDPI AG, pp. 289–335, Mar. 09, 2015. doi: 10.3390/met5010289.  
  
D. Hadka and P. Reed, “Large-scale parallelization of the Borg multiobjective evolutionary algorithm to enhance the management of complex environmental systems”, *Environmental Modelling & Software*, vol. 69. Elsevier BV, pp. 353–369, Jul. 2015. doi: 10.1016/j.envsoft.2014.10.014.  
  
J. D. Herman, P. M. Reed, H. B. Zeffand G. W. Characklis, “How Should Robustness Be Defined for Water Systems Planning under Change?”, *Journal of Water Resources Planning and Management*, vol. 141, no. 10. American Society of Civil Engineers (ASCE), Oct. 2015. doi: 10.1061/(asce)wr.1943-5452.0000509.  
  
J. D. Herman, H. B. Zeff, P. M. Reedand G. W. Characklis, “Beyond optimality: Multistakeholder robustness tradeoffs for regional water portfolio planning under deep uncertainty”, *Water Resources Research*, vol. 50, no. 10. American Geophysical Union (AGU), pp. 7692–7713, Oct. 2014. doi: 10.1002/2014wr015338.  
  
H. B. Zeff, J. R. Kasprzyk, J. D. Herman, P. M. Reedand G. W. Characklis, “Navigating financial and supply reliability tradeoffs in regional drought management portfolios”, *Water Resources Research*, vol. 50, no. 6. American Geophysical Union (AGU), pp. 4906–4923, Jun. 2014. doi: 10.1002/2013wr015126.  
  
W. Chang, K.-H. Ding, L. Tsangand X. Xu, “Microwave Scattering and Medium Characterization for Terrestrial Snow With QCA–Mie and Bicontinuous Models: Comparison Studies”, *IEEE Transactions on Geoscience and Remote Sensing*, vol. 54, no. 6. Institute of Electrical and Electronics Engineers (IEEE), pp. 3637–3648, Jun. 2016. doi: 10.1109/tgrs.2016.2522438.  
  
Kun-Shan Chen, Leung Tsang, Kuan-Liang Chen, Tien Hao Liaoand Jong-Sen Lee, “Polarimetric Simulations of SAR at L-Band Over Bare Soil Using Scattering Matrices of Random Rough Surfaces From Numerical Three-Dimensional Solutions of Maxwell Equations”, *IEEE Transactions on Geoscience and Remote Sensing*, vol. 52, no. 11. Institute of Electrical and Electronics Engineers (IEEE), pp. 7048–7058, Nov. 2014. doi: 10.1109/tgrs.2014.2306922.  
  
H. Huang, “Coherent Model of L-Band Radar Scattering by Soybean Plants: Model Development, Evaluation, and Retrieval”, *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 9, no. 1. Institute of Electrical and Electronics Engineers (IEEE), pp. 272–284, Jan. 2016. doi: 10.1109/jstars.2015.2469717.  
  
S. Huang and L. Tsang, “Electromagnetic Scattering of Randomly Rough Soil Surfaces Based on Numerical Solutions of Maxwell Equations in Three-Dimensional Simulations Using a Hybrid UV/PBTG/SMCG Method”, *IEEE Transactions on Geoscience and Remote Sensing*, vol. 50, no. 10. Institute of Electrical and Electronics Engineers (IEEE), pp. 4025–4035, Oct. 2012. doi: 10.1109/tgrs.2012.2189776.  
  
K. C. Jezek, “Radiometric Approach for Estimating Relative Changes in Intraglacier Average Temperature”, *IEEE Transactions on Geoscience and Remote Sensing*, vol. 53, no. 1. Institute of Electrical and Electronics Engineers (IEEE), pp. 134–143, Jan. 2015. doi: 10.1109/tgrs.2014.2319265.  
  
S.-B. Kim, M. Moghaddam, L. Tsang, M. Burgin, X. Xuand E. G. Njoku, “Models of L-Band Radar Backscattering Coefficients Over Global Terrain for Soil Moisture Retrieval”, *IEEE Transactions on Geoscience and Remote Sensing*, vol. 52, no. 2. Institute of Electrical and Electronics Engineers (IEEE), pp. 1381–1396, Feb. 2014. doi: 10.1109/tgrs.2013.2250980.  
  
T.-H. Liao, S.-B. Kim, S. Tan, L. Tsang, C. Suand T. J. Jackson, “Multiple Scattering Effects With Cyclical Correction in Active Remote Sensing of Vegetated Surface Using Vector Radiative Transfer Theory”, *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 9, no. 4. Institute of Electrical and Electronics Engineers (IEEE), pp. 1414–1429, Apr. 2016. doi: 10.1109/jstars.2015.2505638.  
  
T.-H. Liao and L. Tsang, “Simulations of scattering matrix and coherency matrix for Pol-SAR applications of soil and vegetated surfaces using 3-D numerical solutions of Maxwell equation (NMM3D)”, *2015 IEEE International Geoscience and Remote Sensing Symposium (IGARSS)*. IEEE, Jul. 2015. doi: 10.1109/igarss.2015.7325861.  
  
T.-H. Liao, “Copolarized and Cross-Polarized Backscattering From Random Rough Soil Surfaces From L-Band to Ku-Band Using Numerical Solutions of Maxwell’s Equations With Near-Field Precondition”, *IEEE Transactions on Geoscience and Remote Sensing*, vol. 54, no. 2. Institute of Electrical and Electronics Engineers (IEEE), pp. 651–662, Feb. 2016. doi: 10.1109/tgrs.2015.2451671.  
  
T. Qiao, T.-H. Liaoand L. Tsang, “Accuracy studies of scattering by soil and ocean surfaces based on numerical simulations using Nystrom method”, *2016 IEEE International Geoscience and Remote Sensing Symposium (IGARSS)*. IEEE, Jul. 2016. doi: 10.1109/igarss.2016.7729959.  
  
M. Sanamzadeh, L. Tsang, J. T. Johnson, R. J. Burkholderand S. Tan, “Scattering of electromagnetic waves from 3D multilayer random rough surfaces based on the second-order small perturbation method: energy conservation, reflectivity, and emissivity”, *Journal of the Optical Society of America A*, vol. 34, no. 3. The Optical Society, p. 395, Feb. 22, 2017. doi: 10.1364/josaa.34.000395.  
  
Tai Qiao, T.-H. Liao, L. Tsang, D. Vandemarkand S. Yueh, “Radar backscattering from dielectric random rough surfaces using 3D numerical simulation of Maxwell’s equation”, *2016 Progress in Electromagnetic Research Symposium (PIERS)*. IEEE, Aug. 2016. doi: 10.1109/piers.2016.7735534.  
  
S. Tan, “Physical Models of Layered Polar Firn Brightness Temperatures From 0.5 to 2 GHz”, *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 8, no. 7. Institute of Electrical and Electronics Engineers (IEEE), pp. 3681–3691, Jul. 2015. doi: 10.1109/jstars.2015.2403286.  
  
S. Tan, W. Chang, L. Tsang, J. Lemmetyinenand M. Proksch, “Modeling Both Active and Passive Microwave Remote Sensing of Snow Using Dense Media Radiative Transfer (DMRT) Theory With Multiple Scattering and Backscattering Enhancement”, *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 8, no. 9. Institute of Electrical and Electronics Engineers (IEEE), pp. 4418–4430, Sep. 2015. doi: 10.1109/jstars.2015.2469290.  
  
S. Tan, Jiyue Zhu, L. Tsangand S. V. Nghiem, “Numerical simulation of Maxwell’s equation in 3D (NMM3D) applied to active and passive remote sensing of terrestrial snow and snow on sea ice”, *2016 Progress in Electromagnetic Research Symposium (PIERS)*. IEEE, Aug. 2016. doi: 10.1109/piers.2016.7735538.  
  
S. Tan, C. Xiongand L. Tsang, “Modeling snow anisotropy and backscattering co-polarization phase difference using bicontinuous media and numerical solutions of Maxwell equations”, *2016 IEEE International Geoscience and Remote Sensing Symposium (IGARSS)*. IEEE, Jul. 2016. doi: 10.1109/igarss.2016.7730374.  
  
L. Tsang, K.-H. Ding, S. Huangand X. Xu, “Electromagnetic Computation in Scattering of Electromagnetic Waves by Random Rough Surface and Dense Media in Microwave Remote Sensing of Land Surfaces”, *Proceedings of the IEEE*, vol. 101, no. 2. Institute of Electrical and Electronics Engineers (IEEE), pp. 255–279, Feb. 2013. doi: 10.1109/jproc.2012.2214011.  
  
L. Tsang, “Studies of the influence of deep subwavelength surface roughness on fields of plasmonic thin film based on Lippmann–Schwinger equation in the spectral domain”, *Journal of the Optical Society of America B*, vol. 32, no. 5. The Optical Society, p. 878, Apr. 23, 2015. doi: 10.1364/josab.32.000878.  
  
L. Tsang, “Active and Passive Vegetated Surface Models With Rough Surface Boundary Conditions From NMM3D”, *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 6, no. 3. Institute of Electrical and Electronics Engineers (IEEE), pp. 1698–1709, Jun. 2013. doi: 10.1109/jstars.2013.2257694.  
  
R. I. Petersen, D. R. Stegmanand P. J. Tackley, “A regime diagram of mobile lid convection with plate-like behavior”, *Physics of the Earth and Planetary Interiors*, vol. 241. Elsevier BV, pp. 65–76, Apr. 2015. doi: 10.1016/j.pepi.2015.01.002.  
  
E. Mehnert, “Basin-scale modeling for CO2 sequestration in the basal sandstone reservoir of the Illinois Basin—Improving the geologic model”, *Energy Procedia*, vol. 63. Elsevier BV, pp. 2949–2960, 2014. doi: 10.1016/j.egypro.2014.11.317.  
  
W. R. Roy, E. Mehnert, P. M. Berger, J. R. Damicoand R. T. Okwen, “Transport modeling at multiple scales for the Illinois Basin - Decatur Project”, *Greenhouse Gases: Science and Technology*, vol. 4, no. 5. Wiley, pp. 645–661, Apr. 21, 2014. doi: 10.1002/ghg.1424.  
  
Y. Fan, H. Liand G. Miguez-Macho, “Global Patterns of Groundwater Table Depth”, *Science*, vol. 339, no. 6122. American Association for the Advancement of Science (AAAS), pp. 940–943, Feb. 22, 2013. doi: 10.1126/science.1229881.  
  
L. Liu and D. R. Stegman, “Segmentation of the Farallon slab”, *Earth and Planetary Science Letters*, vol. 311, no. 1–2. Elsevier BV, pp. 1–10, Nov. 2011. doi: 10.1016/j.epsl.2011.09.027.  
  
L. Liu and D. R. Stegman, “Origin of Columbia River flood basalt controlled by propagating rupture of the Farallon slab”, *Nature*, vol. 482, no. 7385. Springer Science and Business Media LLC, pp. 386–389, Feb. 2012. doi: 10.1038/nature10749.  
  
R. I. Petersen, D. R. Stegmanand P. J. Tackley, “The subduction dichotomy of strong plates and weak slabs”, *Solid Earth*, vol. 8, no. 2. Copernicus GmbH, pp. 339–350, Mar. 24, 2017. doi: 10.5194/se-8-339-2017.  
  
M. P. Moschetti, S. Hartzell, L. Ramírez‐Guzmán, A. D. Frankel, S. J. Angsterand W. J. Stephenson, “3D Ground‐Motion Simulations of *M* w  7 Earthquakes on the Salt Lake City Segment of the Wasatch Fault Zone: Variability of Long‐Period ( *T* ≥1  s) Ground Motions and Sensitivity to Kinematic Rupture Parameters”, *Bulletin of the Seismological Society of America*. Seismological Society of America (SSA), Jun. 20, 2017. doi: 10.1785/0120160307.  
  
A. S. Bhaskar, C. Jantz, C. Welty, S. A. Drzyzgaand A. J. Miller, “Coupling of the Water Cycle with Patterns of Urban Growth in the Baltimore Metropolitan Region, United States”, *JAWRA Journal of the American Water Resources Association*, vol. 52, no. 6. Wiley, pp. 1509–1523, Nov. 03, 2016. doi: 10.1111/1752-1688.12479.  
  
M. D. Ballmer, G. Ito, C. J. Wolfeand S. C. Solomon, “Double layering of a thermochemical plume in the upper mantle beneath Hawaii”, *Earth and Planetary Science Letters*, vol. 376. Elsevier BV, pp. 155–164, Aug. 2013. doi: 10.1016/j.epsl.2013.06.022.  
  
Y. Fialko and J. Pearse, “Sombrero Uplift Above the Altiplano-Puna Magma Body: Evidence of a Ballooning Mid-Crustal Diapir”, *Science*, vol. 338, no. 6104. American Association for the Advancement of Science (AAAS), pp. 250–252, Oct. 12, 2012. doi: 10.1126/science.1226358.  
  
E. O. Lindsey and Y. Fialko, “Geodetic constraints on frictional properties and earthquake hazard in the Imperial Valley, Southern California”, *Journal of Geophysical Research: Solid Earth*, vol. 121, no. 2. American Geophysical Union (AGU), pp. 1097–1113, Feb. 2016. doi: 10.1002/2015jb012516.  
  
R. L. Weaver, “On the retrieval of attenuation and site amplifications from ambient noise on linear arrays: further numerical simulations”, *Geophysical Journal International*, vol. 193, no. 3. Oxford University Press (OUP), pp. 1644–1657, Mar. 20, 2013. doi: 10.1093/gji/ggt063.  
  
L. Leonard and C. J. Duffy, “Automating data-model workflows at a level 12 HUC scale: Watershed modeling in a distributed computing environment”, *Environmental Modelling & Software*, vol. 61. Elsevier BV, pp. 174–190, Nov. 2014. doi: 10.1016/j.envsoft.2014.07.015.  
  
L. Leonard and C. Duffy, “Visualization workflows for level-12 HUC scales: Towards an expert system for watershed analysis in a distributed computing environment”, *Environmental Modelling & Software*, vol. 78. Elsevier BV, pp. 163–178, Apr. 2016. doi: 10.1016/j.envsoft.2016.01.001.  
  
Y. Y. Liu, D. R. Maidment, D. G. Tarboton, X. Zhengand S. Wang, “A CyberGIS Integration and Computation Framework for High‐Resolution Continental‐Scale Flood Inundation Mapping”, *JAWRA Journal of the American Water Resources Association*, vol. 54, no. 4. Wiley, pp. 770–784, Jun. 12, 2018. doi: 10.1111/1752-1688.12660.  
  
Y. Liu, “A CyberGIS Approach to Generating High-resolution Height Above Nearest Drainage (HAND) Raster for National Flood Mapping”, *Unpublished*, 2016, doi: 10.13140/RG.2.2.24234.41925/1.  
  
K. Survila, A. A. Yιldιrιm, T. Li, Y. Y. Liu, D. G. Tarbotonand S. Wang, “A Scalable High-performance Topographic Flow Direction Algorithm for Hydrological Information Analysis”, *Proceedings of the XSEDE16 Conference on Diversity, Big Data, and Science at Scale*. ACM, Jul. 17, 2016. doi: 10.1145/2949550.2949571.  
  
A. A. Yιldιrιm, D. Tarboton, Y. Liu, N. S. Saziband S. Wang, “Accelerating TauDEM for Extracting Hydrology Information from National-Scale High Resolution Topographic Dataset”, *Proceedings of the XSEDE16 Conference on Diversity, Big Data, and Science at Scale*. ACM, Jul. 17, 2016. doi: 10.1145/2949550.2949582.  
  
M. Chen, F. Niu, Q. Liu, J. Trompand X. Zheng, “Multiparameter adjoint tomography of the crust and upper mantle beneath East Asia: 1. Model construction and comparisons”, *Journal of Geophysical Research: Solid Earth*, vol. 120, no. 3. American Geophysical Union (AGU), pp. 1762–1786, Mar. 2015. doi: 10.1002/2014jb011638.  
  
M. Chen, “Lithospheric foundering and underthrusting imaged beneath Tibet”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Jun. 06, 2017. doi: 10.1038/ncomms15659.  
  
Y. Liu, F. Niu, M. Chenand W. Yang, “3-D crustal and uppermost mantle structure beneath NE China revealed by ambient noise adjoint tomography”, *Earth and Planetary Science Letters*, vol. 461. Elsevier BV, pp. 20–29, Mar. 2017. doi: 10.1016/j.epsl.2016.12.029.  
  
K. Tao, S. P. Grandand F. Niu, “Full-waveform inversion of triplicated data using a normalized-correlation-coefficient-based misfit function”, *Geophysical Journal International*, vol. 210, no. 3. Oxford University Press (OUP), pp. 1517–1524, Jun. 07, 2017. doi: 10.1093/gji/ggx249.  
  
K. Tao, S. P. Grandand F. Niu, “Seismic Structure of the Upper Mantle Beneath Eastern Asia From Full Waveform Seismic Tomography”, *Geochemistry, Geophysics, Geosystems*, vol. 19, no. 8. American Geophysical Union (AGU), pp. 2732–2763, Aug. 2018. doi: 10.1029/2018gc007460.  
  
M. Chen, V. C. Manea, F. Niu, S. S. Weiand E. Kiser, “Genesis of Intermediate‐Depth and Deep Intraslab Earthquakes beneath Japan Constrained by Seismic Tomography, Seismicity, and Thermal Modeling”, *Geophysical Research Letters*, vol. 46, no. 4. American Geophysical Union (AGU), pp. 2025–2036, Feb. 21, 2019. doi: 10.1029/2018gl080025.  
  
M. Chen, F. Niu, Q. Liuand J. Tromp, “Mantle‐driven uplift of Hangai Dome: New seismic constraints from adjoint tomography”, *Geophysical Research Letters*, vol. 42, no. 17. American Geophysical Union (AGU), pp. 6967–6974, Sep. 03, 2015. doi: 10.1002/2015gl065018.  
  
M. Chen, H. Huang, H. Yao, R. van der Hilstand F. Niu, “Low wave speed zones in the crust beneath SE Tibet revealed by ambient noise adjoint tomography”, *Geophysical Research Letters*, vol. 41, no. 2. American Geophysical Union (AGU), pp. 334–340, Jan. 22, 2014. doi: 10.1002/2013gl058476.  
  
M. L. Barnes and C. Welty, “Quantifying Water Balance Components at a Permeable Pavement Site Using a Coupled Groundwater–Surface Water Model”, *Journal of Hydrologic Engineering*, vol. 24, no. 7. American Society of Civil Engineers (ASCE), Jul. 2019. doi: 10.1061/(asce)he.1943-5584.0001789.  
  
T. C. Lim and C. Welty, “Assessing Variability and Uncertainty in Green Infrastructure Planning Using a High-Resolution Surface-Subsurface Hydrological Model and Site-Monitored Flow Data”, *Frontiers in Built Environment*, vol. 4. Frontiers Media SA, Dec. 04, 2018. doi: 10.3389/fbuil.2018.00071.  
  
H. Xu, Y. Cui, J. H. Dieterich, K. Richards-Dinger, E. Poyrazand D. J. Choi, “Aftershock sequence simulations using synthetic earthquakes and rate-state seismicity formulation”, *Earthquake Science*, vol. 27, no. 4. Elsevier BV, pp. 401–410, Jul. 11, 2014. doi: 10.1007/s11589-014-0087-7.  
  
E. Poyraz, H. Xuand Y. Cui, “Application-specific I/O Optimizations on Petascale Supercomputers”, *Procedia Computer Science*, vol. 29. Elsevier BV, pp. 910–923, 2014. doi: 10.1016/j.procs.2014.05.082.  
  
K. Key, S. Constable, L. Liuand A. Pommier, “Electrical image of passive mantle upwelling beneath the northern East Pacific Rise”, *Nature*, vol. 495, no. 7442. Springer Science and Business Media LLC, pp. 499–502, Mar. 2013. doi: 10.1038/nature11932.  
  
L. Liu, “Rejuvenation of Appalachian topography caused by subsidence-induced differential erosion”, *Nature Geoscience*, vol. 7, no. 7. Springer Science and Business Media LLC, pp. 518–523, Jun. 15, 2014. doi: 10.1038/ngeo2187.  
  
L. Liu, “Constraining Cretaceous subduction polarity in eastern Pacific from seismic tomography and geodynamic modeling”, *Geophysical Research Letters*, vol. 41, no. 22. American Geophysical Union (AGU), pp. 8029–8036, Nov. 22, 2014. doi: 10.1002/2014gl061988.  
  
L. Liu and J. S. Zhang, “Differential contraction of subducted lithosphere layers generates deep earthquakes”, *Earth and Planetary Science Letters*, vol. 421. Elsevier BV, pp. 98–106, Jul. 2015. doi: 10.1016/j.epsl.2015.03.053.  
  
L. Liu and Q. Zhou, “Deep recycling of oceanic asthenosphere material during subduction”, *Geophysical Research Letters*, vol. 42, no. 7. American Geophysical Union (AGU), pp. 2204–2211, Apr. 08, 2015. doi: 10.1002/2015gl063633.  
  
M. S. Avery, C. G. Constable, C. J. Daviesand D. Gubbins, “Spectral methods for analyzing energy balances in geodynamo simulations”, *Physics of the Earth and Planetary Interiors*, vol. 286. Elsevier BV, pp. 127–137, Jan. 2019. doi: 10.1016/j.pepi.2018.10.002.  
  
A. Chourasia, “Visualization of Geodynamo Simulations”, *Proceedings of the XSEDE16 Conference on Diversity, Big Data, and Science at Scale*. ACM, Jul. 17, 2016. doi: 10.1145/2949550.2952772.  
  
X. Meng and Z. Peng, “Seismicity rate changes in the Salton Sea Geothermal Field and the San Jacinto Fault Zone after the 2010 Mw 7.2 El Mayor-Cucapah earthquake”, *Geophysical Journal International*, vol. 197, no. 3. Oxford University Press (OUP), pp. 1750–1762, Apr. 21, 2014. doi: 10.1093/gji/ggu085.  
  
X. Meng and Z. Peng, “Increasing lengths of aftershock zones with depths of moderate-size earthquakes on the San Jacinto Fault suggests triggering of deep creep in the middle crust”, *Geophysical Journal International*, vol. 204, no. 1. Oxford University Press (OUP), pp. 250–261, Nov. 23, 2015. doi: 10.1093/gji/ggv445.  
  
J. I. Walter, X. Meng, Z. Peng, S. Y. Schwartz, A. V. Newmanand M. Protti, “Far-field triggering of foreshocks near the nucleation zone of the 5 September 2012 (MW 7.6) Nicoya Peninsula, Costa Rica earthquake”, *Earth and Planetary Science Letters*, vol. 431. Elsevier BV, pp. 75–86, Dec. 2015. doi: 10.1016/j.epsl.2015.09.017.  
  
G. Xing, F. Niu, M. Chenand Y. Yang, “Effects of shallow density structure on the inversion for crustal shear wave speeds in surface wave tomography”, *Geophysical Journal International*, vol. 205, no. 2. Oxford University Press (OUP), pp. 1144–1152, Mar. 03, 2016. doi: 10.1093/gji/ggw064.  
  
P. L. Falkingham and S. M. Gatesy, “The birth of a dinosaur footprint: Subsurface 3D motion reconstruction and discrete element simulation reveal track ontogeny”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 51. Proceedings of the National Academy of Sciences, pp. 18279–18284, Dec. 08, 2014. doi: 10.1073/pnas.1416252111.  
  
G. W. Bergantz, J. M. Schleicherand A. Burgisser, “Open-system dynamics and mixing in magma mushes”, *Nature Geoscience*, vol. 8, no. 10. Springer Science and Business Media LLC, pp. 793–796, Sep. 07, 2015. doi: 10.1038/ngeo2534.  
  
S. Pokhrel, B. Nguyen, M. Rodriguez, E. Bernabeuand J. J. Simpson, “A Finite Difference Time Domain Investigation of Electric Field Enhancements Along Ocean‐Continent Boundaries During Space Weather Events”, *Journal of Geophysical Research: Space Physics*, vol. 123, no. 6. American Geophysical Union (AGU), pp. 5033–5046, Jun. 2018. doi: 10.1029/2017ja024648.  
  
S. Saha and U. Becker, “The effect of the aliphatic carboxylate linkers on the electronic structures, chemical bonding and optical properties of the uranium-based metal–organic frameworks”, *RSC Advances*, vol. 5, no. 34. Royal Society of Chemistry (RSC), pp. 26735–26748, 2015. doi: 10.1039/c5ra01335f.  
  
S. M. Walker, M. C. Marcano, S. Kim, S. D. Taylorand U. Becker, “Understanding Calcite Wettability Alteration through Surface Potential Measurements and Molecular Simulations”, *The Journal of Physical Chemistry C*, vol. 121, no. 50. American Chemical Society (ACS), pp. 28017–28030, Nov. 22, 2017. doi: 10.1021/acs.jpcc.7b09565.  
  
J. Dufek, “The Fluid Mechanics of Pyroclastic Density Currents”, *Annual Review of Fluid Mechanics*, vol. 48, no. 1. Annual Reviews, pp. 459–485, Jan. 03, 2016. doi: 10.1146/annurev-fluid-122414-034252.  
  
R. Maguire, J. Ritsema, M. Bonnin, P. E. van Kekenand S. Goes, “Evaluating the Resolution of Deep Mantle Plumes in Teleseismic Traveltime Tomography”, *Journal of Geophysical Research: Solid Earth*, vol. 123, no. 1. American Geophysical Union (AGU), pp. 384–400, Jan. 2018. doi: 10.1002/2017jb014730.  
  
M.-J. Noh and I. M. Howat, “Automated stereo-photogrammetric DEM generation at high latitudes: Surface Extraction with TIN-based Search-space Minimization (SETSM) validation and demonstration over glaciated regions”, *GIScience & Remote Sensing*, vol. 52, no. 2. Informa UK Limited, pp. 198–217, Feb. 19, 2015. doi: 10.1080/15481603.2015.1008621.  
  
R. I. Citron, M. Mangaand E. Tan, “A hybrid origin of the Martian crustal dichotomy: Degree-1 convection antipodal to a giant impact”, *Earth and Planetary Science Letters*, vol. 491. Elsevier BV, pp. 58–66, Jun. 2018. doi: 10.1016/j.epsl.2018.03.031.  
  
K. Yuan and B. Romanowicz, “Seismic evidence for partial melting at the root of major hot spot plumes”, *Science*, vol. 357, no. 6349. American Association for the Advancement of Science (AAAS), pp. 393–397, Jul. 28, 2017. doi: 10.1126/science.aan0760.  
  
A. Nayak and D. S. Dreger, “Source Inversion of Seismic Events Associated with the Sinkhole at Napoleonville Salt Dome, Louisiana using a 3D Velocity Model”, *Geophysical Journal International*. Oxford University Press (OUP), May 21, 2018. doi: 10.1093/gji/ggy202.  
  
D. Tang, C. Ma, Y. Wangand X. Xu, “Multiscale evaluation of NCEP and CRUNCEP data sets at 90 large U.S. cities”, *Journal of Geophysical Research: Atmospheres*, vol. 122, no. 14. American Geophysical Union (AGU), pp. 7433–7444, Jul. 26, 2017. doi: 10.1002/2016jd026165.  
  
A. DAMSGAARD, J. SUCKALE, J. A. PIOTROWSKI, M. HOUSSAIS, M. R. SIEGFRIEDand H. A. FRICKER, “Sediment behavior controls equilibrium width of subglacial channels”, *Journal of Glaciology*, vol. 63, no. 242. Cambridge University Press (CUP), pp. 1034–1048, Nov. 27, 2017. doi: 10.1017/jog.2017.71.  
  
S. Lu, “Hall effect control of magnetotail dawn‐dusk asymmetry: A three‐dimensional global hybrid simulation”, *Journal of Geophysical Research: Space Physics*, vol. 121, no. 12. American Geophysical Union (AGU), Dec. 2016. doi: 10.1002/2016ja023325.  
  
T. L. Swetnam, “Considerations for Achieving Cross-Platform Point Cloud Data Fusion across Different Dryland Ecosystem Structural States”, *Frontiers in Plant Science*, vol. 8. Frontiers Media SA, Jan. 10, 2018. doi: 10.3389/fpls.2017.02144.  
  
Y. Chen, Y. Li, A. J. Valocchiand K. T. Christensen, “Lattice Boltzmann simulations of liquid CO2 displacing water in a 2D heterogeneous micromodel at reservoir pressure conditions”, *Journal of Contaminant Hydrology*, vol. 212. Elsevier BV, pp. 14–27, May 2018. doi: 10.1016/j.jconhyd.2017.09.005.  
  
Y. Chen, A. J. Valocchi, Q. Kangand H. S. Viswanathan, “Inertial Effects During the Process of Supercritical CO 2 Displacing Brine in a Sandstone: Lattice Boltzmann Simulations Based on the Continuum‐Surface‐Force and Geometrical Wetting Models”, *Water Resources Research*, vol. 55, no. 12. American Geophysical Union (AGU), pp. 11144–11165, Dec. 2019. doi: 10.1029/2019wr025746.  
  
J. Jiménez‐Martínez, “Homogenization of Dissolution and Enhanced Precipitation Induced by Bubbles in Multiphase Flow Systems”, *Geophysical Research Letters*, vol. 47, no. 7. American Geophysical Union (AGU), Apr. 06, 2020. doi: 10.1029/2020gl087163.  
  
J. Tudek, “In situ contact angle measurements of liquid CO2, brine, and Mount Simon sandstone core using micro X-ray CT imaging, sessile drop, and Lattice Boltzmann modeling”, *Journal of Petroleum Science and Engineering*, vol. 155. Elsevier BV, pp. 3–10, Jul. 2017. doi: 10.1016/j.petrol.2017.01.047.  
  
B. Zhao, “Comprehensive comparison of pore-scale models for multiphase flow in porous media”, *Proceedings of the National Academy of Sciences*, vol. 116, no. 28. Proceedings of the National Academy of Sciences, pp. 13799–13806, Jun. 21, 2019. doi: 10.1073/pnas.1901619116.  
  
M. Mookherjee, D. Mainprice, K. Maheshwari, O. Heinonen, D. Pateland A. Hariharan, “Pressure induced elastic softening in framework aluminosilicate- albite (NaAlSi3O8)”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Oct. 13, 2016. doi: 10.1038/srep34815.  
  
J. S. Salinas, M. Shringarpure, M. I. Canteroand S. Balachandar, “Mixing at a sediment concentration interface in turbulent open channel flow”, *Environmental Fluid Mechanics*, vol. 18, no. 1. Springer Science and Business Media LLC, pp. 173–200, Mar. 08, 2017. doi: 10.1007/s10652-017-9521-4.  
  
S. Klesse, “Continental‐scale tree‐ring‐based projection of Douglas‐fir growth: Testing the limits of space‐for‐time substitution”, *Global Change Biology*, vol. 26, no. 9. Wiley, pp. 5146–5163, Jun. 30, 2020. doi: 10.1111/gcb.15170.  
  
T. L. Swetnam, P. D. Brooks, H. R. Barnard, A. A. Harpoldand E. L. Gallo, “Topographically driven differences in energy and water constrain climatic control on forest carbon sequestration”, *Ecosphere*, vol. 8, no. 4. Wiley, Apr. 2017. doi: 10.1002/ecs2.1797.  
  
A. Madson, E. Fielding, Y. Shengand K. Cavanaugh, “High-Resolution Spaceborne, Airborne and In Situ Landslide Kinematic Measurements of the Slumgullion Landslide in Southwest Colorado”, *Remote Sensing*, vol. 11, no. 3. MDPI AG, p. 265, Jan. 29, 2019. doi: 10.3390/rs11030265.  
  
K. Wang and Y. Fialko, “Observations and Modeling of Coseismic and Postseismic Deformation Due To the 2015 *M w* 7.8 Gorkha (Nepal) Earthquake”, *Journal of Geophysical Research: Solid Earth*, vol. 123, no. 1. American Geophysical Union (AGU), pp. 761–779, Jan. 2018. doi: 10.1002/2017jb014620.  
  
K. Wang, X. Xuand Y. Fialko, “Improving Burst Alignment in TOPS Interferometry With Bivariate Enhanced Spectral Diversity”, *IEEE Geoscience and Remote Sensing Letters*, vol. 14, no. 12. Institute of Electrical and Electronics Engineers (IEEE), pp. 2423–2427, Dec. 2017. doi: 10.1109/lgrs.2017.2767575.  
  
C. Roy and B. A. Romanowicz, “On the Implications of A Priori Constraints in Transdimensional Bayesian Inversion for Continental Lithospheric Layering”, *Journal of Geophysical Research: Solid Earth*, vol. 122, no. 12. American Geophysical Union (AGU), pp. 10, 118–10, 131, Dec. 2017. doi: 10.1002/2017jb014968.  
  
J. D. Gardiner, K. A. Tomko, M.-J. Nohand I. M. Howat, “Code Optimization and Stabilization for a High-Resolution Terrain Generation Application”, *Proceedings of the Practice and Experience on Advanced Research Computing*. ACM, Jul. 22, 2018. doi: 10.1145/3219104.3229241.  
  
J. D. Kubicki, N. Kabengi, M. Chrysochoouand N. Bompoti, “Density functional theory modeling of chromate adsorption onto ferrihydrite nanoparticles”, *Geochemical Transactions*, vol. 19, no. 1. Springer Science and Business Media LLC, Mar. 01, 2018. doi: 10.1186/s12932-018-0053-8.  
  
R. Zhang, “Imaging Hydraulic Fractures Under Energized Steel Casing by Convolutional Neural Networks”, *IEEE Transactions on Geoscience and Remote Sensing*, vol. 58, no. 12. Institute of Electrical and Electronics Engineers (IEEE), pp. 8831–8839, Dec. 2020. doi: 10.1109/tgrs.2020.2991011.  
  
R. Zhang, “Memory-Efficient 3-D LWD Solver With the Flipped Total Field/Scattered Field-Based DGFD Method”, *IEEE Geoscience and Remote Sensing Letters*, vol. 17, no. 9. Institute of Electrical and Electronics Engineers (IEEE), pp. 1498–1502, Sep. 2020. doi: 10.1109/lgrs.2019.2950659.  
  
M. Li and S. Zhong, “Lateral Motion of Mantle Plumes in 3‐D Geodynamic Models”, *Geophysical Research Letters*, vol. 46, no. 9. American Geophysical Union (AGU), pp. 4685–4693, May 15, 2019. doi: 10.1029/2018gl081404.  
  
J. R. Dierauer and C. Zhu, “Drought in the Twenty-First Century in a Water-Rich Region: Modeling Study of the Wabash River Watershed, USA”, *Water*, vol. 12, no. 1. MDPI AG, p. 181, Jan. 08, 2020. doi: 10.3390/w12010181.  
  
C. Chu, “Spatially separating redox centers on 2D carbon nitride with cobalt single atom for photocatalytic H 2 O 2 production”, *Proceedings of the National Academy of Sciences*, vol. 117, no. 12. Proceedings of the National Academy of Sciences, pp. 6376–6382, Mar. 11, 2020. doi: 10.1073/pnas.1913403117.  
  
G. Petropoulos and G. L. Fenves, “Interprocessor communication for high performance, explicit time integration”, *Engineering with Computers*, vol. 26, no. 2. Springer Science and Business Media LLC, pp. 149–157, Jan. 28, 2010. doi: 10.1007/s00366-010-0174-x.  
  
X. S. Liu, “Fast Trabecular Bone Strength Predictions of HR-pQCT and Individual Trabeculae Segmentation-Based Plate and Rod Finite Element Model Discriminate Postmenopausal Vertebral Fractures”, *Journal of Bone and Mineral Research*, vol. 28, no. 7. Wiley, pp. 1666–1678, Jun. 18, 2013. doi: 10.1002/jbmr.1919.  
  
J. Wang, G. J. Kazakia, B. Zhou, X. T. Shiand X. E. Guo, “Distinct Tissue Mineral Density in Plate‐ and Rod‐like Trabeculae of Human Trabecular Bone”, *Journal of Bone and Mineral Research*, vol. 30, no. 9. Wiley, pp. 1641–1650, Jun. 11, 2015. doi: 10.1002/jbmr.2498.  
  
J. Wang, “Trabecular plates and rods determine elastic modulus and yield strength of human trabecular bone”, *Bone*, vol. 72. Elsevier BV, pp. 71–80, Mar. 2015. doi: 10.1016/j.bone.2014.11.006.  
  
B. Zhou, X. Sherry Liu, J. Wang, X. Lucas Lu, A. J. Fieldsand X. Edward Guo, “Dependence of mechanical properties of trabecular bone on plate–rod microstructure determined by individual trabecula segmentation (ITS)”, *Journal of Biomechanics*, vol. 47, no. 3. Elsevier BV, pp. 702–708, Feb. 2014. doi: 10.1016/j.jbiomech.2013.11.039.  
  
B. Zhou, “Bone density, microarchitecture and stiffness in Caucasian and Caribbean Hispanic postmenopausal American women”, *Bone Research*, vol. 2, no. 1. Springer Science and Business Media LLC, Sep. 16, 2014. doi: 10.1038/boneres.2014.16.  
  
B. Zhou, “High-resolution peripheral quantitative computed tomography (HR-pQCT) can assess microstructural and biomechanical properties of both human distal radius and tibia: Ex vivo computational and experimental validations”, *Bone*, vol. 86. Elsevier BV, pp. 58–67, May 2016. doi: 10.1016/j.bone.2016.02.016.  
  
M. Eshraghi, S. D. Felicelliand B. Jelinek, “Three dimensional simulation of solutal dendrite growth using lattice Boltzmann and cellular automaton methods”, *Journal of Crystal Growth*, vol. 354, no. 1. Elsevier BV, pp. 129–134, Sep. 2012. doi: 10.1016/j.jcrysgro.2012.06.002.  
  
P.-H. Chang, M. S. Bahramy, N. Nagaosaand B. K. Nikolić, “Giant Thermoelectric Effect in Graphene-Based Topological Insulators with Heavy Adatoms and Nanopores”, *Nano Letters*, vol. 14, no. 7. American Chemical Society (ACS), pp. 3779–3784, Jun. 23, 2014. doi: 10.1021/nl500755m.  
  
P.-H. Chang, H. Liuand B. K. Nikolić, “First-principles versus semi-empirical modeling of global and local electronic transport properties of graphene nanopore-based sensors for DNA sequencing”, *Journal of Computational Electronics*, vol. 13, no. 4. Springer Science and Business Media LLC, pp. 847–856, Sep. 03, 2014. doi: 10.1007/s10825-014-0614-8.  
  
P.-H. Chang, T. Markussen, S. Smidstrup, K. Stokbroand B. K. Nikolić, “Nonequilibrium spin texture within a thin layer below the surface of current-carrying topological insulator: A first-principles quantum transport study”, *Physical Review B*, vol. 92, no. 20. American Physical Society (APS), Nov. 10, 2015. doi: 10.1103/physrevb.92.201406.  
  
K. Dolui and B. K. Nikolić, “Spin-memory loss due to spin-orbit coupling at ferromagnet/heavy-metal interfaces: *Ab initio* spin-density matrix approach”, *Physical Review B*, vol. 96, no. 22. American Physical Society (APS), Dec. 12, 2017. doi: 10.1103/physrevb.96.220403.  
  
J. M. Marmolejo-Tejada, “Proximity Band Structure and Spin Textures on Both Sides of Topological-Insulator/Ferromagnetic-Metal Interface and Their Charge Transport Probes”, *Nano Letters*, vol. 17, no. 9. American Chemical Society (ACS), pp. 5626–5633, Aug. 16, 2017. doi: 10.1021/acs.nanolett.7b02511.  
  
K. K. Saha and B. K. Nikolić, “Negative differential resistance in graphene-nanoribbon–carbon-nanotube crossbars: a first-principles multiterminal quantum transport study”, *Journal of Computational Electronics*, vol. 12, no. 4. Springer Science and Business Media LLC, pp. 542–552, Nov. 23, 2013. doi: 10.1007/s10825-013-0534-z.  
  
X.-L. Sheng and B. K. Nikolić, “Monolayer of the transition metal trichloride : A playground for two-dimensional magnetism, room-temperature quantum anomalous Hall effect, and topological phase transitions”, *Physical Review B*, vol. 95, no. 20. American Physical Society (APS), May 03, 2017. doi: 10.1103/physrevb.95.201402.  
  
H. Babaee, P. Perdikaris, C. Chryssostomidisand G. E. Karniadakis, “Multi-fidelity modelling of mixed convection based on experimental correlations and numerical simulations”, *Journal of Fluid Mechanics*, vol. 809. Cambridge University Press (CUP), pp. 895–917, Nov. 21, 2016. doi: 10.1017/jfm.2016.718.  
  
H. Babaee and T. P. Sapsis, “A minimization principle for the description of modes associated with finite-time instabilities”, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 472, no. 2186. The Royal Society, p. 20150779, Feb. 2016. doi: 10.1098/rspa.2015.0779.  
  
A. Russakoff, Y. Li, S. Heand K. Varga, “Accuracy and computational efficiency of real-time subspace propagation schemes for the time-dependent density functional theory”, *The Journal of Chemical Physics*, vol. 144, no. 20. AIP Publishing, p. 204125, May 28, 2016. doi: 10.1063/1.4952646.  
  
D. Kidd, C. Covington, Y. Liand K. Varga, “Volkov basis for simulation of interaction of strong laser pulses and solids”, *Physical Review B*, vol. 97, no. 2. American Physical Society (APS), Jan. 09, 2018. doi: 10.1103/physrevb.97.024303.  
  
J. Wang, “Hollow PtPdRh Nanocubes with Enhanced Catalytic Activities for In Vivo Clearance of Radiation‐Induced ROS via Surface‐Mediated Bond Breaking”, *Small*, vol. 14, no. 13. Wiley, p. 1703736, Feb. 09, 2018. doi: 10.1002/smll.201703736.  
  
M. J. Fisher and J. Apt, “Emissions and Economics of Behind-the-Meter Electricity Storage”, *Environmental Science & Technology*, vol. 51, no. 3. American Chemical Society (ACS), pp. 1094–1101, Jan. 11, 2017. doi: 10.1021/acs.est.6b03536.  
  
M. Fisher, J. Aptand F. Sowell, “The economics of commercial demand response for spinning reserve”, *Energy Systems*, vol. 9, no. 1. Springer Science and Business Media LLC, pp. 3–23, Mar. 17, 2017. doi: 10.1007/s12667-017-0236-x.  
  
M. A. Eftekhar, “Versatile supercontinuum generation in parabolic multimode optical fibers”, *Optics Express*, vol. 25, no. 8. The Optical Society, p. 9078, Apr. 10, 2017. doi: 10.1364/oe.25.009078.  
  
Z. Sanjabi Eznaveh, “Tailoring frequency generation in uniform and concatenated multimode fibers”, *Optics Letters*, vol. 42, no. 5. The Optical Society, p. 1015, Mar. 01, 2017. doi: 10.1364/ol.42.001015.  
  
A. O’Hara, R. E. Kahn, Y.-Y. Zhangand S. T. Pantelides, “Defect-mediated leakage in lithium intercalated bilayer graphene”, *AIP Advances*, vol. 7, no. 4. AIP Publishing, p. 045205, Apr. 2017. doi: 10.1063/1.4980052.  
  
M. A. Eftekhar, “Broadband supercontinuum generation in tapered multimode graded-index optical fibers”, *Conference on Lasers and Electro-Optics*. OSA, 2017. doi: 10.1364/cleo\_si.2017.sth1k.7.  
  
M. A. Eftekhar, “Accelerating nonlinear interactions in tapered multimode fibers”, *Conference on Lasers and Electro-Optics*. OSA, 2018. doi: 10.1364/cleo\_qels.2018.fth1m.3.  
  
M. A. Eftekhar, Z. Sanjabi-Eznaveh, J. E. Antonio-Lopez, F. W. Wise, D. N. Christodoulidesand R. Amezcua-Correa, “Instant and efficient second-harmonic generation and downconversion in unprepared graded-index multimode fibers”, *Optics Letters*, vol. 42, no. 17. The Optical Society, p. 3478, Aug. 30, 2017. doi: 10.1364/ol.42.003478.  
  
Y. Chu, “Superior Performance of 5-nm Gate Length GaN Nanowire nFET for Digital Logic Applications”, *IEEE Electron Device Letters*, vol. 40, no. 6. Institute of Electrical and Electronics Engineers (IEEE), pp. 874–877, Jun. 2019. doi: 10.1109/led.2019.2894416.  
  
S.-C. Lu, “Design Guidelines and Limitations of Multilayer Two-dimensional Vertical Tunneling FETs for UltraLow Power Logic Applications”, *2018 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)*. IEEE, Sep. 2018. doi: 10.1109/sispad.2018.8551731.  
  
A. Venugopal, T. Quand R. H. Victora, “Manipulation of nonlinear magnon effects using a secondary microwave frequency”, *Applied Physics Letters*, vol. 117, no. 15. AIP Publishing, p. 152404, Oct. 12, 2020. doi: 10.1063/5.0022227.  
  
J. A. Hernandez, A. Gamezand I. L. Al-Qadi, “Effect of Wide-Base Tires on Nationwide Flexible Pavement Systems: Numerical Modeling”, *Transportation Research Record: Journal of the Transportation Research Board*, vol. 2590, no. 1. SAGE Publications, pp. 104–112, Jan. 2016. doi: 10.3141/2590-12.  
  
J. A. Hernandez, A. Gamez, I. L. Al-Qadiand M. De Beer, “Analytical Approach for Predicting Three-Dimensional Tire–Pavement Contact Load”, *Transportation Research Record: Journal of the Transportation Research Board*, vol. 2456, no. 1. SAGE Publications, pp. 75–84, Jan. 2014. doi: 10.3141/2456-08.  
  
A. Oskooi, “Texturing the cathode of white organic light-emitting diodes with a lattice of nanoscale scatterers for enhanced light out-coupling”, *Applied Physics Letters*, vol. 106, no. 4. AIP Publishing, p. 041111, Jan. 26, 2015. doi: 10.1063/1.4907253.  
  
Z. Yin, K. R. Reddyand P. A. Durbin, “On the dynamic computation of the model constant in delayed detached eddy simulation”, *Physics of Fluids*, vol. 27, no. 2. AIP Publishing, p. 025105, Feb. 2015. doi: 10.1063/1.4907746.  
  
M. Nekouei and S. A. Vanapalli, “Volume-of-fluid simulations in microfluidic T-junction devices: Influence of viscosity ratio on droplet size”, *Physics of Fluids*, vol. 29, no. 3. AIP Publishing, p. 032007, Mar. 2017. doi: 10.1063/1.4978801.  
  
Q. Li, “Reconstructing the Surface of Gold Nanoclusters by Cadmium Doping”, *Journal of the American Chemical Society*, vol. 139, no. 49. American Chemical Society (ACS), pp. 17779–17782, Dec. 04, 2017. doi: 10.1021/jacs.7b11491.  
  
S. Salehyar, Y. Liand Q. Zhu, “Fully-coupled time-domain simulations of the response of a floating wind turbine to non-periodic disturbances”, *Renewable Energy*, vol. 111. Elsevier BV, pp. 214–226, Oct. 2017. doi: 10.1016/j.renene.2017.04.017.  
  
E. M. Rathje, “DesignSafe: New Cyberinfrastructure for Natural Hazards Engineering”, *Natural Hazards Review*, vol. 18, no. 3. American Society of Civil Engineers (ASCE), Aug. 2017. doi: 10.1061/(asce)nh.1527-6996.0000246.  
  
N. Austin, J. Yeand G. Mpourmpakis, “CO2 activation on Cu-based Zr-decorated nanoparticles”, *Catalysis Science & Technology*, vol. 7, no. 11. Royal Society of Chemistry (RSC), pp. 2245–2251, 2017. doi: 10.1039/c6cy02628a.  
  
N. Austin, S. Zhao, J. R. McKone, R. Jinand G. Mpourmpakis, “Elucidating the active sites for CO2 electroreduction on ligand-protected Au25 nanoclusters”, *Catalysis Science & Technology*, vol. 8, no. 15. Royal Society of Chemistry (RSC), pp. 3795–3805, 2018. doi: 10.1039/c8cy01099d.  
  
J. Chung, I. Granja, M. G. Taylor, G. Mpourmpakis, J. R. Asplinand J. D. Rimer, “Molecular modifiers reveal a mechanism of pathological crystal growth inhibition”, *Nature*, vol. 536, no. 7617. Springer Science and Business Media LLC, pp. 446–450, Aug. 2016. doi: 10.1038/nature19062.  
  
J. Chung, M. G. Taylor, I. Granja, J. R. Asplin, G. Mpourmpakisand J. D. Rimer, “Factors Differentiating the Effectiveness of Polyprotic Acids as Inhibitors of Calcium Oxalate Crystallization in Kidney Stone Disease”, *Crystal Growth & Design*, vol. 18, no. 9. American Chemical Society (ACS), pp. 5617–5627, Jul. 27, 2018. doi: 10.1021/acs.cgd.8b00945.  
  
J. Dean, Y. Yang, N. Austin, G. Veserand G. Mpourmpakis, “Design of Copper‐Based Bimetallic Nanoparticles for Carbon Dioxide Adsorption and Activation”, *ChemSusChem*, vol. 11, no. 7. Wiley, pp. 1169–1178, Feb. 28, 2018. doi: 10.1002/cssc.201702342.  
  
M. G. Taylor and G. Mpourmpakis, “Thermodynamic stability of ligand-protected metal nanoclusters”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Jul. 07, 2017. doi: 10.1038/ncomms15988.  
  
S. Zhao, “Influence of Atomic-Level Morphology on Catalysis: The Case of Sphere and Rod-Like Gold Nanoclusters for CO2 Electroreduction”, *ACS Catalysis*, vol. 8, no. 6. American Chemical Society (ACS), pp. 4996–5001, Apr. 26, 2018. doi: 10.1021/acscatal.8b00365.  
  
H. L. Kline and J. J. Alonso, “Adjoint of Generalized Outflow-Based Functionals Applied to Hypersonic Inlet Design”, *AIAA Journal*, vol. 55, no. 11. American Institute of Aeronautics and Astronautics (AIAA), pp. 3903–3915, Nov. 2017. doi: 10.2514/1.j055863.  
  
M. K. Hasan and A. Gross, “Numerical Investigation of Radial Flow in Solar Chimney Power Plant Collector”, *55th AIAA Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 05, 2017. doi: 10.2514/6.2017-1010.  
  
A. Bleem and V. Daggett, “Structural and functional diversity among amyloid proteins: Agents of disease, building blocks of biology, and implications for molecular engineering”, *Biotechnology and Bioengineering*, vol. 114, no. 1. Wiley, pp. 7–20, Aug. 23, 2016. doi: 10.1002/bit.26059.  
  
Z. Lavrich, Z. Taie, S. Menon, S. Daly, D. Hallidayand C. Hagen, “Internal Combustion Engines as Fluidized Bed Reactors”, *Volume 1: Large Bore Engines; Fuels; Advanced Combustion*. American Society of Mechanical Engineers, Oct. 15, 2017. doi: 10.1115/icef2017-3524.  
  
Z. Lavrich, D. R. Wagner, Z. Taie, D. Hallidayand C. L. Hagen, “Design considerations for small scale rotating fluidized beds in static geometry with screens for fine particles”, *Chemical Engineering Research and Design*, vol. 137. Elsevier BV, pp. 89–100, Sep. 2018. doi: 10.1016/j.cherd.2018.06.044.  
  
S. I. Allec and B. M. Wong, “Inconsistencies in the Electronic Properties of Phosphorene Nanotubes: New Insights from Large-Scale DFT Calculations”, *The Journal of Physical Chemistry Letters*, vol. 7, no. 21. American Chemical Society (ACS), pp. 4340–4345, Oct. 21, 2016. doi: 10.1021/acs.jpclett.6b02271.  
  
L. N. Anderson, F. W. Aquino, A. E. Raeber, X. Chenand B. M. Wong, “Halogen Bonding Interactions: Revised Benchmarks and a New Assessment of Exchange vs Dispersion”, *Journal of Chemical Theory and Computation*, vol. 14, no. 1. American Chemical Society (ACS), pp. 180–190, Dec. 22, 2017. doi: 10.1021/acs.jctc.7b01078.  
  
L. N. Anderson, M. B. Oviedoand B. M. Wong, “Accurate Electron Affinities and Orbital Energies of Anions from a Nonempirically Tuned Range-Separated Density Functional Theory Approach”, *Journal of Chemical Theory and Computation*, vol. 13, no. 4. American Chemical Society (ACS), pp. 1656–1666, Mar. 31, 2017. doi: 10.1021/acs.jctc.6b01249.  
  
M. Emami Khansari, “Anion Complexation Studies of 3-Nitrophenyl-Substituted Tripodal Thiourea Receptor: A Naked-Eye Detection of Sulfate via Fluoride Displacement Assay”, *ACS Omega*, vol. 2, no. 12. American Chemical Society (ACS), pp. 9057–9066, Dec. 18, 2017. doi: 10.1021/acsomega.7b01485.  
  
N. V. Ilawe, M. B. Oviedoand B. M. Wong, “Real-Time Quantum Dynamics of Long-Range Electronic Excitation Transfer in Plasmonic Nanoantennas”, *Journal of Chemical Theory and Computation*, vol. 13, no. 8. American Chemical Society (ACS), pp. 3442–3454, Jul. 17, 2017. doi: 10.1021/acs.jctc.7b00423.  
  
S. Pari, I. A. Wang, H. Liuand B. M. Wong, “Sulfate radical oxidation of aromatic contaminants: a detailed assessment of density functional theory and high-level quantum chemical methods”, *Environmental Science: Processes & Impacts*, vol. 19, no. 3. Royal Society of Chemistry (RSC), pp. 395–404, 2017. doi: 10.1039/c7em00009j.  
  
H. DorMohammadi, Q. Pang, L. Árnadóttirand O. Burkan Isgor, “Atomistic simulation of initial stages of iron corrosion in pure water using reactive molecular dynamics”, *Computational Materials Science*, vol. 145. Elsevier BV, pp. 126–133, Apr. 2018. doi: 10.1016/j.commatsci.2017.12.044.  
  
A. K. Chew and R. C. Van Lehn, “Effect of Core Morphology on the Structural Asymmetry of Alkanethiol Monolayer-Protected Gold Nanoparticles”, *The Journal of Physical Chemistry C*, vol. 122, no. 45. American Chemical Society (ACS), pp. 26288–26297, Oct. 29, 2018. doi: 10.1021/acs.jpcc.8b09323.  
  
H. Casquero, Y. J. Zhang, C. Bona-Casas, L. Dalcinand H. Gomez, “Non-body-fitted fluid–structure interaction: Divergence-conforming B-splines, fully-implicit dynamics, and variational formulation”, *Journal of Computational Physics*, vol. 374. Elsevier BV, pp. 625–653, Dec. 2018. doi: 10.1016/j.jcp.2018.07.020.  
  
A. Li, X. Chai, G. Yangand Y. Jessica Zhang, “An Isogeometric Analysis Computational Platform for Material Transport Simulation in Complex Neurite Networks”, *Molecular & Cellular Biomechanics*, vol. 16, no. 2. Computers, Materials and Continua (Tech Science Press), pp. 123–140, 2019. doi: 10.32604/mcb.2019.06479.  
  
A. Pawar, Y. J. Zhang, C. Anitescuand T. Rabczuk, “Joint image segmentation and registration based on a dynamic level set approach using truncated hierarchical B-splines”, *Computers & Mathematics with Applications*, vol. 78, no. 10. Elsevier BV, pp. 3250–3267, Nov. 2019. doi: 10.1016/j.camwa.2019.04.026.  
  
E. Holzenthal and D. F. Hill, “NUMERICAL WAVE DISSIPATION OVER IDEALIZED MARSH PLATFORM”, *Coastal Engineering Proceedings*, no. 36. Coastal Engineering Research Council, p. 104, Dec. 30, 2018. doi: 10.9753/icce.v36.papers.104.  
  
J. Palmore Jr and O. Desjardins, “A volume of fluid framework for interface-resolved simulations of vaporizing liquid-gas flows”, *Journal of Computational Physics*, vol. 399. Elsevier BV, p. 108954, Dec. 2019. doi: 10.1016/j.jcp.2019.108954.  
  
Z. Huang, C. Xuand S. Huang, “A CFD simulation of wave loads on a pile-type oscillating-water-column device”, *Journal of Hydrodynamics*, vol. 31, no. 1. Springer Science and Business Media LLC, pp. 41–49, Jan. 21, 2019. doi: 10.1007/s42241-019-0015-3.  
  
C. Xu and Z. Huang, “Three-dimensional CFD simulation of a circular OWC with a nonlinear power-takeoff: Model validation and a discussion on resonant sloshing inside the pneumatic chamber”, *Ocean Engineering*, vol. 176. Elsevier BV, pp. 184–198, Mar. 2019. doi: 10.1016/j.oceaneng.2019.02.010.  
  
Z. Huang, S. Huangand C. Xu, “Characteristics of the flow around a circular OWC-type wave energy converter supported by a bottom-sitting C-shaped structure”, *Applied Ocean Research*, vol. 101. Elsevier BV, p. 102228, Aug. 2020. doi: 10.1016/j.apor.2020.102228.  
  
M. Belgin, “A data‐driven support strategy for a sustainable research software repository”, *Concurrency and Computation: Practice and Experience*, vol. 31, no. 20. Wiley, May 17, 2019. doi: 10.1002/cpe.5338.  
  
M. Belgin, “A data‐driven support strategy for a sustainable research software repository”, *Concurrency and Computation: Practice and Experience*, vol. 31, no. 20. Wiley, May 17, 2019. doi: 10.1002/cpe.5338.  
  
S. Sarajlic, Neranjan Edirisinghe, Y. Lukinov, M. Walters, B. Davisand Gregori Faroux, *HPC Strategic Model for Georgia State University: Discovery Environment for HPC Research and Bridging XSEDE Resources*. figshare, 2016. doi: 10.6084/M9.FIGSHARE.3969375.V4.  
  
S. Sarajlic, N. Edirisinghe, Y. Wu, Y. Jiangand G. Faroux, “Training-based Workforce Development in Advanced Computing for Research and Education (ACoRE)”, *Proceedings of the Practice and Experience in Advanced Research Computing 2017 on Sustainability, Success and Impact*. ACM, Jul. 09, 2017. doi: 10.1145/3093338.3104178.  
  
T. L. Swetnam, “Scaling GIS analysis tasks from the desktop to the cloud utilizing contemporary distributed computing and data management approaches”, *Proceedings of the XSEDE16 Conference on Diversity, Big Data, and Science at Scale*. ACM, Jul. 17, 2016. doi: 10.1145/2949550.2949573.  
  
M. A. Rajib, V. Merwade, I. L. Kim, L. Zhao, C. Songand S. Zhe, “SWATShare – A web platform for collaborative research and education through online sharing, simulation and visualization of SWAT models”, *Environmental Modelling & Software*, vol. 75. Elsevier BV, pp. 498–512, Jan. 2016. doi: 10.1016/j.envsoft.2015.10.032.  
  
A. Abbaspour-Tamijani, “DFT and thermodynamics calculations of surface cation release in LiCoO2”, *Applied Surface Science*, vol. 515. Elsevier BV, p. 145865, Jun. 2020. doi: 10.1016/j.apsusc.2020.145865.  
  
H. A. Alalwan, S. E. Mason, V. H. Grassianand D. M. Cwiertny, “α-Fe2O3 Nanoparticles as Oxygen Carriers for Chemical Looping Combustion: An Integrated Materials Characterization Approach to Understanding Oxygen Carrier Performance, Reduction Mechanism, and Particle Size Effects”, *Energy & Fuels*, vol. 32, no. 7. American Chemical Society (ACS), pp. 7959–7970, Jun. 17, 2018. doi: 10.1021/acs.energyfuels.8b01539.  
  
J. W. Bennett, J. L. Bjorklund, T. Z. Forbesand S. E. Mason, “Systematic Study of Aluminum Nanoclusters and Anion Adsorbates”, *Inorganic Chemistry*, vol. 56, no. 21. American Chemical Society (ACS), pp. 13014–13028, Oct. 19, 2017. doi: 10.1021/acs.inorgchem.7b01803.  
  
J. W. Bennett, X. Huang, Y. Fang, D. M. Cwiertny, V. H. Grassianand S. E. Mason, “Methane Dissociation on α-Fe2O3(0001) and Fe3O4(111) Surfaces: First-Principles Insights into Chemical Looping Combustion”, *The Journal of Physical Chemistry C*, vol. 123, no. 11. American Chemical Society (ACS), pp. 6450–6463, Feb. 20, 2019. doi: 10.1021/acs.jpcc.8b08675.  
  
J. W. Bennett, “A systematic determination of hubbard U using the GBRV ultrasoft pseudopotential set”, *Computational Materials Science*, vol. 170. Elsevier BV, p. 109137, Dec. 2019. doi: 10.1016/j.commatsci.2019.109137.  
  
J. W. Bennett, D. T. Jones, R. J. Hamersand S. E. Mason, “First-Principles and Thermodynamics Study of Compositionally Tuned Complex Metal Oxides: Cation Release from the (001) Surface of Mn-Rich Lithium Nickel Manganese Cobalt Oxide”, *Inorganic Chemistry*, vol. 57, no. 21. American Chemical Society (ACS), pp. 13300–13311, Oct. 16, 2018. doi: 10.1021/acs.inorgchem.8b01855.  
  
J. W. Bennett, D. Jones, X. Huang, R. J. Hamersand S. E. Mason, “Dissolution of Complex Metal Oxides from First-Principles and Thermodynamics: Cation Removal from the (001) Surface of Li(Ni1/3Mn1/3Co1/3)O2”, *Environmental Science & Technology*, vol. 52, no. 10. American Chemical Society (ACS), pp. 5792–5802, Apr. 13, 2018. doi: 10.1021/acs.est.8b00054.  
  
J. W. Bennett, D. T. Jones, B. G. Hudson, J. Melendez-Rivera, R. J. Hamersand S. E. Mason, “Emerging investigator series: first-principles and thermodynamics comparison of compositionally-tuned delafossites: cation release from the (001) surface of complex metal oxides”, *Environmental Science: Nano*, vol. 7, no. 6. Royal Society of Chemistry (RSC), pp. 1642–1651, 2020. doi: 10.1039/c9en01304k.  
  
J. Bennett, M. Raglione, S. Oburn, L. MacGillivray, M. Arnoldand S. Mason, “DFT Computed Dielectric Response and THz Spectra of Organic Co-Crystals and Their Constituent Components”, *Molecules*, vol. 24, no. 5. MDPI AG, p. 959, Mar. 08, 2019. doi: 10.3390/molecules24050959.  
  
J. L. Bjorklund, J. W. Bennett, T. Z. Forbesand S. E. Mason, “Modeling of *M*Al12 Keggin Heteroatom Reactivity by Anion Adsorption”, *Crystal Growth & Design*, vol. 19, no. 5. American Chemical Society (ACS), pp. 2820–2829, Mar. 20, 2019. doi: 10.1021/acs.cgd.9b00044.  
  
J. T. Buchman, “Nickel enrichment of next-generation NMC nanomaterials alters material stability, causing unexpected dissolution behavior and observed toxicity to *S. oneidensis* MR-1 and *D. magna*”, *Environmental Science: Nano*, vol. 7, no. 2. Royal Society of Chemistry (RSC), pp. 571–587, 2020. doi: 10.1039/c9en01074b.  
  
K. Corum, A. Abbaspour Tamijaniand S. Mason, “Density Functional Theory Study of Arsenate Adsorption onto Alumina Surfaces”, *Minerals*, vol. 8, no. 3. MDPI AG, p. 91, Mar. 01, 2018. doi: 10.3390/min8030091.  
  
K. W. Corum, X. Huang, J. W. Bennettand S. E. Mason, “Systematic density functional theory study of the structural and electronic properties of constrained and fully relaxed (0 0 1) surfaces of alumina and hematite”, *Molecular Simulation*, vol. 43, no. 5–6. Informa UK Limited, pp. 406–419, Feb. 14, 2017. doi: 10.1080/08927022.2017.1285402.  
  
A. Hailu, A. A. Tamijani, S. E. Masonand S. K. Shaw, “Efficient Conversion of CO2 to Formate Using Inexpensive and Easily Prepared Post-Transition Metal Alloy Catalysts”, *Energy & Fuels*, vol. 34, no. 3. American Chemical Society (ACS), pp. 3467–3476, Jan. 28, 2020. doi: 10.1021/acs.energyfuels.9b03783.  
  
X. Huang, J. W. Bennett, M. N. Hang, E. D. Laudadio, R. J. Hamersand S. E. Mason, “*Ab Initio* Atomistic Thermodynamics Study of the (001) Surface of LiCoO2 in a Water Environment and Implications for Reactivity under Ambient Conditions”, *The Journal of Physical Chemistry C*, vol. 121, no. 9. American Chemical Society (ACS), pp. 5069–5080, Feb. 28, 2017. doi: 10.1021/acs.jpcc.6b12163.  
  
S. K. Bajgain and M. Mookherjee, “Structure and Properties of Albite Melt at High Pressures”, *ACS Earth and Space Chemistry*, vol. 4, no. 1. American Chemical Society (ACS), pp. 1–13, Dec. 06, 2019. doi: 10.1021/acsearthspacechem.9b00187.  
  
S. K. Bajgain, M. Mookherjee, R. Dasgupta, D. B. Ghoshand B. B. Karki, “Nitrogen Content in the Earth’s Outer Core”, *Geophysical Research Letters*, vol. 46, no. 1. American Geophysical Union (AGU), pp. 89–98, Jan. 03, 2019. doi: 10.1029/2018gl080555.  
  
S. K. Bajgain, Y. Peng, M. Mookherjee, Z. Jingand M. Solomon, “Properties of Hydrous Aluminosilicate Melts at High Pressures”, *ACS Earth and Space Chemistry*, vol. 3, no. 3. American Chemical Society (ACS), pp. 390–402, Feb. 08, 2019. doi: 10.1021/acsearthspacechem.8b00157.  
  
A. Basu, P. Murphy, M. Mookherjee, B. Haberland R. Boehler, “High-pressure behavior of a linear chain alkane, tricosane”, *Journal of Applied Physics*, vol. 127, no. 10. AIP Publishing, p. 105901, Mar. 14, 2020. doi: 10.1063/1.5143450.  
  
M. Mookherjee, W. R. Panero, B. Wunderand S. Jahn, “Anomalous elastic behavior of phase egg, AlSiO3(OH), at high pressures”, *American Mineralogist*, vol. 104, no. 1. Mineralogical Society of America, pp. 130–139, Jan. 01, 2019. doi: 10.2138/am-2019-6694.  
  
Y. Peng and M. Mookherjee, “Thermoelasticity of tremolite amphibole: Geophysical implications”, *American Mineralogist*, vol. 105, no. 6. Mineralogical Society of America, pp. 904–916, Jun. 01, 2020. doi: 10.2138/am-2020-7189.  
  
S. Tennakoon, “Single crystal elasticity of natural topaz at high-temperatures”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, Jan. 22, 2018. doi: 10.1038/s41598-017-17856-3.  
  
S. Tennakoon, “Single crystal elasticity of natural topaz at high-temperatures”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, Jan. 22, 2018. doi: 10.1038/s41598-017-17856-3.  
  
M. Xu, “High-pressure elastic properties of dolomite melt supporting carbonate-induced melting in deep upper mantle”, *Proceedings of the National Academy of Sciences*, vol. 117, no. 31. Proceedings of the National Academy of Sciences, pp. 18285–18291, Jul. 20, 2020. doi: 10.1073/pnas.2004347117.  
  
C. Meng, “Extending Esh3D Code to Solve Interacting Eshelby’s Inhomogeneity Problems”, *Earth and Space Science*, vol. 6, no. 8. American Geophysical Union (AGU), pp. 1569–1577, Aug. 2019. doi: 10.1029/2019ea000594.  
  
C. Meng, “Esh3D, an Analytical and Numerical Hybrid Code for Full Space and Half‐Space Eshelby’s Inclusion Problems”, *Earth and Space Science*, vol. 6, no. 3. American Geophysical Union (AGU), pp. 505–514, Mar. 2019. doi: 10.1029/2018ea000442.  
  
C. Meng, C. Guand B. Hager, “An Eshelby Solution‐Based Finite‐Element Approach to Heterogeneous Fault‐Zone Modeling”, *Seismological Research Letters*, vol. 91, no. 1. Seismological Society of America (SSA), pp. 465–474, Oct. 16, 2019. doi: 10.1785/0220190083.  
  
C. Meng and B. Hager, “A Crosslink Constraint Method for Modeling Episodic Dynamic Rupture on Intersecting Faults”, *Seismological Research Letters*, vol. 91, no. 2A. Seismological Society of America (SSA), pp. 1030–1041, Feb. 12, 2020. doi: 10.1785/0220190234.  
  
C. Meng and H. Wang, “A finite element and finite difference mixed approach for modeling fault rupture and ground motion”, *Computers & Geosciences*, vol. 113. Elsevier BV, pp. 54–69, Apr. 2018. doi: 10.1016/j.cageo.2018.01.015.  
  
A. H. Kohanpur, M. Rahromostaqim, A. J. Valocchiand M. Sahimi, “Two-phase flow of CO2-brine in a heterogeneous sandstone: Characterization of the rock and comparison of the lattice-Boltzmann, pore-network, and direct numerical simulation methods”, *Advances in Water Resources*, vol. 135. Elsevier BV, p. 103469, Jan. 2020. doi: 10.1016/j.advwatres.2019.103469.  
  
A. Langmead, P. Rodriguez, S. P. Satheesanand A. Craig, “Extracting Meaningful Data from Decomposing Bodies”, *Proceedings of the Practice and Experience in Advanced Research Computing 2017 on Sustainability, Success and Impact*. ACM, Jul. 09, 2017. doi: 10.1145/3093338.3093368.  
  
V. Kuhn, A. Craigand R. Arora, “Multiple concurrent queries on demand”, *Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment: Bridging from the eXtreme to the campus and beyond*. ACM, Jul. 16, 2012. doi: 10.1145/2335755.2335825.  
  
V. Kuhn, A. Craig, M. Simeone, S. P. Satheesanand L. Marini, “The VAT”, *Proceedings of the 2015 XSEDE Conference on Scientific Advancements Enabled by Enhanced Cyberinfrastructure - XSEDE ’15*. ACM Press, 2015. doi: 10.1145/2792745.2792756.  
  
V. Kuhn, “MOVIE”, *Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment*. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616529.  
  
J. Pustejovsky, “Enhancing Access to Digital Media”, *Proceedings of the Practice and Experience in Advanced Research Computing 2017 on Sustainability, Success and Impact*. ACM, Jul. 09, 2017. doi: 10.1145/3093338.3104171.  
  
J. Bragard, “Shock-induced termination of reentrant cardiac arrhythmias: Comparing monophasic and biphasic shock protocols”, *Chaos: An Interdisciplinary Journal of Nonlinear Science*, vol. 23, no. 4. AIP Publishing, p. 043119, Dec. 2013. doi: 10.1063/1.4829632.  
  
A. Bueno-Orovio, E. M. Cherry, S. J. Evansand F. H. Fenton, “Basis for the Induction of Tissue-Level Phase-2 Reentry as a Repolarization Disorder in the Brugada Syndrome”, *BioMed Research International*, vol. 2015. Hindawi Limited, pp. 1–12, 2015. doi: 10.1155/2015/197586.  
  
M. M. Elshrif and E. M. Cherry, “A Quantitative Comparison of the Behavior of Human Ventricular Cardiac Electrophysiology Models in Tissue”, *PLoS ONE*, vol. 9, no. 1. Public Library of Science (PLoS), p. e84401, Jan. 08, 2014. doi: 10.1371/journal.pone.0084401.  
  
E. M. Cherry and F. H. Fenton, “Contribution of the Purkinje network to wave propagation in the canine ventricle: insights from a combined electrophysiological-anatomical model”, *Nonlinear Dynamics*, vol. 68, no. 3. Springer Science and Business Media LLC, pp. 365–379, Oct. 27, 2011. doi: 10.1007/s11071-011-0221-1.  
  
E. M. Cherry and F. H. Fenton, “Effects of boundaries and geometry on the spatial distribution of action potential duration in cardiac tissue”, *Journal of Theoretical Biology*, vol. 285, no. 1. Elsevier BV, pp. 164–176, Sep. 2011. doi: 10.1016/j.jtbi.2011.06.039.  
  
E. M. Cherry, F. H. Fentonand R. F. Gilmour Jr., “Mechanisms of ventricular arrhythmias: a dynamical systems-based perspective”, *American Journal of Physiology-Heart and Circulatory Physiology*, vol. 302, no. 12. American Physiological Society, pp. H2451–H2463, Jun. 15, 2012. doi: 10.1152/ajpheart.00770.2011.  
  
R. H. Clayton, “Models of cardiac tissue electrophysiology: Progress, challenges and open questions”, *Progress in Biophysics and Molecular Biology*, vol. 104, no. 1–3. Elsevier BV, pp. 22–48, Jan. 2011. doi: 10.1016/j.pbiomolbio.2010.05.008.  
  
P. Ganesan, E. M. Cherry, D. T. Huang, A. M. Pertsovand B. Ghoraani, “Locating Atrial Fibrillation Rotor and Focal Sources Using Iterative Navigation of Multipole Diagnostic Catheters”, *Cardiovascular Engineering and Technology*, vol. 10, no. 2. Springer Science and Business Media LLC, pp. 354–366, Apr. 15, 2019. doi: 10.1007/s13239-019-00414-5.  
  
M. J. Hoffman, N. S. LaVigne, S. T. Scorse, F. H. Fentonand E. M. Cherry, “Reconstructing three-dimensional reentrant cardiac electrical wave dynamics using data assimilation”, *Chaos: An Interdisciplinary Journal of Nonlinear Science*, vol. 26, no. 1. AIP Publishing, p. 013107, Jan. 2016. doi: 10.1063/1.4940238.  
  
S. Luther, “Low-energy control of electrical turbulence in the heart”, *Nature*, vol. 475, no. 7355. Springer Science and Business Media LLC, pp. 235–239, Jul. 2011. doi: 10.1038/nature10216.  
  
S. A. Niederer, “Verification of cardiac tissue electrophysiology simulators using an *N* -version benchmark”, *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 369, no. 1954. The Royal Society, pp. 4331–4351, Nov. 13, 2011. doi: 10.1098/rsta.2011.0139.  
  
J. N. Ulysses, “An Optimization-Based Algorithm for the Construction of Cardiac Purkinje Network Models”, *IEEE Transactions on Biomedical Engineering*, vol. 65, no. 12. Institute of Electrical and Electronics Engineers (IEEE), pp. 2760–2768, Dec. 2018. doi: 10.1109/tbme.2018.2815504.  
  
S. A. Neymotin, S. Dura-Bernal, P. Lakatos, T. D. Sangerand W. W. Lytton, “Multitarget Multiscale Simulation for Pharmacological Treatment of Dystonia in Motor Cortex”, *Frontiers in Pharmacology*, vol. 7. Frontiers Media SA, Jun. 14, 2016. doi: 10.3389/fphar.2016.00157.  
  
O. E. Kadri, V. D. Chandran, M. Surblyteand R. S. Voronov, “In vivo measurement of blood clot mechanics from computational fluid dynamics based on intravital microscopy images”, *Computers in Biology and Medicine*, vol. 106. Elsevier BV, pp. 1–11, Mar. 2019. doi: 10.1016/j.compbiomed.2019.01.001.  
  
R. P. Duncan, “Dynamic recruitment of amino acid transporters to the insect/symbiont interface”, *Molecular Ecology*, vol. 23, no. 6. Wiley, pp. 1608–1623, Feb. 16, 2014. doi: 10.1111/mec.12627.  
  
W. L. Mondy, “The Basement Membrane: Key to the Reverse Engineering Biological Tissues”, *Computer-Aided Design and Applications*, vol. 8, no. 1. CAD Solutions, LLC, pp. 59–70, Jan. 2011. doi: 10.3722/cadaps.2011.59-70.  
  
W. L. Mondy, C. Casteleyn, D. V. Loo, M. Raja, C. Singletonand J. G. Jacot, “Osmium Tetroxide Labeling of (Poly)Methyl Methacrylate Corrosion Casts for Enhancement of Micro-CT Microvascular Imaging”, *Microscopy and Microanalysis*, vol. 19, no. 6. Oxford University Press (OUP), pp. 1416–1427, Oct. 08, 2013. doi: 10.1017/s1431927613013421.  
  
A. Alhourani, “Magnetoencephalography-based identification of functional connectivity network disruption following mild traumatic brain injury”, *Journal of Neurophysiology*, vol. 116, no. 4. American Physiological Society, pp. 1840–1847, Oct. 01, 2016. doi: 10.1152/jn.00513.2016.  
  
D. Krieger, M. McNeil, J. Zhang, W. Schneider, X. Liand D. O. Okonkwo, “Referee consensus”, *Proceedings of the Conference on Extreme Science and Engineering Discovery Environment: Gateway to Discovery*. ACM, Jul. 22, 2013. doi: 10.1145/2484762.2484789.  
  
N. Y. Feng, D. J. Fergusand A. H. Bass, “Neural transcriptome reveals molecular mechanisms for temporal control of vocalization across multiple timescales”, *BMC Genomics*, vol. 16, no. 1. Springer Science and Business Media LLC, May 27, 2015. doi: 10.1186/s12864-015-1577-2.  
  
D. J. Fergus, N. Y. Fengand A. H. Bass, “Gene expression underlying enhanced, steroid-dependent auditory sensitivity of hair cell epithelium in a vocal fish”, *BMC Genomics*, vol. 16, no. 1. Springer Science and Business Media LLC, Oct. 14, 2015. doi: 10.1186/s12864-015-1940-3.  
  
P. Gleeson, “Open Source Brain: A Collaborative Resource for Visualizing, Analyzing, Simulating, and Developing Standardized Models of Neurons and Circuits”, *Neuron*, vol. 103, no. 3. Elsevier BV, pp. 395–411.e5, Aug. 2019. doi: 10.1016/j.neuron.2019.05.019.  
  
R. Martínez-Cancino, “The open EEGLAB portal Interface: High-Performance computing with EEGLAB”, *NeuroImage*, vol. 224. Elsevier BV, p. 116778, Jan. 2021. doi: 10.1016/j.neuroimage.2020.116778.  
  
M. J. Bezaire, I. Raikov, K. Burk, D. Vyasand I. Soltesz, “Interneuronal mechanisms of hippocampal theta oscillations in a full-scale model of the rodent CA1 circuit”, *eLife*, vol. 5. eLife Sciences Publications, Ltd, Dec. 23, 2016. doi: 10.7554/elife.18566.  
  
C. Rennó‐Costa, D. G. Teixeiraand I. Soltesz, “Regulation of gamma‐frequency oscillation by feedforward inhibition: A computational modeling study”, *Hippocampus*, vol. 29, no. 10. Wiley, pp. 957–970, Apr. 16, 2019. doi: 10.1002/hipo.23093.  
  
J. W. Goodliffe, “Differential changes to D1 and D2 medium spiny neurons in the 12-month-old Q175+/- mouse model of Huntington’s Disease”, *PLOS ONE*, vol. 13, no. 8. Public Library of Science (PLoS), p. e0200626, Aug. 17, 2018. doi: 10.1371/journal.pone.0200626.  
  
T. H. Rumbell, D. Draguljić, A. Yadav, P. R. Hof, J. I. Luebkeand C. M. Weaver, “Automated evolutionary optimization of ion channel conductances and kinetics in models of young and aged rhesus monkey pyramidal neurons”, *Journal of Computational Neuroscience*, vol. 41, no. 1. Springer Science and Business Media LLC, pp. 65–90, Apr. 22, 2016. doi: 10.1007/s10827-016-0605-9.  
  
D. E. Crocker, J. I. Khudyakovand C. D. Champagne, “Oxidative stress in northern elephant seals: Integration of omics approaches with ecological and experimental studies”, *Comparative Biochemistry and Physiology Part A: Molecular & Integrative Physiology*, vol. 200. Elsevier BV, pp. 94–103, Oct. 2016. doi: 10.1016/j.cbpa.2016.02.011.  
  
J. S. Deyarmin, “Blubber transcriptome responses to repeated ACTH administration in a marine mammal”, *Scientific Reports*, vol. 9, no. 1. Springer Science and Business Media LLC, Feb. 25, 2019. doi: 10.1038/s41598-019-39089-2.  
  
J. I. Khudyakov, “Expression of obesity-related adipokine genes during fasting in a naturally obese marine mammal”, *American Journal of Physiology-Regulatory, Integrative and Comparative Physiology*, vol. 317, no. 4. American Physiological Society, pp. R521–R529, Oct. 01, 2019. doi: 10.1152/ajpregu.00182.2019.  
  
B. Martinez, J. Khudyakov, K. Rutherford, D. E. Crocker, N. Gemmelland R. M. Ortiz, “Adipose transcriptome analysis provides novel insights into molecular regulation of prolonged fasting in northern elephant seal pups”, *Physiological Genomics*, vol. 50, no. 7. American Physiological Society, pp. 495–503, Jul. 01, 2018. doi: 10.1152/physiolgenomics.00002.2018.  
  
R. A. Cameron, P. Kudtarkar, S. M. Gordon, K. C. Worleyand R. A. Gibbs, “Do echinoderm genomes measure up?”, *Marine Genomics*, vol. 22. Elsevier BV, pp. 1–9, Aug. 2015. doi: 10.1016/j.margen.2015.02.004.  
  
I. Venkatesh, V. Mehra, Z. Wang, B. Califfand M. G. Blackmore, “Developmental chromatin restriction of pro-growth gene networks acts as an epigenetic barrier to axon regeneration in cortical neurons”, *[]*. Cold Spring Harbor Laboratory, Feb. 03, 2018. doi: 10.1101/259408.  
  
Z. Wang, “KLF6 and STAT3 co-occupy regulatory DNA and functionally synergize to promote axon growth in CNS neurons”, *[]*. Cold Spring Harbor Laboratory, Jan. 31, 2018. doi: 10.1101/257022.  
  
J. Cha, “Effects of Serotonin Transporter Gene Variation on Impulsivity Mediated by Default Mode Network: A Family Study of Depression”, *Cerebral Cortex*, vol. 28, no. 6. Oxford University Press (OUP), pp. 1911–1921, Apr. 21, 2017. doi: 10.1093/cercor/bhx097.  
  
J. Cha, “Effects of Serotonin Transporter Gene Variation on Impulsivity Mediated by Default Mode Network: A Family Study of Depression”, *Cerebral Cortex*, vol. 28, no. 6. Oxford University Press (OUP), pp. 1911–1921, Apr. 21, 2017. doi: 10.1093/cercor/bhx097.  
  
C. Lugo-Candelas, “Associations Between Brain Structure and Connectivity in Infants and Exposure to Selective Serotonin Reuptake Inhibitors During Pregnancy”, *JAMA Pediatrics*, vol. 172, no. 6. American Medical Association (AMA), p. 525, Jun. 01, 2018. doi: 10.1001/jamapediatrics.2017.5227.  
  
Y. Wang, “Diagnosis and Prognosis Using Machine Learning Trained on Brain Morphometry and White Matter Connectomes”, *[]*. Cold Spring Harbor Laboratory, Jan. 30, 2018. doi: 10.1101/255141.  
  
F. Feng, “Gamma Oscillations in the Basolateral Amygdala: Biophysical Mechanisms and Computational Consequences”, *eneuro*, vol. 6, no. 1. Society for Neuroscience, pp. ENEURO.0388–18.2018, Jan. 2019. doi: 10.1523/eneuro.0388-18.2018.  
  
S. Deitrich, “Applying iRODS to the Brain Image Library”, *Proceedings of the Practice and Experience on Advanced Research Computing*. ACM, Jul. 22, 2018. doi: 10.1145/3219104.3229266.  
  
H. R. de Bézieux, “Improving replicability in single-cell RNA-Seq cell type discovery with Dune”, *[]*. Cold Spring Harbor Laboratory, Mar. 04, 2020. doi: 10.1101/2020.03.03.974220.  
  
D. van der Meer, “Understanding the genetic determinants of the brain with MOSTest”, *Nature Communications*, vol. 11, no. 1. Springer Science and Business Media LLC, Jul. 14, 2020. doi: 10.1038/s41467-020-17368-1.  
  
J. A. Burger, “Safety and activity of ibrutinib plus rituximab for patients with high-risk chronic lymphocytic leukaemia: a single-arm, phase 2 study”, *The Lancet Oncology*, vol. 15, no. 10. Elsevier BV, pp. 1090–1099, Sep. 2014. doi: 10.1016/s1470-2045(14)70335-3.  
  
J. A. Burger, “Leukemia cell proliferation and death in chronic lymphocytic leukemia patients on therapy with the BTK inhibitor ibrutinib”, *JCI Insight*, vol. 2, no. 2. American Society for Clinical Investigation, Jan. 26, 2017. doi: 10.1172/jci.insight.89904.  
  
D. Wodarz, “Kinetics of CLL cells in tissues and blood during therapy with the BTK inhibitor ibrutinib”, *Blood*, vol. 123, no. 26. American Society of Hematology, pp. 4132–4135, Jun. 26, 2014. doi: 10.1182/blood-2014-02-554220.  
  
D. H. Brann, “Non-neuronal expression of SARS-CoV-2 entry genes in the olfactory system suggests mechanisms underlying COVID-19-associated anosmia”, *[]*. Cold Spring Harbor Laboratory, Mar. 27, 2020. doi: 10.1101/2020.03.25.009084.  
  
C. L. Roark and L. L. Holt, “Long-term priors constrain category learning in the context of short-term statistical regularities”, *[]*. Center for Open Science, Oct. 09, 2020. doi: 10.31234/osf.io/sdf7y.  
  
C. L. Roark, K. Smaydaand B. Chandrasekaran, “Auditory and visual category learning in musicians and non-musicians”, *[]*. Center for Open Science, Oct. 09, 2020. doi: 10.31234/osf.io/q9gxw.  
  
F.-C. Yeh, “Shape analysis of the human association pathways”, *NeuroImage*, vol. 223. Elsevier BV, p. 117329, Dec. 2020. doi: 10.1016/j.neuroimage.2020.117329.  
  
E. Coulter, J. Fischer, B. Hallock, R. Knepperand C. Stewart, “Implementation of Simple XSEDE-Like Clusters”, *Proceedings of the XSEDE16 Conference on Diversity, Big Data, and Science at Scale*. ACM, Jul. 17, 2016. doi: 10.1145/2949550.2949570.  
  
J. Fischer, E. Coulter, R. Knepper, C. Peckand C. A. Stewart, “XCBC and XNIT - Tools for Cluster Implementation and Management in Research and Training”, *2015 IEEE International Conference on Cluster Computing*. IEEE, Sep. 2015. doi: 10.1109/cluster.2015.143.  
  
B. Hallock, R. Knepper, J. Fergusonand C. Stewart, “XSEDE Campus Bridging Pilot Case Study”, *Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment*. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616570.  
  
R. Knepper, “The shape of the TeraGrid”, *Proceedings of the 2011 TeraGrid Conference: Extreme Digital Discovery*. ACM, Jul. 18, 2011. doi: 10.1145/2016741.2016799.  
  
J. P. Navarro, C. A. Stewart, R. Knepper, L. Liming, D. Lifkaand M. Dahan, “The Community Software Repository from XSEDE”, *Proceedings of the Practice and Experience in Advanced Research Computing 2017 on Sustainability, Success and Impact*. ACM, Jul. 09, 2017. doi: 10.1145/3093338.3093373.  
  
C. A. Stewart, R. Knepper, M. R. Link, M. Pierce, E. Wernertand N. Wilkins-Diehr, “Cyberinfrastructure, Science Gateways, Campus Bridging, and Cloud Computing”, *Encyclopedia of Information Science and Technology, Third Edition*. IGI Global, pp. 6562–6572, Jul. 31, 2014. doi: 10.4018/978-1-4666-5888-2.ch645.  
  
Y. Chen, “AI-PLAX: AI-based placental assessment and examination using photos”, *Computerized Medical Imaging and Graphics*, vol. 84. Elsevier BV, p. 101744, Sep. 2020. doi: 10.1016/j.compmedimag.2020.101744.  
  
A. V. Vo and D. F. Laefer, “A BIG DATA APPROACH FOR COMPREHENSIVE URBAN SHADOW ANALYSIS FROM AIRBORNE LASER SCANNING POINT CLOUDS”, *ISPRS Annals of the Photogrammetry, Remote Sensing and Spatial Information Sciences*, vol. IV–4/W8. Copernicus GmbH, pp. 131–137, Sep. 23, 2019. doi: 10.5194/isprs-annals-iv-4-w8-131-2019.  
  
J. Shao, S. Ji, A. O. Glova, Y. Qiao, T. Yangand T. Sherwood, “Index Obfuscation for Oblivious Document Retrieval in a Trusted Execution Environment”, *Proceedings of the 29th ACM International Conference on Information & Knowledge Management*. ACM, Oct. 19, 2020. doi: 10.1145/3340531.3412035.  
  
J. Shao, S. Jiand T. Yang, “Privacy-aware Document Ranking with Neural Signals”, *Proceedings of the 42nd International ACM SIGIR Conference on Research and Development in Information Retrieval*. ACM, Jul. 18, 2019. doi: 10.1145/3331184.3331189.  
  
S. K. Easley, M. T. Chang, D. Shindich, C. J. Hernandezand T. M. Keaveny, “Biomechanical effects of simulated resorption cavities in cancellous bone across a wide range of bone volume fractions”, *Journal of Bone and Mineral Research*, vol. 27, no. 9. Wiley, pp. 1927–1935, Aug. 17, 2012. doi: 10.1002/jbmr.1657.  
  
S. K. Easley, M. G. Jekir, A. J. Burghardt, M. Liand T. M. Keaveny, “Contribution of the intra-specimen variations in tissue mineralization to PTH- and raloxifene-induced changes in stiffness of rat vertebrae”, *Bone*, vol. 46, no. 4. Elsevier BV, pp. 1162–1169, Apr. 2010. doi: 10.1016/j.bone.2009.12.009.  
  
A. J. Fields, G. L. Leeand T. M. Keaveny, “Mechanisms of initial endplate failure in the human vertebral body”, *Journal of Biomechanics*, vol. 43, no. 16. Elsevier BV, pp. 3126–3131, Dec. 2010. doi: 10.1016/j.jbiomech.2010.08.002.  
  
A. J. Fields, G. L. Lee, X. S. Liu, M. G. Jekir, X. E. Guoand T. M. Keaveny, “Influence of vertical trabeculae on the compressive strength of the human vertebra”, *Journal of Bone and Mineral Research*, vol. 26, no. 2. Wiley, pp. 263–269, Jan. 20, 2011. doi: 10.1002/jbmr.207.  
  
A. J. Fields, “Vertebral fragility and structural redundancy”, *Journal of Bone and Mineral Research*, vol. 27, no. 10. Wiley, pp. 2152–2158, Sep. 18, 2012. doi: 10.1002/jbmr.1664.  
  
S. Nawathe, H. Akhlaghpour, M. L. Bouxseinand T. M. Keaveny, “Microstructural Failure Mechanisms in the Human Proximal Femur for Sideways Fall Loading”, *Journal of Bone and Mineral Research*, vol. 29, no. 2. Wiley, pp. 507–515, Jan. 17, 2014. doi: 10.1002/jbmr.2033.  
  
S. Nawathe, F. Juillardand T. M. Keaveny, “Theoretical bounds for the influence of tissue-level ductility on the apparent-level strength of human trabecular bone”, *Journal of Biomechanics*, vol. 46, no. 7. Elsevier BV, pp. 1293–1299, Apr. 2013. doi: 10.1016/j.jbiomech.2013.02.011.  
  
S. Nawathe, B. P. Nguyen, N. Barzanian, H. Akhlaghpour, M. L. Bouxseinand T. M. Keaveny, “Cortical and trabecular load sharing in the human femoral neck”, *Journal of Biomechanics*, vol. 48, no. 5. Elsevier BV, pp. 816–822, Mar. 2015. doi: 10.1016/j.jbiomech.2014.12.022.  
  
M. M. Pendleton, S. Sadoughi, A. Li, G. D. O’Connell, J. S. Alwoodand T. M. Keaveny, “High-precision method for cyclic loading of small-animal vertebrae to assess bone quality”, *Bone Reports*, vol. 9. Elsevier BV, pp. 165–172, Dec. 2018. doi: 10.1016/j.bonr.2018.10.002.  
  
A. Sanyal, A. Gupta, H. H. Bayraktar, R. Y. Kwonand T. M. Keaveny, “Shear strength behavior of human trabecular bone”, *Journal of Biomechanics*, vol. 45, no. 15. Elsevier BV, pp. 2513–2519, Oct. 2012. doi: 10.1016/j.jbiomech.2012.07.023.  
  
A. Sanyal and T. M. Keaveny, “Biaxial Normal Strength Behavior in the Axial-Transverse Plane for Human Trabecular Bone—Effects of Bone Volume Fraction, Microarchitecture, and Anisotropy”, *Journal of Biomechanical Engineering*, vol. 135, no. 12. ASME International, Nov. 06, 2013. doi: 10.1115/1.4025679.  
  
A. Sanyal, J. Scheffelinand T. M. Keaveny, “The Quartic Piecewise-Linear Criterion for the Multiaxial Yield Behavior of Human Trabecular Bone”, *Journal of Biomechanical Engineering*, vol. 137, no. 1. ASME International, Jan. 01, 2015. doi: 10.1115/1.4029109.  
  
H. Yang, S. Nawathe, A. J. Fieldsand T. M. Keaveny, “Micromechanics of the human vertebral body for forward flexion”, *Journal of Biomechanics*, vol. 45, no. 12. Elsevier BV, pp. 2142–2148, Aug. 2012. doi: 10.1016/j.jbiomech.2012.05.044.  
  
D. B. Fielding, C. F. McKee, A. Socrates, A. J. Cunninghamand R. I. Klein, “The turbulent origin of spin–orbit misalignment in planetary systems”, *Monthly Notices of the Royal Astronomical Society*, vol. 450, no. 3. Oxford University Press (OUP), pp. 3306–3318, May 13, 2015. doi: 10.1093/mnras/stv836.  
  
A. T. Lee, A. J. Cunningham, C. F. McKeeand R. I. Klein, “BONDI-HOYLE ACCRETION IN AN ISOTHERMAL MAGNETIZED PLASMA”, *The Astrophysical Journal*, vol. 783, no. 1. American Astronomical Society, p. 50, Feb. 12, 2014. doi: 10.1088/0004-637x/783/1/50.  
  
A. T. Lee, S. S. R. Offner, K. M. Kratter, R. A. Smullenand P. S. Li, “The Formation and Evolution of Wide-orbit Stellar Multiples In Magnetized Clouds”, *The Astrophysical Journal*, vol. 887, no. 2. American Astronomical Society, p. 232, Dec. 23, 2019. doi: 10.3847/1538-4357/ab584b.  
  
P. S. Li, R. I. Kleinand C. F. McKee, “Formation of stellar clusters in magnetized, filamentary infrared dark clouds”, *Monthly Notices of the Royal Astronomical Society*, vol. 473, no. 3. Oxford University Press (OUP), pp. 4220–4241, Nov. 18, 2017. doi: 10.1093/mnras/stx2611.  
  
A. L. Rosen, P. S. Li, Q. Zhangand B. Burkhart, “Massive-star Formation via the Collapse of Subvirial and Virialized Turbulent Massive Cores”, *The Astrophysical Journal*, vol. 887, no. 2. American Astronomical Society, p. 108, Dec. 16, 2019. doi: 10.3847/1538-4357/ab54c6.  
  
J. Fallica, K.-F. Liu, J. Liangand G. Wang, “Coupling to Multihadron States with Chiral Fermions”, *Proceedings of The 36th Annual International Symposium on Lattice Field Theory — PoS(LATTICE2018)*. Sissa Medialab, May 29, 2019. doi: 10.22323/1.334.0080.  
  
A. S. Kronfeld, “Lattice QCD and neutrino-nucleus scattering”, *The European Physical Journal A*, vol. 55, no. 11. Springer Science and Business Media LLC, Nov. 2019. doi: 10.1140/epja/i2019-12916-x.  
  
J. Liang, K.-F. Liuand Y.-B. Yang, “Lattice calculation of hadronic tensor of the nucleon”, *EPJ Web of Conferences*, vol. 175. EDP Sciences, p. 14014, 2018. doi: 10.1051/epjconf/201817514014.  
  
H.-W. Lin, “Parton distributions and lattice QCD calculations: A community white paper”, *Progress in Particle and Nuclear Physics*, vol. 100. Elsevier BV, pp. 107–160, May 2018. doi: 10.1016/j.ppnp.2018.01.007.  
  
K.-F. Liu and C. Lorcé, “The parton orbital angular momentum: Status and prospects”, *The European Physical Journal A*, vol. 52, no. 6. Springer Science and Business Media LLC, Jun. 2016. doi: 10.1140/epja/i2016-16160-8.  
  
C. Lorcé and K.-F. Liu, “Quark and Gluon Orbital Angular Momentum: Where Are We?”, *Few-Body Systems*, vol. 57, no. 6. Springer Science and Business Media LLC, pp. 379–384, Feb. 08, 2016. doi: 10.1007/s00601-016-1043-y.  
  
G. Wang, J. Liang, T. Draper, K.-F. Liuand Y.-B. Yang, “Pion Form Factor with Overlap Fermion”, *Proceedings of The 36th Annual International Symposium on Lattice Field Theory — PoS(LATTICE2018)*. Sissa Medialab, May 29, 2019. doi: 10.22323/1.334.0127.  
  
Y.-B. Yang, “Charm and strange quark masses andfrom overlap fermions”, *Physical Review D*, vol. 92, no. 3. American Physical Society (APS), Aug. 26, 2015. doi: 10.1103/physrevd.92.034517.  
  
Y.-B. Yang, Y. Chen, T. Draper, J. Liangand K.-F. Liu, “Proton mass decomposition”, *EPJ Web of Conferences*, vol. 175. EDP Sciences, p. 14002, 2018. doi: 10.1051/epjconf/201817514002.  
  
Y. Zhao, K.-F. Liuand Y.-B. Yang, “Orbital angular momentum and generalized transverse momentum distribution”, *Physical Review D*, vol. 93, no. 5. American Physical Society (APS), Mar. 03, 2016. doi: 10.1103/physrevd.93.054006.  
  
Z.-Y. Fan, Y.-B. Yang, A. Anthony, H.-W. Linand K.-F. Liu, “Gluon Quasi-Parton-Distribution Functions from Lattice QCD”, *Physical Review Letters*, vol. 121, no. 24. American Physical Society (APS), Dec. 11, 2018. doi: 10.1103/physrevlett.121.242001.  
  
K.-F. Liu, J. Liangand Y.-B. Yang, “Variance reduction and cluster decomposition”, *Physical Review D*, vol. 97, no. 3. American Physical Society (APS), Feb. 15, 2018. doi: 10.1103/physrevd.97.034507.  
  
Y.-B. Yang, “Proton Mass Decomposition from the QCD Energy Momentum Tensor”, *Physical Review Letters*, vol. 121, no. 21. American Physical Society (APS), Nov. 19, 2018. doi: 10.1103/physrevlett.121.212001.  
  
N. K. Banavali, “Analyzing the Relationship between Single Base Flipping and Strand Slippage near DNA Duplex Termini”, *The Journal of Physical Chemistry B*, vol. 117, no. 46. American Chemical Society (ACS), pp. 14320–14328, Nov. 11, 2013. doi: 10.1021/jp408957c.  
  
Y. Chen, S. Kale, J. Weare, A. R. Dinnerand B. Roux, “Multiple Time-Step Dual-Hamiltonian Hybrid Molecular Dynamics – Monte Carlo Canonical Propagation Algorithm”, *Journal of Chemical Theory and Computation*, vol. 12, no. 4. American Chemical Society (ACS), pp. 1449–1458, Mar. 25, 2016. doi: 10.1021/acs.jctc.5b00706.  
  
J. Chowdhary, E. Harder, P. E. M. Lopes, L. Huang, A. D. MacKerell Jr.and B. Roux, “A Polarizable Force Field of Dipalmitoylphosphatidylcholine Based on the Classical Drude Model for Molecular Dynamics Simulations of Lipids”, *The Journal of Physical Chemistry B*, vol. 117, no. 31. American Chemical Society (ACS), pp. 9142–9160, Jul. 30, 2013. doi: 10.1021/jp402860e.  
  
A. Das, H. Rui, R. Nakamotoand B. Roux, “Conformational Transitions and Alternating-Access Mechanism in the Sarcoplasmic Reticulum Calcium Pump”, *Journal of Molecular Biology*, vol. 429, no. 5. Elsevier BV, pp. 647–666, Mar. 2017. doi: 10.1016/j.jmb.2017.01.007.  
  
B. Dhakshnamoorthy, A. Rohaim, H. Rui, L. Blachowiczand B. Roux, “Structural and functional characterization of a calcium-activated cation channel from Tsukamurella paurometabola”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Sep. 28, 2016. doi: 10.1038/ncomms12753.  
  
B. Dhakshnamoorthy, B. K. Ziervogel, L. Blachowiczand B. Roux, “A Structural Study of Ion Permeation in OmpF Porin from Anomalous X-ray Diffraction and Molecular Dynamics Simulations”, *Journal of the American Chemical Society*, vol. 135, no. 44. American Chemical Society (ACS), pp. 16561–16568, Oct. 29, 2013. doi: 10.1021/ja407783a.  
  
B. Egwolf, Y. Luo, D. E. Waltersand B. Roux, “Ion Selectivity of α-Hemolysin with β-Cyclodextrin Adapter. II. Multi-Ion Effects Studied with Grand Canonical Monte Carlo/Brownian Dynamics Simulations”, *The Journal of Physical Chemistry B*, vol. 114, no. 8. American Chemical Society (ACS), pp. 2901–2909, Feb. 10, 2010. doi: 10.1021/jp906791b.  
  
M. Fajer, Y. Mengand B. Roux, “The Activation of c-Src Tyrosine Kinase: Conformational Transition Pathway and Free Energy Landscape”, *The Journal of Physical Chemistry B*, vol. 121, no. 15. American Chemical Society (ACS), pp. 3352–3363, Oct. 28, 2016. doi: 10.1021/acs.jpcb.6b08409.  
  
J. C. Gumbart, B. Rouxand C. Chipot, “Efficient Determination of Protein–Protein Standard Binding Free Energies from First Principles”, *Journal of Chemical Theory and Computation*, vol. 9, no. 8. American Chemical Society (ACS), pp. 3789–3798, Aug. 01, 2013. doi: 10.1021/ct400273t.  
  
J. Herrou, G. Rotskoff, Y. Luo, B. Rouxand S. Crosson, “Structural basis of a protein partner switch that regulates the general stress response of α-proteobacteria”, *Proceedings of the National Academy of Sciences*, vol. 109, no. 21. Proceedings of the National Academy of Sciences, May 2012. doi: 10.1073/pnas.1116887109.  
  
L. Huang and B. Roux, “Automated Force Field Parameterization for Nonpolarizable and Polarizable Atomic Models Based on Ab Initio Target Data”, *Journal of Chemical Theory and Computation*, vol. 9, no. 8. American Chemical Society (ACS), pp. 3543–3556, Jul. 25, 2013. doi: 10.1021/ct4003477.  
  
S. M. Islam, R. A. Stein, H. S. Mchaouraband B. Roux, “Structural Refinement from Restrained-Ensemble Simulations Based on EPR/DEER Data: Application to T4 Lysozyme”, *The Journal of Physical Chemistry B*, vol. 117, no. 17. American Chemical Society (ACS), pp. 4740–4754, Apr. 11, 2013. doi: 10.1021/jp311723a.  
  
W. Jiang, “Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD”, *Computer Physics Communications*, vol. 185, no. 3. Elsevier BV, pp. 908–916, Mar. 2014. doi: 10.1016/j.cpc.2013.12.014.  
  
S. Jo, D. Suh, Z. He, C. Chipotand B. Roux, “Leveraging the Information from Markov State Models To Improve the Convergence of Umbrella Sampling Simulations”, *The Journal of Physical Chemistry B*, vol. 120, no. 33. American Chemical Society (ACS), pp. 8733–8742, Aug. 03, 2016. doi: 10.1021/acs.jpcb.6b05125.  
  
K. Kazmier, “Conformational dynamics of ligand-dependent alternating access in LeuT”, *Nature Structural & Molecular Biology*, vol. 21, no. 5. Springer Science and Business Media LLC, pp. 472–479, Apr. 20, 2014. doi: 10.1038/nsmb.2816.  
  
F. Khalili-Araghi, B. Ziervogel, J. C. Gumbartand B. Roux, “Molecular dynamics simulations of membrane proteins under asymmetric ionic concentrations”, *Journal of General Physiology*, vol. 142, no. 4. Rockefeller University Press, pp. 465–475, Sep. 30, 2013. doi: 10.1085/jgp.201311014.  
  
B. Lev, B. Rouxand S. Y. Noskov, “Relative Free Energies for Hydration of Monovalent Ions from QM and QM/MM Simulations”, *Journal of Chemical Theory and Computation*, vol. 9, no. 9. American Chemical Society (ACS), pp. 4165–4175, Aug. 26, 2013. doi: 10.1021/ct400296w.  
  
J. Li, J. Ostmeyer, E. Boulanger, H. Rui, E. Perozoand B. Roux, “Chemical substitutions in the selectivity filter of potassium channels do not rule out constricted-like conformations for C-type inactivation”, *Proceedings of the National Academy of Sciences*, vol. 114, no. 42. Proceedings of the National Academy of Sciences, pp. 11145–11150, Oct. 02, 2017. doi: 10.1073/pnas.1706983114.  
  
Y.-L. Lin, A. Aleksandrov, T. Simonsonand B. Roux, “An Overview of Electrostatic Free Energy Computations for Solutions and Proteins”, *Journal of Chemical Theory and Computation*, vol. 10, no. 7. American Chemical Society (ACS), pp. 2690–2709, Jun. 05, 2014. doi: 10.1021/ct500195p.  
  
Y.-L. Lin, Y. Meng, L. Huangand B. Roux, “Computational Study of Gleevec and G6G Reveals Molecular Determinants of Kinase Inhibitor Selectivity”, *Journal of the American Chemical Society*, vol. 136, no. 42. American Chemical Society (ACS), pp. 14753–14762, Oct. 07, 2014. doi: 10.1021/ja504146x.  
  
Y.-L. Lin, Y. Meng, W. Jiangand B. Roux, “Explaining why Gleevec is a specific and potent inhibitor of Abl kinase”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 5. Proceedings of the National Academy of Sciences, pp. 1664–1669, Jan. 14, 2013. doi: 10.1073/pnas.1214330110.  
  
Y.-L. Lin and B. Roux, “Computational Analysis of the Binding Specificity of Gleevec to Abl, c-Kit, Lck, and c-Src Tyrosine Kinases”, *Journal of the American Chemical Society*, vol. 135, no. 39. American Chemical Society (ACS), pp. 14741–14753, Sep. 20, 2013. doi: 10.1021/ja405939x.  
  
P. E. M. Lopes, “Polarizable Force Field for Peptides and Proteins Based on the Classical Drude Oscillator”, *Journal of Chemical Theory and Computation*, vol. 9, no. 12. American Chemical Society (ACS), pp. 5430–5449, Nov. 05, 2013. doi: 10.1021/ct400781b.  
  
J. D. Lueck, “Atomic mutagenesis in ion channels with engineered stoichiometry”, *eLife*, vol. 5. eLife Sciences Publications, Ltd, Oct. 06, 2016. doi: 10.7554/elife.18976.  
  
Y. Luo, B. Egwolf, D. E. Waltersand B. Roux, “Ion Selectivity of α-Hemolysin with a β-Cyclodextrin Adapter. I. Single Ion Potential of Mean Force and Diffusion Coefficient”, *The Journal of Physical Chemistry B*, vol. 114, no. 2. American Chemical Society (ACS), pp. 952–958, Dec. 30, 2009. doi: 10.1021/jp906790f.  
  
D. Medovoy, E. Perozoand B. Roux, “Multi-ion free energy landscapes underscore the microscopic mechanism of ion selectivity in the KcsA channel”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1858, no. 7. Elsevier BV, pp. 1722–1732, Jul. 2016. doi: 10.1016/j.bbamem.2016.02.019.  
  
Y. Meng, M. P. Pondand B. Roux, “Tyrosine Kinase Activation and Conformational Flexibility: Lessons from Src-Family Tyrosine Kinases”, *Accounts of Chemical Research*, vol. 50, no. 5. American Chemical Society (ACS), pp. 1193–1201, Apr. 20, 2017. doi: 10.1021/acs.accounts.7b00012.  
  
Y. Meng and B. Roux, “Locking the Active Conformation of c-Src Kinase through the Phosphorylation of the Activation Loop”, *Journal of Molecular Biology*, vol. 426, no. 2. Elsevier BV, pp. 423–435, Jan. 2014. doi: 10.1016/j.jmb.2013.10.001.  
  
Y. Meng and B. Roux, “Computational study of the W260A activating mutant of Src tyrosine kinase”, *Protein Science*, vol. 25, no. 1. Wiley, pp. 219–230, Jul. 18, 2015. doi: 10.1002/pro.2731.  
  
B. K. Radak, “Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems”, *Journal of Chemical Theory and Computation*, vol. 13, no. 12. American Chemical Society (ACS), pp. 5933–5944, Nov. 22, 2017. doi: 10.1021/acs.jctc.7b00875.  
  
H. Raghuraman, S. M. Islam, S. Mukherjee, B. Rouxand E. Perozo, “Dynamics transitions at the outer vestibule of the KcsA potassium channel during gating”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 5. Proceedings of the National Academy of Sciences, pp. 1831–1836, Jan. 15, 2014. doi: 10.1073/pnas.1314875111.  
  
S. Riahi, B. Rouxand C. N. Rowley, “QM/MM molecular dynamics simulations of the hydration of Mg(II) and Zn(II) ions”, *Canadian Journal of Chemistry*, vol. 91, no. 7. Canadian Science Publishing, pp. 552–558, Jul. 2013. doi: 10.1139/cjc-2012-0515.  
  
“Correction for Raghuraman et al., Dynamics transitions at the outer vestibule of the KcsA potassium channel during gating”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 12. Proceedings of the National Academy of Sciences, pp. 4644–4644, Feb. 14, 2014. doi: 10.1073/pnas.1402205111.  
  
B. Roux and S. M. Islam, “Restrained-Ensemble Molecular Dynamics Simulations Based on Distance Histograms from Double Electron–Electron Resonance Spectroscopy”, *The Journal of Physical Chemistry B*, vol. 117, no. 17. American Chemical Society (ACS), pp. 4733–4739, Apr. 11, 2013. doi: 10.1021/jp3110369.  
  
C. N. Rowley and B. Roux, “A computational study of barium blockades in the KcsA potassium channel based on multi-ion potential of mean force calculations and free energy perturbation”, *Journal of General Physiology*, vol. 142, no. 4. Rockefeller University Press, pp. 451–463, Sep. 16, 2013. doi: 10.1085/jgp.201311049.  
  
H. Rui, P. Artigasand B. Roux, “The selectivity of the Na+/K+-pump is controlled by binding site protonation and self-correcting occlusion”, *eLife*, vol. 5. eLife Sciences Publications, Ltd, Aug. 04, 2016. doi: 10.7554/elife.16616.  
  
D. Suh, B. K. Radak, C. Chipotand B. Roux, “Enhanced configurational sampling with hybrid non-equilibrium molecular dynamics–Monte Carlo propagator”, *The Journal of Chemical Physics*, vol. 148, no. 1. AIP Publishing, p. 014101, Jan. 07, 2018. doi: 10.1063/1.5004154.  
  
R. M. Venable, Y. Luo, K. Gawrisch, B. Rouxand R. W. Pastor, “Simulations of Anionic Lipid Membranes: Development of Interaction-Specific Ion Parameters and Validation Using NMR Data”, *The Journal of Physical Chemistry B*, vol. 117, no. 35. American Chemical Society (ACS), pp. 10183–10192, Aug. 22, 2013. doi: 10.1021/jp401512z.  
  
M. Weingarth, E. A. W. van der Cruijsen, J. Ostmeyer, S. Lievestro, B. Rouxand M. Baldus, “Quantitative Analysis of the Water Occupancy around the Selectivity Filter of a K+ Channel in Different Gating Modes”, *Journal of the American Chemical Society*, vol. 136, no. 5. American Chemical Society (ACS), pp. 2000–2007, Jan. 22, 2014. doi: 10.1021/ja411450y.  
  
W. Wojtas-Niziurski, Y. Meng, B. Rouxand S. Bernèche, “Self-Learning Adaptive Umbrella Sampling Method for the Determination of Free Energy Landscapes in Multiple Dimensions”, *Journal of Chemical Theory and Computation*, vol. 9, no. 4. American Chemical Society (ACS), pp. 1885–1895, Mar. 27, 2013. doi: 10.1021/ct300978b.  
  
B. K. Ziervogel and B. Roux, “The Binding of Antibiotics in OmpF Porin”, *Structure*, vol. 21, no. 1. Elsevier BV, pp. 76–87, Jan. 2013. doi: 10.1016/j.str.2012.10.014.  
  
M. C. Bennett, A. H. Kulahliogluand L. Mitas, “A quantum Monte Carlo study of mono(benzene) TM and bis(benzene) TM systems”, *Chemical Physics Letters*, vol. 667. Elsevier BV, pp. 74–78, Jan. 2017. doi: 10.1016/j.cplett.2016.11.032.  
  
M. C. Bennett, C. A. Melton, A. Annaberdiyev, G. Wang, L. Shulenburgerand L. Mitas, “A new generation of effective core potentials for correlated calculations”, *The Journal of Chemical Physics*, vol. 147, no. 22. AIP Publishing, p. 224106, Dec. 14, 2017. doi: 10.1063/1.4995643.  
  
J. Kim, “QMCPACK: an open source*ab initio*quantum Monte Carlo package for the electronic structure of atoms, molecules and solids”, *Journal of Physics: Condensed Matter*, vol. 30, no. 19. IOP Publishing, p. 195901, Apr. 19, 2018. doi: 10.1088/1361-648x/aab9c3.  
  
C. A. Melton, M. C. Bennettand L. Mitas, “Projector quantum Monte Carlo with averaged vs explicit spin-orbit effects: Applications to tungsten molecular systems”, *Journal of Physics and Chemistry of Solids*, vol. 128. Elsevier BV, pp. 367–373, May 2019. doi: 10.1016/j.jpcs.2017.12.033.  
  
C. A. Melton and L. Mitas, “Fixed-Node and Fixed-Phase Approximations and Their Relationship to Variable Spins in Quantum Monte Carlo”, *ACS Symposium Series*. American Chemical Society, pp. 1–13, Jan. 2016. doi: 10.1021/bk-2016-1234.ch001.  
  
C. A. Melton and L. Mitas, “Quantum Monte Carlo with variable spins: Fixed-phase and fixed-node approximations”, *Physical Review E*, vol. 96, no. 4. American Physical Society (APS), Oct. 10, 2017. doi: 10.1103/physreve.96.043305.  
  
Q. Niu, “Global‐view coefficients: a data management solution for parallel quantum Monte Carlo applications”, *Concurrency and Computation: Practice and Experience*, vol. 28, no. 13. Wiley, pp. 3655–3671, Jan. 28, 2016. doi: 10.1002/cpe.3748.  
  
M. Dubecký, R. Derian, P. Jurečka, L. Mitas, P. Hobzaand M. Otyepka, “Quantum Monte Carlo for noncovalent interactions: an efficient protocol attaining benchmark accuracy”, *Physical Chemistry Chemical Physics*, vol. 16, no. 38. Royal Society of Chemistry (RSC), pp. 20915–20923, 2014. doi: 10.1039/c4cp02093f.  
  
L. Horváthová, R. Derian, L. Mitasand I. Štich, “Quantum Monte Carlo study of one-dimensional transition-metal organometallic cluster systems and their suitability as spin filters”, *Physical Review B*, vol. 90, no. 11. American Physical Society (APS), Sep. 11, 2014. doi: 10.1103/physrevb.90.115414.  
  
A. H. Kulahlioglu and L. Mitas, “A quantum Monte Carlo study of zinc-porphyrin: Vertical excitation between the singlet ground state and the lowest-lying singlet excited state”, *Computational and Theoretical Chemistry*, vol. 1046. Elsevier BV, pp. 6–9, Oct. 2014. doi: 10.1016/j.comptc.2014.07.006.  
  
A. H. Kulahlioglu, K. Rasch, S. Huand L. Mitas, “Density dependence of fixed-node errors in diffusion quantum Monte Carlo: Triplet pair correlations”, *Chemical Physics Letters*, vol. 591. Elsevier BV, pp. 170–174, Jan. 2014. doi: 10.1016/j.cplett.2013.11.033.  
  
K. M. Rasch, S. Huand L. Mitas, “Communication: Fixed-node errors in quantum Monte Carlo: Interplay of electron density and node nonlinearities”, *The Journal of Chemical Physics*, vol. 140, no. 4. AIP Publishing, p. 041102, Jan. 28, 2014. doi: 10.1063/1.4862496.  
  
C. Bergonzo, N. M. Henriksen, D. R. Roe, J. M. Swails, A. E. Roitbergand T. E. Cheatham III, “Multidimensional Replica Exchange Molecular Dynamics Yields a Converged Ensemble of an RNA Tetranucleotide”, *Journal of Chemical Theory and Computation*, vol. 10, no. 1. American Chemical Society (ACS), pp. 492–499, Nov. 22, 2013. doi: 10.1021/ct400862k.  
  
R. Galindo-Murillo and T. E. Cheatham III, “DNA Binding Dynamics and Energetics of Cobalt, Nickel, and Copper Metallopeptides”, *ChemMedChem*, vol. 9, no. 6. Wiley, pp. 1252–1259, May 02, 2014. doi: 10.1002/cmdc.201402020.  
  
R. Galindo-Murillo, J. C. Garcia-Ramos, L. Ruiz-Azuara, T. E. Cheathamand F. Cortes-Guzman, “Intercalation processes of copper complexes in DNA”, *Nucleic Acids Research*, vol. 43, no. 11. Oxford University Press (OUP), pp. 5364–5376, May 09, 2015. doi: 10.1093/nar/gkv467.  
  
R. Galindo-Murillo, D. R. Roeand T. E. Cheatham III, “Convergence and reproducibility in molecular dynamics simulations of the DNA duplex d(GCACGAACGAACGAACGC)”, *Biochimica et Biophysica Acta (BBA) - General Subjects*, vol. 1850, no. 5. Elsevier BV, pp. 1041–1058, May 2015. doi: 10.1016/j.bbagen.2014.09.007.  
  
N. M. Henriksen, H. S. Hayatshahi, D. R. Davisand T. E. Cheatham III, “Structural and Energetic Analysis of 2-Aminobenzimidazole Inhibitors in Complex with the Hepatitis C Virus IRES RNA Using Molecular Dynamics Simulations”, *Journal of Chemical Information and Modeling*, vol. 54, no. 6. American Chemical Society (ACS), pp. 1758–1772, Jun. 03, 2014. doi: 10.1021/ci500132c.  
  
Z. Lin, “Oxazinin A, a Pseudodimeric Natural Product of Mixed Biosynthetic Origin from a Filamentous Fungus”, *Organic Letters*, vol. 16, no. 18. American Chemical Society (ACS), pp. 4774–4777, Sep. 04, 2014. doi: 10.1021/ol502227x.  
  
A. Okal, S. Cornillie, S. J. Matissek, K. J. Matissek, T. E. Cheatham IIIand C. S. Lim, “Re-Engineered p53 Chimera with Enhanced Homo-Oligomerization That Maintains Tumor Suppressor Activity”, *Molecular Pharmaceutics*, vol. 11, no. 7. American Chemical Society (ACS), pp. 2442–2452, May 29, 2014. doi: 10.1021/mp500202p.  
  
M. Pasi, “μABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA”, *Nucleic Acids Research*, vol. 42, no. 19. Oxford University Press (OUP), pp. 12272–12283, Sep. 26, 2014. doi: 10.1093/nar/gku855.  
  
D. R. Roe, C. Bergonzoand T. E. Cheatham III, “Evaluation of Enhanced Sampling Provided by Accelerated Molecular Dynamics with Hamiltonian Replica Exchange Methods”, *The Journal of Physical Chemistry B*, vol. 118, no. 13. American Chemical Society (ACS), pp. 3543–3552, Mar. 25, 2014. doi: 10.1021/jp4125099.  
  
J. Šponer, A. Mládek, N. Špačková, X. Cang, T. E. Cheatham IIIand S. Grimme, “Relative Stability of Different DNA Guanine Quadruplex Stem Topologies Derived Using Large-Scale Quantum-Chemical Computations”, *Journal of the American Chemical Society*, vol. 135, no. 26. American Chemical Society (ACS), pp. 9785–9796, Jun. 19, 2013. doi: 10.1021/ja402525c.  
  
J. C. Thibault, T. E. Cheatham IIIand J. C. Facelli, “iBIOMES Lite: Summarizing Biomolecular Simulation Data in Limited Settings”, *Journal of Chemical Information and Modeling*, vol. 54, no. 6. American Chemical Society (ACS), pp. 1810–1819, Jun. 09, 2014. doi: 10.1021/ci500173w.  
  
J. C. Thibault, D. R. Roe, J. C. Facelliand T. E. Cheatham III, “Data model, dictionaries, and desiderata for biomolecular simulation data indexing and sharing”, *Journal of Cheminformatics*, vol. 6, no. 1. Springer Science and Business Media LLC, Jan. 30, 2014. doi: 10.1186/1758-2946-6-4.  
  
C. Bergonzo and T. E. Cheatham III, “Improved Force Field Parameters Lead to a Better Description of RNA Structure”, *Journal of Chemical Theory and Computation*, vol. 11, no. 9. American Chemical Society (ACS), pp. 3969–3972, Aug. 18, 2015. doi: 10.1021/acs.jctc.5b00444.  
  
C. Bergonzo, K. B. Halland T. E. Cheatham III, “Stem-Loop V of Varkud Satellite RNA Exhibits Characteristics of the Mg2+ Bound Structure in the Presence of Monovalent Ions”, *The Journal of Physical Chemistry B*, vol. 119, no. 38. American Chemical Society (ACS), pp. 12355–12364, Sep. 14, 2015. doi: 10.1021/acs.jpcb.5b05190.  
  
C. Bergonzo, K. B. Halland T. E. Cheatham III, “Divalent Ion Dependent Conformational Changes in an RNA Stem-Loop Observed by Molecular Dynamics”, *Journal of Chemical Theory and Computation*, vol. 12, no. 7. American Chemical Society (ACS), pp. 3382–3389, Jun. 28, 2016. doi: 10.1021/acs.jctc.6b00173.  
  
T. E. Cheatham and D. R. Roe, “The Impact of Heterogeneous Computing on Workflows for Biomolecular Simulation and Analysis”, *Computing in Science & Engineering*, vol. 17, no. 2. Institute of Electrical and Electronics Engineers (IEEE), pp. 30–39, Mar. 2015. doi: 10.1109/mcse.2015.7.  
  
R. Galindo-Murillo, D. R. Davisand T. E. Cheatham III, “Probing the influence of hypermodified residues within the tRNA3Lys anticodon stem loop interacting with the A-loop primer sequence from HIV-1”, *Biochimica et Biophysica Acta (BBA) - General Subjects*, vol. 1860, no. 3. Elsevier BV, pp. 607–617, Mar. 2016. doi: 10.1016/j.bbagen.2015.11.009.  
  
R. Galindo-Murillo, “Assessing the Current State of Amber Force Field Modifications for DNA”, *Journal of Chemical Theory and Computation*, vol. 12, no. 8. American Chemical Society (ACS), pp. 4114–4127, Jul. 07, 2016. doi: 10.1021/acs.jctc.6b00186.  
  
Z. Heidari, D. R. Roe, R. Galindo-Murillo, J. B. Ghasemiand T. E. Cheatham III, “Using Wavelet Analysis To Assist in Identification of Significant Events in Molecular Dynamics Simulations”, *Journal of Chemical Information and Modeling*, vol. 56, no. 7. American Chemical Society (ACS), pp. 1282–1291, Jun. 22, 2016. doi: 10.1021/acs.jcim.5b00727.  
  
J. C. Robertson and T. E. Cheatham III, “DNA Backbone BI/BII Distribution and Dynamics in E2 Protein-Bound Environment Determined by Molecular Dynamics Simulations”, *The Journal of Physical Chemistry B*, vol. 119, no. 44. American Chemical Society (ACS), pp. 14111–14119, Oct. 27, 2015. doi: 10.1021/acs.jpcb.5b08486.  
  
A. C. Simmonett, F. C. Pickard IV, Y. Shao, T. E. Cheatham IIIand B. R. Brooks, “Efficient treatment of induced dipoles”, *The Journal of Chemical Physics*, vol. 143, no. 7. AIP Publishing, p. 074115, Aug. 21, 2015. doi: 10.1063/1.4928530.  
  
J. C. Thibault, D. R. Roe, K. Eilbeck, T. E. Cheatham IIIand J. C. Facelli, “Development of an informatics infrastructure for data exchange of biomolecular simulations: Architecture, data models and ontology”, *SAR and QSAR in Environmental Research*, vol. 26, no. 7–9. Informa UK Limited, pp. 577–593, Sep. 02, 2015. doi: 10.1080/1062936x.2015.1076515.  
  
M. Zgarbová, J. Šponer, M. Otyepka, T. E. Cheatham III, R. Galindo-Murilloand P. Jurečka, “Refinement of the Sugar–Phosphate Backbone Torsion Beta for AMBER Force Fields Improves the Description of Z- and B-DNA”, *Journal of Chemical Theory and Computation*, vol. 11, no. 12. American Chemical Society (ACS), pp. 5723–5736, Nov. 20, 2015. doi: 10.1021/acs.jctc.5b00716.  
  
A. Alexandru and I. Horváth, “Chiral symmetry breaking and chiral polarization: Tests for finite temperature and many flavors”, *Nuclear Physics B*, vol. 891. Elsevier BV, pp. 1–41, Feb. 2015. doi: 10.1016/j.nuclphysb.2014.11.018.  
  
K.-F. Liu, “From nuclear structure to nucleon structure”, *Nuclear Physics A*, vol. 928. Elsevier BV, pp. 99–109, Aug. 2014. doi: 10.1016/j.nuclphysa.2014.04.011.  
  
S. Buddhiraju and S. Fan, “Theory of solar cell light trapping through a nonequilibrium Green’s function formulation of Maxwell’s equations”, *Physical Review B*, vol. 96, no. 3. American Physical Society (APS), Jul. 14, 2017. doi: 10.1103/physrevb.96.035304.  
  
S. Buddhiraju, P. Santhanamand S. Fan, “Thermodynamic limits of energy harvesting from outgoing thermal radiation”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 16. Proceedings of the National Academy of Sciences, Apr. 02, 2018. doi: 10.1073/pnas.1717595115.  
  
Y. Buyukalp, P. B. Catrysse, W. Shinand S. Fan, “Planar, Ultrathin, Subwavelength Spectral Light Separator for Efficient, Wide-Angle Spectral Imaging”, *ACS Photonics*, vol. 4, no. 3. American Chemical Society (ACS), pp. 525–535, Mar. 06, 2017. doi: 10.1021/acsphotonics.6b00705.  
  
L. Cai, “Spectrally Selective Nanocomposite Textile for Outdoor Personal Cooling”, *Advanced Materials*, vol. 30, no. 35. Wiley, p. 1802152, Jul. 17, 2018. doi: 10.1002/adma.201802152.  
  
L. Cai, “Warming up human body by nanoporous metallized polyethylene textile”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Sep. 19, 2017. doi: 10.1038/s41467-017-00614-4.  
  
A. Cerjan and S. Fan, “Achieving Arbitrary Control over Pairs of Polarization States Using Complex Birefringent Metamaterials”, *Physical Review Letters*, vol. 118, no. 25. American Physical Society (APS), Jun. 22, 2017. doi: 10.1103/physrevlett.118.253902.  
  
A. Cerjan, A. Ramanand S. Fan, “Exceptional Contours and Band Structure Design in Parity-Time Symmetric Photonic Crystals”, *Physical Review Letters*, vol. 116, no. 20. American Physical Society (APS), May 20, 2016. doi: 10.1103/physrevlett.116.203902.  
  
A. Cerjan, M. Xiao, L. Yuanand S. Fan, “Effects of non-Hermitian perturbations on Weyl Hamiltonians with arbitrary topological charges”, *Physical Review B*, vol. 97, no. 7. American Physical Society (APS), Feb. 13, 2018. doi: 10.1103/physrevb.97.075128.  
  
K. Chen, B. Zhaoand S. Fan, “MESH: A free electromagnetic solver for far-field and near-field radiative heat transfer for layered periodic structures”, *Computer Physics Communications*, vol. 231. Elsevier BV, pp. 163–172, Oct. 2018. doi: 10.1016/j.cpc.2018.04.032.  
  
Z. Chen, L. Zhu, A. Ramanand S. Fan, “Radiative cooling to deep sub-freezing temperatures through a 24-h day–night cycle”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Dec. 13, 2016. doi: 10.1038/ncomms13729.  
  
S. Fan and A. Raman, “Metamaterials for radiative sky cooling”, *National Science Review*, vol. 5, no. 2. Oxford University Press (OUP), pp. 132–133, Jan. 20, 2018. doi: 10.1093/nsr/nwy012.  
  
S. Fan, Y. Shiand Q. Lin, “Nonreciprocal Photonics Without Magneto-Optics”, *IEEE Antennas and Wireless Propagation Letters*, vol. 17, no. 11. Institute of Electrical and Electronics Engineers (IEEE), pp. 1948–1952, Nov. 2018. doi: 10.1109/lawp.2018.2856258.  
  
V. Fernández-Hurtado, F. J. García-Vidal, S. Fanand J. C. Cuevas, “Enhancing Near-Field Radiative Heat Transfer with Si-based Metasurfaces”, *Physical Review Letters*, vol. 118, no. 20. American Physical Society (APS), May 15, 2017. doi: 10.1103/physrevlett.118.203901.  
  
C. Guo, M. Xiao, M. Minkov, Y. Shiand S. Fan, “Photonic crystal slab Laplace operator for image differentiation”, *Optica*, vol. 5, no. 3. The Optical Society, p. 251, Feb. 27, 2018. doi: 10.1364/optica.5.000251.  
  
P.-C. Hsu, “Radiative human body cooling by nanoporous polyethylene textile”, *Science*, vol. 353, no. 6303. American Association for the Advancement of Science (AAAS), pp. 1019–1023, Sep. 02, 2016. doi: 10.1126/science.aaf5471.  
  
T. W. Hughes and S. Fan, “Plasmonic Circuit Theory for Multiresonant Light Funneling to a Single Spatial Hot Spot”, *Nano Letters*, vol. 16, no. 9. American Chemical Society (ACS), pp. 5764–5769, Aug. 22, 2016. doi: 10.1021/acs.nanolett.6b02474.  
  
T. W. Hughes, M. Minkov, Y. Shiand S. Fan, “Training of photonic neural networks through in situ backpropagation and gradient measurement”, *Optica*, vol. 5, no. 7. The Optical Society, p. 864, Jul. 19, 2018. doi: 10.1364/optica.5.000864.  
  
T. Hughes, G. Veronis, K. P. Wootton, R. Joel Englandand S. Fan, “Method for computationally efficient design of dielectric laser accelerator structures”, *Optics Express*, vol. 25, no. 13. The Optical Society, p. 15414, Jun. 22, 2017. doi: 10.1364/oe.25.015414.  
  
O. Isabella, R. Vismara, D. N. P. Linssen, K. X. Wang, S. Fanand M. Zeman, “Advanced light trapping scheme in decoupled front and rear textured thin-film silicon solar cells”, *Solar Energy*, vol. 162. Elsevier BV, pp. 344–356, Mar. 2018. doi: 10.1016/j.solener.2018.01.040.  
  
I. Karakasoglu, M. Xiaoand S. Fan, “Polarization control with dielectric helix metasurfaces and arrays”, *Optics Express*, vol. 26, no. 17. The Optical Society, p. 21664, Aug. 07, 2018. doi: 10.1364/oe.26.021664.  
  
S. J. Kim, “Anti-Hermitian photodetector facilitating efficient subwavelength photon sorting”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Jan. 22, 2018. doi: 10.1038/s41467-017-02496-y.  
  
J.-. long . Kou, Z. Jurado, Z. Chen, S. Fanand A. J. Minnich, “Daytime Radiative Cooling Using Near-Black Infrared Emitters”, *ACS Photonics*, vol. 4, no. 3. American Chemical Society (ACS), pp. 626–630, Feb. 15, 2017. doi: 10.1021/acsphotonics.6b00991.  
  
Q. Lin, X.-Q. Sun, M. Xiao, S.-C. Zhangand S. Fan, “A three-dimensional photonic topological insulator using a two-dimensional ring resonator lattice with a synthetic frequency dimension”, *Science Advances*, vol. 4, no. 10. American Association for the Advancement of Science (AAAS), Oct. 05, 2018. doi: 10.1126/sciadv.aat2774.  
  
Q. Lin, M. Xiao, L. Yuanand S. Fan, “Photonic Weyl point in a two-dimensional resonator lattice with a synthetic frequency dimension”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Dec. 15, 2016. doi: 10.1038/ncomms13731.  
  
H. Liu, “Enhanced high-harmonic generation from an all-dielectric metasurface”, *Nature Physics*, vol. 14, no. 10. Springer Science and Business Media LLC, pp. 1006–1010, Aug. 06, 2018. doi: 10.1038/s41567-018-0233-6.  
  
S.-C. Liu, “Size Scaling of Photonic Crystal Surface Emitting Lasers on Silicon Substrates”, *IEEE Photonics Journal*, vol. 10, no. 3. Institute of Electrical and Electronics Engineers (IEEE), pp. 1–6, Jun. 2018. doi: 10.1109/jphot.2018.2829900.  
  
W. Li and S. Fan, “Nanophotonic control of thermal radiation for energy applications [Invited]”, *Optics Express*, vol. 26, no. 12. The Optical Society, p. 15995, Jun. 08, 2018. doi: 10.1364/oe.26.015995.  
  
W. Li, Y. Shi, K. Chen, L. Zhuand S. Fan, “A Comprehensive Photonic Approach for Solar Cell Cooling”, *ACS Photonics*, vol. 4, no. 4. American Chemical Society (ACS), pp. 774–782, Mar. 17, 2017. doi: 10.1021/acsphotonics.7b00089.  
  
W. Li, Y. Shi, Z. Chenand S. Fan, “Photonic thermal management of coloured objects”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Oct. 12, 2018. doi: 10.1038/s41467-018-06535-0.  
  
Y. Li, “Thermal meta-device in analogue of zero-index photonics”, *Nature Materials*, vol. 18, no. 1. Springer Science and Business Media LLC, pp. 48–54, Dec. 03, 2018. doi: 10.1038/s41563-018-0239-6.  
  
D. A. B. Miller, L. Zhuand S. Fan, “Universal modal radiation laws for all thermal emitters”, *Proceedings of the National Academy of Sciences*, vol. 114, no. 17. Proceedings of the National Academy of Sciences, pp. 4336–4341, Apr. 10, 2017. doi: 10.1073/pnas.1701606114.  
  
M. Minkov and S. Fan, “Unidirectional light transport in dynamically modulated waveguides”, *Physical Review Applied*, vol. 10, no. 4. American Physical Society (APS), Oct. 10, 2018. doi: 10.1103/physrevapplied.10.044028.  
  
M. Minkov, Y. Shiand S. Fan, “Exact solution to the steady-state dynamics of a periodically modulated resonator”, *APL Photonics*, vol. 2, no. 7. AIP Publishing, p. 076101, Jul. 2017. doi: 10.1063/1.4985381.  
  
M. Ono, K. Chen, W. Liand S. Fan, “Self-adaptive radiative cooling based on phase change materials”, *Optics Express*, vol. 26, no. 18. The Optical Society, p. A777, Jul. 24, 2018. doi: 10.1364/oe.26.00a777.  
  
Y. Peng, “Nanoporous polyethylene microfibres for large-scale radiative cooling fabric”, *Nature Sustainability*, vol. 1, no. 2. Springer Science and Business Media LLC, pp. 105–112, Feb. 09, 2018. doi: 10.1038/s41893-018-0023-2.  
  
C. Qin, L. Yuan, B. Wang, S. Fanand P. Lu, “Effective electric-field force for a photon in a synthetic frequency lattice created in a waveguide modulator”, *Physical Review A*, vol. 97, no. 6. American Physical Society (APS), Jun. 18, 2018. doi: 10.1103/physreva.97.063838.  
  
Y. Shen, G. Fang, A. Cerjan, Z. Chi, S. Fanand C. Jin, “Slanted gold mushroom array: a switchable bi/tridirectional surface plasmon polariton splitter”, *Nanoscale*, vol. 8, no. 34. Royal Society of Chemistry (RSC), pp. 15505–15513, 2016. doi: 10.1039/c6nr03488h.  
  
W. Shin, W. Cai, P. B. Catrysse, G. Veronis, M. L. Brongersmaand S. Fan, “Broadband Sharp 90-degree Bends and T-Splitters in Plasmonic Coaxial Waveguides”, *Nano Letters*, vol. 13, no. 10. American Chemical Society (ACS), pp. 4753–4758, Sep. 04, 2013. doi: 10.1021/nl402335x.  
  
Y. Shi, A. Cerjanand S. Fan, “Invited Article: Acousto-optic finite-difference frequency-domain algorithm for first-principles simulations of on-chip acousto-optic devices”, *APL Photonics*, vol. 2, no. 2. AIP Publishing, p. 020801, Feb. 2017. doi: 10.1063/1.4975002.  
  
Y. Shi, S. Hanand S. Fan, “Optical Circulation and Isolation Based on Indirect Photonic Transitions of Guided Resonance Modes”, *ACS Photonics*, vol. 4, no. 7. American Chemical Society (ACS), pp. 1639–1645, Jul. 03, 2017. doi: 10.1021/acsphotonics.7b00420.  
  
Y. Shi, Q. Lin, M. Minkovand S. Fan, “Nonreciprocal Optical Dissipation Based on Direction-Dependent Rabi Splitting”, *IEEE Journal of Selected Topics in Quantum Electronics*, vol. 24, no. 6. Institute of Electrical and Electronics Engineers (IEEE), pp. 1–7, Nov. 2018. doi: 10.1109/jstqe.2018.2814792.  
  
Y. Shi, W. Li, A. Ramanand S. Fan, “Optimization of Multilayer Optical Films with a Memetic Algorithm and Mixed Integer Programming”, *ACS Photonics*, vol. 5, no. 3. American Chemical Society (ACS), pp. 684–691, Dec. 15, 2017. doi: 10.1021/acsphotonics.7b01136.  
  
Y. Shi, W. Shinand S. Fan, “Multi-frequency finite-difference frequency-domain algorithm for active nanophotonic device simulations”, *Optica*, vol. 3, no. 11. The Optical Society, p. 1256, Oct. 25, 2016. doi: 10.1364/optica.3.001256.  
  
A. Y. Song, P. B. Catrysseand S. Fan, “Broadband Control of Topological Nodes in Electromagnetic Fields”, *Physical Review Letters*, vol. 120, no. 19. American Physical Society (APS), May 11, 2018. doi: 10.1103/physrevlett.120.193903.  
  
R. St-Gelais, G. R. Bhatt, L. Zhu, S. Fanand M. Lipson, “Hot Carrier-Based Near-Field Thermophotovoltaic Energy Conversion”, *ACS Nano*, vol. 11, no. 3. American Chemical Society (ACS), pp. 3001–3009, Mar. 16, 2017. doi: 10.1021/acsnano.6b08597.  
  
X.-Q. Sun, M. Xiao, T. Bzdušek, S.-C. Zhangand S. Fan, “Three-Dimensional Chiral Lattice Fermion in Floquet Systems”, *Physical Review Letters*, vol. 121, no. 19. American Physical Society (APS), Nov. 07, 2018. doi: 10.1103/physrevlett.121.196401.  
  
N. H. Thomas, Z. Chen, S. Fanand A. J. Minnich, “Semiconductor-based Multilayer Selective Solar Absorber for Unconcentrated Solar Thermal Energy Conversion”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Jul. 13, 2017. doi: 10.1038/s41598-017-05235-x.  
  
R. Trivedi, K. Fischer, S. Xu, S. Fanand J. Vuckovic, “Few-photon scattering and emission from low-dimensional quantum systems”, *Physical Review B*, vol. 98, no. 14. American Physical Society (APS), Oct. 29, 2018. doi: 10.1103/physrevb.98.144112.  
  
S. Verweij and S. Fan, “Understanding search behavior via search landscape analysis in design optimization of optical structures”, *Journal of the Optical Society of America B*, vol. 33, no. 12. The Optical Society, p. 2457, Nov. 10, 2016. doi: 10.1364/josab.33.002457.  
  
S. Verweij and S. Fan, “Objective-trait-bias metaheuristics for design optimization of optical structures”, *Journal of the Optical Society of America B*, vol. 34, no. 7. The Optical Society, p. 1551, Jun. 29, 2017. doi: 10.1364/josab.34.001551.  
  
J. Wang, Y. Shi, T. Hughes, Z. Zhaoand S. Fan, “Adjoint-based optimization of active nanophotonic devices”, *Optics Express*, vol. 26, no. 3. The Optical Society, p. 3236, Jan. 30, 2018. doi: 10.1364/oe.26.003236.  
  
K. Wang, Y. Shi, A. S. Solntsev, S. Fan, A. A. Sukhorukovand D. N. Neshev, “Non-reciprocal geometric phase in nonlinear frequency conversion”, *Optics Letters*, vol. 42, no. 10. The Optical Society, p. 1990, May 12, 2017. doi: 10.1364/ol.42.001990.  
  
M. Xiao, Q. Linand S. Fan, “Hyperbolic Weyl Point in Reciprocal Chiral Metamaterials”, *Physical Review Letters*, vol. 117, no. 5. American Physical Society (APS), Jul. 27, 2016. doi: 10.1103/physrevlett.117.057401.  
  
S. Xu and S. Fan, “Generalized cluster decomposition principle illustrated in waveguide quantum electrodynamics”, *Physical Review A*, vol. 95, no. 6. American Physical Society (APS), Jun. 09, 2017. doi: 10.1103/physreva.95.063809.  
  
S. Yi, “Subwavelength angle-sensing photodetectors inspired by directional hearing in small animals”, *Nature Nanotechnology*, vol. 13, no. 12. Springer Science and Business Media LLC, pp. 1143–1147, Oct. 29, 2018. doi: 10.1038/s41565-018-0278-9.  
  
L. Yuan, Q. Lin, M. Xiaoand S. Fan, “Synthetic dimension in photonics”, *Optica*, vol. 5, no. 11. The Optical Society, p. 1396, Oct. 31, 2018. doi: 10.1364/optica.5.001396.  
  
L. Yuan, D.-. wei . Wangand S. Fan, “Synthetic gauge potential and effective magnetic field in a Raman medium undergoing molecular modulation”, *Physical Review A*, vol. 95, no. 3. American Physical Society (APS), Mar. 01, 2017. doi: 10.1103/physreva.95.033801.  
  
L. Yuan, M. Xiao, Q. Linand S. Fan, “Synthetic space with arbitrary dimensions in a few rings undergoing dynamic modulation”, *Physical Review B*, vol. 97, no. 10. American Physical Society (APS), Mar. 19, 2018. doi: 10.1103/physrevb.97.104105.  
  
M. Zhang, “Electronically programmable photonic molecule”, *Nature Photonics*, vol. 13, no. 1. Springer Science and Business Media LLC, pp. 36–40, Dec. 14, 2018. doi: 10.1038/s41566-018-0317-y.  
  
B. Zhao, B. Guizal, Z. M. Zhang, S. Fanand M. Antezza, “Near-field heat transfer between graphene/hBN multilayers”, *Physical Review B*, vol. 95, no. 24. American Physical Society (APS), Jun. 30, 2017. doi: 10.1103/physrevb.95.245437.  
  
B. Zhao, P. Santhanam, K. Chen, S. Buddhirajuand S. Fan, “Near-Field Thermophotonic Systems for Low-Grade Waste-Heat Recovery”, *Nano Letters*, vol. 18, no. 8. American Chemical Society (ACS), pp. 5224–5230, Jul. 17, 2018. doi: 10.1021/acs.nanolett.8b02184.  
  
N. Zhao, S. Verweij, W. Shinand S. Fan, “Accelerating convergence of an iterative solution of finite difference frequency domain problems via schur complement domain decomposition”, *Optics Express*, vol. 26, no. 13. The Optical Society, p. 16925, Jun. 18, 2018. doi: 10.1364/oe.26.016925.  
  
Z. Zhao, “Design of a tapered slot waveguide dielectric laser accelerator for sub-relativistic electrons”, *Optics Express*, vol. 26, no. 18. The Optical Society, p. 22801, Aug. 21, 2018. doi: 10.1364/oe.26.022801.  
  
Z. Zhao, Y. Shi, K. Chenand S. Fan, “Relation between absorption and emission directivities for dipoles coupled with optical antennas”, *Physical Review A*, vol. 98, no. 1. American Physical Society (APS), Jul. 27, 2018. doi: 10.1103/physreva.98.013845.  
  
Z. Zhao, K. X. Wangand S. Fan, “Analysis of an anti-reflecting nanowire transparent electrode for solar cells”, *Journal of Applied Physics*, vol. 121, no. 11. AIP Publishing, p. 113109, Mar. 21, 2017. doi: 10.1063/1.4978769.  
  
L. Zhu and S. Fan, “Persistent Directional Current at Equilibrium in Nonreciprocal Many-Body Near Field Electromagnetic Heat Transfer”, *Physical Review Letters*, vol. 117, no. 13. American Physical Society (APS), Sep. 23, 2016. doi: 10.1103/physrevlett.117.134303.  
  
L. Zhu, Y. Guoand S. Fan, “Theory of many-body radiative heat transfer without the constraint of reciprocity”, *Physical Review B*, vol. 97, no. 9. American Physical Society (APS), Mar. 07, 2018. doi: 10.1103/physrevb.97.094302.  
  
T. Zhu, “Plasmonic computing of spatial differentiation”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, May 19, 2017. doi: 10.1038/ncomms15391.  
  
J. Bielak, H. Karaogluand R. Taborda, “Memory-efficient displacement-based internal friction for wave propagation simulation”, *GEOPHYSICS*, vol. 76, no. 6. Society of Exploration Geophysicists, pp. T131–T145, Nov. 2011. doi: 10.1190/geo2011-0019.1.  
  
S. Callaghan, “Scaling up workflow-based applications”, *Journal of Computer and System Sciences*, vol. 76, no. 6. Elsevier BV, pp. 428–446, Sep. 2010. doi: 10.1016/j.jcss.2009.11.005.  
  
S. Callaghan, “Metrics for heterogeneous scientific workflows: A case study of an earthquake science application”, *The International Journal of High Performance Computing Applications*, vol. 25, no. 3. SAGE Publications, pp. 274–285, Jun. 29, 2011. doi: 10.1177/1094342011414743.  
  
X. Chen, J. Haffener, T. H. W. Goebel, X. Meng, Z. Pengand J. C. Chang, “Temporal Correlation Between Seismic Moment and Injection Volume for an Induced Earthquake Sequence in Central Oklahoma”, *Journal of Geophysical Research: Solid Earth*, vol. 123, no. 4. American Geophysical Union (AGU), pp. 3047–3064, Apr. 2018. doi: 10.1002/2017jb014694.  
  
E. Deelman, “Pegasus, a workflow management system for science automation”, *Future Generation Computer Systems*, vol. 46. Elsevier BV, pp. 17–35, May 2015. doi: 10.1016/j.future.2014.10.008.  
  
D. S. Dreger and T. H. Jordan, “Introduction to the Focus Section on Validation of the SCEC Broadband Platform V14.3 Simulation Methods”, *Seismological Research Letters*, vol. 86, no. 1. Seismological Society of America (SSA), pp. 15–16, Dec. 17, 2014. doi: 10.1785/0220140233.  
  
E. H. Field, “Uniform California Earthquake Rupture Forecast, Version 3 (UCERF3)–The Time-Independent Model”, *Bulletin of the Seismological Society of America*, vol. 104, no. 3. Seismological Society of America (SSA), pp. 1122–1180, Jun. 01, 2014. doi: 10.1785/0120130164.  
  
E. H. Field, “Long‐Term Time‐Dependent Probabilities for the Third Uniform California Earthquake Rupture Forecast (UCERF3)”, *Bulletin of the Seismological Society of America*, vol. 105, no. 2A. Seismological Society of America (SSA), pp. 511–543, Mar. 10, 2015. doi: 10.1785/0120140093.  
  
E. H. Field, “A Synoptic View of the Third Uniform California Earthquake Rupture Forecast (UCERF3)”, *Seismological Research Letters*, vol. 88, no. 5. Seismological Society of America (SSA), pp. 1259–1267, Jul. 12, 2017. doi: 10.1785/0220170045.  
  
E. H. Field, “A Spatiotemporal Clustering Model for the Third Uniform California Earthquake Rupture Forecast (UCERF3‐ETAS): Toward an Operational Earthquake Forecast”, *Bulletin of the Seismological Society of America*, vol. 107, no. 3. Seismological Society of America (SSA), pp. 1049–1081, Feb. 28, 2017. doi: 10.1785/0120160173.  
  
E. Field, K. Porterand K. Milner, “A Prototype Operational Earthquake Loss Model for California Based on UCERF3-ETAS – A First Look at Valuation”, *Earthquake Spectra*, vol. 33, no. 4. SAGE Publications, pp. 1279–1299, Nov. 2017. doi: 10.1193/011817eqs017m.  
  
R. Graves, “CyberShake: A Physics-Based Seismic Hazard Model for Southern California”, *Pure and Applied Geophysics*, vol. 168, no. 3–4. Springer Science and Business Media LLC, pp. 367–381, May 18, 2010. doi: 10.1007/s00024-010-0161-6.  
  
P. J. Maechling, F. Silva, S. Callaghanand T. H. Jordan, “SCEC Broadband Platform: System Architecture and Software Implementation”, *Seismological Research Letters*, vol. 86, no. 1. Seismological Society of America (SSA), pp. 27–38, Dec. 17, 2014. doi: 10.1785/0220140125.  
  
M. Rynge, “Enabling large-scale scientific workflows on petascale resources using MPI master/worker”, *Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment: Bridging from the eXtreme to the campus and beyond*. ACM, Jul. 16, 2012. doi: 10.1145/2335755.2335846.  
  
B. E. Shaw, “A physics-based earthquake simulator replicates seismic hazard statistics across California”, *Science Advances*, vol. 4, no. 8. American Association for the Advancement of Science (AAAS), Aug. 03, 2018. doi: 10.1126/sciadv.aau0688.  
  
J. H. Shaw, “Unified Structural Representation of the southern California crust and upper mantle”, *Earth and Planetary Science Letters*, vol. 415. Elsevier BV, pp. 1–15, Apr. 2015. doi: 10.1016/j.epsl.2015.01.016.  
  
J. H. Shaw, “Unified Structural Representation of the southern California crust and upper mantle”, *Earth and Planetary Science Letters*, vol. 415. Elsevier BV, pp. 1–15, Apr. 2015. doi: 10.1016/j.epsl.2015.01.016.  
  
J. H. Shaw, “Unified Structural Representation of the southern California crust and upper mantle”, *Earth and Planetary Science Letters*, vol. 415. Elsevier BV, pp. 1–15, Apr. 2015. doi: 10.1016/j.epsl.2015.01.016.  
  
Z. Shi and S. M. Day, “Rupture dynamics and ground motion from 3-D rough-fault simulations”, *Journal of Geophysical Research: Solid Earth*, vol. 118, no. 3. American Geophysical Union (AGU), pp. 1122–1141, Mar. 2013. doi: 10.1002/jgrb.50094.  
  
P. Small, “The SCEC Unified Community Velocity Model Software Framework”, *Seismological Research Letters*, vol. 88, no. 6. Seismological Society of America (SSA), pp. 1539–1552, Sep. 06, 2017. doi: 10.1785/0220170082.  
  
R. Taborda and J. Bielak, “Ground‐Motion Simulation and Validation of the 2008 Chino Hills, California, Earthquake”, *Bulletin of the Seismological Society of America*, vol. 103, no. 1. Seismological Society of America (SSA), pp. 131–156, Feb. 2013. doi: 10.1785/0120110325.  
  
R. Taborda and J. Bielak, “Ground-Motion Simulation and Validation of the 2008 Chino Hills, California, Earthquake Using Different Velocity Models”, *Bulletin of the Seismological Society of America*, vol. 104, no. 4. Seismological Society of America (SSA), pp. 1876–1898, Jul. 01, 2014. doi: 10.1785/0120130266.  
  
R. Taborda, J. Bielakand D. Restrepo, “Earthquake Ground-Motion Simulation including Nonlinear Soil Effects under Idealized Conditions with Application to Two Case Studies”, *Seismological Research Letters*, vol. 83, no. 6. Seismological Society of America (SSA), pp. 1047–1060, Nov. 01, 2012. doi: 10.1785/0220120079.  
  
J. Tobin, A. Breuer, A. Heinecke, C. Yountand Y. Cui, “Accelerating Seismic Simulations Using the Intel Xeon Phi Knights Landing Processor”, *Lecture Notes in Computer Science*. Springer International Publishing, pp. 139–157, 2017. doi: 10.1007/978-3-319-58667-0\_8.  
  
D. Yao, “Detailed spatiotemporal evolution of microseismicity and repeating earthquakes following the 2012*Mw*7.6 Nicoya earthquake”, *Journal of Geophysical Research: Solid Earth*, vol. 122, no. 1. American Geophysical Union (AGU), pp. 524–542, Jan. 2017. doi: 10.1002/2016jb013632.  
  
J. D. Zechar, “The Collaboratory for the Study of Earthquake Predictability perspective on computational earthquake science”, *Concurrency and Computation: Practice and Experience*, vol. 22, no. 12. Wiley, pp. 1836–1847, Sep. 30, 2009. doi: 10.1002/cpe.1519.  
  
L. Abbo, “Slow Solar Wind: Observations and Modeling”, *Space Science Reviews*, vol. 201, no. 1–4. Springer Science and Business Media LLC, pp. 55–108, Jun. 29, 2016. doi: 10.1007/s11214-016-0264-1.  
  
R. M. Caplan, J. A. Linker, Z. Mikić, C. Downs, T. Törökand V. S. Titov, “GPU Acceleration of an Established Solar MHD Code using OpenACC”, *Journal of Physics: Conference Series*, vol. 1225, no. 1. IOP Publishing, p. 012012, May 01, 2019. doi: 10.1088/1742-6596/1225/1/012012.  
  
X. Cheng, “Initiation and Early Kinematic Evolution of Solar Eruptions”, *The Astrophysical Journal*, vol. 894, no. 2. American Astronomical Society, p. 85, May 01, 2020. doi: 10.3847/1538-4357/ab886a.  
  
P. Lamy, O. Floyd, Z. Mikićand P. Riley, “Validation of MHD Model Predictions of the Corona with LASCO-C2 Polarized Brightness Images”, *Solar Physics*, vol. 294, no. 11. Springer Science and Business Media LLC, Nov. 2019. doi: 10.1007/s11207-019-1549-9.  
  
J. A. Linker, “Coupled MHD-Focused Transport Simulations for Modeling Solar Particle Events”, *Journal of Physics: Conference Series*, vol. 1225, no. 1. IOP Publishing, p. 012007, May 01, 2019. doi: 10.1088/1742-6596/1225/1/012007.  
  
R. Lionello, “Ion Charge States in a Time-Dependent Wave-Turbulence-Driven Model of the Solar Wind”, *Solar Physics*, vol. 294, no. 1. Springer Science and Business Media LLC, Jan. 2019. doi: 10.1007/s11207-019-1401-2.  
  
R. Lionello, V. S. Titov, Z. Mikićand J. A. Linker, “Slip-back Mapping as a Tracker of Topological Changes in Evolving Magnetic Configurations”, *The Astrophysical Journal*, vol. 891, no. 1. American Astronomical Society, p. 14, Feb. 27, 2020. doi: 10.3847/1538-4357/ab68d9.  
  
M. Owens, “A Computationally Efficient, Time-Dependent Model of the Solar Wind for Use as a Surrogate to Three-Dimensional Numerical Magnetohydrodynamic Simulations”, *Solar Physics*, vol. 295, no. 3. Springer Science and Business Media LLC, Mar. 2020. doi: 10.1007/s11207-020-01605-3.  
  
M. J. Owens, M. Lang, P. Riley, M. Lockwoodand A. S. Lawless, “Quantifying the latitudinal representivity of in situ solar wind observations”, *Journal of Space Weather and Space Climate*, vol. 10. EDP Sciences, p. 8, 2020. doi: 10.1051/swsc/2020009.  
  
M. J. Owens, M. Lang, P. Rileyand D. Stansby, “Towards Construction of a Solar Wind “Reanalysis” Dataset: Application to the First Perihelion Pass of Parker Solar Probe”, *Solar Physics*, vol. 294, no. 6. Springer Science and Business Media LLC, Jun. 2019. doi: 10.1007/s11207-019-1479-6.  
  
K. K. Reeves, T. Török, Z. Mikić, J. Linkerand N. A. Murphy, “Exploring Plasma Heating in the Current Sheet Region in a Three-dimensional Coronal Mass Ejection Simulation”, *The Astrophysical Journal*, vol. 887, no. 1. American Astronomical Society, p. 103, Dec. 13, 2019. doi: 10.3847/1538-4357/ab4ce8.  
  
M. A. Reiss, “Forecasting the Ambient Solar Wind with Numerical Models. II. An Adaptive Prediction System for Specifying Solar Wind Speed near the Sun”, *The Astrophysical Journal*, vol. 891, no. 2. American Astronomical Society, p. 165, Mar. 17, 2020. doi: 10.3847/1538-4357/ab78a0.  
  
P. Riley, C. Downs, J. A. Linker, Z. Mikic, R. Lionelloand R. M. Caplan, “Predicting the Structure of the Solar Corona and Inner Heliosphere during *Parker Solar Probe* ’s First Perihelion Pass”, *The Astrophysical Journal*, vol. 874, no. 2. American Astronomical Society, p. L15, Mar. 28, 2019. doi: 10.3847/2041-8213/ab0ec3.  
  
P. Riley, J. A. Linker, Z. Mikic, R. M. Caplan, C. Downsand J.-L. Thumm, “Can an Unobserved Concentration of Magnetic Flux Above the Poles of the Sun Resolve the Open Flux Problem?”, *The Astrophysical Journal*, vol. 884, no. 1. American Astronomical Society, p. 18, Oct. 08, 2019. doi: 10.3847/1538-4357/ab3a98.  
  
A. Szabo, “The Heliospheric Current Sheet in the Inner Heliosphere Observed by the *Parker Solar Probe*”, *The Astrophysical Journal Supplement Series*, vol. 246, no. 2. American Astronomical Society, p. 47, Feb. 03, 2020. doi: 10.3847/1538-4365/ab5dac.  
  
S. R. Cranmer, S. E. Gibsonand P. Riley, “Origins of the Ambient Solar Wind: Implications for Space Weather”, *Space Science Reviews*, vol. 212, no. 3–4. Springer Science and Business Media LLC, pp. 1345–1384, Oct. 02, 2017. doi: 10.1007/s11214-017-0416-y.  
  
S. Dacie, “Sequential Eruptions Triggered by Flux Emergence: Observations and Modeling”, *The Astrophysical Journal*, vol. 862, no. 2. American Astronomical Society, p. 117, Jul. 30, 2018. doi: 10.3847/1538-4357/aacce3.  
  
S. Dacie, “Sequential Eruptions Triggered by Flux Emergence: Observations and Modeling”, *The Astrophysical Journal*, vol. 862, no. 2. American Astronomical Society, p. 117, Jul. 30, 2018. doi: 10.3847/1538-4357/aacce3.  
  
S. Dacie, “Sequential Eruptions Triggered by Flux Emergence: Observations and Modeling”, *The Astrophysical Journal*, vol. 862, no. 2. American Astronomical Society, p. 117, Jul. 30, 2018. doi: 10.3847/1538-4357/aacce3.  
  
G. I. Dima, J. R. Kuhn, D. Mickeyand C. Downs, “Using a New Infrared Si x Coronal Emission Line for Discriminating between Magnetohydrodynamic Models of the Solar Corona During the 2006 Solar Eclipse”, *The Astrophysical Journal*, vol. 852, no. 1. American Astronomical Society, p. 23, Jan. 02, 2018. doi: 10.3847/1538-4357/aa9e87.  
  
G. I. Dima, J. R. Kuhn, D. Mickeyand C. Downs, “Using a New Infrared Si x Coronal Emission Line for Discriminating between Magnetohydrodynamic Models of the Solar Corona During the 2006 Solar Eclipse”, *The Astrophysical Journal*, vol. 852, no. 1. American Astronomical Society, p. 23, Jan. 02, 2018. doi: 10.3847/1538-4357/aa9e87.  
  
C. Froment, “Long-period Intensity Pulsations in Coronal Loops Explained by Thermal Non-equilibrium Cycles”, *The Astrophysical Journal*, vol. 835, no. 2. American Astronomical Society, p. 272, Feb. 01, 2017. doi: 10.3847/1538-4357/835/2/272.  
  
C. Froment, “On the Occurrence of Thermal Nonequilibrium in Coronal Loops”, *The Astrophysical Journal*, vol. 855, no. 1. American Astronomical Society, p. 52, Mar. 07, 2018. doi: 10.3847/1538-4357/aaaf1d.  
  
C. Froment, “On the Occurrence of Thermal Nonequilibrium in Coronal Loops”, *The Astrophysical Journal*, vol. 855, no. 1. American Astronomical Society, p. 52, Mar. 07, 2018. doi: 10.3847/1538-4357/aaaf1d.  
  
L. M. Green, T. Török, B. Vršnak, W. Manchester IVand A. Veronig, “The Origin, Early Evolution and Predictability of Solar Eruptions”, *Space Science Reviews*, vol. 214, no. 1. Springer Science and Business Media LLC, Feb. 2018. doi: 10.1007/s11214-017-0462-5.  
  
L. M. Green, T. Török, B. Vršnak, W. Manchester IVand A. Veronig, “The Origin, Early Evolution and Predictability of Solar Eruptions”, *Space Science Reviews*, vol. 214, no. 1. Springer Science and Business Media LLC, Feb. 2018. doi: 10.1007/s11214-017-0462-5.  
  
Q. Hu, M. G. Linton, B. E. Wood, P. Rileyand T. Nieves-Chinchilla, “The Grad–Shafranov Reconstruction of Toroidal Magnetic Flux Ropes: First Applications”, *Solar Physics*, vol. 292, no. 11. Springer Science and Business Media LLC, Nov. 2017. doi: 10.1007/s11207-017-1195-z.  
  
D. Lario, “The Solar Energetic Particle Event of 2010 August 14: Connectivity with the Solar Source Inferred from Multiple Spacecraft Observations and Modeling”, *The Astrophysical Journal*, vol. 838, no. 1. American Astronomical Society, p. 51, Mar. 23, 2017. doi: 10.3847/1538-4357/aa63e4.  
  
D. Lario, R.-Y. Kwon, P. Rileyand N. E. Raouafi, “On the Link between the Release of Solar Energetic Particles Measured at Widespread Heliolongitudes and the Properties of the Associated Coronal Shocks”, *The Astrophysical Journal*, vol. 847, no. 2. American Astronomical Society, p. 103, Sep. 27, 2017. doi: 10.3847/1538-4357/aa89e3.  
  
W. Liu, M. Jin, C. Downs, L. Ofman, M. C. M. Cheungand N. V. Nitta, “A Truly Global Extreme Ultraviolet Wave from the SOL2017-09-10 X8.2+ Solar Flare-Coronal Mass Ejection”, *The Astrophysical Journal*, vol. 864, no. 2. American Astronomical Society, p. L24, Aug. 31, 2018. doi: 10.3847/2041-8213/aad77b.  
  
W. Liu, M. Jin, C. Downs, L. Ofman, M. C. M. Cheungand N. V. Nitta, “A Truly Global Extreme Ultraviolet Wave from the SOL2017-09-10 X8.2+ Solar Flare-Coronal Mass Ejection”, *The Astrophysical Journal*, vol. 864, no. 2. American Astronomical Society, p. L24, Aug. 31, 2018. doi: 10.3847/2041-8213/aad77b.  
  
W. Liu, M. Jin, C. Downs, L. Ofman, M. C. M. Cheungand N. V. Nitta, “A Truly Global Extreme Ultraviolet Wave from the SOL2017-09-10 X8.2+ Solar Flare-Coronal Mass Ejection”, *The Astrophysical Journal*, vol. 864, no. 2. American Astronomical Society, p. L24, Aug. 31, 2018. doi: 10.3847/2041-8213/aad77b.  
  
Y. Liu, X. Sun, T. Török, V. S. Titovand J. E. Leake, “Electric-current Neutralization, Magnetic Shear, and Eruptive Activity in Solar Active Regions”, *The Astrophysical Journal*, vol. 846, no. 1. American Astronomical Society, p. L6, Aug. 29, 2017. doi: 10.3847/2041-8213/aa861e.  
  
D. M. Long, “Understanding the Physical Nature of Coronal “EIT Waves””, *Solar Physics*, vol. 292, no. 1. Springer Science and Business Media LLC, Dec. 12, 2016. doi: 10.1007/s11207-016-1030-y.  
  
W. Manchester IV, “The Physical Processes of CME/ICME Evolution”, *Space Science Reviews*, vol. 212, no. 3–4. Springer Science and Business Media LLC, pp. 1159–1219, Aug. 03, 2017. doi: 10.1007/s11214-017-0394-0.  
  
R. Ma, R. A. Angryk, P. Rileyand S. F. Boubrahimi, “Coronal Mass Ejection Data Clustering and Visualization of Decision Trees”, *The Astrophysical Journal Supplement Series*, vol. 236, no. 1. American Astronomical Society, p. 14, May 11, 2018. doi: 10.3847/1538-4365/aab76f.  
  
R. Ma, R. A. Angryk, P. Rileyand S. F. Boubrahimi, “Coronal Mass Ejection Data Clustering and Visualization of Decision Trees”, *The Astrophysical Journal Supplement Series*, vol. 236, no. 1. American Astronomical Society, p. 14, May 11, 2018. doi: 10.3847/1538-4365/aab76f.  
  
R. Ma, R. A. Angryk, P. Rileyand S. F. Boubrahimi, “Coronal Mass Ejection Data Clustering and Visualization of Decision Trees”, *The Astrophysical Journal Supplement Series*, vol. 236, no. 1. American Astronomical Society, p. 14, May 11, 2018. doi: 10.3847/1538-4365/aab76f.  
  
Z. Mikić, “Predicting the corona for the 21 August 2017 total solar eclipse”, *Nature Astronomy*, vol. 2, no. 11. Springer Science and Business Media LLC, pp. 913–921, Aug. 27, 2018. doi: 10.1038/s41550-018-0562-5.  
  
Z. Mikić, “Predicting the corona for the 21 August 2017 total solar eclipse”, *Nature Astronomy*, vol. 2, no. 11. Springer Science and Business Media LLC, pp. 913–921, Aug. 27, 2018. doi: 10.1038/s41550-018-0562-5.  
  
Z. Mikić, “Predicting the corona for the 21 August 2017 total solar eclipse”, *Nature Astronomy*, vol. 2, no. 11. Springer Science and Business Media LLC, pp. 913–921, Aug. 27, 2018. doi: 10.1038/s41550-018-0562-5.  
  
M. J. Owens, M. Lockwoodand P. Riley, “Global solar wind variations over the last four centuries”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Jan. 31, 2017. doi: 10.1038/srep41548.  
  
M. J. Owens, P. Rileyand T. S. Horbury, “Probabilistic Solar Wind and Geomagnetic Forecasting Using an Analogue Ensemble or “Similar Day” Approach”, *Solar Physics*, vol. 292, no. 5. Springer Science and Business Media LLC, Apr. 19, 2017. doi: 10.1007/s11207-017-1090-7.  
  
J. C. Raymond, C. Downs, M. M. Knight, K. Battams, S. Giordanoand R. Rosati, “Comet C/2011 W3 (Lovejoy) between 2 and 10 Solar Radii: Physical Parameters of the Comet and the Corona”, *The Astrophysical Journal*, vol. 858, no. 1. American Astronomical Society, p. 19, Apr. 27, 2018. doi: 10.3847/1538-4357/aabade.  
  
J. C. Raymond, C. Downs, M. M. Knight, K. Battams, S. Giordanoand R. Rosati, “Comet C/2011 W3 (Lovejoy) between 2 and 10 Solar Radii: Physical Parameters of the Comet and the Corona”, *The Astrophysical Journal*, vol. 858, no. 1. American Astronomical Society, p. 19, Apr. 27, 2018. doi: 10.3847/1538-4357/aabade.  
  
J. C. Raymond, C. Downs, M. M. Knight, K. Battams, S. Giordanoand R. Rosati, “Comet C/2011 W3 (Lovejoy) between 2 and 10 Solar Radii: Physical Parameters of the Comet and the Corona”, *The Astrophysical Journal*, vol. 858, no. 1. American Astronomical Society, p. 19, Apr. 27, 2018. doi: 10.3847/1538-4357/aabade.  
  
N. Reginald, O. St. Cyr, J. Davila, L. Rastaetterand T. Török, “Evaluating Uncertainties in Coronal Electron Temperature and Radial Speed Measurements Using a Simulation of the Bastille Day Eruption”, *Solar Physics*, vol. 293, no. 5. Springer Science and Business Media LLC, May 2018. doi: 10.1007/s11207-018-1301-x.  
  
N. Reginald, O. St. Cyr, J. Davila, L. Rastaetterand T. Török, “Evaluating Uncertainties in Coronal Electron Temperature and Radial Speed Measurements Using a Simulation of the Bastille Day Eruption”, *Solar Physics*, vol. 293, no. 5. Springer Science and Business Media LLC, May 2018. doi: 10.1007/s11207-018-1301-x.  
  
N. Reginald, O. St. Cyr, J. Davila, L. Rastaetterand T. Török, “Evaluating Uncertainties in Coronal Electron Temperature and Radial Speed Measurements Using a Simulation of the Bastille Day Eruption”, *Solar Physics*, vol. 293, no. 5. Springer Science and Business Media LLC, May 2018. doi: 10.1007/s11207-018-1301-x.  
  
P. Riley, D. Baker, Y. D. Liu, P. Verronen, H. Singerand M. Güdel, “Extreme Space Weather Events: From Cradle to Grave”, *Space Science Reviews*, vol. 214, no. 1. Springer Science and Business Media LLC, Dec. 20, 2017. doi: 10.1007/s11214-017-0456-3.  
  
P. Riley, D. Baker, Y. D. Liu, P. Verronen, H. Singerand M. Güdel, “Extreme Space Weather Events: From Cradle to Grave”, *Space Science Reviews*, vol. 214, no. 1. Springer Science and Business Media LLC, Dec. 20, 2017. doi: 10.1007/s11214-017-0456-3.  
  
A. P. Rouillard, “DERIVING THE PROPERTIES OF CORONAL PRESSURE FRONTS IN 3D: APPLICATION TO THE 2012 MAY 17 GROUND LEVEL ENHANCEMENT”, *The Astrophysical Journal*, vol. 833, no. 1. American Astronomical Society, p. 45, Dec. 07, 2016. doi: 10.3847/1538-4357/833/1/45.  
  
N. A. Schwadron, “Particle Radiation Sources, Propagation and Interactions in Deep Space, at Earth, the Moon, Mars, and Beyond: Examples of Radiation Interactions and Effects”, *Space Science Reviews*, vol. 212, no. 3–4. Springer Science and Business Media LLC, pp. 1069–1106, Jul. 03, 2017. doi: 10.1007/s11214-017-0381-5.  
  
C. Shen, J. C. Raymond, Z. Mikić, J. A. Linker, K. K. Reevesand N. A. Murphy, “Time-dependent Ionization in a Steady Flow in an MHD Model of the Solar Corona and Wind”, *The Astrophysical Journal*, vol. 850, no. 1. American Astronomical Society, p. 26, Nov. 14, 2017. doi: 10.3847/1538-4357/aa93f3.  
  
V. S. Titov, C. Downs, Z. Mikić, T. Török, J. A. Linkerand R. M. Caplan, “Regularized Biot–Savart Laws for Modeling Magnetic Flux Ropes”, *The Astrophysical Journal*, vol. 852, no. 2. American Astronomical Society, p. L21, Jan. 05, 2018. doi: 10.3847/2041-8213/aaa3da.  
  
V. S. Titov, C. Downs, Z. Mikić, T. Török, J. A. Linkerand R. M. Caplan, “Regularized Biot–Savart Laws for Modeling Magnetic Flux Ropes”, *The Astrophysical Journal*, vol. 852, no. 2. American Astronomical Society, p. L21, Jan. 05, 2018. doi: 10.3847/2041-8213/aaa3da.  
  
V. S. Titov, Z. Mikić, T. Török, J. A. Linkerand O. Panasenco, “2010 August 1–2 Sympathetic Eruptions. II. Magnetic Topology of the MHD Background Field”, *The Astrophysical Journal*, vol. 845, no. 2. American Astronomical Society, p. 141, Aug. 21, 2017. doi: 10.3847/1538-4357/aa81ce.  
  
T. Török, “Sun-to-Earth MHD Simulation of the 2000 July 14 “Bastille Day” Eruption”, *The Astrophysical Journal*, vol. 856, no. 1. American Astronomical Society, p. 75, Mar. 27, 2018. doi: 10.3847/1538-4357/aab36d.  
  
T. Török, “Sun-to-Earth MHD Simulation of the 2000 July 14 “Bastille Day” Eruption”, *The Astrophysical Journal*, vol. 856, no. 1. American Astronomical Society, p. 75, Mar. 27, 2018. doi: 10.3847/1538-4357/aab36d.  
  
A. R. Winebarger, R. Lionello, C. Downs, Z. Mikićand J. Linker, “Identifying Observables That Can Differentiate Between Impulsive and Footpoint Heating: Time Lags and Intensity Ratios”, *The Astrophysical Journal*, vol. 865, no. 2. American Astronomical Society, p. 111, Sep. 27, 2018. doi: 10.3847/1538-4357/aad9fb.  
  
A. R. Winebarger, R. Lionello, C. Downs, Z. Mikićand J. Linker, “Identifying Observables That Can Differentiate Between Impulsive and Footpoint Heating: Time Lags and Intensity Ratios”, *The Astrophysical Journal*, vol. 865, no. 2. American Astronomical Society, p. 111, Sep. 27, 2018. doi: 10.3847/1538-4357/aad9fb.  
  
A. R. Winebarger, R. Lionello, C. Downs, Z. Mikićand J. Linker, “Identifying Observables That Can Differentiate Between Impulsive and Footpoint Heating: Time Lags and Intensity Ratios”, *The Astrophysical Journal*, vol. 865, no. 2. American Astronomical Society, p. 111, Sep. 27, 2018. doi: 10.3847/1538-4357/aad9fb.  
  
A. R. Yeates, “Global Non-Potential Magnetic Models of the Solar Corona During the March 2015 Eclipse”, *Space Science Reviews*, vol. 214, no. 5. Springer Science and Business Media LLC, Aug. 2018. doi: 10.1007/s11214-018-0534-1.  
  
A. R. Yeates, “Global Non-Potential Magnetic Models of the Solar Corona During the March 2015 Eclipse”, *Space Science Reviews*, vol. 214, no. 5. Springer Science and Business Media LLC, Aug. 2018. doi: 10.1007/s11214-018-0534-1.  
  
A. R. Yeates, “Global Non-Potential Magnetic Models of the Solar Corona During the March 2015 Eclipse”, *Space Science Reviews*, vol. 214, no. 5. Springer Science and Business Media LLC, Aug. 2018. doi: 10.1007/s11214-018-0534-1.  
  
L. Abbo, R. Lionello, P. Rileyand Y.-M. Wang, “Coronal Pseudo-Streamer and Bipolar Streamer Observed by SOHO/UVCS in March 2008”, *Solar Physics*, vol. 290, no. 7. Springer Science and Business Media LLC, pp. 2043–2054, Jun. 24, 2015. doi: 10.1007/s11207-015-0723-y.  
  
C. Gressl, “Comparative Study of MHD Modeling of the Background Solar Wind”, *Solar Physics*, vol. 289, no. 5. Springer Science and Business Media LLC, pp. 1783–1801, Nov. 09, 2013. doi: 10.1007/s11207-013-0421-6.  
  
M. Kramar, V. Airapetian, Z. Mikićand J. Davila, “3D Coronal Density Reconstruction and Retrieving the Magnetic Field Structure during Solar Minimum”, *Solar Physics*, vol. 289, no. 8. Springer Science and Business Media LLC, pp. 2927–2944, Apr. 11, 2014. doi: 10.1007/s11207-014-0525-7.  
  
A.-E. Lebatard, “Dating the Homo erectus bearing travertine from Kocabaş (Denizli, Turkey) at at least 1.1 Ma”, *Earth and Planetary Science Letters*, vol. 390. Elsevier BV, pp. 8–18, Mar. 2014. doi: 10.1016/j.epsl.2013.12.031.  
  
S. W. McIntosh, “The solar magnetic activity band interaction and instabilities that shape quasi-periodic variability”, *Nature Communications*, vol. 6, no. 1. Springer Science and Business Media LLC, Apr. 07, 2015. doi: 10.1038/ncomms7491.  
  
P. Riley, “A Multi-Observatory Inter-Comparison of Line-of-Sight Synoptic Solar Magnetograms”, *Solar Physics*, vol. 289, no. 3. Springer Science and Business Media LLC, pp. 769–792, Jul. 25, 2013. doi: 10.1007/s11207-013-0353-1.  
  
C. J. Schrijver, “Understanding space weather to shield society: A global road map for 2015–2025 commissioned by COSPAR and ILWS”, *Advances in Space Research*, vol. 55, no. 12. Elsevier BV, pp. 2745–2807, Jun. 2015. doi: 10.1016/j.asr.2015.03.023.  
  
V. Titov, “Three-body problem periodic orbits with vanishing angular momentum”, *Astronomische Nachrichten*, vol. 336, no. 3. Wiley, pp. 271–275, Apr. 2015. doi: 10.1002/asna.201412159.  
  
T. Török, B. Kliem, M. A. Berger, M. G. Linton, P. Démoulinand L. van Driel-Gesztelyi, “The evolution of writhe in kink-unstable flux ropes and erupting filaments”, *Plasma Physics and Controlled Fusion*, vol. 56, no. 6. IOP Publishing, p. 064012, May 08, 2014. doi: 10.1088/0741-3335/56/6/064012.  
  
A. Vourlidas, “The Wide-Field Imager for Solar Probe Plus (WISPR)”, *Space Science Reviews*, vol. 204, no. 1–4. Springer Science and Business Media LLC, pp. 83–130, Feb. 11, 2015. doi: 10.1007/s11214-014-0114-y.  
  
T. Wiegelmann, G. J. D. Petrieand P. Riley, “Coronal Magnetic Field Models”, *Space Science Reviews*, vol. 210, no. 1–4. Springer Science and Business Media LLC, pp. 249–274, Jul. 31, 2015. doi: 10.1007/s11214-015-0178-3.  
  
J. A. Cole, L. Kohler, J. Hedhliand Z. Luthey-Schulten, “Spatially-resolved metabolic cooperativity within dense bacterial colonies”, *BMC Systems Biology*, vol. 9, no. 1. Springer Science and Business Media LLC, Mar. 18, 2015. doi: 10.1186/s12918-015-0155-1.  
  
J. A. Cole and Z. Luthey-Schulten, “Whole Cell Modeling: From Single Cells to Colonies”, *Israel Journal of Chemistry*, vol. 54, no. 8–9. Wiley, pp. 1219–1229, Jul. 31, 2014. doi: 10.1002/ijch.201300147.  
  
T. M. Earnest, J. A. Cole, J. R. Peterson, M. J. Hallock, T. E. Kuhlmanand Z. Luthey‐Schulten, “Ribosome biogenesis in replicating cells: Integration of experiment and theory”, *Biopolymers*, vol. 105, no. 10. Wiley, pp. 735–751, Jul. 22, 2016. doi: 10.1002/bip.22892.  
  
T. M. Earnest, J. Lai, K. Chen, M. J. Hallock, J. R. Williamsonand Z. Luthey-Schulten, “Toward a Whole-Cell Model of Ribosome Biogenesis: Kinetic Modeling of SSU Assembly”, *Biophysical Journal*, vol. 109, no. 6. Elsevier BV, pp. 1117–1135, Sep. 2015. doi: 10.1016/j.bpj.2015.07.030.  
  
Z. Ghaemi, I. Guzman, D. Gnutt, Z. Luthey-Schultenand M. Gruebele, “Role of Electrostatics in Protein–RNA Binding: The Global vs the Local Energy Landscape”, *The Journal of Physical Chemistry B*, vol. 121, no. 36. American Chemical Society (ACS), pp. 8437–8446, Aug. 31, 2017. doi: 10.1021/acs.jpcb.7b04318.  
  
I. Guzman, Z. Ghaemi, A. Baranger, Z. Luthey-Schultenand M. Gruebele, “Native Conformational Dynamics of the Spliceosomal U1A Protein”, *The Journal of Physical Chemistry B*, vol. 119, no. 9. American Chemical Society (ACS), pp. 3651–3661, Feb. 24, 2015. doi: 10.1021/jp511760m.  
  
M. J. Hallock, J. E. Stone, E. Roberts, C. Fryand Z. Luthey-Schulten, “Simulation of reaction diffusion processes over biologically relevant size and time scales using multi-GPU workstations”, *Parallel Computing*, vol. 40, no. 5–6. Elsevier BV, pp. 86–99, May 2014. doi: 10.1016/j.parco.2014.03.009.  
  
H. Kim, “Protein-guided RNA dynamics during early ribosome assembly”, *Nature*, vol. 506, no. 7488. Springer Science and Business Media LLC, pp. 334–338, Feb. 12, 2014. doi: 10.1038/nature13039.  
  
J. Lai, K. Chenand Z. Luthey-Schulten, “Structural Intermediates and Folding Events in the Early Assembly of the Ribosomal Small Subunit”, *The Journal of Physical Chemistry B*, vol. 117, no. 42. American Chemical Society (ACS), pp. 13335–13345, Sep. 30, 2013. doi: 10.1021/jp404106r.  
  
L. Li, S. A. Martinisand Z. Luthey-Schulten, “Capture and Quality Control Mechanisms for Adenosine-5′-triphosphate Binding”, *Journal of the American Chemical Society*, vol. 135, no. 16. American Chemical Society (ACS), pp. 6047–6055, Feb. 13, 2013. doi: 10.1021/ja308044w.  
  
J. R. Peterson, J. A. Cole, J. Fei, T. Haand Z. A. Luthey-Schulten, “Effects of DNA replication on mRNA noise”, *Proceedings of the National Academy of Sciences*, vol. 112, no. 52. Proceedings of the National Academy of Sciences, pp. 15886–15891, Dec. 15, 2015. doi: 10.1073/pnas.1516246112.  
  
J. R. Peterson, “Towards a Computational Model of a Methane Producing Archaeum”, *Archaea*, vol. 2014. Hindawi Limited, pp. 1–18, 2014. doi: 10.1155/2014/898453.  
  
W. Cai, W. Shin, S. Fanand M. L. Brongersma, “Elements for Plasmonic Nanocircuits with Three-Dimensional Slot Waveguides”, *Advanced Materials*, vol. 22, no. 45. Wiley, pp. 5120–5124, Sep. 21, 2010. doi: 10.1002/adma.201001440.  
  
W. Shin and S. Fan, “Choice of the perfectly matched layer boundary condition for frequency-domain Maxwell’s equations solvers”, *Journal of Computational Physics*, vol. 231, no. 8. Elsevier BV, pp. 3406–3431, Apr. 2012. doi: 10.1016/j.jcp.2012.01.013.  
  
A. Black Pyrkosz, J. Eargle, A. Sethiand Z. Luthey-Schulten, “Exit Strategies for Charged tRNA from GluRS”, *Journal of Molecular Biology*, vol. 397, no. 5. Elsevier BV, pp. 1350–1371, Apr. 2010. doi: 10.1016/j.jmb.2010.02.003.  
  
K. Chen, “Assembly of the Five-Way Junction in the Ribosomal Small Subunit Using Hybrid MD-Go̅ Simulations”, *The Journal of Physical Chemistry B*, vol. 116, no. 23. American Chemical Society (ACS), pp. 6819–6831, May 25, 2012. doi: 10.1021/jp212614b.  
  
K. Chen, J. Eargle, K. Sarkar, M. Gruebeleand Z. Luthey-Schulten, “Functional Role of Ribosomal Signatures”, *Biophysical Journal*, vol. 99, no. 12. Elsevier BV, pp. 3930–3940, Dec. 2010. doi: 10.1016/j.bpj.2010.09.062.  
  
J. Asorey, M. Carrasco Kind, I. Sevilla-Noarbe, R. J. Brunnerand J. Thaler, “Galaxy clustering with photometric surveys using PDF redshift information”, *Monthly Notices of the Royal Astronomical Society*, vol. 459, no. 2. Oxford University Press (OUP), pp. 1293–1309, Mar. 28, 2016. doi: 10.1093/mnras/stw721.  
  
M. Carrasco Kind and R. J. Brunner, “TPZ: photometric redshift PDFs and ancillary information by using prediction trees and random forests”, *Monthly Notices of the Royal Astronomical Society*, vol. 432, no. 2. Oxford University Press (OUP), pp. 1483–1501, May 01, 2013. doi: 10.1093/mnras/stt574.  
  
M. Carrasco Kind and R. J. Brunner, “SOMz: photometric redshift PDFs with self-organizing maps and random atlas”, *Monthly Notices of the Royal Astronomical Society*, vol. 438, no. 4. Oxford University Press (OUP), pp. 3409–3421, Jan. 25, 2014. doi: 10.1093/mnras/stt2456.  
  
M. Carrasco Kind and R. J. Brunner, “Sparse representation of photometric redshift probability density functions: preparing for petascale astronomy”, *Monthly Notices of the Royal Astronomical Society*, vol. 441, no. 4. Oxford University Press (OUP), pp. 3550–3561, May 31, 2014. doi: 10.1093/mnras/stu827.  
  
M. Carrasco Kind and R. J. Brunner, “Exhausting the information: novel Bayesian combination of photometric redshift PDFs”, *Monthly Notices of the Royal Astronomical Society*, vol. 442, no. 4. Oxford University Press (OUP), pp. 3380–3399, Jun. 30, 2014. doi: 10.1093/mnras/stu1098.  
  
H. M. Kamdar, M. J. Turkand R. J. Brunner, “Machine learning and cosmological simulations – II. Hydrodynamical simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 457, no. 2. Oxford University Press (OUP), pp. 1162–1179, Feb. 01, 2016. doi: 10.1093/mnras/stv2981.  
  
H. M. Kamdar, M. J. Turkand R. J. Brunner, “Machine learning and cosmological simulations – I. Semi-analytical models”, *Monthly Notices of the Royal Astronomical Society*, vol. 455, no. 1. Oxford University Press (OUP), pp. 642–658, Nov. 05, 2015. doi: 10.1093/mnras/stv2310.  
  
E. J. Kim, R. J. Brunnerand M. Carrasco Kind, “A hybrid ensemble learning approach to star–galaxy classification”, *Monthly Notices of the Royal Astronomical Society*, vol. 453, no. 1. Oxford University Press (OUP), pp. 507–521, Aug. 17, 2015. doi: 10.1093/mnras/stv1608.  
  
Y. Wang and R. J. Brunner, “On the clustering of compact galaxy pairs in dark matter haloes”, *Monthly Notices of the Royal Astronomical Society*, vol. 444, no. 3. Oxford University Press (OUP), pp. 2854–2869, Sep. 12, 2014. doi: 10.1093/mnras/stu1562.  
  
P. H. Constantino, M. Vlysidis, P. Smadbeckand Y. N. Kaznessis, “Modeling stochasticity in biochemical reaction networks”, *Journal of Physics D: Applied Physics*, vol. 49, no. 9. IOP Publishing, p. 093001, Feb. 01, 2016. doi: 10.1088/0022-3727/49/9/093001.  
  
B. Ekblad, P. K. Kyriakou, C. Oppegård, J. Nissen-Meyer, Y. N. Kaznessisand P. E. Kristiansen, “Structure–Function Analysis of the Two-Peptide Bacteriocin Plantaricin EF”, *Biochemistry*, vol. 55, no. 36. American Chemical Society (ACS), pp. 5106–5116, Aug. 31, 2016. doi: 10.1021/acs.biochem.6b00588.  
  
B. Forkus, S. Ritter, M. Vlysidis, K. Geldartand Y. N. Kaznessis, “Antimicrobial Probiotics Reduce Salmonella enterica in Turkey Gastrointestinal Tracts”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Jan. 17, 2017. doi: 10.1038/srep40695.  
  
K. Geldart and Y. N. Kaznessis, “Characterization of Class IIa Bacteriocin Resistance in Enterococcus faecium”, *Antimicrobial Agents and Chemotherapy*, vol. 61, no. 4. American Society for Microbiology, Apr. 2017. doi: 10.1128/aac.02033-16.  
  
P.-K. Lai and Y. N. Kaznessis, “Free Energy Calculations of Microcin J25 Variants Binding to the FhuA Receptor”, *Journal of Chemical Theory and Computation*, vol. 13, no. 7. American Chemical Society (ACS), pp. 3413–3423, Jun. 28, 2017. doi: 10.1021/acs.jctc.7b00417.  
  
P. Smadbeck and Y. N. Kaznessis, “A closure scheme for chemical master equations”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 35. Proceedings of the National Academy of Sciences, pp. 14261–14265, Aug. 12, 2013. doi: 10.1073/pnas.1306481110.  
  
T. Afroz, K. Biliouris, K. E. Boykin, Y. Kaznessisand C. L. Beisel, “Trade-offs in Engineering Sugar Utilization Pathways for Titratable Control”, *ACS Synthetic Biology*, vol. 4, no. 2. American Chemical Society (ACS), pp. 141–149, Apr. 28, 2014. doi: 10.1021/sb400162z.  
  
T. Afroz, K. Biliouris, Y. Kaznessisand C. L. Beisel, “Bacterial sugar utilization gives rise to distinct single-cell behaviours”, *Molecular Microbiology*. Wiley, p. n/a–n/a, Jul. 16, 2014. doi: 10.1111/mmi.12695.  
  
J. Borrero, Y. Chen, G. M. Dunnyand Y. N. Kaznessis, “Modified Lactic Acid Bacteria Detect and Inhibit Multiresistant Enterococci”, *ACS Synthetic Biology*, vol. 4, no. 3. American Chemical Society (ACS), pp. 299–306, Jun. 16, 2014. doi: 10.1021/sb500090b.  
  
K. Geldart, J. Borreroand Y. N. Kaznessis, “Chloride-Inducible Expression Vector for Delivery of Antimicrobial Peptides Targeting Antibiotic-Resistant Enterococcus faecium”, *Applied and Environmental Microbiology*, vol. 81, no. 11. American Society for Microbiology, pp. 3889–3897, Jun. 2015. doi: 10.1128/aem.00227-15.  
  
M. K. McClintock, Y. N. Kaznessisand B. J. Hackel, “Enterocin A mutants identified by saturation mutagenesis enhance potency towards vancomycin‐resistant *Enterococci*”, *Biotechnology and Bioengineering*, vol. 113, no. 2. Wiley, pp. 414–423, Sep. 03, 2015. doi: 10.1002/bit.25710.  
  
G. Sfyroera, “Rare Loss-of-Function Mutation in Complement Component C3 Provides Insight into Molecular and Pathophysiological Determinants of Complement Activity”, *The Journal of Immunology*, vol. 194, no. 7. The American Association of Immunologists, pp. 3305–3316, Apr. 01, 2015. doi: 10.4049/jimmunol.1402781.  
  
P. Smadbeck and Y. N. Kaznessis, “Chemical Master Equation Closure for Computer-Aided Synthetic Biology”, *Methods in Molecular Biology*. Springer New York, pp. 179–191, Nov. 13, 2014. doi: 10.1007/978-1-4939-1878-2\_9.  
  
P. Smadbeck and Y. N. Kaznessis, “On a theory of stability for nonlinear stochastic chemical reaction networks”, *The Journal of Chemical Physics*, vol. 142, no. 18. AIP Publishing, p. 184101, May 14, 2015. doi: 10.1063/1.4919834.  
  
K. Volzing, J. Borrero, M. J. Sadowskyand Y. N. Kaznessis, “Antimicrobial Peptides Targeting Gram-negative Pathogens, Produced and Delivered by Lactic Acid Bacteria”, *ACS Synthetic Biology*, vol. 2, no. 11. American Chemical Society (ACS), pp. 643–650, Jul. 10, 2013. doi: 10.1021/sb4000367.  
  
A. Arsiccio, J. McCarty, R. Pisanoand J.-E. Shea, “Effect of Surfactants on Surface-Induced Denaturation of Proteins: Evidence of an Orientation-Dependent Mechanism”, *The Journal of Physical Chemistry B*, vol. 122, no. 49. American Chemical Society (ACS), pp. 11390–11399, Aug. 17, 2018. doi: 10.1021/acs.jpcb.8b07368.  
  
W. F. D. Bennett, J.-E. Sheaand D. P. Tieleman, “Phospholipid Chain Interactions with Cholesterol Drive Domain Formation in Lipid Membranes”, *Biophysical Journal*, vol. 114, no. 11. Elsevier BV, pp. 2595–2605, Jun. 2018. doi: 10.1016/j.bpj.2018.04.022.  
  
C. Bleiholder, “Ion Mobility Spectrometry Reveals the Mechanism of Amyloid Formation of Aβ(25–35) and Its Modulation by Inhibitors at the Molecular Level: Epigallocatechin Gallate and *Scyllo*-inositol”, *Journal of the American Chemical Society*, vol. 135, no. 45. American Chemical Society (ACS), pp. 16926–16937, Nov. 01, 2013. doi: 10.1021/ja406197f.  
  
S. Das, “Molecularly Smooth Self-Assembled Monolayer for High-Mobility Organic Field-Effect Transistors”, *Nano Letters*, vol. 16, no. 10. American Chemical Society (ACS), pp. 6709–6715, Sep. 29, 2016. doi: 10.1021/acs.nanolett.6b03860.  
  
N. E. C. de Almeida, “Opposing Effects of Cucurbit[7]uril and 1,2,3,4,6-Penta-*O*-galloyl-β-d-glucopyranose on Amyloid β25–35 Assembly”, *ACS Chemical Neuroscience*, vol. 7, no. 2. American Chemical Society (ACS), pp. 218–226, Dec. 10, 2015. doi: 10.1021/acschemneuro.5b00280.  
  
T. D. Do, “Elucidation of the Aggregation Pathways of Helix–Turn–Helix Peptides: Stabilization at the Turn Region Is Critical for Fibril Formation”, *Biochemistry*, vol. 54, no. 26. American Chemical Society (ACS), pp. 4050–4062, Jun. 24, 2015. doi: 10.1021/acs.biochem.5b00414.  
  
T. D. Do, J. W. Checco, M. Tro, J.-E. Shea, M. T. Bowersand J. V. Sweedler, “Conformational investigation of the structure–activity relationship of GdFFD and its analogues on an achatin-like neuropeptide receptor of *Aplysia californica* involved in the feeding circuit”, *Physical Chemistry Chemical Physics*, vol. 20, no. 34. Royal Society of Chemistry (RSC), pp. 22047–22057, 2018. doi: 10.1039/c8cp03661f.  
  
T. D. Do, N. J. Economou, A. Chamas, S. K. Buratto, J.-E. Sheaand M. T. Bowers, “Interactions between Amyloid-β and Tau Fragments Promote Aberrant Aggregates: Implications for Amyloid Toxicity”, *The Journal of Physical Chemistry B*, vol. 118, no. 38. American Chemical Society (ACS), pp. 11220–11230, Sep. 15, 2014. doi: 10.1021/jp506258g.  
  
T. D. Do, “Effects of pH and Charge State on Peptide Assembly: The YVIFL Model System”, *The Journal of Physical Chemistry B*, vol. 117, no. 37. American Chemical Society (ACS), pp. 10759–10768, Sep. 04, 2013. doi: 10.1021/jp406066d.  
  
T. D. Do, “Amyloid β-Protein C-Terminal Fragments: Formation of Cylindrins and β-Barrels”, *Journal of the American Chemical Society*, vol. 138, no. 2. American Chemical Society (ACS), pp. 549–557, Jan. 06, 2016. doi: 10.1021/jacs.5b09536.  
  
P. Ganguly, “Tau Assembly: The Dominant Role of PHF6 (VQIVYK) in Microtubule Binding Region Repeat R3”, *The Journal of Physical Chemistry B*, vol. 119, no. 13. American Chemical Society (ACS), pp. 4582–4593, Mar. 24, 2015. doi: 10.1021/acs.jpcb.5b00175.  
  
P. Ganguly, T. Hajari, J.-E. Sheaand N. F. A. van der Vegt, “Mutual Exclusion of Urea and Trimethylamine *N*-Oxide from Amino Acids in Mixed Solvent Environment”, *The Journal of Physical Chemistry Letters*, vol. 6, no. 4. American Chemical Society (ACS), pp. 581–585, Jan. 28, 2015. doi: 10.1021/jz502634k.  
  
P. Ganguly and J.-E. Shea, “Distinct and Nonadditive Effects of Urea and Guanidinium Chloride on Peptide Solvation”, *The Journal of Physical Chemistry Letters*, vol. 10, no. 23. American Chemical Society (ACS), pp. 7406–7413, Nov. 13, 2019. doi: 10.1021/acs.jpclett.9b03004.  
  
A. I. Ilitchev, “Human Islet Amyloid Polypeptide N-Terminus Fragment Self-Assembly: Effect of Conserved Disulfide Bond on Aggregation Propensity”, *Journal of the American Society for Mass Spectrometry*, vol. 27, no. 6. American Chemical Society (ACS), pp. 1010–1018, Feb. 19, 2016. doi: 10.1007/s13361-016-1347-7.  
  
L. Larini, “Initiation of assembly of tau(273-284) and its ΔK280 mutant: an experimental and computational study”, *Physical Chemistry Chemical Physics*, vol. 15, no. 23. Royal Society of Chemistry (RSC), p. 8916, 2013. doi: 10.1039/c3cp00063j.  
  
L. Larini and J.-E. Shea, “Coarse-Grained Modeling of Simple Molecules at Different Resolutions in the Absence of Good Sampling”, *The Journal of Physical Chemistry B*, vol. 116, no. 29. American Chemical Society (ACS), pp. 8337–8349, Mar. 02, 2012. doi: 10.1021/jp2097263.  
  
L. Larini and J.-E. Shea, “Role of β-Hairpin Formation in Aggregation: The Self-Assembly of the Amyloid-β(25–35) Peptide”, *Biophysical Journal*, vol. 103, no. 3. Elsevier BV, pp. 576–586, Aug. 2012. doi: 10.1016/j.bpj.2012.06.027.  
  
L. Larini and J.-E. Shea, “Double Resolution Model for Studying TMAO/Water Effective Interactions”, *The Journal of Physical Chemistry B*, vol. 117, no. 42. American Chemical Society (ACS), pp. 13268–13277, Jul. 08, 2013. doi: 10.1021/jp403635g.  
  
Z. A. Levine, S. A. Fischer, J.-E. Sheaand J. Pfaendtner, “Trp-Cage Folding on Organic Surfaces”, *The Journal of Physical Chemistry B*, vol. 119, no. 33. American Chemical Society (ACS), pp. 10417–10425, Aug. 05, 2015. doi: 10.1021/acs.jpcb.5b04213.  
  
Z. A. Levine, L. Larini, N. E. LaPointe, S. C. Feinsteinand J.-E. Shea, “Regulation and aggregation of intrinsically disordered peptides”, *Proceedings of the National Academy of Sciences*, vol. 112, no. 9. Proceedings of the National Academy of Sciences, pp. 2758–2763, Feb. 17, 2015. doi: 10.1073/pnas.1418155112.  
  
Z. A. Levine, “Surface force measurements and simulations of mussel-derived peptide adhesives on wet organic surfaces”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 16. Proceedings of the National Academy of Sciences, pp. 4332–4337, Mar. 28, 2016. doi: 10.1073/pnas.1603065113.  
  
Z. A. Levine and J.-E. Shea, “Simulations of disordered proteins and systems with conformational heterogeneity”, *Current Opinion in Structural Biology*, vol. 43. Elsevier BV, pp. 95–103, Apr. 2017. doi: 10.1016/j.sbi.2016.11.006.  
  
Z. A. Levine, “Determination of Biomembrane Bending Moduli in Fully Atomistic Simulations”, *Journal of the American Chemical Society*, vol. 136, no. 39. American Chemical Society (ACS), pp. 13582–13585, Sep. 16, 2014. doi: 10.1021/ja507910r.  
  
Y. Lin, “Narrow equilibrium window for complex coacervation of tau and RNA under cellular conditions”, *eLife*, vol. 8. eLife Sciences Publications, Ltd, Apr. 05, 2019. doi: 10.7554/elife.42571.  
  
J. McCarty, K. T. Delaney, S. P. O. Danielsen, G. H. Fredricksonand J.-E. Shea, “Complete Phase Diagram for Liquid–Liquid Phase Separation of Intrinsically Disordered Proteins”, *The Journal of Physical Chemistry Letters*, vol. 10, no. 8. American Chemical Society (ACS), pp. 1644–1652, Mar. 15, 2019. doi: 10.1021/acs.jpclett.9b00099.  
  
E. K. Peter, M. Agarwal, B. Kim, I. V. Pivkinand J.-E. Shea, “How water layers on graphene affect folding and adsorption of TrpZip2”, *The Journal of Chemical Physics*, vol. 141, no. 22. AIP Publishing, pp. 22D511, Dec. 14, 2014. doi: 10.1063/1.4896984.  
  
E. K. Peter, I. V. Pivkinand J.-E. Shea, “A kMC-MD method with generalized move-sets for the simulation of folding of *α*-helical and *β*-stranded peptides”, *The Journal of Chemical Physics*, vol. 142, no. 14. AIP Publishing, p. 144903, Apr. 14, 2015. doi: 10.1063/1.4915919.  
  
E. K. Peter and J.-E. Shea, “A hybrid MD-kMC algorithm for folding proteins in explicit solvent”, *Physical Chemistry Chemical Physics*, vol. 16, no. 14. Royal Society of Chemistry (RSC), p. 6430, 2014. doi: 10.1039/c3cp55251a.  
  
E. K. Peter and J.-E. Shea, “An adaptive bias – hybrid MD/kMC algorithm for protein folding and aggregation”, *Physical Chemistry Chemical Physics*, vol. 19, no. 26. Royal Society of Chemistry (RSC), pp. 17373–17382, 2017. doi: 10.1039/c7cp03035e.  
  
S. Seo, “Significant Performance Enhancement of Polymer Resins by Bioinspired Dynamic Bonding”, *Advanced Materials*, vol. 29, no. 39. Wiley, p. 1703026, Aug. 18, 2017. doi: 10.1002/adma.201703026.  
  
J.-E. Shea and Z. A. Levine, “Studying the Early Stages of Protein Aggregation Using Replica Exchange Molecular Dynamics Simulations”, *Methods in Molecular Biology*. Springer New York, pp. 225–250, 2016. doi: 10.1007/978-1-4939-2978-8\_15.  
  
A. C. Susa, “Defining the Molecular Basis of Amyloid Inhibitors: Human Islet Amyloid Polypeptide–Insulin Interactions”, *Journal of the American Chemical Society*, vol. 136, no. 37. American Chemical Society (ACS), pp. 12912–12919, Sep. 04, 2014. doi: 10.1021/ja504031d.  
  
X. Wang, “The Linker between the Dimerization and Catalytic Domains of the CheA Histidine Kinase Propagates Changes in Structure and Dynamics That Are Important for Enzymatic Activity”, *Biochemistry*, vol. 53, no. 5. American Chemical Society (ACS), pp. 855–861, Jan. 28, 2014. doi: 10.1021/bi4012379.  
  
A. G. Wong, C. Wu, E. Hannaberry, M. D. Watson, J.-E. Sheaand D. P. Raleigh, “Analysis of the Amyloidogenic Potential of Pufferfish (*Takifugu rubripes*) Islet Amyloid Polypeptide Highlights the Limitations of Thioflavin-T Assays and the Difficulties in Defining Amyloidogenicity”, *Biochemistry*, vol. 55, no. 3. American Chemical Society (ACS), pp. 510–518, Jan. 13, 2016. doi: 10.1021/acs.biochem.5b01107.  
  
C. Wu and J.-E. Shea, “Structural Similarities and Differences between Amyloidogenic and Non-Amyloidogenic Islet Amyloid Polypeptide (IAPP) Sequences and Implications for the Dual Physiological and Pathological Activities of These Peptides”, *PLoS Computational Biology*, vol. 9, no. 8. Public Library of Science (PLoS), p. e1003211, Aug. 29, 2013. doi: 10.1371/journal.pcbi.1003211.  
  
G. H. Zerze, R. G. Mullen, Z. A. Levine, J.-E. Sheaand J. Mittal, “To What Extent Does Surface Hydrophobicity Dictate Peptide Folding and Stability near Surfaces?”, *Langmuir*, vol. 31, no. 44. American Chemical Society (ACS), pp. 12223–12230, Oct. 28, 2015. doi: 10.1021/acs.langmuir.5b03814.  
  
X. Zheng, “Mechanism of C-Terminal Fragments of Amyloid β-Protein as Aβ Inhibitors: Do C-Terminal Interactions Play a Key Role in Their Inhibitory Activity?”, *The Journal of Physical Chemistry B*, vol. 120, no. 8. American Chemical Society (ACS), pp. 1615–1623, Oct. 16, 2015. doi: 10.1021/acs.jpcb.5b08177.  
  
S. Banerjee, “Slowing DNA Transport Using Graphene-DNA Interactions”, *Advanced Functional Materials*, vol. 25, no. 6. Wiley, pp. 936–946, Dec. 22, 2014. doi: 10.1002/adfm.201403719.  
  
M. Belkin and A. Aksimentiev, “Molecular Dynamics Simulation of DNA Capture and Transport in Heated Nanopores”, *ACS Applied Materials & Interfaces*, vol. 8, no. 20. American Chemical Society (ACS), pp. 12599–12608, Mar. 21, 2016. doi: 10.1021/acsami.6b00463.  
  
M. Belkin, S.-H. Chao, G. Giannettiand A. Aksimentiev, “Modeling thermophoretic effects in solid-state nanopores”, *Journal of Computational Electronics*, vol. 13, no. 4. Springer Science and Business Media LLC, pp. 826–838, Jul. 17, 2014. doi: 10.1007/s10825-014-0594-8.  
  
M. Belkin, S.-H. Chao, M. P. Jonsson, C. Dekkerand A. Aksimentiev, “Plasmonic Nanopores for Trapping, Controlling Displacement, and Sequencing of DNA”, *ACS Nano*, vol. 9, no. 11. American Chemical Society (ACS), pp. 10598–10611, Oct. 01, 2015. doi: 10.1021/acsnano.5b04173.  
  
M. Belkin, C. Maffeo, D. B. Wellsand A. Aksimentiev, “Stretching and Controlled Motion of Single-Stranded DNA in Locally Heated Solid-State Nanopores”, *ACS Nano*, vol. 7, no. 8. American Chemical Society (ACS), pp. 6816–6824, Jul. 26, 2013. doi: 10.1021/nn403575n.  
  
C. R. Benson, “Inchworm movement of two rings switching onto a thread by biased Brownian diffusion represent a three-body problem”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 38. Proceedings of the National Academy of Sciences, pp. 9391–9396, May 07, 2018. doi: 10.1073/pnas.1719539115.  
  
S. Bhattacharya, J. Yooand A. Aksimentiev, “Water Mediates Recognition of DNA Sequence *via* Ionic Current Blockade in a Biological Nanopore”, *ACS Nano*, vol. 10, no. 4. American Chemical Society (ACS), pp. 4644–4651, Apr. 15, 2016. doi: 10.1021/acsnano.6b00940.  
  
S. Carson, J. Wilson, A. Aksimentiev, P. R. Weigeleand M. Wanunu, “Hydroxymethyluracil modifications enhance the flexibility and hydrophilicity of double-stranded DNA”, *Nucleic Acids Research*, vol. 44, no. 5. Oxford University Press (OUP), pp. 2085–2092, Nov. 17, 2015. doi: 10.1093/nar/gkv1199.  
  
S.-H. Chao, S. S. Matthews, R. Paxman, A. Aksimentiev, M. Gruebeleand J. L. Price, “Two Structural Scenarios for Protein Stabilization by PEG”, *The Journal of Physical Chemistry B*, vol. 118, no. 28. American Chemical Society (ACS), pp. 8388–8395, Jun. 02, 2014. doi: 10.1021/jp502234s.  
  
J. Comer and A. Aksimentiev, “Predicting the DNA Sequence Dependence of Nanopore Ion Current Using Atomic-Resolution Brownian Dynamics”, *The Journal of Physical Chemistry C*, vol. 116, no. 5. American Chemical Society (ACS), pp. 3376–3393, Jan. 31, 2012. doi: 10.1021/jp210641j.  
  
J. Comer and A. Aksimentiev, “Predicting the DNA Sequence Dependence of Nanopore Ion Current Using Atomic-Resolution Brownian Dynamics”, *The Journal of Physical Chemistry C*, vol. 116, no. 5. American Chemical Society (ACS), pp. 3376–3393, Jan. 31, 2012. doi: 10.1021/jp210641j.  
  
J. Comer and A. Aksimentiev, “DNA sequence-dependent ionic currents in ultra-small solid-state nanopores”, *Nanoscale*, vol. 8, no. 18. Royal Society of Chemistry (RSC), pp. 9600–9613, 2016. doi: 10.1039/c6nr01061j.  
  
J. Comer, A. Hoand A. Aksimentiev, “Toward detection of DNA-bound proteins using solid-state nanopores: Insights from computer simulations”, *ELECTROPHORESIS*, vol. 33, no. 23. Wiley, pp. 3466–3479, Nov. 12, 2012. doi: 10.1002/elps.201200164.  
  
K. Decker, M. Page, A. Boyd, I. MacAllister, M. Ginsbergand A. Aksimentiev, “Selective Permeability of Truncated Aquaporin 1 in Silico”, *ACS Biomaterials Science & Engineering*, vol. 3, no. 3. American Chemical Society (ACS), pp. 342–348, Jan. 12, 2017. doi: 10.1021/acsbiomaterials.6b00583.  
  
T. Gamble, “Rectification of Ion Current in Nanopores Depends on the Type of Monovalent Cations: Experiments and Modeling”, *The Journal of Physical Chemistry C*, vol. 118, no. 18. American Chemical Society (ACS), pp. 9809–9819, Apr. 23, 2014. doi: 10.1021/jp501492g.  
  
K. Göpfrich, “Ion Channels Made from a Single Membrane-Spanning DNA Duplex”, *Nano Letters*, vol. 16, no. 7. American Chemical Society (ACS), pp. 4665–4669, Jun. 29, 2016. doi: 10.1021/acs.nanolett.6b02039.  
  
K. Göpfrich, “Large-Conductance Transmembrane Porin Made from DNA Origami”, *ACS Nano*, vol. 10, no. 9. American Chemical Society (ACS), pp. 8207–8214, Aug. 23, 2016. doi: 10.1021/acsnano.6b03759.  
  
S. Bhattacharya, I. M. Derrington, M. Pavlenok, M. Niederweis, J. H. Gundlachand A. Aksimentiev, “Molecular Dynamics Study of MspA Arginine Mutants Predicts Slow DNA Translocations and Ion Current Blockades Indicative of DNA Sequence”, *ACS Nano*, vol. 6, no. 8. American Chemical Society (ACS), pp. 6960–6968, Jul. 13, 2012. doi: 10.1021/nn3019943.  
  
S. W. Kowalczyk, D. B. Wells, A. Aksimentievand C. Dekker, “Slowing down DNA Translocation through a Nanopore in Lithium Chloride”, *Nano Letters*, vol. 12, no. 2. American Chemical Society (ACS), pp. 1038–1044, Jan. 27, 2012. doi: 10.1021/nl204273h.  
  
C.-Y. Li, “Ionic Conductivity, Structural Deformation, and Programmable Anisotropy of DNA Origami in Electric Field”, *ACS Nano*, vol. 9, no. 2. American Chemical Society (ACS), pp. 1420–1433, Jan. 30, 2015. doi: 10.1021/nn505825z.  
  
B. Luan, R. Carr, M. Caffreyand A. Aksimentiev, “The effect of calcium on the conformation of cobalamin transporter BtuB”, *Proteins: Structure, Function, and Bioinformatics*, vol. 78, no. 5. Wiley, pp. 1153–1162, Oct. 16, 2009. doi: 10.1002/prot.22635.  
  
C. Maffeo, S. Bhattacharya, J. Yoo, D. Wellsand A. Aksimentiev, “Modeling and Simulation of Ion Channels”, *Chemical Reviews*, vol. 112, no. 12. American Chemical Society (ACS), pp. 6250–6284, Oct. 04, 2012. doi: 10.1021/cr3002609.  
  
C. Maffeo, B. Luanand A. Aksimentiev, “End-to-end attraction of duplex DNA”, *Nucleic Acids Research*, vol. 40, no. 9. Oxford University Press (OUP), pp. 3812–3821, Jan. 11, 2012. doi: 10.1093/nar/gkr1220.  
  
C. Maffeo, T. T. M. Ngo, T. Haand A. Aksimentiev, “A Coarse-Grained Model of Unstructured Single-Stranded DNA Derived from Atomistic Simulation and Single-Molecule Experiment”, *Journal of Chemical Theory and Computation*, vol. 10, no. 8. American Chemical Society (ACS), pp. 2891–2896, Jun. 09, 2014. doi: 10.1021/ct500193u.  
  
C. Maffeo, J. Yooand A. Aksimentiev, “*De novo*reconstruction of DNA origami structures through atomistic molecular dynamics simulation”, *Nucleic Acids Research*, vol. 44, no. 7. Oxford University Press (OUP), pp. 3013–3019, Mar. 14, 2016. doi: 10.1093/nar/gkw155.  
  
C. Maffeo, J. Yoo, J. Comer, D. B. Wells, B. Luanand A. Aksimentiev, “Close encounters with DNA”, *Journal of Physics: Condensed Matter*, vol. 26, no. 41. IOP Publishing, p. 413101, Sep. 19, 2014. doi: 10.1088/0953-8984/26/41/413101.  
  
S. Bhattacharya, “Rectification of the Current in α-Hemolysin Pore Depends on the Cation Type: The Alkali Series Probed by Molecular Dynamics Simulations and Experiments”, *The Journal of Physical Chemistry C*, vol. 115, no. 10. American Chemical Society (ACS), pp. 4255–4264, Feb. 21, 2011. doi: 10.1021/jp111441p.  
  
U. Mirsaidov, J. Comer, V. Dimitrov, A. Aksimentievand G. Timp, “Slowing the translocation of double-stranded DNA using a nanopore smaller than the double helix”, *Nanotechnology*, vol. 21, no. 39. IOP Publishing, p. 395501, Sep. 01, 2010. doi: 10.1088/0957-4484/21/39/395501.  
  
T. T. M. Ngo, “Effects of cytosine modifications on DNA flexibility and nucleosome mechanical stability”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Feb. 24, 2016. doi: 10.1038/ncomms10813.  
  
A. Ohmann, “Outperforming nature: synthetic enzyme built from DNA flips lipids of biological membranes at record rates”, *[]*. Cold Spring Harbor Laboratory, Dec. 30, 2017. doi: 10.1101/241166.  
  
S. Pud, “Mechanical Trapping of DNA in a Double-Nanopore System”, *Nano Letters*, vol. 16, no. 12. American Chemical Society (ACS), pp. 8021–8028, Dec. 01, 2016. doi: 10.1021/acs.nanolett.6b04642.  
  
A. D. Radadia, “Control of Nanoscale Environment to Improve Stability of Immobilized Proteins on Diamond Surfaces”, *Advanced Functional Materials*, vol. 21, no. 6. Wiley, pp. 1040–1050, Feb. 08, 2011. doi: 10.1002/adfm.201002251.  
  
M. Shankla and A. Aksimentiev, “Conformational transitions and stop-and-go nanopore transport of single-stranded DNA on charged graphene”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, Oct. 09, 2014. doi: 10.1038/ncomms6171.  
  
M. Shankla and A. Aksimentiev, “Modulation of Molecular Flux Using a Graphene Nanopore Capacitor”, *The Journal of Physical Chemistry B*, vol. 121, no. 15. American Chemical Society (ACS), pp. 3724–3733, Jan. 17, 2017. doi: 10.1021/acs.jpcb.6b10574.  
  
Y.-. xiao . Shen, “Highly permeable artificial water channels that can self-assemble into two-dimensional arrays”, *Proceedings of the National Academy of Sciences*, vol. 112, no. 32. Proceedings of the National Academy of Sciences, pp. 9810–9815, Jul. 27, 2015. doi: 10.1073/pnas.1508575112.  
  
X. Shi, “Dynamics of a Molecular Plug Docked onto a Solid-State Nanopore”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 16. American Chemical Society (ACS), pp. 4686–4694, Jul. 30, 2018. doi: 10.1021/acs.jpclett.8b01755.  
  
S. M. Slone, C.-Y. Li, J. Yooand A. Aksimentiev, “Molecular mechanics of DNA bricks:*in situ*structure, mechanical properties and ionic conductivity”, *New Journal of Physics*, vol. 18, no. 5. IOP Publishing, p. 055012, May 27, 2016. doi: 10.1088/1367-2630/18/5/055012.  
  
C. Stavis, “Surface functionalization of thin-film diamond for highly stable and selective biological interfaces”, *Proceedings of the National Academy of Sciences*, vol. 108, no. 3. Proceedings of the National Academy of Sciences, pp. 983–988, Sep. 30, 2010. doi: 10.1073/pnas.1006660107.  
  
K. Tian, K. Decker, A. Aksimentievand L.-Q. Gu, “Interference-Free Detection of Genetic Biomarkers Using Synthetic Dipole-Facilitated Nanopore Dielectrophoresis”, *ACS Nano*, vol. 11, no. 2. American Chemical Society (ACS), pp. 1204–1213, Jan. 06, 2017. doi: 10.1021/acsnano.6b07570.  
  
W. Timp, J. Comerand A. Aksimentiev, “DNA Base-Calling from a Nanopore Using a Viterbi Algorithm”, *Biophysical Journal*, vol. 102, no. 10. Elsevier BV, pp. L37–L39, May 2012. doi: 10.1016/j.bpj.2012.04.009.  
  
M. Wanunu, S. Bhattacharya, Y. Xie, Y. Tor, A. Aksimentievand M. Drndic, “Nanopore Analysis of Individual RNA/Antibiotic Complexes”, *ACS Nano*, vol. 5, no. 12. American Chemical Society (ACS), pp. 9345–9353, Nov. 16, 2011. doi: 10.1021/nn203764j.  
  
B. M. Venkatesan, “Lipid bilayer coated Al2O3 nanopore sensors: towards a hybrid biological solid-state nanopore”, *Biomedical Microdevices*, vol. 13, no. 4. Springer Science and Business Media LLC, pp. 671–682, Apr. 13, 2011. doi: 10.1007/s10544-011-9537-3.  
  
B. M. Venkatesan, “Lipid bilayer coated Al2O3 nanopore sensors: towards a hybrid biological solid-state nanopore”, *Biomedical Microdevices*, vol. 13, no. 4. Springer Science and Business Media LLC, pp. 671–682, Apr. 13, 2011. doi: 10.1007/s10544-011-9537-3.  
  
D. B. Wells and A. Aksimentiev, “Mechanical Properties of a Complete Microtubule Revealed through Molecular Dynamics Simulation”, *Biophysical Journal*, vol. 99, no. 2. Elsevier BV, pp. 629–637, Jul. 2010. doi: 10.1016/j.bpj.2010.04.038.  
  
D. B. Wells, M. Belkin, J. Comerand A. Aksimentiev, “Assessing Graphene Nanopores for Sequencing DNA”, *Nano Letters*, vol. 12, no. 8. American Chemical Society (ACS), pp. 4117–4123, Jul. 17, 2012. doi: 10.1021/nl301655d.  
  
J. Wilson, L. Sloman, Z. Heand A. Aksimentiev, “Graphene Nanopores for Protein Sequencing”, *Advanced Functional Materials*, vol. 26, no. 27. Wiley, pp. 4830–4838, Jun. 09, 2016. doi: 10.1002/adfm.201601272.  
  
J. Yoo and A. Aksimentiev, “Improved Parametrization of Li+, Na+, K+, and Mg2+ Ions for All-Atom Molecular Dynamics Simulations of Nucleic Acid Systems”, *The Journal of Physical Chemistry Letters*, vol. 3, no. 1. American Chemical Society (ACS), pp. 45–50, Dec. 13, 2011. doi: 10.1021/jz201501a.  
  
J. Yoo and A. Aksimentiev, “Improved Parametrization of Li+, Na+, K+, and Mg2+ Ions for All-Atom Molecular Dynamics Simulations of Nucleic Acid Systems”, *The Journal of Physical Chemistry Letters*, vol. 3, no. 1. American Chemical Society (ACS), pp. 45–50, Dec. 13, 2011. doi: 10.1021/jz201501a.  
  
J. Yoo and A. Aksimentiev, “Competitive Binding of Cations to Duplex DNA Revealed through Molecular Dynamics Simulations”, *The Journal of Physical Chemistry B*, vol. 116, no. 43. American Chemical Society (ACS), pp. 12946–12954, Oct. 19, 2012. doi: 10.1021/jp306598y.  
  
J. Yoo and A. Aksimentiev, “In situ structure and dynamics of DNA origami determined through molecular dynamics simulations”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 50. Proceedings of the National Academy of Sciences, pp. 20099–20104, Nov. 25, 2013. doi: 10.1073/pnas.1316521110.  
  
J. Yoo and A. Aksimentiev, “Molecular Dynamics of Membrane-Spanning DNA Channels: Conductance Mechanism, Electro-Osmotic Transport, and Mechanical Gating”, *The Journal of Physical Chemistry Letters*, vol. 6, no. 23. American Chemical Society (ACS), pp. 4680–4687, Nov. 12, 2015. doi: 10.1021/acs.jpclett.5b01964.  
  
J. Yoo and A. Aksimentiev, “Improved Parameterization of Amine–Carboxylate and Amine–Phosphate Interactions for Molecular Dynamics Simulations Using the CHARMM and AMBER Force Fields”, *Journal of Chemical Theory and Computation*, vol. 12, no. 1. American Chemical Society (ACS), pp. 430–443, Dec. 16, 2015. doi: 10.1021/acs.jctc.5b00967.  
  
J. Yoo and A. Aksimentiev, “The structure and intermolecular forces of DNA condensates”, *Nucleic Acids Research*, vol. 44, no. 5. Oxford University Press (OUP), pp. 2036–2046, Feb. 15, 2016. doi: 10.1093/nar/gkw081.  
  
J. Yoo and A. Aksimentiev, “Refined Parameterization of Nonbonded Interactions Improves Conformational Sampling and Kinetics of Protein Folding Simulations”, *The Journal of Physical Chemistry Letters*, vol. 7, no. 19. American Chemical Society (ACS), pp. 3812–3818, Sep. 14, 2016. doi: 10.1021/acs.jpclett.6b01747.  
  
J. Yoo, H. Kim, A. Aksimentievand T. Ha, “Direct evidence for sequence-dependent attraction between double-stranded DNA controlled by methylation”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Mar. 22, 2016. doi: 10.1038/ncomms11045.  
  
J. Yoo, J. Wilsonand A. Aksimentiev, “Improved model of hydrated calcium ion for molecular dynamics simulations using classical biomolecular force fields”, *Biopolymers*, vol. 105, no. 10. Wiley, pp. 752–763, Jul. 22, 2016. doi: 10.1002/bip.22868.  
  
H.-Y. K. Yang, S. Bhattacharyaand P. M. Ricker, “THE IMPACT OF CLUSTER STRUCTURE AND DYNAMICAL STATE ON SCATTER IN THE SUNYAEV-ZEL’DOVICH FLUX-MASS RELATION”, *The Astrophysical Journal*, vol. 725, no. 1. American Astronomical Society, pp. 1124–1136, Nov. 23, 2010. doi: 10.1088/0004-637x/725/1/1124.  
  
P. S. Iyer and K. Mahesh, “A numerical study of shear layer characteristics of low-speed transverse jets”, *Journal of Fluid Mechanics*, vol. 790. Cambridge University Press (CUP), pp. 275–307, Feb. 03, 2016. doi: 10.1017/jfm.2016.7.  
  
K. Mahesh, “The Interaction of Jets with Crossflow”, *Annual Review of Fluid Mechanics*, vol. 45, no. 1. Annual Reviews, pp. 379–407, Jan. 03, 2013. doi: 10.1146/annurev-fluid-120710-101115.  
  
I. Cerovečki and M. R. Mazloff, “The Spatiotemporal Structure of Diabatic Processes Governing the Evolution of Subantarctic Mode Water in the Southern Ocean”, *Journal of Physical Oceanography*, vol. 46, no. 2. American Meteorological Society, pp. 683–710, Feb. 2016. doi: 10.1175/jpo-d-14-0243.1.  
  
J. Masich, T. K. Chereskinand M. R. Mazloff, “Topographic form stress in the S outhern O cean S tate E stimate”, *Journal of Geophysical Research: Oceans*, vol. 120, no. 12. American Geophysical Union (AGU), pp. 7919–7933, Dec. 2015. doi: 10.1002/2015jc011143.  
  
J. Green, “Up, down, and strange nucleon axial form factors from lattice QCD”, *Physical Review D*, vol. 95, no. 11. American Physical Society (APS), Jun. 14, 2017. doi: 10.1103/physrevd.95.114502.  
  
J. Green, “High-precision calculation of the strange nucleon electromagnetic form factors”, *Physical Review D*, vol. 92, no. 3. American Physical Society (APS), Aug. 26, 2015. doi: 10.1103/physrevd.92.031501.  
  
K. Blancato, S. Geneland G. Bryan, “Implications of Galaxy Buildup for Putative IMF Variations in Massive Galaxies”, *The Astrophysical Journal*, vol. 845, no. 2. American Astronomical Society, p. 136, Aug. 18, 2017. doi: 10.3847/1538-4357/aa7b84.  
  
C. Brummel-Smith, “ENZO: An Adaptive Mesh Refinement Code for Astrophysics (Version 2.6)”, *Journal of Open Source Software*, vol. 4, no. 42. The Open Journal, p. 1636, Oct. 03, 2019. doi: 10.21105/joss.01636.  
  
J. Chen, G. L. Bryanand M. Salem, “Cosmological simulations of dwarf galaxies with cosmic ray feedback”, *Monthly Notices of the Royal Astronomical Society*, vol. 460, no. 3. Oxford University Press (OUP), pp. 3335–3344, May 20, 2016. doi: 10.1093/mnras/stw1197.  
  
D. DeFelippis, S. Genel, G. L. Bryanand S. M. Fall, “The Impact of Galactic Winds on the Angular Momentum of Disk Galaxies in the Illustris Simulation”, *The Astrophysical Journal*, vol. 841, no. 1. American Astronomical Society, p. 16, May 18, 2017. doi: 10.3847/1538-4357/aa6dfc.  
  
A. Emerick, G. L. Bryan, M.-M. M. Low, B. Côté, K. V. Johnstonand B. W. O’Shea, “Metal Mixing and Ejection in Dwarf Galaxies Are Dependent on Nucleosynthetic Source”, *The Astrophysical Journal*, vol. 869, no. 2. American Astronomical Society, p. 94, Dec. 14, 2018. doi: 10.3847/1538-4357/aaec7d.  
  
A. Emerick, G. L. Bryanand M.-M. Mac Low, “Stellar Radiation Is Critical for Regulating Star Formation and Driving Outflows in Low-mass Dwarf Galaxies”, *The Astrophysical Journal*, vol. 865, no. 2. American Astronomical Society, p. L22, Oct. 01, 2018. doi: 10.3847/2041-8213/aae315.  
  
A. Emerick, G. L. Bryanand M.-M. Mac Low, “Simulating an isolated dwarf galaxy with multichannel feedback and chemical yields from individual stars”, *Monthly Notices of the Royal Astronomical Society*, vol. 482, no. 1. Oxford University Press (OUP), pp. 1304–1329, Oct. 04, 2018. doi: 10.1093/mnras/sty2689.  
  
R. Fernandez and G. L. Bryan, “Slow cooling in low-metallicity clouds: an origin of globular cluster bimodality?”, *Monthly Notices of the Royal Astronomical Society*, vol. 479, no. 1. Oxford University Press (OUP), pp. 200–210, May 23, 2018. doi: 10.1093/mnras/sty1361.  
  
R. Fernandez, G. L. Bryan, Z. Haimanand M. Li, “H2 suppression with shocking inflows: testing a pathway for supermassive black hole formation”, *Monthly Notices of the Royal Astronomical Society*, vol. 439, no. 4. Oxford University Press (OUP), pp. 3798–3807, Feb. 26, 2014. doi: 10.1093/mnras/stu230.  
  
Y. Fujimoto, G. L. Bryan, E. J. Tasker, A. Habeand C. M. Simpson, “GMC evolution in a barred spiral galaxy with star formation and thermal feedback”, *Monthly Notices of the Royal Astronomical Society*, vol. 461, no. 2. Oxford University Press (OUP), pp. 1684–1700, Jun. 20, 2016. doi: 10.1093/mnras/stw1461.  
  
S. Genel, “A Quantification of the Butterfly Effect in Cosmological Simulations and Implications for Galaxy Scaling Relations”, *The Astrophysical Journal*, vol. 871, no. 1. American Astronomical Society, p. 21, Jan. 18, 2019. doi: 10.3847/1538-4357/aaf4bb.  
  
C. B. Hummels, G. L. Bryan, B. D. Smithand M. J. Turk, “Constraints on hydrodynamical subgrid models from quasar absorption line studies of the simulated circumgalactic medium”, *Monthly Notices of the Royal Astronomical Society*, vol. 430, no. 3. Oxford University Press (OUP), pp. 1548–1565, Feb. 09, 2013. doi: 10.1093/mnras/sts702.  
  
M. Li, G. L. Bryanand J. P. Ostriker, “Quantifying Supernovae-driven Multiphase Galactic Outflows”, *The Astrophysical Journal*, vol. 841, no. 2. American Astronomical Society, p. 101, May 31, 2017. doi: 10.3847/1538-4357/aa7263.  
  
X. Li, L. Huiand G. L. Bryan, “Numerical and perturbative computations of the fuzzy dark matter model”, *Physical Review D*, vol. 99, no. 6. American Physical Society (APS), Mar. 12, 2019. doi: 10.1103/physrevd.99.063509.  
  
Y. Li, G. L. Bryan, M. Ruszkowski, G. M. Voit, B. W. O’Sheaand M. Donahue, “COOLING, AGN FEEDBACK, AND STAR FORMATION IN SIMULATED COOL-CORE GALAXY CLUSTERS”, *The Astrophysical Journal*, vol. 811, no. 2. American Astronomical Society, p. 73, Sep. 24, 2015. doi: 10.1088/0004-637x/811/2/73.  
  
Y. Li, M. Ruszkowskiand G. L. Bryan, “AGN Heating in Simulated Cool-core Clusters”, *The Astrophysical Journal*, vol. 847, no. 2. American Astronomical Society, p. 106, Sep. 27, 2017. doi: 10.3847/1538-4357/aa88c1.  
  
M. Li (李邈), J. P. Ostriker, R. Cen, G. L. Bryanand T. Naab, “SUPERNOVA FEEDBACK AND THE HOT GAS FILLING FRACTION OF THE INTERSTELLAR MEDIUM”, *The Astrophysical Journal*, vol. 814, no. 1. American Astronomical Society, p. 4, Nov. 10, 2015. doi: 10.1088/0004-637x/814/1/4.  
  
N. Melso, G. L. Bryanand M. Li, “Simulating Gas Inflow at the Disk–Halo Interface”, *The Astrophysical Journal*, vol. 872, no. 1. American Astronomical Society, p. 47, Feb. 08, 2019. doi: 10.3847/1538-4357/aafaf5.  
  
J.-C. Passy and G. L. Bryan, “AN ADAPTIVE PARTICLE-MESH GRAVITY SOLVER FOR ENZO”, *The Astrophysical Journal Supplement Series*, vol. 215, no. 1. American Astronomical Society, p. 8, Oct. 20, 2014. doi: 10.1088/0067-0049/215/1/8.  
  
M. Salem, G. Besla, G. Bryan, M. Putman, R. P. van der Mareland S. Tonnesen, “RAM PRESSURE STRIPPING OF THE LARGE MAGELLANIC CLOUD’S DISK AS A PROBE OF THE MILKY WAY’S CIRCUMGALACTIC MEDIUM”, *The Astrophysical Journal*, vol. 815, no. 1. American Astronomical Society, p. 77, Dec. 10, 2015. doi: 10.1088/0004-637x/815/1/77.  
  
M. Salem and G. L. Bryan, “Cosmic ray driven outflows in global galaxy disc models”, *Monthly Notices of the Royal Astronomical Society*, vol. 437, no. 4. Oxford University Press (OUP), pp. 3312–3330, Nov. 28, 2013. doi: 10.1093/mnras/stt2121.  
  
M. Salem, G. L. Bryanand L. Corlies, “Role of cosmic rays in the circumgalactic medium”, *Monthly Notices of the Royal Astronomical Society*, vol. 456, no. 1. Oxford University Press (OUP), pp. 582–601, Dec. 16, 2015. doi: 10.1093/mnras/stv2641.  
  
C. M. Simpson, G. L. Bryan, C. Hummelsand J. P. Ostriker, “KINETIC ENERGY FROM SUPERNOVA FEEDBACK IN HIGH-RESOLUTION GALAXY SIMULATIONS”, *The Astrophysical Journal*, vol. 809, no. 1. American Astronomical Society, p. 69, Aug. 11, 2015. doi: 10.1088/0004-637x/809/1/69.  
  
C. M. Simpson, “The effect of feedback and reionization on star formation in low-mass dwarf galaxy haloes”, *Monthly Notices of the Royal Astronomical Society*, vol. 432, no. 3. Oxford University Press (OUP), pp. 1989–2011, May 09, 2013. doi: 10.1093/mnras/stt474.  
  
B. D. Smith, “grackle: a chemistry and cooling library for astrophysics”, *Monthly Notices of the Royal Astronomical Society*, vol. 466, no. 2. Oxford University Press (OUP), pp. 2217–2234, Dec. 17, 2016. doi: 10.1093/mnras/stw3291.  
  
S. Tonnesen and G. L. Bryan, “Star formation in ram pressure stripped galactic tails”, *Monthly Notices of the Royal Astronomical Society*, vol. 422, no. 2. Oxford University Press (OUP), pp. 1609–1624, Mar. 09, 2012. doi: 10.1111/j.1365-2966.2012.20737.x.  
  
E. Visbal, G. L. Bryanand Z. Haiman, “What is the maximum mass of a Population III galaxy?”, *Monthly Notices of the Royal Astronomical Society*, vol. 469, no. 2. Oxford University Press (OUP), pp. 1456–1465, Apr. 17, 2017. doi: 10.1093/mnras/stx909.  
  
E. Visbal, Z. Haimanand G. L. Bryan, “A no-go theorem for direct collapse black holes without a strong ultraviolet background”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 442, no. 1. Oxford University Press (OUP), pp. L100–L104, Jun. 10, 2014. doi: 10.1093/mnrasl/slu063.  
  
E. Visbal, Z. Haimanand G. L. Bryan, “Direct collapse black hole formation from synchronized pairs of atomic cooling haloes”, *Monthly Notices of the Royal Astronomical Society*, vol. 445, no. 1. Oxford University Press (OUP), pp. 1056–1063, Oct. 08, 2014. doi: 10.1093/mnras/stu1794.  
  
E. Visbal, Z. Haimanand G. L. Bryan, “Limits on Population III star formation in minihaloes implied by*Planck*”, *Monthly Notices of the Royal Astronomical Society*, vol. 453, no. 4. Oxford University Press (OUP), pp. 4457–4467, Sep. 17, 2015. doi: 10.1093/mnras/stv1941.  
  
E. Visbal, Z. Haimanand G. L. Bryan, “Looking for Population III stars with He ii line intensity mapping”, *Monthly Notices of the Royal Astronomical Society*, vol. 450, no. 3. Oxford University Press (OUP), pp. 2506–2513, May 06, 2015. doi: 10.1093/mnras/stv785.  
  
E. Visbal, Z. Haimanand G. L. Bryan, “Formation of massive Population III galaxies through photoionization feedback: a possible explanation for CR 7”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 460, no. 1. Oxford University Press (OUP), pp. L59–L63, Apr. 14, 2016. doi: 10.1093/mnrasl/slw071.  
  
E. Visbal, Z. Haimanand G. L. Bryan, “Self-consistent semi-analytic models of the first stars”, *Monthly Notices of the Royal Astronomical Society*, vol. 475, no. 4. Oxford University Press (OUP), pp. 5246–5256, Jan. 17, 2018. doi: 10.1093/mnras/sty142.  
  
E. Visbal, Z. Haiman, B. Terrazas, G. L. Bryanand R. Barkana, “High-redshift star formation in a time-dependent Lyman–Werner background”, *Monthly Notices of the Royal Astronomical Society*, vol. 445, no. 1. Oxford University Press (OUP), pp. 107–114, Sep. 22, 2014. doi: 10.1093/mnras/stu1710.  
  
G. M. Voit, G. L. Bryan, B. W. O’Sheaand M. Donahue, “PRECIPITATION-REGULATED STAR FORMATION IN GALAXIES”, *The Astrophysical Journal*, vol. 808, no. 1. American Astronomical Society, p. L30, Jul. 23, 2015. doi: 10.1088/2041-8205/808/1/l30.  
  
G. M. Voit, M. Donahue, G. L. Bryanand M. McDonald, “Regulation of star formation in giant galaxies by precipitation, feedback and conduction”, *Nature*, vol. 519, no. 7542. Springer Science and Business Media LLC, pp. 203–206, Mar. 2015. doi: 10.1038/nature14167.  
  
G. M. Voit, M. Donahue, B. W. O’Shea, G. L. Bryan, M. Sunand N. Werner, “SUPERNOVA SWEEPING AND BLACK HOLE FEEDBACK IN ELLIPTICAL GALAXIES”, *The Astrophysical Journal*, vol. 803, no. 2. American Astronomical Society, p. L21, Apr. 16, 2015. doi: 10.1088/2041-8205/803/2/l21.  
  
G. M. Voit, “Circumgalactic Pressure Profiles Indicate Precipitation-limited Atmospheres for *M* \* ∼ 109–1011.5 *M* ⊙”, *The Astrophysical Journal*, vol. 879, no. 1. American Astronomical Society, p. L1, Jun. 25, 2019. doi: 10.3847/2041-8213/ab2766.  
  
G. M. Voit, G. Meece, Y. Li, B. W. O’Shea, G. L. Bryanand M. Donahue, “A Global Model for Circumgalactic and Cluster-core Precipitation”, *The Astrophysical Journal*, vol. 845, no. 1. American Astronomical Society, p. 80, Aug. 10, 2017. doi: 10.3847/1538-4357/aa7d04.  
  
M. M. Ameen and J. Abraham, “RANS and LES Study of Lift-Off Physics in Reacting Diesel Jets”, *SAE Technical Paper Series*. SAE International, Apr. 01, 2014. doi: 10.4271/2014-01-1118.  
  
M. M. Ameen and J. Abraham, “A priori evaluation of subgrid-scale combustion models for diesel engine applications”, *Fuel*, vol. 153. Elsevier BV, pp. 612–619, Aug. 2015. doi: 10.1016/j.fuel.2015.03.036.  
  
M. M. Ameen and J. Abraham, “Evaluation of scalar dissipation rate sub-models for modeling unsteady reacting jets in engines”, *Chemical Engineering Science*, vol. 127. Elsevier BV, pp. 334–343, May 2015. doi: 10.1016/j.ces.2015.01.055.  
  
C. Bajaj, M. Ameenand J. Abraham, “Evaluation of an Unsteady Flamelet Progress Variable Model for Autoignition and Flame Lift-Off in Diesel Jets”, *Combustion Science and Technology*, vol. 185, no. 3. Informa UK Limited, pp. 454–472, Feb. 27, 2013. doi: 10.1080/00102202.2012.726667.  
  
Z. Wang and J. Abraham, “Fundamental physics of flame development in an autoigniting dual fuel mixture”, *Proceedings of the Combustion Institute*, vol. 35, no. 1. Elsevier BV, pp. 1041–1048, 2015. doi: 10.1016/j.proci.2014.06.079.  
  
Y. O. Ahn, “Conformational coupling between the active site and residues within the K C -channel of the *Vibrio cholerae cbb* 3 -type (C-family) oxygen reductase”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 42. Proceedings of the National Academy of Sciences, Oct. 06, 2014. doi: 10.1073/pnas.1411676111.  
  
M. J. Arcario, C. G. Mayneand E. Tajkhorshid, “Atomistic Models of General Anesthetics for Use in in Silico Biological Studies”, *The Journal of Physical Chemistry B*, vol. 118, no. 42. American Chemical Society (ACS), pp. 12075–12086, Oct. 10, 2014. doi: 10.1021/jp502716m.  
  
M. J. Arcario, C. G. Mayneand E. Tajkhorshid, “A membrane-embedded pathway delivers general anesthetics to two interacting binding sites in the Gloeobacter violaceus ion channel”, *Journal of Biological Chemistry*, vol. 292, no. 23. Elsevier BV, pp. 9480–9492, Jul. 2017. doi: 10.1074/jbc.m117.780197.  
  
M. J. Arcario, Y. Z. Ohkuboand E. Tajkhorshid, “Capturing Spontaneous Partitioning of Peripheral Proteins Using a Biphasic Membrane-Mimetic Model”, *The Journal of Physical Chemistry B*, vol. 115, no. 21. American Chemical Society (ACS), pp. 7029–7037, May 11, 2011. doi: 10.1021/jp109631y.  
  
M. J. Arcario and E. Tajkhorshid, “Membrane-Induced Structural Rearrangement and Identification of a Novel Membrane Anchor in Talin F2F3”, *Biophysical Journal*, vol. 107, no. 9. Elsevier BV, pp. 2059–2069, Nov. 2014. doi: 10.1016/j.bpj.2014.09.022.  
  
W. R. Arnold, J. L. Baylon, E. Tajkhorshidand A. Das, “Asymmetric Binding and Metabolism of Polyunsaturated Fatty Acids (PUFAs) by CYP2J2 Epoxygenase”, *Biochemistry*, vol. 55, no. 50. American Chemical Society (ACS), pp. 6969–6980, Dec. 05, 2016. doi: 10.1021/acs.biochem.6b01037.  
  
W. R. Arnold, J. L. Baylon, E. Tajkhorshidand A. Das, “Arachidonic Acid Metabolism by Human Cardiovascular CYP2J2 Is Modulated by Doxorubicin”, *Biochemistry*, vol. 56, no. 51. American Chemical Society (ACS), pp. 6700–6712, Dec. 12, 2017. doi: 10.1021/acs.biochem.7b01025.  
  
A. Aster, “Tuning symmetry breaking charge separation in perylene bichromophores by conformational control”, *Chemical Science*, vol. 10, no. 45. Royal Society of Chemistry (RSC), pp. 10629–10639, 2019. doi: 10.1039/c9sc03913a.  
  
A. Barati Farimani, N. R. Aluruand E. Tajkhorshid, “Thermodynamic insight into spontaneous hydration and rapid water permeation in aquaporins”, *Applied Physics Letters*, vol. 105, no. 8. AIP Publishing, p. 083702, Aug. 25, 2014. doi: 10.1063/1.4893782.  
  
S. Barrick, J. Li, X. Kong, A. Ray, E. Tajkhorshidand D. Leckband, “Salt bridges gate α-catenin activation at intercellular junctions”, *Molecular Biology of the Cell*, vol. 29, no. 2. American Society for Cell Biology (ASCB), pp. 111–122, Jan. 15, 2018. doi: 10.1091/mbc.e17-03-0168.  
  
J. L. Baylon and E. Tajkhorshid, “Capturing Spontaneous Membrane Insertion of the Influenza Virus Hemagglutinin Fusion Peptide”, *The Journal of Physical Chemistry B*, vol. 119, no. 25. American Chemical Society (ACS), pp. 7882–7893, Jun. 08, 2015. doi: 10.1021/acs.jpcb.5b02135.  
  
H. M. Berman, “Federating Structural Models and Data: Outcomes from A Workshop on Archiving Integrative Structures”, *Structure*, vol. 27, no. 12. Elsevier BV, pp. 1745–1759, Dec. 2019. doi: 10.1016/j.str.2019.11.002.  
  
A. E. Blanchard, M. J. Arcario, K. Schultenand E. Tajkhorshid, “A Highly Tilted Membrane Configuration for the Prefusion State of Synaptobrevin”, *Biophysical Journal*, vol. 107, no. 9. Elsevier BV, pp. 2112–2121, Nov. 2014. doi: 10.1016/j.bpj.2014.09.013.  
  
A. K. S. Camara, Y. Zhou, P.-C. Wen, E. Tajkhorshidand W.-M. Kwok, “Mitochondrial VDAC1: A Key Gatekeeper as Potential Therapeutic Target”, *Frontiers in Physiology*, vol. 8. Frontiers Media SA, Jun. 30, 2017. doi: 10.3389/fphys.2017.00460.  
  
L. N. Carnevale, A. S. Arango, W. R. Arnold, E. Tajkhorshidand A. Das, “Endocannabinoid Virodhamine Is an Endogenous Inhibitor of Human Cardiovascular CYP2J2 Epoxygenase”, *Biochemistry*, vol. 57, no. 46. American Chemical Society (ACS), pp. 6489–6499, Oct. 04, 2018. doi: 10.1021/acs.biochem.8b00691.  
  
A. Chakravarti, “Reconstitution and substrate specificity for isopentenyl pyrophosphate of the antiviral radical SAM enzyme viperin”, *Journal of Biological Chemistry*, vol. 293, no. 36. Elsevier BV, pp. 14122–14133, Sep. 2018. doi: 10.1074/jbc.ra118.003998.  
  
S. Chen, Y. Zhao, Y. Wang, M. Shekhar, E. Tajkhorshidand E. Gouaux, “Activation and Desensitization Mechanism of AMPA Receptor-TARP Complex by Cryo-EM”, *Cell*, vol. 170, no. 6. Elsevier BV, pp. 1234–1246.e14, Sep. 2017. doi: 10.1016/j.cell.2017.07.045.  
  
J. A. Coleman, “Serotonin transporter–ibogaine complexes illuminate mechanisms of inhibition and transport”, *Nature*, vol. 569, no. 7754. Springer Science and Business Media LLC, pp. 141–145, Apr. 24, 2019. doi: 10.1038/s41586-019-1135-1.  
  
I. G. Denisov, J. L. Baylon, Y. V. Grinkova, E. Tajkhorshidand S. G. Sligar, “Drug–Drug Interactions between Atorvastatin and Dronedarone Mediated by Monomeric CYP3A4”, *Biochemistry*, vol. 57, no. 5. American Chemical Society (ACS), pp. 805–816, Dec. 14, 2017. doi: 10.1021/acs.biochem.7b01012.  
  
I. G. Denisov, Y. V. Grinkova, J. L. Baylon, E. Tajkhorshidand S. G. Sligar, “Mechanism of Drug–Drug Interactions Mediated by Human Cytochrome P450 CYP3A4 Monomer”, *Biochemistry*, vol. 54, no. 13. American Chemical Society (ACS), pp. 2227–2239, Mar. 25, 2015. doi: 10.1021/acs.biochem.5b00079.  
  
I. G. Denisov, Y. V. Grinkova, P. Nandigrami, M. Shekhar, E. Tajkhorshidand S. G. Sligar, “Allosteric Interactions in Human Cytochrome P450 CYP3A4: The Role of Phenylalanine 213”, *Biochemistry*, vol. 58, no. 10. American Chemical Society (ACS), pp. 1411–1422, Feb. 20, 2019. doi: 10.1021/acs.biochem.8b01268.  
  
G. Enkavi, “Simulation Studies of the Mechanism of Membrane Transporters”, *Methods in Molecular Biology*. Humana Press, pp. 361–405, Aug. 18, 2012. doi: 10.1007/978-1-62703-017-5\_14.  
  
S. W. Fanning, “The SERM/SERD bazedoxifene disrupts ESR1 helix 12 to overcome acquired hormone resistance in breast cancer cells”, *eLife*, vol. 7. eLife Sciences Publications, Ltd, Nov. 29, 2018. doi: 10.7554/elife.37161.  
  
S. W. Fanning, “Estrogen receptor alpha somatic mutations Y537S and D538G confer breast cancer endocrine resistance by stabilizing the activating function-2 binding conformation”, *eLife*, vol. 5. eLife Sciences Publications, Ltd, Feb. 02, 2016. doi: 10.7554/elife.12792.  
  
G. Gonzalez-Gutierrez, Y. Wang, G. D. Cymes, E. Tajkhorshidand C. Grosman, “Chasing the open-state structure of pentameric ligand-gated ion channels”, *Journal of General Physiology*, vol. 149, no. 12. Rockefeller University Press, pp. 1119–1138, Oct. 31, 2017. doi: 10.1085/jgp.201711803.  
  
W. Han, R. C. Cheng, M. C. Madukeand E. Tajkhorshid, “Water access points and hydration pathways in CLC H + /Cl − transporters”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 5. Proceedings of the National Academy of Sciences, pp. 1819–1824, Dec. 30, 2013. doi: 10.1073/pnas.1317890111.  
  
B. J. Henderson, “Menthol Stereoisomers Exhibit Different Effects on α4β2 nAChR Upregulation and Dopamine Neuron Spontaneous Firing”, *eneuro*, vol. 5, no. 6. Society for Neuroscience, pp. ENEURO.0465–18.2018, Nov. 2018. doi: 10.1523/eneuro.0465-18.2018.  
  
P. Hosseinzadeh, “Enhancing Mn(II)-Binding and Manganese Peroxidase Activity in a Designed Cytochrome *c* Peroxidase through Fine-Tuning Secondary-Sphere Interactions”, *Biochemistry*, vol. 55, no. 10. American Chemical Society (ACS), pp. 1494–1502, Mar. 02, 2016. doi: 10.1021/acs.biochem.5b01299.  
  
R. E. Hulse, J. R. Sachleben, P.-C. Wen, M. Moradi, E. Tajkhorshidand E. Perozo, “Conformational Dynamics at the Inner Gate of KcsA during Activation”, *Biochemistry*, vol. 53, no. 16. American Chemical Society (ACS), pp. 2557–2559, Apr. 18, 2014. doi: 10.1021/bi500168u.  
  
D. T. Infield, “Main-chain mutagenesis reveals intrahelical coupling in an ion channel voltage-sensor”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Nov. 29, 2018. doi: 10.1038/s41467-018-07477-3.  
  
T. Jiang, W. Han, M. Madukeand E. Tajkhorshid, “Molecular Basis for Differential Anion Binding and Proton Coupling in the Cl–/H+ Exchanger ClC-ec1”, *Journal of the American Chemical Society*, vol. 138, no. 9. American Chemical Society (ACS), pp. 3066–3075, Feb. 26, 2016. doi: 10.1021/jacs.5b12062.  
  
T. Jiang, “Computational Dissection of Membrane Transport at a Microscopic Level”, *Trends in Biochemical Sciences*, vol. 45, no. 3. Elsevier BV, pp. 202–216, Mar. 2020. doi: 10.1016/j.tibs.2019.09.001.  
  
T. Jiang, K. Yu, H. C. Hartzelland E. Tajkhorshid, “Lipids and ions traverse the membrane by the same physical pathway in the nhTMEM16 scramblase”, *eLife*, vol. 6. eLife Sciences Publications, Ltd, Sep. 16, 2017. doi: 10.7554/elife.28671.  
  
X. Jiang, “Multivalent Polymer–Peptide Conjugates: A General Platform for Inhibiting Amyloid Beta Peptide Aggregation”, *ACS Macro Letters*, vol. 8, no. 10. American Chemical Society (ACS), pp. 1365–1371, Sep. 30, 2019. doi: 10.1021/acsmacrolett.9b00559.  
  
M. R. Kalani, A. Moradi, M. Moradiand E. Tajkhorshid, “Characterizing a Histidine Switch Controlling pH-Dependent Conformational Changes of the Influenza Virus Hemagglutinin”, *Biophysical Journal*, vol. 105, no. 4. Elsevier BV, pp. 993–1003, Aug. 2013. doi: 10.1016/j.bpj.2013.06.047.  
  
D. Kerr, G. T. Tietjen, Z. Gong, E. Tajkhorshid, E. J. Adamsand K. Y. C. Lee, “Sensitivity of peripheral membrane proteins to the membrane context: A case study of phosphatidylserine and the TIM proteins”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1860, no. 10. Elsevier BV, pp. 2126–2133, Oct. 2018. doi: 10.1016/j.bbamem.2018.06.010.  
  
C. M. Khantwal, “Revealing an outward-facing open conformational state in a CLC Cl–/H+ exchange transporter”, *eLife*, vol. 5. eLife Sciences Publications, Ltd, Jan. 22, 2016. doi: 10.7554/elife.11189.  
  
P. Kumar, “Cryo-EM structures of a lipid-sensitive pentameric ligand-gated ion channel embedded in a phosphatidylcholine-only bilayer”, *Proceedings of the National Academy of Sciences*, vol. 117, no. 3. Proceedings of the National Academy of Sciences, pp. 1788–1798, Jan. 07, 2020. doi: 10.1073/pnas.1906823117.  
  
J. Li, “Structural Determinants of the Mechanical Stability of α-Catenin”, *Journal of Biological Chemistry*, vol. 290, no. 31. Elsevier BV, pp. 18890–18903, Jul. 2015. doi: 10.1074/jbc.m115.647941.  
  
J. Li, S. A. Shaikh, G. Enkavi, P.-C. Wen, Z. Huangand E. Tajkhorshid, “Transient formation of water-conducting states in membrane transporters”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 19. Proceedings of the National Academy of Sciences, pp. 7696–7701, Apr. 22, 2013. doi: 10.1073/pnas.1218986110.  
  
J. Li and E. Tajkhorshid, “A gate-free pathway for substrate release from the inward-facing state of the Na+-galactose transporter”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1818, no. 2. Elsevier BV, pp. 263–271, Feb. 2012. doi: 10.1016/j.bbamem.2011.09.011.  
  
J. Li, P.-C. Wen, M. Moradiand E. Tajkhorshid, “Computational characterization of structural dynamics underlying function in active membrane transporters”, *Current Opinion in Structural Biology*, vol. 31. Elsevier BV, pp. 96–105, Apr. 2015. doi: 10.1016/j.sbi.2015.04.001.  
  
J. Li, Z. Zhaoand E. Tajkhorshid, “Locking Two Rigid-body Bundles in an Outward-Facing Conformation: The Ion-coupling Mechanism in a LeuT-fold Transporter”, *Scientific Reports*, vol. 9, no. 1. Springer Science and Business Media LLC, Dec. 20, 2019. doi: 10.1038/s41598-019-55722-6.  
  
M. Macchione, “A Chalcogen‐Bonding Cascade Switch for Planarizable Push–Pull Probes”, *Angewandte Chemie International Edition*, vol. 58, no. 44. Wiley, pp. 15752–15756, Sep. 20, 2019. doi: 10.1002/anie.201909741.  
  
J. J. Madsen, Y. Z. Ohkubo, G. H. Peters, J. H. Faber, E. Tajkhorshidand O. H. Olsen, “Membrane Interaction of the Factor VIIIa Discoidin Domains in Atomistic Detail”, *Biochemistry*, vol. 54, no. 39. American Chemical Society (ACS), pp. 6123–6131, Sep. 21, 2015. doi: 10.1021/acs.biochem.5b00417.  
  
M. Mahdavi, A. Fattahi, E. Tajkhorshidand S. Nouranian, “Molecular Insights into the Loading and Dynamics of Doxorubicin on PEGylated Graphene Oxide Nanocarriers”, *ACS Applied Bio Materials*, vol. 3, no. 3. American Chemical Society (ACS), pp. 1354–1363, Feb. 12, 2020. doi: 10.1021/acsabm.9b00956.  
  
P. Mahinthichaichan, R. B. Gennisand E. Tajkhorshid, “All the O2 Consumed by *Thermus thermophilus* Cytochrome ba3 Is Delivered to the Active Site through a Long, Open Hydrophobic Tunnel with Entrances within the Lipid Bilayer”, *Biochemistry*, vol. 55, no. 8. American Chemical Society (ACS), pp. 1265–1278, Feb. 18, 2016. doi: 10.1021/acs.biochem.5b01255.  
  
P. Mahinthichaichan, R. B. Gennisand E. Tajkhorshid, “Bacterial denitrifying nitric oxide reductases and aerobic respiratory terminal oxidases use similar delivery pathways for their molecular substrates”, *Biochimica et Biophysica Acta (BBA) - Bioenergetics*, vol. 1859, no. 9. Elsevier BV, pp. 712–724, Sep. 2018. doi: 10.1016/j.bbabio.2018.06.002.  
  
P. Mahinthichaichan, R. B. Gennisand E. Tajkhorshid, “Cytochrome *aa*3 Oxygen Reductase Utilizes the Tunnel Observed in the Crystal Structures To Deliver O2 for Catalysis”, *Biochemistry*, vol. 57, no. 14. American Chemical Society (ACS), pp. 2150–2161, Mar. 16, 2018. doi: 10.1021/acs.biochem.7b01194.  
  
P. Mahinthichaichan, D. M. Morris, Y. Wang, G. J. Jensenand E. Tajkhorshid, “Selective Permeability of Carboxysome Shell Pores to Anionic Molecules”, *The Journal of Physical Chemistry B*, vol. 122, no. 39. American Chemical Society (ACS), pp. 9110–9118, Sep. 07, 2018. doi: 10.1021/acs.jpcb.8b06822.  
  
S. E. Mansoor, W. Lü, W. Oosterheert, M. Shekhar, E. Tajkhorshidand E. Gouaux, “X-ray structures define human P2X3 receptor gating cycle and antagonist action”, *Nature*, vol. 538, no. 7623. Springer Science and Business Media LLC, pp. 66–71, Sep. 14, 2016. doi: 10.1038/nature19367.  
  
C. Martens, “Direct protein-lipid interactions shape the conformational landscape of secondary transporters”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Oct. 08, 2018. doi: 10.1038/s41467-018-06704-1.  
  
C. Martens, M. Shekhar, A. M. Lau, E. Tajkhorshidand A. Politis, “Integrating hydrogen–deuterium exchange mass spectrometry with molecular dynamics simulations to probe lipid-modulated conformational changes in membrane proteins”, *Nature Protocols*, vol. 14, no. 11. Springer Science and Business Media LLC, pp. 3183–3204, Oct. 11, 2019. doi: 10.1038/s41596-019-0219-6.  
  
C. G. Mayne, “The cellular membrane as a mediator for small molecule interaction with membrane proteins”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1858, no. 10. Elsevier BV, pp. 2290–2304, Oct. 2016. doi: 10.1016/j.bbamem.2016.04.016.  
  
D. R. McDougle, “Incorporation of charged residues in the CYP2J2 F-G loop disrupts CYP2J2–lipid bilayer interactions”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1848, no. 10. Elsevier BV, pp. 2460–2470, Oct. 2015. doi: 10.1016/j.bbamem.2015.07.015.  
  
C. Misra, “Aberrant Expression of a Non-muscle RBFOX2 Isoform Triggers Cardiac Conduction Defects in Myotonic Dystrophy”, *Developmental Cell*, vol. 52, no. 6. Elsevier BV, pp. 748–763.e6, Mar. 2020. doi: 10.1016/j.devcel.2020.01.037.  
  
S. K. Misra, “Pro-Nifuroxazide Self-Assembly Leads to Triggerable Nanomedicine for Anti-cancer Therapy”, *ACS Applied Materials & Interfaces*, vol. 11, no. 20. American Chemical Society (ACS), pp. 18074–18089, Apr. 23, 2019. doi: 10.1021/acsami.9b01343.  
  
M. Moradi, G. Enkaviand E. Tajkhorshid, “Atomic-level characterization of transport cycle thermodynamics in the glycerol-3-phosphate:phosphate antiporter”, *Nature Communications*, vol. 6, no. 1. Springer Science and Business Media LLC, Sep. 29, 2015. doi: 10.1038/ncomms9393.  
  
M. Moradi and E. Tajkhorshid, “Mechanistic picture for conformational transition of a membrane transporter at atomic resolution”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 47. Proceedings of the National Academy of Sciences, pp. 18916–18921, Nov. 04, 2013. doi: 10.1073/pnas.1313202110.  
  
M. Moradi and E. Tajkhorshid, “Driven Metadynamics: Reconstructing Equilibrium Free Energies from Driven Adaptive-Bias Simulations”, *The Journal of Physical Chemistry Letters*, vol. 4, no. 11. American Chemical Society (ACS), pp. 1882–1887, May 21, 2013. doi: 10.1021/jz400816x.  
  
M. Moradi and E. Tajkhorshid, “Computational Recipe for Efficient Description of Large-Scale Conformational Changes in Biomolecular Systems”, *Journal of Chemical Theory and Computation*, vol. 10, no. 7. American Chemical Society (ACS), pp. 2866–2880, Jun. 11, 2014. doi: 10.1021/ct5002285.  
  
M. P. Muller, “Characterization of Lipid–Protein Interactions and Lipid-Mediated Modulation of Membrane Protein Function through Molecular Simulation”, *Chemical Reviews*, vol. 119, no. 9. American Chemical Society (ACS), pp. 6086–6161, Apr. 12, 2019. doi: 10.1021/acs.chemrev.8b00608.  
  
M. P. Muller, Y. Wang, J. H. Morrisseyand E. Tajkhorshid, “Lipid specificity of the membrane binding domain of coagulation factor X”, *Journal of Thrombosis and Haemostasis*, vol. 15, no. 10. Elsevier BV, pp. 2005–2016, Oct. 2017. doi: 10.1111/jth.13788.  
  
P. S. Padayatti, “Structural Insights into the Lipid A Transport Pathway in MsbA”, *Structure*, vol. 27, no. 7. Elsevier BV, pp. 1114–1123.e3, Jul. 2019. doi: 10.1016/j.str.2019.04.007.  
  
P. S. Padayatti, “Critical Role of Water Molecules in Proton Translocation by the Membrane-Bound Transhydrogenase”, *Structure*, vol. 25, no. 7. Elsevier BV, pp. 1111–1119.e3, Jul. 2017. doi: 10.1016/j.str.2017.05.022.  
  
S. Pant and E. Tajkhorshid, “Microscopic Characterization of GRP1 PH Domain Interaction with Anionic Membranes”, *Journal of Computational Chemistry*, vol. 41, no. 6. Wiley, pp. 489–499, Nov. 25, 2019. doi: 10.1002/jcc.26109.  
  
M. Reza Kalani and E. Tajkhorshid, “Molecular Dynamics: The Computational Molecular Microscope”, *Razavi International Journal of Medicine*, vol. 2, no. 3. Kowsar Medical Institute, Aug. 25, 2014. doi: 10.5812/rijm.20117.  
  
M. Scheurer, “PyContact: Rapid, Customizable, and Visual Analysis of Noncovalent Interactions in MD Simulations”, *Biophysical Journal*, vol. 114, no. 3. Elsevier BV, pp. 577–583, Feb. 2018. doi: 10.1016/j.bpj.2017.12.003.  
  
R. Shahoei and E. Tajkhorshid, “Menthol Binding to the Human α4β2 Nicotinic Acetylcholine Receptor Facilitated by Its Strong Partitioning in the Membrane”, *The Journal of Physical Chemistry B*, vol. 124, no. 10. American Chemical Society (ACS), pp. 1866–1880, Feb. 12, 2020. doi: 10.1021/acs.jpcb.9b10092.  
  
S. A. Shaikh, J. Li, G. Enkavi, P.-C. Wen, Z. Huangand E. Tajkhorshid, “Visualizing Functional Motions of Membrane Transporters with Molecular Dynamics Simulations”, *Biochemistry*, vol. 52, no. 4. American Chemical Society (ACS), pp. 569–587, Jan. 17, 2013. doi: 10.1021/bi301086x.  
  
S. A. Shaikh, P.-C. Wen, G. Enkavi, Z. Huangand E. Tajkhorshid, “Capturing Functional Motions of Membrane Channels and Transporters with Molecular Dynamics Simulation”, *Journal of Computational and Theoretical Nanoscience*, vol. 7, no. 12. American Scientific Publishers, pp. 2481–2500, Dec. 01, 2010. doi: 10.1166/jctn.2010.1636.  
  
A. Singharoy, A. M. Barragan, S. Thangapandian, E. Tajkhorshidand K. Schulten, “Binding Site Recognition and Docking Dynamics of a Single Electron Transport Protein: Cytochrome *c*2”, *Journal of the American Chemical Society*, vol. 138, no. 37. American Chemical Society (ACS), pp. 12077–12089, Sep. 07, 2016. doi: 10.1021/jacs.6b01193.  
  
A. Singharoy, “Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism”, *Cell*, vol. 179, no. 5. Elsevier BV, pp. 1098–1111.e23, Nov. 2019. doi: 10.1016/j.cell.2019.10.021.  
  
J. W. Smith, “Polymer−Peptide Conjugates Convert Amyloid into Protein Nanobundles through Fragmentation and Lateral Association”, *ACS Applied Nano Materials*, vol. 3, no. 2. American Chemical Society (ACS), pp. 937–945, Sep. 10, 2019. doi: 10.1021/acsanm.9b01331.  
  
R. P. Sparks, “A small-molecule competitive inhibitor of phosphatidic acid binding by the AAA+ protein NSF/Sec18 blocks the SNARE-priming stage of vacuole fusion”, *Journal of Biological Chemistry*, vol. 294, no. 46. Elsevier BV, pp. 17168–17185, Nov. 2019. doi: 10.1074/jbc.ra119.008865.  
  
T. E. Speltz, “Stapled Peptides with γ‐Methylated Hydrocarbon Chains for the Estrogen Receptor/Coactivator Interaction”, *Angewandte Chemie International Edition*, vol. 55, no. 13. Wiley, pp. 4252–4255, Mar. 2016. doi: 10.1002/anie.201510557.  
  
M. L. Starr, “Phosphatidic acid induces conformational changes in Sec18 protomers that prevent SNARE priming”, *Journal of Biological Chemistry*, vol. 294, no. 9. Elsevier BV, pp. 3100–3116, Mar. 2019. doi: 10.1074/jbc.ra118.006552.  
  
C. Sun, “Structure of the alternative complex III in a supercomplex with cytochrome oxidase”, *Nature*, vol. 557, no. 7703. Springer Science and Business Media LLC, pp. 123–126, Apr. 25, 2018. doi: 10.1038/s41586-018-0061-y.  
  
C. Sun, “Q-Band Electron-Nuclear Double Resonance Reveals Out-of-Plane Hydrogen Bonds Stabilize an Anionic Ubisemiquinone in Cytochrome *bo*3 from *Escherichia coli*”, *Biochemistry*, vol. 55, no. 40. American Chemical Society (ACS), pp. 5714–5725, Sep. 28, 2016. doi: 10.1021/acs.biochem.6b00669.  
  
E. Tajkhorshid and C. Chipot, “Tribute to Klaus Schulten”, *The Journal of Physical Chemistry B*, vol. 121, no. 15. American Chemical Society (ACS), pp. 3203–3205, Apr. 20, 2017. doi: 10.1021/acs.jpcb.7b02140.  
  
K. Terekhova, “Binding partner- and force-promoted changes in αE-catenin conformation probed by native cysteine labeling”, *Scientific Reports*, vol. 9, no. 1. Springer Science and Business Media LLC, Oct. 25, 2019. doi: 10.1038/s41598-019-51816-3.  
  
S. Thangapandian, K. Kapoorand E. Tajkhorshid, “Probing cholesterol binding and translocation in P-glycoprotein”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1862, no. 1. Elsevier BV, p. 183090, Jan. 2020. doi: 10.1016/j.bbamem.2019.183090.  
  
G. T. Tietjen, “Coupling X-Ray Reflectivity and In Silico Binding to Yield Dynamics of Membrane Recognition by Tim1”, *Biophysical Journal*, vol. 113, no. 7. Elsevier BV, pp. 1505–1519, Oct. 2017. doi: 10.1016/j.bpj.2017.08.003.  
  
B. Verhalen, “Energy transduction and alternating access of the mammalian ABC transporter P-glycoprotein”, *Nature*, vol. 543, no. 7647. Springer Science and Business Media LLC, pp. 738–741, Mar. 2017. doi: 10.1038/nature21414.  
  
J. V. Vermaas, “Efficient Exploration of Membrane-Associated Phenomena at Atomic Resolution”, *The Journal of Membrane Biology*, vol. 248, no. 3. Springer Science and Business Media LLC, pp. 563–582, May 22, 2015. doi: 10.1007/s00232-015-9806-9.  
  
J. V. Vermaas, D. J. Hardy, J. E. Stone, E. Tajkhorshidand A. Kohlmeyer, “TopoGromacs: Automated Topology Conversion from CHARMM to GROMACS within VMD”, *Journal of Chemical Information and Modeling*, vol. 56, no. 6. American Chemical Society (ACS), pp. 1112–1116, Jun. 01, 2016. doi: 10.1021/acs.jcim.6b00103.  
  
J. V. Vermaas, S. B. Rempeand E. Tajkhorshid, “Electrostatic lock in the transport cycle of the multidrug resistance transporter EmrE”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 32. Proceedings of the National Academy of Sciences, Jul. 19, 2018. doi: 10.1073/pnas.1722399115.  
  
J. V. Vermaas, A. T. Taguchi, S. A. Dikanov, C. A. Wraightand E. Tajkhorshid, “Redox Potential Tuning through Differential Quinone Binding in the Photosynthetic Reaction Center of *Rhodobacter sphaeroides*”, *Biochemistry*, vol. 54, no. 12. American Chemical Society (ACS), pp. 2104–2116, Mar. 23, 2015. doi: 10.1021/acs.biochem.5b00033.  
  
J. V. Vermaas and E. Tajkhorshid, “A Microscopic View of Phospholipid Insertion into Biological Membranes”, *The Journal of Physical Chemistry B*, vol. 118, no. 7. American Chemical Society (ACS), pp. 1754–1764, Dec. 16, 2013. doi: 10.1021/jp409854w.  
  
J. V. Vermaas and E. Tajkhorshid, “Conformational heterogeneity of α -synuclein in membrane”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1838, no. 12. Elsevier BV, pp. 3107–3117, Dec. 2014. doi: 10.1016/j.bbamem.2014.08.012.  
  
J. V. Vermaas, “Microscopic Characterization of Membrane Transporter Function by In Silico Modeling and Simulation”, *Methods in Enzymology*. Elsevier, pp. 373–428, 2016. doi: 10.1016/bs.mie.2016.05.042.  
  
Y. Wang, “Constructing atomic structural models into cryo-EM densities using molecular dynamics – Pros and cons”, *Journal of Structural Biology*, vol. 204, no. 2. Elsevier BV, pp. 319–328, Nov. 2018. doi: 10.1016/j.jsb.2018.08.003.  
  
D. A. Weisz, “Mass spectrometry-based cross-linking study shows that the Psb28 protein binds to cytochrome *b* 559 in Photosystem II”, *Proceedings of the National Academy of Sciences*, vol. 114, no. 9. Proceedings of the National Academy of Sciences, pp. 2224–2229, Feb. 13, 2017. doi: 10.1073/pnas.1620360114.  
  
P.-C. Wen, “Microscopic view of lipids and their diverse biological functions”, *Current Opinion in Structural Biology*, vol. 51. Elsevier BV, pp. 177–186, Aug. 2018. doi: 10.1016/j.sbi.2018.07.003.  
  
P.-C. Wen and E. Tajkhorshid, “Conformational Coupling of the Nucleotide-Binding and the Transmembrane Domains in ABC Transporters”, *Biophysical Journal*, vol. 101, no. 3. Elsevier BV, pp. 680–690, Aug. 2011. doi: 10.1016/j.bpj.2011.06.031.  
  
P.-C. Wen, J. M. Vanegas, S. B. Rempeand E. Tajkhorshid, “Probing key elements of teixobactin–lipid II interactions in membranes”, *Chemical Science*, vol. 9, no. 34. Royal Society of Chemistry (RSC), pp. 6997–7008, 2018. doi: 10.1039/c8sc02616e.  
  
A. K. Yadav, “An Activity‐Based Sensing Approach for the Detection of Cyclooxygenase‐2 in Live Cells”, *Angewandte Chemie International Edition*, vol. 59, no. 8. Wiley, pp. 3307–3314, Feb. 06, 2020. doi: 10.1002/anie.201914845.  
  
K. Yu, T. Jiang, Y. Cui, E. Tajkhorshidand H. C. Hartzell, “A network of phosphatidylinositol 4,5-bisphosphate binding sites regulates gating of the Ca 2+ -activated Cl − channel ANO1 (TMEM16A)”, *Proceedings of the National Academy of Sciences*, vol. 116, no. 40. Proceedings of the National Academy of Sciences, pp. 19952–19962, Sep. 12, 2019. doi: 10.1073/pnas.1904012116.  
  
X. Yu, “Dimeric structure of the uracil:proton symporter UraA provides mechanistic insights into the SLC4/23/26 transporters”, *Cell Research*, vol. 27, no. 8. Springer Science and Business Media LLC, pp. 1020–1033, Jun. 16, 2017. doi: 10.1038/cr.2017.83.  
  
N. Trebesch, J. V. Vermaasand E. Tajkhorshid, “Chapter 7. Computational Characterization of Molecular Mechanisms of Membrane Transporter Function”, *Theoretical and Computational Chemistry Series*. Royal Society of Chemistry, pp. 197–236, 2016. doi: 10.1039/9781782626695-00197.  
  
J. V. Vermaas and E. Tajkhorshid, “Differential Membrane Binding Mechanics of Synaptotagmin Isoforms Observed in Atomic Detail”, *Biochemistry*, vol. 56, no. 1. American Chemical Society (ACS), pp. 281–293, Dec. 20, 2016. doi: 10.1021/acs.biochem.6b00468.  
  
F. Zeng, “Structural basis of co-translational quality control by ArfA and RF2 bound to ribosome”, *Nature*, vol. 541, no. 7638. Springer Science and Business Media LLC, pp. 554–557, Jan. 11, 2017. doi: 10.1038/nature21053.  
  
S. R. Beane, “Nucleon-nucleon scattering parameters in the limit of SU(3) flavor symmetry”, *Physical Review C*, vol. 88, no. 2. American Physical Society (APS), Aug. 21, 2013. doi: 10.1103/physrevc.88.024003.  
  
D. V. Kotov, H. C. Yee, A. A. Wray, B. Sjögreenand A. G. Kritsuk, “Numerical dissipation control in high order shock-capturing schemes for LES of low speed flows”, *Journal of Computational Physics*, vol. 307. Elsevier BV, pp. 189–202, Feb. 2016. doi: 10.1016/j.jcp.2015.11.029.  
  
A. G. Kritsuk, “Energy Transfer and Spectra in Simulations of Two-Dimensional Compressible Turbulence”, *Turbulent Cascades II*. Springer International Publishing, pp. 61–70, 2019. doi: 10.1007/978-3-030-12547-9\_8.  
  
A. G. Kritsuk, C. T. Leeand M. L. Norman, “A supersonic turbulence origin of Larson’s laws”, *Monthly Notices of the Royal Astronomical Society*, vol. 436, no. 4. Oxford University Press (OUP), pp. 3247–3261, Oct. 17, 2013. doi: 10.1093/mnras/stt1805.  
  
A. G. Kritsuk, S. D. Ustyugovand M. L. Norman, “The structure and statistics of interstellar turbulence”, *New Journal of Physics*, vol. 19, no. 6. IOP Publishing, p. 065003, Jun. 15, 2017. doi: 10.1088/1367-2630/aa7156.  
  
A. G. Kritsuk, H. C. Yee, B. Sjögreenand D. Kotov, “Comparative study of high order methods for subsonic turbulence simulation with stochastic forcing”, *Journal of Physics: Conference Series*, vol. 1623, no. 1. IOP Publishing, p. 012010, Sep. 01, 2020. doi: 10.1088/1742-6596/1623/1/012010.  
  
R. Wagner, G. Falkovich, A. G. Kritsukand M. L. Norman, “Flux correlations in supersonic isothermal turbulence”, *Journal of Fluid Mechanics*, vol. 713. Cambridge University Press (CUP), pp. 482–490, Oct. 17, 2012. doi: 10.1017/jfm.2012.470.  
  
S. Choi, J. Choiand C.-L. Lin, “Contributions of Kinetic Energy and Viscous Dissipation to Airway Resistance in Pulmonary Inspiratory and Expiratory Airflows in Successive Symmetric Airway Models With Various Bifurcation Angles”, *Journal of Biomechanical Engineering*, vol. 140, no. 1. ASME International, Nov. 09, 2017. doi: 10.1115/1.4038163.  
  
S. Miyawaki, S. Choi, E. A. Hoffmanand C.-L. Lin, “A 4DCT imaging-based breathing lung model with relative hysteresis”, *Journal of Computational Physics*, vol. 326. Elsevier BV, pp. 76–90, Dec. 2016. doi: 10.1016/j.jcp.2016.08.039.  
  
S. Miyawaki, E. A. Hoffmanand C.-L. Lin, “Effect of static vs. dynamic imaging on particle transport in CT-based numerical models of human central airways”, *Journal of Aerosol Science*, vol. 100. Elsevier BV, pp. 129–139, Oct. 2016. doi: 10.1016/j.jaerosci.2016.07.006.  
  
S. Miyawaki, E. A. Hoffmanand C.-L. Lin, “Numerical simulations of aerosol delivery to the human lung with an idealized laryngeal model, image-based airway model, and automatic meshing algorithm”, *Computers & Fluids*, vol. 148. Elsevier BV, pp. 1–9, Apr. 2017. doi: 10.1016/j.compfluid.2017.02.008.  
  
S. Miyawaki, M. H. Tawhai, E. A. Hoffmanand C.-L. Lin, “Effect of Carrier Gas Properties on Aerosol Distribution in a CT-based Human Airway Numerical Model”, *Annals of Biomedical Engineering*, vol. 40, no. 7. Springer Science and Business Media LLC, pp. 1495–1507, Jan. 14, 2012. doi: 10.1007/s10439-011-0503-2.  
  
S. Miyawaki, M. H. Tawhai, E. A. Hoffman, S. E. Wenzeland C.-L. Lin, “Automatic construction of subject-specific human airway geometry including trifurcations based on a CT-segmented airway skeleton and surface”, *Biomechanics and Modeling in Mechanobiology*, vol. 16, no. 2. Springer Science and Business Media LLC, pp. 583–596, Oct. 04, 2016. doi: 10.1007/s10237-016-0838-6.  
  
P. K. Rajaraman, “Transport and deposition of hygroscopic particles in asthmatic subjects with and without airway narrowing”, *Journal of Aerosol Science*, vol. 146. Elsevier BV, p. 105581, Aug. 2020. doi: 10.1016/j.jaerosci.2020.105581.  
  
D. Wu, R. C. Boucher, B. Button, T. Elstonand C.-L. Lin, “An integrated mathematical epithelial cell model for airway surface liquid regulation by mechanical forces”, *Journal of Theoretical Biology*, vol. 438. Elsevier BV, pp. 34–45, Feb. 2018. doi: 10.1016/j.jtbi.2017.11.010.  
  
D. Wu, S. Miyawaki, M. H. Tawhai, E. A. Hoffmanand C.-L. Lin, “A Numerical Study of Water Loss Rate Distributions in MDCT-Based Human Airway Models”, *Annals of Biomedical Engineering*, vol. 43, no. 11. Springer Science and Business Media LLC, pp. 2708–2721, Apr. 14, 2015. doi: 10.1007/s10439-015-1318-3.  
  
D. Wu, M. H. Tawhai, E. A. Hoffmanand C.-L. Lin, “A Numerical Study of Heat and Water Vapor Transfer in MDCT-Based Human Airway Models”, *Annals of Biomedical Engineering*, vol. 42, no. 10. Springer Science and Business Media LLC, pp. 2117–2131, Aug. 01, 2014. doi: 10.1007/s10439-014-1074-9.  
  
C. Andersen, J. Bulava, B. Hörzand C. Morningstar, “The I = 1 pion–pion scattering amplitude and timelike pion form factor from Nf = 2 + 1 lattice QCD”, *Nuclear Physics B*, vol. 939. Elsevier BV, pp. 145–173, Feb. 2019. doi: 10.1016/j.nuclphysb.2018.12.018.  
  
R. Brett, J. Bulava, J. Fallica, A. Hanlon, B. Hörzand C. Morningstar, “Determination of s- and p-wave I = 1/2 Kπ scattering amplitudes in Nf = 2 + 1 lattice QCD”, *Nuclear Physics B*, vol. 932. Elsevier BV, pp. 29–51, Jul. 2018. doi: 10.1016/j.nuclphysb.2018.05.008.  
  
C. Morningstar, “Estimating the two-particle K-matrix for multiple partial waves and decay channels from finite-volume energies”, *Nuclear Physics B*, vol. 924. Elsevier BV, pp. 477–507, Nov. 2017. doi: 10.1016/j.nuclphysb.2017.09.014.  
  
P. Cessi and C. L. Wolfe, “Adiabatic Eastern Boundary Currents”, *Journal of Physical Oceanography*, vol. 43, no. 6. American Meteorological Society, pp. 1127–1149, Jun. 01, 2013. doi: 10.1175/jpo-d-12-0211.1.  
  
P. Cessi, C. L. Wolfeand B. C. Ludka, “Eastern-Boundary Contribution to the Residual and Meridional Overturning Circulations”, *Journal of Physical Oceanography*, vol. 40, no. 9. American Meteorological Society, pp. 2075–2090, Sep. 01, 2010. doi: 10.1175/2010jpo4426.1.  
  
C. L. Wolfe and P. Cessi, “What Sets the Strength of the Middepth Stratification and Overturning Circulation in Eddying Ocean Models?”, *Journal of Physical Oceanography*, vol. 40, no. 7. American Meteorological Society, pp. 1520–1538, Jul. 01, 2010. doi: 10.1175/2010jpo4393.1.  
  
C. L. Wolfe and P. Cessi, “The Adiabatic Pole-to-Pole Overturning Circulation”, *Journal of Physical Oceanography*, vol. 41, no. 9. American Meteorological Society, pp. 1795–1810, Sep. 01, 2011. doi: 10.1175/2011jpo4570.1.  
  
A. M. DeStefano and J. Heerikhuisen, “Charge-exchange source terms in magnetohydrodynamic plasmas”, *Journal of Physics: Conference Series*, vol. 837. IOP Publishing, p. 012013, May 30, 2017. doi: 10.1088/1742-6596/837/1/012013.  
  
R. L. Fermo, N. V. Pogorelovand L. F. Burlaga, “Transient shocks beyond the heliopause”, *Journal of Physics: Conference Series*, vol. 642. IOP Publishing, p. 012008, Sep. 2015. doi: 10.1088/1742-6596/642/1/012008.  
  
J. Heerikhuisen, K. V. Gamayunov, E. J. Zirnsteinand N. V. Pogorelov, “NEUTRAL ATOM PROPERTIES IN THE DIRECTION OF THE*IBEX*RIBBON”, *The Astrophysical Journal*, vol. 831, no. 2. American Astronomical Society, p. 137, Nov. 03, 2016. doi: 10.3847/0004-637x/831/2/137.  
  
J. C. Kasper, “Solar Wind Electrons Alphas and Protons (SWEAP) Investigation: Design of the Solar Wind and Coronal Plasma Instrument Suite for Solar Probe Plus”, *Space Science Reviews*, vol. 204, no. 1–4. Springer Science and Business Media LLC, pp. 131–186, Oct. 29, 2015. doi: 10.1007/s11214-015-0206-3.  
  
T. K. Kim, N. V. Pogorelov, S. N. Borovikov, J. M. Clover, B. V. Jacksonand H.-S. Yu, “Time-dependent MHD simulations of the solar wind outflow using interplanetary scintillation observations”, *AIP Conference Proceedings*. AIP, 2012. doi: 10.1063/1.4768757.  
  
T. K. Kim, N. V. Pogorelovand L. F. Burlaga, “Modeling Shocks Detected by *Voyager 1* in the Local Interstellar Medium”, *The Astrophysical Journal*, vol. 843, no. 2. American Astronomical Society, p. L32, Jul. 11, 2017. doi: 10.3847/2041-8213/aa7b2b.  
  
T. K. Kim, N. V. Pogorelov, G. P. Zank, H. A. Elliottand D. J. McComas, “MODELING THE SOLAR WIND AT THE*ULYSSES*,*VOYAGER*, AND*NEW HORIZONS*SPACECRAFT”, *The Astrophysical Journal*, vol. 832, no. 1. American Astronomical Society, p. 72, Nov. 18, 2016. doi: 10.3847/0004-637x/832/1/72.  
  
L. Lamy, “The aurorae of Uranus past equinox”, *Journal of Geophysical Research: Space Physics*, vol. 122, no. 4. American Geophysical Union (AGU), pp. 3997–4008, Apr. 2017. doi: 10.1002/2017ja023918.  
  
L. Lamy, “Saturn’s Northern Aurorae at Solstice From HST Observations Coordinated With Cassini’s Grand Finale”, *Geophysical Research Letters*, vol. 45, no. 18. American Geophysical Union (AGU), pp. 9353–9362, Sep. 23, 2018. doi: 10.1029/2018gl078211.  
  
J. A. Linker, “An Empirically Driven Time-Dependent Model of the Solar Wind”, *Journal of Physics: Conference Series*, vol. 719. IOP Publishing, p. 012012, May 2016. doi: 10.1088/1742-6596/719/1/012012.  
  
V. López-Barquero, S. Xu, P. Desiati, A. Lazarian, N. V. Pogorelovand H. Yan, “TeV Cosmic-Ray Anisotropy from the Magnetic Field at the Heliospheric Boundary”, *The Astrophysical Journal*, vol. 842, no. 1. American Astronomical Society, p. 54, Jun. 14, 2017. doi: 10.3847/1538-4357/aa74d1.  
  
X. Luo, M. S. Potgieter, M. Zhang, N. V. Pogorelov, X. Fengand R. du Toit Strauss, “A NUMERICAL SIMULATION OF COSMIC RAY MODULATION NEAR THE HELIOPAUSE. II. SOME PHYSICAL INSIGHTS”, *The Astrophysical Journal*, vol. 826, no. 2. American Astronomical Society, p. 182, Jul. 29, 2016. doi: 10.3847/0004-637x/826/2/182.  
  
X. Luo, M. Zhang, M. Potgieter, X. Fengand N. V. Pogorelov, “A NUMERICAL SIMULATION OF COSMIC-RAY MODULATION NEAR THE HELIOPAUSE”, *The Astrophysical Journal*, vol. 808, no. 1. American Astronomical Society, p. 82, Jul. 21, 2015. doi: 10.1088/0004-637x/808/1/82.  
  
X. Luo, M. Zhang, M. S. Potgieter, X. Fengand N. V. Pogorelov, “Study cosmic ray modulation near the heliopause: A numerical approach”, *SOLAR WIND 14: Proceedings of the Fourteenth International Solar Wind Conference*. AIP Publishing, 2016. doi: 10.1063/1.4943842.  
  
P. Manoharan, T. Kim, N. V. Pogorelov, C. N. Argeand P. K. Manoharan, “Modeling solar wind with boundary conditions from interplanetary scintillations”, *Journal of Physics: Conference Series*, vol. 642. IOP Publishing, p. 012016, Sep. 2015. doi: 10.1088/1742-6596/642/1/012016.  
  
D. J. McComas, “Heliosphere Responds to a Large Solar Wind Intensification: Decisive Observations from *IBEX*”, *The Astrophysical Journal*, vol. 856, no. 1. American Astronomical Society, p. L10, Mar. 23, 2018. doi: 10.3847/2041-8213/aab611.  
  
N. V. Pogorelov, “The Heliotail: Theory and Modeling”, *Journal of Physics: Conference Series*, vol. 719. IOP Publishing, p. 012013, May 2016. doi: 10.1088/1742-6596/719/1/012013.  
  
N. V. Pogorelov, M. C. Bedford, I. A. Kryukovand G. P. Zank, “Pickup Ion Effect of the Solar Wind Interaction with the Local Interstellar Medium”, *Journal of Physics: Conference Series*, vol. 767. IOP Publishing, p. 012020, Nov. 2016. doi: 10.1088/1742-6596/767/1/012020.  
  
N. V. Pogorelov, S. N. Borovikov, J. Heerikhuisenand M. Zhang, “THE HELIOTAIL”, *The Astrophysical Journal*, vol. 812, no. 1. American Astronomical Society, p. L6, Oct. 06, 2015. doi: 10.1088/2041-8205/812/1/l6.  
  
N. V. Pogorelov, “Modeling Coronal Mass Ejections with the Multi-Scale Fluid-Kinetic Simulation Suite”, *Journal of Physics: Conference Series*, vol. 837. IOP Publishing, p. 012014, May 30, 2017. doi: 10.1088/1742-6596/837/1/012014.  
  
N. V. Pogorelov, “Heliosheath Processes and the Structure of the Heliopause: Modeling Energetic Particles, Cosmic Rays, and Magnetic Fields”, *Space Science Reviews*, vol. 212, no. 1–2. Springer Science and Business Media LLC, pp. 193–248, Apr. 06, 2017. doi: 10.1007/s11214-017-0354-8.  
  
N. V. Pogorelov, J. Heerikhuisen, V. Roytershteyn, L. F. Burlaga, D. A. Gurnettand W. S. Kurth, “Three-dimensional Features of the Outer Heliosphere Due to Coupling between the Interstellar and Heliospheric Magnetic Field. V. The Bow Wave, Heliospheric Boundary Layer, Instabilities, and Magnetic Reconnection”, *The Astrophysical Journal*, vol. 845, no. 1. American Astronomical Society, p. 9, Aug. 04, 2017. doi: 10.3847/1538-4357/aa7d4f.  
  
M. S. Yalim, N. Pogorelovand Y. Liu, “A data-driven MHD model of the global solar corona within Multi-Scale Fluid-Kinetic Simulation Suite (MS-FLUKSS)”, *Journal of Physics: Conference Series*, vol. 837. IOP Publishing, p. 012015, May 30, 2017. doi: 10.1088/1742-6596/837/1/012015.  
  
M. Zhang, X. Luoand N. Pogorelov, “Where is the cosmic-ray modulation boundary of the heliosphere?”, *Physics of Plasmas*, vol. 22, no. 9. AIP Publishing, p. 091501, Aug. 20, 2015. doi: 10.1063/1.4928945.  
  
E. J. Zirnstein, J. Heerikhuisen, H. O. Funsten, G. Livadiotis, D. J. McComasand N. V. Pogorelov, “LOCAL INTERSTELLAR MAGNETIC FIELD DETERMINED FROM THE *INTERSTELLAR BOUNDARY EXPLORER* RIBBON”, *The Astrophysical Journal*, vol. 818, no. 1. American Astronomical Society, p. L18, Feb. 09, 2016. doi: 10.3847/2041-8205/818/1/l18.  
  
E. J. Zirnstein, J. Heerikhuisen, D. J. McComas, N. V. Pogorelov, D. B. Reisenfeldand J. R. Szalay, “Simulation of the Solar Wind Dynamic Pressure Increase in 2014 and Its Effect on Energetic Neutral Atom Fluxes from the Heliosphere”, *The Astrophysical Journal*, vol. 859, no. 2. American Astronomical Society, p. 104, May 30, 2018. doi: 10.3847/1538-4357/aac016.  
  
E. J. Zirnstein, J. Heerikhuisen, N. V. Pogorelov, D. J. McComasand M. A. Dayeh, “SIMULATIONS OF A DYNAMIC SOLAR CYCLE AND ITS EFFECTS ON THE*INTERSTELLAR BOUNDARY EXPLORER*RIBBON AND GLOBALLY DISTRIBUTED ENERGETIC NEUTRAL ATOM FLUX”, *The Astrophysical Journal*, vol. 804, no. 1. American Astronomical Society, p. 5, Apr. 23, 2015. doi: 10.1088/0004-637x/804/1/5.  
  
E. J. Zirnstein, “Structure of the Heliotail from *Interstellar Boundary Explorer* Observations: Implications for the 11-year Solar Cycle and Pickup Ions in the Heliosheath”, *The Astrophysical Journal*, vol. 836, no. 2. American Astronomical Society, p. 238, Feb. 23, 2017. doi: 10.3847/1538-4357/aa5cb2.  
  
S. N. Borovikov and N. V. Pogorelov, “*VOYAGER 1* NEAR THE HELIOPAUSE”, *The Astrophysical Journal*, vol. 783, no. 1. American Astronomical Society, p. L16, Feb. 18, 2014. doi: 10.1088/2041-8205/783/1/l16.  
  
S. N. Borovikov, N. V. Pogorelov, L. F. Burlagaand J. D. Richardson, “PLASMA NEAR THE HELIOSHEATH: OBSERVATIONS AND MODELING”, *The Astrophysical Journal*, vol. 728, no. 1. American Astronomical Society, p. L21, Jan. 24, 2011. doi: 10.1088/2041-8205/728/1/l21.  
  
S. N. Borovikov, N. V. Pogorelovand R. W. Ebert, “SOLAR ROTATION EFFECTS ON THE HELIOSHEATH FLOW NEAR SOLAR MINIMA”, *The Astrophysical Journal*, vol. 750, no. 1. American Astronomical Society, p. 42, Apr. 13, 2012. doi: 10.1088/0004-637x/750/1/42.  
  
M. I. Desai, “LATITUDINAL AND ENERGY DEPENDENCE OF ENERGETIC NEUTRAL ATOM SPECTRAL INDICES MEASURED BY THE*INTERSTELLAR BOUNDARY EXPLORER*”, *The Astrophysical Journal*, vol. 802, no. 2. American Astronomical Society, p. 100, Mar. 31, 2015. doi: 10.1088/0004-637x/802/2/100.  
  
V. Florinski, S. E. S. Ferreiraand N. V. Pogorelov, “Galactic Cosmic Rays in the Outer Heliosphere: Theory and Models”, *Space Science Reviews*, vol. 176, no. 1–4. Springer Science and Business Media LLC, pp. 147–163, Mar. 03, 2011. doi: 10.1007/s11214-011-9756-1.  
  
P. C. Frisch, “CAN*IBEX*IDENTIFY VARIATIONS IN THE GALACTIC ENVIRONMENT OF THE SUN USING ENERGETIC NEUTRAL ATOMS?”, *The Astrophysical Journal*, vol. 719, no. 2. American Astronomical Society, pp. 1984–1992, Aug. 04, 2010. doi: 10.1088/0004-637x/719/2/1984.  
  
K. V. Gamayunov, M. Zhang, N. V. Pogorelov, J. Heerikhuisenand H. K. Rassoul, “SELF-CONSISTENT MODEL OF THE INTERSTELLAR PICKUP PROTONS, ALFVÉNIC TURBULENCE, AND CORE SOLAR WIND IN THE OUTER HELIOSPHERE”, *The Astrophysical Journal*, vol. 757, no. 1. American Astronomical Society, p. 74, Sep. 05, 2012. doi: 10.1088/0004-637x/757/1/74.  
  
J. Heerikhuisen and N. V. Pogorelov, “AN ESTIMATE OF THE NEARBY INTERSTELLAR MAGNETIC FIELD USING NEUTRAL ATOMS”, *The Astrophysical Journal*, vol. 738, no. 1. American Astronomical Society, p. 29, Aug. 10, 2011. doi: 10.1088/0004-637x/738/1/29.  
  
J. Heerikhuisen, “Modeling Neutral Hydrogen in the Heliospheric Interface”, *AIP Conference Proceedings*. AIP, 2010. doi: 10.1063/1.3395922.  
  
J. Heerikhuisen, E. J. Zirnstein, H. O. Funsten, N. V. Pogorelovand G. P. Zank, “THE EFFECT OF NEW INTERSTELLAR MEDIUM PARAMETERS ON THE HELIOSPHERE AND ENERGETIC NEUTRAL ATOMS FROM THE INTERSTELLAR BOUNDARY”, *The Astrophysical Journal*, vol. 784, no. 1. American Astronomical Society, p. 73, Mar. 05, 2014. doi: 10.1088/0004-637x/784/1/73.  
  
T. K. Kim, N. V. Pogorelov, S. N. Borovikov, B. V. Jackson, H. ‐S . Yuand M. Tokumaru, “MHD heliosphere with boundary conditions from a tomographic reconstruction using interplanetary scintillation data”, *Journal of Geophysical Research: Space Physics*, vol. 119, no. 10. American Geophysical Union (AGU), pp. 7981–7997, Oct. 2014. doi: 10.1002/2013ja019755.  
  
H. Kucharek, “THE SOLAR WIND AS A POSSIBLE SOURCE OF FAST TEMPORAL VARIATIONS OF THE HELIOSPHERIC RIBBON”, *The Astrophysical Journal*, vol. 776, no. 2. American Astronomical Society, p. 109, Oct. 04, 2013. doi: 10.1088/0004-637x/776/2/109.  
  
D. J. McComas, “The Heliosphere’s Interstellar Interaction: No Bow Shock”, *Science*, vol. 336, no. 6086. American Association for the Advancement of Science (AAAS), pp. 1291–1293, Jun. 08, 2012. doi: 10.1126/science.1221054.  
  
N. V. Pogorelov, “Transient Phenomena in the Distant Solar Wind and in the Heliosheath”, *AIP Conference Proceedings*. AIP, 2010. doi: 10.1063/1.3395926.  
  
N. V. Pogorelov, S. N. Borovikov, G. P. Zank, L. F. Burlaga, R. A. Deckerand E. C. Stone, “RADIAL VELOCITY ALONG THE *VOYAGER 1* TRAJECTORY: THE EFFECT OF SOLAR CYCLE”, *The Astrophysical Journal*, vol. 750, no. 1. American Astronomical Society, p. L4, Apr. 09, 2012. doi: 10.1088/2041-8205/750/1/l4.  
  
N. V. Pogorelov, J. Heerikhuisen, G. P. Zank, S. N. Borovikov, P. C. Frischand D. J. McComas, “*INTERSTELLAR BOUNDARY EXPLORER*MEASUREMENTS AND MAGNETIC FIELD IN THE VICINITY OF THE HELIOPAUSE”, *The Astrophysical Journal*, vol. 742, no. 2. American Astronomical Society, p. 104, Nov. 14, 2011. doi: 10.1088/0004-637x/742/2/104.  
  
N. V. Pogorelov, S. T. Suess, S. N. Borovikov, R. W. Ebert, D. J. McComasand G. P. Zank, “THREE-DIMENSIONAL FEATURES OF THE OUTER HELIOSPHERE DUE TO COUPLING BETWEEN THE INTERSTELLAR AND INTERPLANETARY MAGNETIC FIELDS. IV. SOLAR CYCLE MODEL BASED ON*ULYSSES*OBSERVATIONS”, *The Astrophysical Journal*, vol. 772, no. 1. American Astronomical Society, p. 2, Jun. 26, 2013. doi: 10.1088/0004-637x/772/1/2.  
  
J. D. Slavin, “Exclusion of Tiny Interstellar Dust Grains From the Heliosphere”, *AIP Conference Proceedings*. AIP, 2010. doi: 10.1063/1.3396301.  
  
G. P. Zank, J. Heerikhuisen, B. E. Wood, N. V. Pogorelov, E. Zirnsteinand D. J. McComas, “HELIOSPHERIC STRUCTURE: THE BOW WAVE AND THE HYDROGEN WALL”, *The Astrophysical Journal*, vol. 763, no. 1. American Astronomical Society, p. 20, Dec. 28, 2012. doi: 10.1088/0004-637x/763/1/20.  
  
M. Zhang, P. Zuoand N. Pogorelov, “HELIOSPHERIC INFLUENCE ON THE ANISOTROPY OF TeV COSMIC RAYS”, *The Astrophysical Journal*, vol. 790, no. 1. American Astronomical Society, p. 5, Jun. 26, 2014. doi: 10.1088/0004-637x/790/1/5.  
  
E. J. Zirnstein, J. Heerikhuisen, G. P. Zank, N. V. Pogorelov, D. J. McComasand M. I. Desai, “CHARGE-EXCHANGE COUPLING BETWEEN PICKUP IONS ACROSS THE HELIOPAUSE AND ITS EFFECT ON ENERGETIC NEUTRAL HYDROGEN FLUX”, *The Astrophysical Journal*, vol. 783, no. 2. American Astronomical Society, p. 129, Feb. 24, 2014. doi: 10.1088/0004-637x/783/2/129.  
  
M. Luisier and G. Klimeck, “Phonon-limited mobility and injection velocity in n- and p-doped ultrascaled nanowire field-effect transistors with different crystal orientations”, *2010 International Electron Devices Meeting*. IEEE, Dec. 2010. doi: 10.1109/iedm.2010.5703324.  
  
J. Hong, S. P. Persaud, S. Horvath, P. M. Allen, B. D. Evavoldand C. Zhu, “Force-Regulated In Situ TCR–Peptide-Bound MHC Class II Kinetics Determine Functions of CD4+ T Cells”, *The Journal of Immunology*, vol. 195, no. 8. The American Association of Immunologists, pp. 3557–3564, Oct. 15, 2015. doi: 10.4049/jimmunol.1501407.  
  
L. Ju, Y. Chen, F. Zhou, H. Lu, M. A. Cruzand C. Zhu, “Von Willebrand factor-A1 domain binds platelet glycoprotein Ibα in multiple states with distinctive force-dependent dissociation kinetics”, *Thrombosis Research*, vol. 136, no. 3. Elsevier BV, pp. 606–612, Sep. 2015. doi: 10.1016/j.thromres.2015.06.019.  
  
L. Ju, J. Qianand C. Zhu, “Transport Regulation of Two-Dimensional Receptor-Ligand Association”, *Biophysical Journal*, vol. 108, no. 7. Elsevier BV, pp. 1773–1784, Apr. 2015. doi: 10.1016/j.bpj.2015.02.023.  
  
B. Liu, W. Chen, K. Natarajan, Z. Li, D. H. Marguliesand C. Zhu, “The cellular environment regulates in situ kinetics of T-cell receptor interaction with peptide major histocompatibility complex”, *European Journal of Immunology*, vol. 45, no. 7. Wiley, pp. 2099–2110, May 22, 2015. doi: 10.1002/eji.201445358.  
  
F. Rosetti, “A Lupus-Associated Mac-1 Variant Has Defects in Integrin Allostery and Interaction with Ligands under Force”, *Cell Reports*, vol. 10, no. 10. Elsevier BV, pp. 1655–1664, Mar. 2015. doi: 10.1016/j.celrep.2015.02.037.  
  
J. Mondal, R. A. Friesnerand B. J. Berne, “Role of Desolvation in Thermodynamics and Kinetics of Ligand Binding to a Kinase”, *Journal of Chemical Theory and Computation*, vol. 10, no. 12. American Chemical Society (ACS), pp. 5696–5705, Nov. 26, 2014. doi: 10.1021/ct500584n.  
  
P. Tiwary and B. J. Berne, “Kramers turnover: From energy diffusion to spatial diffusion using metadynamics”, *The Journal of Chemical Physics*, vol. 144, no. 13. AIP Publishing, p. 134103, Apr. 07, 2016. doi: 10.1063/1.4944577.  
  
P. Tiwary and B. J. Berne, “Spectral gap optimization of order parameters for sampling complex molecular systems”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 11. Proceedings of the National Academy of Sciences, pp. 2839–2844, Feb. 29, 2016. doi: 10.1073/pnas.1600917113.  
  
P. Tiwary and B. J. Berne, “How wet should be the reaction coordinate for ligand unbinding?”, *The Journal of Chemical Physics*, vol. 145, no. 5. AIP Publishing, p. 054113, Aug. 07, 2016. doi: 10.1063/1.4959969.  
  
P. Tiwary and B. J. Berne, “Predicting reaction coordinates in energy landscapes with diffusion anisotropy”, *The Journal of Chemical Physics*, vol. 147, no. 15. AIP Publishing, p. 152701, Oct. 21, 2017. doi: 10.1063/1.4983727.  
  
P. Tiwary, J. Mondaland B. J. Berne, “How and when does an anticancer drug leave its binding site?”, *Science Advances*, vol. 3, no. 5. American Association for the Advancement of Science (AAAS), May 05, 2017. doi: 10.1126/sciadv.1700014.  
  
P. Tiwary, J. Mondal, J. A. Morroneand B. J. Berne, “Role of water and steric constraints in the kinetics of cavity–ligand unbinding”, *Proceedings of the National Academy of Sciences*, vol. 112, no. 39. Proceedings of the National Academy of Sciences, pp. 12015–12019, Sep. 14, 2015. doi: 10.1073/pnas.1516652112.  
  
P. Tiwary, “Molecular Determinants and Bottlenecks in the Dissociation Dynamics of Biotin–Streptavidin”, *The Journal of Physical Chemistry B*, vol. 121, no. 48. American Chemical Society (ACS), pp. 10841–10849, Nov. 21, 2017. doi: 10.1021/acs.jpcb.7b09510.  
  
B. N. Olsen, P. H. Schlesinger, D. S. Oryand N. A. Baker, “25-Hydroxycholesterol Increases the Availability of Cholesterol in Phospholipid Membranes”, *Biophysical Journal*, vol. 100, no. 4. Elsevier BV, pp. 948–956, Feb. 2011. doi: 10.1016/j.bpj.2010.12.3728.  
  
J. Beckvermit, T. Harman, A. Bezdjianand C. Wight, “Modeling Deflagration in Energetic Materials using the Uintah Computational Framework”, *Procedia Computer Science*, vol. 51. Elsevier BV, pp. 552–561, 2015. doi: 10.1016/j.procs.2015.05.321.  
  
M. Berzins, J. Luitjens, Q. Meng, T. Harman, C. A. Wightand J. R. Peterson, “Uintah”, *Proceedings of the 2010 TeraGrid Conference*. ACM, Aug. 02, 2010. doi: 10.1145/1838574.1838577.  
  
M. Hall, J. C. Beckvermit, C. A. Wight, T. Harmanand M. Berzins, “The influence of an applied heat flux on the violence of reaction of an explosive device”, *Proceedings of the Conference on Extreme Science and Engineering Discovery Environment: Gateway to Discovery*. ACM, Jul. 22, 2013. doi: 10.1145/2484762.2484786.  
  
Q. Meng, A. Humphrey, J. Schmidtand M. Berzins, “Investigating applications portability with the Uintah DAG-based runtime system on PetaScale supercomputers”, *Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis*. ACM, Nov. 17, 2013. doi: 10.1145/2503210.2503250.  
  
Q. Meng, A. Humphrey, J. Schmidtand M. Berzins, “Preliminary experiences with the uintah framework on Intel Xeon Phi and stampede”, *Proceedings of the Conference on Extreme Science and Engineering Discovery Environment: Gateway to Discovery*. ACM, Jul. 22, 2013. doi: 10.1145/2484762.2484779.  
  
J. R. Peterson, J. C. Beckvermit, T. Harman, M. Berzinsand C. A. Wight, “Multiscale modeling of high explosives for transportation accidents”, *Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment: Bridging from the eXtreme to the campus and beyond*. ACM, Jul. 16, 2012. doi: 10.1145/2335755.2335828.  
  
J. R. Peterson and C. A. Wight, “An Eulerian–Lagrangian computational model for deflagration and detonation of high explosives”, *Combustion and Flame*, vol. 159, no. 7. Elsevier BV, pp. 2491–2499, Jul. 2012. doi: 10.1016/j.combustflame.2012.02.006.  
  
H. Chen, “Reversible Modulation of Orbital Occupations via an Interface-Induced Polar State in Metallic Manganites”, *Nano Letters*, vol. 14, no. 9. American Chemical Society (ACS), pp. 4965–4970, Aug. 28, 2014. doi: 10.1021/nl501209p.  
  
O. E. Dagdeviren, “Suppression of the spectral weight of topological surface states on the nanoscale via local symmetry breaking”, *Physical Review Materials*, vol. 2, no. 11. American Physical Society (APS), Nov. 20, 2018. doi: 10.1103/physrevmaterials.2.114205.  
  
O. E. Dagdeviren, “Length Scale and Dimensionality of Defects in Epitaxial SnTe Topological Crystalline Insulator Films”, *Advanced Materials Interfaces*, vol. 4, no. 2. Wiley, p. 1601011, Jan. 2017. doi: 10.1002/admi.201601011.  
  
A. S. Disa, “Control of hidden ground-state order in superlattices”, *Physical Review Materials*, vol. 1, no. 2. American Physical Society (APS), Jul. 27, 2017. doi: 10.1103/physrevmaterials.1.024410.  
  
A. S. Disa, “Orbital Engineering in Symmetry-Breaking Polar Heterostructures”, *Physical Review Letters*, vol. 114, no. 2. American Physical Society (APS), Jan. 12, 2015. doi: 10.1103/physrevlett.114.026801.  
  
M. Dogan, “Single Atomic Layer Ferroelectric on Silicon”, *Nano Letters*, vol. 18, no. 1. American Chemical Society (ACS), pp. 241–246, Dec. 26, 2017. doi: 10.1021/acs.nanolett.7b03988.  
  
M. Dogan, N. Gong, T.-P. Maand S. Ismail-Beigi, “Causes of ferroelectricity in HfO2-based thin films: an *ab initio* perspective”, *Physical Chemistry Chemical Physics*, vol. 21, no. 23. Royal Society of Chemistry (RSC), pp. 12150–12162, 2019. doi: 10.1039/c9cp01880h.  
  
M. Dogan and S. Ismail-Beigi, “*Ab initio* study of the interface”, *Physical Review B*, vol. 96, no. 7. American Physical Society (APS), Aug. 01, 2017. doi: 10.1103/physrevb.96.075301.  
  
M. Dogan and S. Ismail-Beigi, “Ferroelectric ZrO2 Monolayers as Buffer Layers between SrTiO3 and Si”, *The Journal of Physical Chemistry C*, vol. 123, no. 24. American Chemical Society (ACS), pp. 15053–15061, May 22, 2019. doi: 10.1021/acs.jpcc.9b03069.  
  
M. Dogan and S. Ismail-Beigi, “Theory of Ferroelectric ZrO2 Monolayers on Si”, *The Journal of Physical Chemistry C*, vol. 123, no. 23. American Chemical Society (ACS), pp. 14350–14361, May 22, 2019. doi: 10.1021/acs.jpcc.9b01073.  
  
K. F. Garrity, A. M. Kolpakand S. Ismail-Beigi, “Growth and interfacial properties of epitaxial oxides on semiconductors: ab initio insights”, *Journal of Materials Science*, vol. 47, no. 21. Springer Science and Business Media LLC, pp. 7417–7438, May 03, 2012. doi: 10.1007/s10853-012-6425-z.  
  
K. Garrity, A. M. Kolpak, S. Ismail-Beigiand E. I. Altman, “Chemistry of Ferroelectric Surfaces”, *Advanced Materials*, vol. 22, no. 26–27. Wiley, pp. 2969–2973, Apr. 23, 2010. doi: 10.1002/adma.200903723.  
  
A. B. Georgescu and S. Ismail-Beigi, “Surface Piezoelectricity of (0001) Sapphire”, *Physical Review Applied*, vol. 11, no. 6. American Physical Society (APS), Jun. 27, 2019. doi: 10.1103/physrevapplied.11.064065.  
  
E. N. Jin, A. Kakekhani, S. Ismail-Beigi, C. H. Ahnand F. J. Walker, “Two-dimensional electron gas oxide remote doping of Si(001)”, *Physical Review Materials*, vol. 2, no. 11. American Physical Society (APS), Nov. 26, 2018. doi: 10.1103/physrevmaterials.2.115001.  
  
A. Kakekhani and S. Ismail-Beigi, “Ferroelectric-Based Catalysis: Switchable Surface Chemistry”, *ACS Catalysis*, vol. 5, no. 8. American Chemical Society (ACS), pp. 4537–4545, Jun. 29, 2015. doi: 10.1021/acscatal.5b00507.  
  
A. Kakekhani and S. Ismail-Beigi, “Polarization-driven catalysis via ferroelectric oxide surfaces”, *Physical Chemistry Chemical Physics*, vol. 18, no. 29. Royal Society of Chemistry (RSC), pp. 19676–19695, 2016. doi: 10.1039/c6cp03170f.  
  
A. Kakekhani and S. Ismail-Beigi, “Ferroelectric oxide surface chemistry: water splitting via pyroelectricity”, *Journal of Materials Chemistry A*, vol. 4, no. 14. Royal Society of Chemistry (RSC), pp. 5235–5246, 2016. doi: 10.1039/c6ta00513f.  
  
D. P. Kumah, “Tuning the Structure of Nickelates to Achieve Two-Dimensional Electron Conduction”, *Advanced Materials*, vol. 26, no. 12. Wiley, pp. 1935–1940, Feb. 03, 2014. doi: 10.1002/adma.201304256.  
  
D. P. Kumah, “Engineered Unique Elastic Modes at aInterface”, *Physical Review Letters*, vol. 116, no. 10. American Physical Society (APS), Mar. 07, 2016. doi: 10.1103/physrevlett.116.106101.  
  
D. P. Kumah, “Effect of Surface Termination on the Electronic Properties ofFilms”, *Physical Review Applied*, vol. 2, no. 5. American Physical Society (APS), Nov. 06, 2014. doi: 10.1103/physrevapplied.2.054004.  
  
S. Lee, “Strong Orbital Polarization in a Cobaltate-Titanate Oxide Heterostructure”, *Physical Review Letters*, vol. 123, no. 11. American Physical Society (APS), Sep. 10, 2019. doi: 10.1103/physrevlett.123.117201.  
  
X. Li, “Controlled Doping of Carbon Nanotubes with Metallocenes for Application in Hybrid Carbon Nanotube/Si Solar Cells”, *Nano Letters*, vol. 14, no. 6. American Chemical Society (ACS), pp. 3388–3394, May 13, 2014. doi: 10.1021/nl500894h.  
  
A. Malashevich, “Controlling Mobility in Perovskite Oxides by Ferroelectric Modulation of Atomic-Scale Interface Structure”, *Nano Letters*, vol. 18, no. 1. American Chemical Society (ACS), pp. 573–578, Dec. 26, 2017. doi: 10.1021/acs.nanolett.7b04715.  
  
M. S. J. Marshall, “Conduction at a Ferroelectric Interface”, *Physical Review Applied*, vol. 2, no. 5. American Physical Society (APS), Nov. 05, 2014. doi: 10.1103/physrevapplied.2.051001.  
  
P. J. Phillips, “Experimental verification of orbital engineering at the atomic scale: Charge transfer and symmetry breaking in nickelate heterostructures”, *Physical Review B*, vol. 95, no. 20. American Physical Society (APS), May 19, 2017. doi: 10.1103/physrevb.95.205131.  
  
H. Tang and S. Ismail-Beigi, “Charge transfer and negative curvature energy in magnesium boride nanotubes”, *Physical Review B*, vol. 94, no. 3. American Physical Society (APS), Jul. 18, 2016. doi: 10.1103/physrevb.94.035425.  
  
R. Wu, “Large-area single-crystal sheets of borophene on Cu(111) surfaces”, *Nature Nanotechnology*, vol. 14, no. 1. Springer Science and Business Media LLC, pp. 44–49, Dec. 03, 2018. doi: 10.1038/s41565-018-0317-6.  
  
C. Zhou, “Structure of a Two-Dimensional Silicate Layer Formed by Reaction with an Alloy Substrate”, *Chemistry of Materials*, vol. 31, no. 3. American Chemical Society (ACS), pp. 851–861, Jan. 02, 2019. doi: 10.1021/acs.chemmater.8b03988.  
  
C. Zhou, “Tuning two-dimensional phase formation through epitaxial strain and growth conditions: silica and silicate on NixPd1−x(111) alloy substrates”, *Nanoscale*, vol. 11, no. 44. Royal Society of Chemistry (RSC), pp. 21340–21353, 2019. doi: 10.1039/c9nr05944j.  
  
K. Zou, “Role of doublelayers at the interface of FeSe/superconductors”, *Physical Review B*, vol. 93, no. 18. American Physical Society (APS), May 16, 2016. doi: 10.1103/physrevb.93.180506.  
  
P. Long, “A tunnel FET design for high-current, 120 mV operation”, *2016 IEEE International Electron Devices Meeting (IEDM)*. IEEE, Dec. 2016. doi: 10.1109/iedm.2016.7838511.  
  
J. Casas, “Ligand-engaged TCR is triggered by Lck not associated with CD8 coreceptor”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, Nov. 27, 2014. doi: 10.1038/ncomms6624.  
  
W. Chen, J. Lou, E. A. Evansand C. Zhu, “Observing force-regulated conformational changes and ligand dissociation from a single integrin on cells”, *Journal of Cell Biology*, vol. 199, no. 3. Rockefeller University Press, pp. 497–512, Oct. 29, 2012. doi: 10.1083/jcb.201201091.  
  
W. Chen and C. Zhu, “Mechanical regulation of T-cell functions”, *Immunological Reviews*, vol. 256, no. 1. Wiley, pp. 160–176, Oct. 10, 2013. doi: 10.1111/imr.12122.  
  
D. K. Cole, “Hotspot autoimmune T cell receptor binding underlies pathogen and insulin peptide cross-reactivity”, *Journal of Clinical Investigation*, vol. 126, no. 6. American Society for Clinical Investigation, pp. 2191–2204, May 16, 2016. doi: 10.1172/jci85679.  
  
V. F. Fiore, L. Ju, Y. Chen, C. Zhuand T. H. Barker, “Dynamic catch of a Thy-1–α5β1+syndecan-4 trimolecular complex”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, Sep. 12, 2014. doi: 10.1038/ncomms5886.  
  
X. Xiang, C.-. yin . Lee, T. Li, W. Chen, J. Louand C. Zhu, “Structural Basis and Kinetics of Force-Induced Conformational Changes of an αA Domain-Containing Integrin”, *PLoS ONE*, vol. 6, no. 11. Public Library of Science (PLoS), p. e27946, Nov. 28, 2011. doi: 10.1371/journal.pone.0027946.  
  
J. D. Hood, V. I. Zarnitsyna, C. Zhuand B. D. Evavold, “Regulatory and T Effector Cells Have Overlapping Low to High Ranges in TCR Affinities for Self during Demyelinating Disease”, *The Journal of Immunology*, vol. 195, no. 9. The American Association of Immunologists, pp. 4162–4170, Nov. 01, 2015. doi: 10.4049/jimmunol.1501464.  
  
L. Ju, J. Lou, Y. Chen, Z. Liand C. Zhu, “Force-Induced Unfolding of Leucine-Rich Repeats of Glycoprotein Ibα Strengthens Ligand Interaction”, *Biophysical Journal*, vol. 109, no. 9. Elsevier BV, pp. 1781–1784, Nov. 2015. doi: 10.1016/j.bpj.2015.08.050.  
  
C.-. yin . Lee, “Actin depolymerization under force is governed by lysine 113:glutamic acid 195-mediated catch-slip bonds”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 13. Proceedings of the National Academy of Sciences, pp. 5022–5027, Mar. 04, 2013. doi: 10.1073/pnas.1218407110.  
  
B. Liu, W. Chen, B. D. Evavoldand C. Zhu, “Accumulation of Dynamic Catch Bonds between TCR and Agonist Peptide-MHC Triggers T Cell Signaling”, *Cell*, vol. 157, no. 2. Elsevier BV, pp. 357–368, Apr. 2014. doi: 10.1016/j.cell.2014.02.053.  
  
B. Liu, W. Chenand C. Zhu, “Molecular Force Spectroscopy on Cells”, *Annual Review of Physical Chemistry*, vol. 66, no. 1. Annual Reviews, pp. 427–451, Apr. 01, 2015. doi: 10.1146/annurev-physchem-040214-121742.  
  
R. J. Mallis, “Pre-TCR ligand binding impacts thymocyte development before αβTCR expression”, *Proceedings of the National Academy of Sciences*, vol. 112, no. 27. Proceedings of the National Academy of Sciences, pp. 8373–8378, Jun. 08, 2015. doi: 10.1073/pnas.1504971112.  
  
W. Chen, J. Lou, J. Hsin, K. Schulten, S. C. Harveyand C. Zhu, “Molecular Dynamics Simulations of Forced Unbending of Integrin αVβ3”, *PLoS Computational Biology*, vol. 7, no. 2. Public Library of Science (PLoS), p. e1001086, Feb. 17, 2011. doi: 10.1371/journal.pcbi.1001086.  
  
S. Pryshchep, V. I. Zarnitsyna, J. Hong, B. D. Evavoldand C. Zhu, “Accumulation of Serial Forces on TCR and CD8 Frequently Applied by Agonist Antigenic Peptides Embedded in MHC Molecules Triggers Calcium in T Cells”, *The Journal of Immunology*, vol. 193, no. 1. The American Association of Immunologists, pp. 68–76, Jul. 01, 2014. doi: 10.4049/jimmunol.1303436.  
  
Y. Zhang, C. Ge, C. Zhuand K. Salaita, “DNA-based digital tension probes reveal integrin forces during early cell adhesion”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, Oct. 24, 2014. doi: 10.1038/ncomms6167.  
  
B. M. Byington, N. H. Brummell, J. M. Stoneand D. O. Gough, “Stoked nondynamos: sustaining field in magnetically non-closed systems”, *New Journal of Physics*, vol. 16, no. 8. IOP Publishing, p. 083002, Aug. 01, 2014. doi: 10.1088/1367-2630/16/8/083002.  
  
L. Korre, N. Brummelland P. Garaud, “Boussinesq convection in a gaseous spherical shell”, *EAS Publications Series*, vol. 82. EDP Sciences, pp. 373–382, 2019. doi: 10.1051/eas/1982033.  
  
L. Korre, P. Garaudand N. H. Brummell, “Convective overshooting and penetration in a Boussinesq spherical shell”, *Monthly Notices of the Royal Astronomical Society*, vol. 484, no. 1. Oxford University Press (OUP), pp. 1220–1237, Jan. 07, 2019. doi: 10.1093/mnras/stz047.  
  
B. Manek, N. Brummelland D. Lee, “The Rise of a Magnetic Flux Tube in a Background Field: Solar Helicity Selection Rules”, *The Astrophysical Journal*, vol. 859, no. 2. American Astronomical Society, p. L27, Jun. 04, 2018. doi: 10.3847/2041-8213/aac723.  
  
B. Manek, N. Brummelland D. Lee, “Solar Hemispheric Helicity Rules: A New Explanation”, *Astrophysics and Space Science Proceedings*. Springer International Publishing, pp. 133–135, 2020. doi: 10.1007/978-3-030-55336-4\_18.  
  
T. S. Wood and N. H. Brummell, “A Self-consistent Model of the Solar Tachocline”, *The Astrophysical Journal*, vol. 853, no. 2. American Astronomical Society, p. 97, Jan. 26, 2018. doi: 10.3847/1538-4357/aaa6d5.  
  
F. Bertoni, A. Castelletti, M. Giulianiand P. M. Reed, “Discovering Dependencies, Trade‐Offs, and Robustness in Joint Dam Design and Operation: An Ex‐Post Assessment of the Kariba Dam”, *Earth’s Future*, vol. 7, no. 12. American Geophysical Union (AGU), pp. 1367–1390, Dec. 2019. doi: 10.1029/2019ef001235.  
  
M. Giuliani, J. D. Quinn, J. D. Herman, A. Castellettiand P. M. Reed, “Scalable Multiobjective Control for Large-Scale Water Resources Systems Under Uncertainty”, *IEEE Transactions on Control Systems Technology*, vol. 26, no. 4. Institute of Electrical and Electronics Engineers (IEEE), pp. 1492–1499, Jul. 2018. doi: 10.1109/tcst.2017.2705162.  
  
D. F. Gold, P. M. Reed, B. C. Trindadeand G. W. Characklis, “Identifying Actionable Compromises: Navigating Multi‐City Robustness Conflicts to Discover Cooperative Safe Operating Spaces for Regional Water Supply Portfolios”, *Water Resources Research*, vol. 55, no. 11. American Geophysical Union (AGU), pp. 9024–9050, Nov. 2019. doi: 10.1029/2019wr025462.  
  
A. Hadjimichael, “Defining Robustness, Vulnerabilities, and Consequential Scenarios for Diverse Stakeholder Interests in Institutionally Complex River Basins”, *Earth’s Future*, vol. 8, no. 7. American Geophysical Union (AGU), Jul. 2020. doi: 10.1029/2020ef001503.  
  
J. D. Quinn, P. M. Reed, M. Giulianiand A. Castelletti, “Rival framings: A framework for discovering how problem formulation uncertainties shape risk management trade‐offs in water resources systems”, *Water Resources Research*, vol. 53, no. 8. American Geophysical Union (AGU), pp. 7208–7233, Aug. 2017. doi: 10.1002/2017wr020524.  
  
J. D. Quinn, P. M. Reed, M. Giulianiand A. Castelletti, “What Is Controlling Our Control Rules? Opening the Black Box of Multireservoir Operating Policies Using Time‐Varying Sensitivity Analysis”, *Water Resources Research*, vol. 55, no. 7. American Geophysical Union (AGU), pp. 5962–5984, Jul. 2019. doi: 10.1029/2018wr024177.  
  
J. D. Quinn, P. M. Reed, M. Giuliani, A. Castelletti, J. W. Oylerand R. E. Nicholas, “Exploring How Changing Monsoonal Dynamics and Human Pressures Challenge Multireservoir Management for Flood Protection, Hydropower Production, and Agricultural Water Supply”, *Water Resources Research*, vol. 54, no. 7. American Geophysical Union (AGU), pp. 4638–4662, Jul. 2018. doi: 10.1029/2018wr022743.  
  
B. C. Trindade, D. F. Gold, P. M. Reed, H. B. Zeffand G. W. Characklis, “Water pathways: An open source stochastic simulation system for integrated water supply portfolio management and infrastructure investment planning”, *Environmental Modelling & Software*, vol. 132. Elsevier BV, p. 104772, Oct. 2020. doi: 10.1016/j.envsoft.2020.104772.  
  
B. C. Trindade, P. M. Reedand G. W. Characklis, “Deeply uncertain pathways: Integrated multi-city regional water supply infrastructure investment and portfolio management”, *Advances in Water Resources*, vol. 134. Elsevier BV, p. 103442, Dec. 2019. doi: 10.1016/j.advwatres.2019.103442.  
  
B. C. Trindade, P. M. Reed, J. D. Herman, H. B. Zeffand G. W. Characklis, “Reducing regional drought vulnerabilities and multi-city robustness conflicts using many-objective optimization under deep uncertainty”, *Advances in Water Resources*, vol. 104. Elsevier BV, pp. 195–209, Jun. 2017. doi: 10.1016/j.advwatres.2017.03.023.  
  
H. B. Zeff, J. D. Herman, P. M. Reedand G. W. Characklis, “Cooperative drought adaptation: Integrating infrastructure development, conservation, and water transfers into adaptive policy pathways”, *Water Resources Research*, vol. 52, no. 9. American Geophysical Union (AGU), pp. 7327–7346, Sep. 2016. doi: 10.1002/2016wr018771.  
  
J. A. Ciezak-Jenkins, B. A. Steele, G. M. Borstadand I. I. Oleynik, “Structural and spectroscopic studies of nitrogen-carbon monoxide mixtures: Photochemical response and observation of a novel phase”, *The Journal of Chemical Physics*, vol. 146, no. 18. AIP Publishing, p. 184309, May 14, 2017. doi: 10.1063/1.4983040.  
  
K. N. Cong, B. A. Steele, A. C. Landervilleand I. I. Oleynik, “First-principles investigation of iron pentacarbonyl molecular solid phases at high pressure”, *AIP Conference Proceedings*. Author(s), 2017. doi: 10.1063/1.4971606.  
  
J. C. Crowhurst, J. M. Zaug, H. B. Radousky, B. A. Steele, A. C. Landervilleand I. I. Oleynik, “Ammonium Azide under High Pressure: A Combined Theoretical and Experimental Study”, *The Journal of Physical Chemistry A*, vol. 118, no. 38. American Chemical Society (ACS), pp. 8695–8700, Sep. 16, 2014. doi: 10.1021/jp502619n.  
  
J. M. Gonzalez, A. C. Landervilleand I. I. Oleynik, “Vibrational and thermophysical properties of PETN from first principles”, *AIP Conference Proceedings*. Author(s), 2017. doi: 10.1063/1.4971597.  
  
J. M. Gonzalez, K. Nguyen-Cong, B. A. Steeleand I. I. Oleynik, “Novel phases and superconductivity of tin sulfide compounds”, *The Journal of Chemical Physics*, vol. 148, no. 19. AIP Publishing, p. 194701, May 21, 2018. doi: 10.1063/1.5018434.  
  
J. M. Gonzalez and I. I. Oleynik, “Layer-dependent properties ofandtwo-dimensional materials”, *Physical Review B*, vol. 94, no. 12. American Physical Society (APS), Sep. 29, 2016. doi: 10.1103/physrevb.94.125443.  
  
N. A. Inogamov, “Surface nano-structuring produced by spallation of metal irradiated by an ultrashort laser pulse”, *Journal of Physics: Conference Series*, vol. 500, no. 11. IOP Publishing, p. 112070, May 07, 2014. doi: 10.1088/1742-6596/500/11/112070.  
  
N. A. Inogamov, “Surface nanodeformations caused by ultrashort laser pulse”, *Engineering Failure Analysis*, vol. 47. Elsevier BV, pp. 328–337, Jan. 2015. doi: 10.1016/j.engfailanal.2013.12.009.  
  
N. A. Inogamov, “Ultrafast lasers and solids in highly excited states: results of hydrodynamics and molecular dynamics simulations”, *Journal of Physics: Conference Series*, vol. 510. IOP Publishing, p. 012041, May 15, 2014. doi: 10.1088/1742-6596/510/1/012041.  
  
N. A. Inogamov, V. V. Zhakhovsky, V. A. Khokhlov, B. J. Demaske, K. V. Khishchenkoand I. I. Oleynik, “Two-temperature hydrodynamic expansion and coupling of strong elastic shock with supersonic melting front produced by ultrashort laser pulse”, *Journal of Physics: Conference Series*, vol. 500, no. 19. IOP Publishing, p. 192023, May 07, 2014. doi: 10.1088/1742-6596/500/19/192023.  
  
N. A. Inogamov, “Electron-Ion Relaxation, Phase Transitions, and Surface Nano-Structuring Produced by Ultrashort Laser Pulses in Metals”, *Contributions to Plasma Physics*, vol. 53, no. 10. Wiley, pp. 796–810, Dec. 2013. doi: 10.1002/ctpp.201310049.  
  
M. A. Kozhushner, V. L. Bodneva, I. I. Oleynik, T. V. Belysheva, M. I. Ikimand L. I. Trakhtenberg, “Sensor Effect in Oxide Films with a Large Concentration of Conduction Electrons”, *The Journal of Physical Chemistry C*, vol. 121, no. 12. American Chemical Society (ACS), pp. 6940–6945, Mar. 21, 2017. doi: 10.1021/acs.jpcc.6b10956.  
  
M. A. Kozhushner, B. V. Lidskii, I. I. Oleynik, V. S. Posvyanskiiand L. I. Trakhtenberg, “Inhomogeneous Charge Distribution in Semiconductor Nanoparticles”, *The Journal of Physical Chemistry C*, vol. 119, no. 28. American Chemical Society (ACS), pp. 16286–16292, Jul. 01, 2015. doi: 10.1021/acs.jpcc.5b01410.  
  
M. A. Kozhushner, L. I. Trakhtenberg, V. L. Bodneva, T. V. Belisheva, A. C. Landervilleand I. I. Oleynik, “Effect of Temperature and Nanoparticle Size on Sensor Properties of Nanostructured Tin Dioxide Films”, *The Journal of Physical Chemistry C*, vol. 118, no. 21. American Chemical Society (ACS), pp. 11440–11444, May 19, 2014. doi: 10.1021/jp501989k.  
  
M. A. Kozhushner, L. I. Trakhtenberg, A. C. Landervilleand I. I. Oleynik, “Theory of Sensing Response of Nanostructured Tin-Dioxide Thin Films to Reducing Hydrogen Gas”, *The Journal of Physical Chemistry C*, vol. 117, no. 22. American Chemical Society (ACS), pp. 11562–11568, May 23, 2013. doi: 10.1021/jp311847j.  
  
A. C. Landerville, J. C. Crowhurst, C. D. Grant, J. M. Zaugand I. Oleynik, “Experimental and theoretical investigation of pressure-dependent Raman spectra of triaminotrinitrobenzene (TATB) at high pressures”, *AIP Conference Proceedings*. Author(s), 2017. doi: 10.1063/1.4971499.  
  
A. C. Landerville and I. I. Oleynik, “Vibrational and thermal properties of β-HMX and TATB from dispersion corrected density functional theory”, *AIP Conference Proceedings*. Author(s), 2017. doi: 10.1063/1.4971541.  
  
A. C. Landerville, B. A. Steeleand I. I. Oleynik, “Ammonium azide under hydrostatic compression”, *Journal of Physics: Conference Series*, vol. 500, no. 16. IOP Publishing, p. 162006, May 07, 2014. doi: 10.1088/1742-6596/500/16/162006.  
  
K. Nguyen-Cong, J. M. Gonzalez, B. A. Steeleand I. I. Oleynik, “Tin–Selenium Compounds at Ambient and High Pressures”, *The Journal of Physical Chemistry C*, vol. 122, no. 32. American Chemical Society (ACS), pp. 18274–18281, Jul. 11, 2018. doi: 10.1021/acs.jpcc.8b04881.  
  
R. Perriot, V. V. Zhakhovsky, N. A. Inogamovand I. I. Oleynik, “Evolution of elastic precursor and plastic shock wave in copper via molecular dynamics simulations”, *Journal of Physics: Conference Series*, vol. 500, no. 17. IOP Publishing, p. 172008, May 07, 2014. doi: 10.1088/1742-6596/500/17/172008.  
  
B. A. Steele, A. C. Landervilleand I. I. Oleynik, “Density functional theory investigation of sodium azide at high pressure”, *Journal of Physics: Conference Series*, vol. 500, no. 16. IOP Publishing, p. 162005, May 07, 2014. doi: 10.1088/1742-6596/500/16/162005.  
  
B. A. Steele and I. I. Oleynik, “New phase of ammonium nitrate: A monoclinic distortion of AN-IV”, *The Journal of Chemical Physics*, vol. 143, no. 23. AIP Publishing, p. 234705, Dec. 21, 2015. doi: 10.1063/1.4937420.  
  
B. A. Steele and I. I. Oleynik, “Sodium pentazolate: A nitrogen rich high energy density material”, *Chemical Physics Letters*, vol. 643. Elsevier BV, pp. 21–26, Jan. 2016. doi: 10.1016/j.cplett.2015.11.008.  
  
B. A. Steele and I. I. Oleynik, “New crystal phase of ammonium nitrate: First-principles prediction and characterization”, *AIP Conference Proceedings*. Author(s), 2017. doi: 10.1063/1.4971719.  
  
B. A. Steele and I. I. Oleynik, “Pentazole and Ammonium Pentazolate: Crystalline Hydro-Nitrogens at High Pressure”, *The Journal of Physical Chemistry A*, vol. 121, no. 8. American Chemical Society (ACS), pp. 1808–1813, Feb. 16, 2017. doi: 10.1021/acs.jpca.6b12900.  
  
B. A. Steele and I. I. Oleynik, “First principles investigation of nitrogen-rich energetic materials”, *AIP Conference Proceedings*. Author(s), 2018. doi: 10.1063/1.5044992.  
  
N. Goldman, Ed., *Computational Approaches for Chemistry Under Extreme Conditions*. Springer International Publishing, 2019. doi: 10.1007/978-3-030-05600-1.  
  
B. A. Steele, E. Stavrou, J. C. Crowhurst, J. M. Zaug, V. B. Prakapenkaand I. I. Oleynik, “High-Pressure Synthesis of a Pentazolate Salt”, *Chemistry of Materials*, vol. 29, no. 2. American Chemical Society (ACS), pp. 735–741, Dec. 19, 2016. doi: 10.1021/acs.chemmater.6b04538.  
  
B. A. Steele, “Cesium pentazolate: A new nitrogen-rich energetic material”, *AIP Conference Proceedings*. Author(s), 2017. doi: 10.1063/1.4971510.  
  
V. V. Zhakhovsky, M. M. Budzevich, A. C. Landerville, I. I. Oleynikand C. T. White, “Nano-scale spinning detonation in a condensed phase energetic material”, *Journal of Physics: Conference Series*, vol. 500, no. 17. IOP Publishing, p. 172006, May 07, 2014. doi: 10.1088/1742-6596/500/17/172006.  
  
V. V. Zhakhovsky, M. M. Budzevich, A. C. Landerville, I. I. Oleynikand C. T. White, “From laminar to turbulent detonations in energetic materials from molecular dynamics simulations”, *Journal of Physics: Conference Series*, vol. 500, no. 17. IOP Publishing, p. 172005, May 07, 2014. doi: 10.1088/1742-6596/500/17/172005.  
  
V. V. Zhakhovsky, N. A. Inogamov, B. J. Demaske, I. I. Oleynikand C. T. White, “Elastic-plastic collapse of super-elastic shock waves in face-centered-cubic solids”, *Journal of Physics: Conference Series*, vol. 500, no. 17. IOP Publishing, p. 172007, May 07, 2014. doi: 10.1088/1742-6596/500/17/172007.  
  
“Preface: 19th Biennial APS Conference on Shock Compression of Condensed Matter”, *AIP Conference Proceedings*. Author(s), 2017. doi: 10.1063/1.4971455.  
  
B. A. Steele and I. I. Oleynik, “Ternary Inorganic Compounds Containing Carbon, Nitrogen, and Oxygen at High Pressures”, *Inorganic Chemistry*, vol. 56, no. 21. American Chemical Society (ACS), pp. 13321–13328, Oct. 17, 2017. doi: 10.1021/acs.inorgchem.7b02102.  
  
A. S. Williams, B. A. Steeleand I. I. Oleynik, “Novel rubidium poly-nitrogen materials at high pressure”, *The Journal of Chemical Physics*, vol. 147, no. 23. AIP Publishing, p. 234701, Dec. 21, 2017. doi: 10.1063/1.5004416.  
  
V. Balasubramanian, A. Buchel, S. R. Green, L. Lehnerand S. L. Liebling, “Balasubramanian*et al.*Reply:”, *Physical Review Letters*, vol. 115, no. 4. American Physical Society (APS), Jul. 23, 2015. doi: 10.1103/physrevlett.115.049102.  
  
A. Buchel, S. R. Green, L. Lehnerand S. L. Liebling, “Conserved quantities and dual turbulent cascades in anti–de Sitter spacetime”, *Physical Review D*, vol. 91, no. 6. American Physical Society (APS), Mar. 09, 2015. doi: 10.1103/physrevd.91.064026.  
  
M. Kavic, S. L. Liebling, M. Lippertand J. H. Simonetti, “Accessing the axion via compact object binaries”, *Journal of Cosmology and Astroparticle Physics*, vol. 2020, no. 8. IOP Publishing, pp. 005–005, Aug. 04, 2020. doi: 10.1088/1475-7516/2020/08/005.  
  
L. Lehner, “Unequal mass binary neutron star mergers and multimessenger signals”, *Classical and Quantum Gravity*, vol. 33, no. 18. IOP Publishing, p. 184002, Sep. 02, 2016. doi: 10.1088/0264-9381/33/18/184002.  
  
L. Lehner, S. L. Liebling, C. Palenzuelaand P. M. Motl, “instability and gravitational wave signal in binary neutron star mergers”, *Physical Review D*, vol. 94, no. 4. American Physical Society (APS), Aug. 08, 2016. doi: 10.1103/physrevd.94.043003.  
  
S. L. Liebling and G. Khanna, “Scalar collapse in AdS with an OpenCL open source code”, *Classical and Quantum Gravity*, vol. 34, no. 20. IOP Publishing, p. 205012, Sep. 27, 2017. doi: 10.1088/1361-6382/aa8b43.  
  
S. L. Liebling and C. Palenzuela, “Electromagnetic luminosity of the coalescence of charged black hole binaries”, *Physical Review D*, vol. 94, no. 6. American Physical Society (APS), Sep. 19, 2016. doi: 10.1103/physrevd.94.064046.  
  
S. L. Liebling, C. Palenzuelaand L. Lehner, “Toward fidelity and scalability in non-vacuum mergers”, *Classical and Quantum Gravity*, vol. 37, no. 13. IOP Publishing, p. 135006, Jun. 12, 2020. doi: 10.1088/1361-6382/ab8fcd.  
  
Y. Miao, S. E. Nichols, P. M. Gasper, V. T. Metzgerand J. A. McCammon, “Activation and dynamic network of the M2 muscarinic receptor”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 27. Proceedings of the National Academy of Sciences, pp. 10982–10987, Jun. 18, 2013. doi: 10.1073/pnas.1309755110.  
  
Y. Miao, S. E. Nicholsand J. A. McCammon, “Free energy landscape of G-protein coupled receptors, explored by accelerated molecular dynamics”, *Physical Chemistry Chemical Physics*, vol. 16, no. 14. Royal Society of Chemistry (RSC), p. 6398, 2014. doi: 10.1039/c3cp53962h.  
  
Y. Miao, W. Sinko, L. Pierce, D. Bucher, R. C. Walkerand J. A. McCammon, “Improved Reweighting of Accelerated Molecular Dynamics Simulations for Free Energy Calculation”, *Journal of Chemical Theory and Computation*, vol. 10, no. 7. American Chemical Society (ACS), pp. 2677–2689, May 09, 2014. doi: 10.1021/ct500090q.  
  
S. E. Nichols, C. X. Hernández, Y. Wangand J. A. McCammon, “Structure-based network analysis of an evolved G protein-coupled receptor homodimer interface”, *Protein Science*, vol. 22, no. 6. Wiley, pp. 745–754, May 08, 2013. doi: 10.1002/pro.2258.  
  
Y. T. Pang, Y. Miao, Y. Wangand J. A. McCammon, “Gaussian Accelerated Molecular Dynamics in NAMD”, *Journal of Chemical Theory and Computation*, vol. 13, no. 1. American Chemical Society (ACS), pp. 9–19, Dec. 30, 2016. doi: 10.1021/acs.jctc.6b00931.  
  
V. Rao, “PKA Phosphorylation of Cardiac Troponin I Modulates Activation and Relaxation Kinetics of Ventricular Myofibrils”, *Biophysical Journal*, vol. 107, no. 5. Elsevier BV, pp. 1196–1204, Sep. 2014. doi: 10.1016/j.bpj.2014.07.027.  
  
Y. Miao, J. Baudry, J. C. Smithand J. A. McCammon, “General trends of dihedral conformational transitions in a globular protein”, *Proteins: Structure, Function, and Bioinformatics*, vol. 84, no. 4. Wiley, pp. 501–514, Feb. 15, 2016. doi: 10.1002/prot.24996.  
  
Y. Miao and J. A. McCammon, “Graded activation and free energy landscapes of a muscarinic G-protein–coupled receptor”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 43. Proceedings of the National Academy of Sciences, pp. 12162–12167, Oct. 10, 2016. doi: 10.1073/pnas.1614538113.  
  
Y. Miao, A. D. Calimanand J. A. McCammon, “Allosteric Effects of Sodium Ion Binding on Activation of the M3 Muscarinic G-Protein-Coupled Receptor”, *Biophysical Journal*, vol. 108, no. 7. Elsevier BV, pp. 1796–1806, Apr. 2015. doi: 10.1016/j.bpj.2015.03.003.  
  
G. Palermo, “Protospacer Adjacent Motif-Induced Allostery Activates CRISPR-Cas9”, *Journal of the American Chemical Society*, vol. 139, no. 45. American Chemical Society (ACS), pp. 16028–16031, Aug. 07, 2017. doi: 10.1021/jacs.7b05313.  
  
Y. Cheng, “Troponin I Mutations R146G and R21C Alter Cardiac Troponin Function, Contractile Properties, and Modulation by Protein Kinase A (PKA)-mediated Phosphorylation”, *Journal of Biological Chemistry*, vol. 290, no. 46. Elsevier BV, pp. 27749–27766, Nov. 2015. doi: 10.1074/jbc.m115.683045.  
  
K. Kappel, Y. Miaoand J. A. McCammon, “Accelerated molecular dynamics simulations of ligand binding to a muscarinic G-protein-coupled receptor”, *Quarterly Reviews of Biophysics*, vol. 48, no. 4. Cambridge University Press (CUP), pp. 479–487, Jul. 16, 2015. doi: 10.1017/s0033583515000153.  
  
M. O. Kim, P. G. Blachlyand J. A. McCammon, “Conformational Dynamics and Binding Free Energies of Inhibitors of BACE-1: From the Perspective of Protonation Equilibria”, *PLOS Computational Biology*, vol. 11, no. 10. Public Library of Science (PLoS), p. e1004341, Oct. 27, 2015. doi: 10.1371/journal.pcbi.1004341.  
  
S. Lindert, Y. Cheng, P. Kekenes-Huskey, M. Regnierand J. A. McCammon, “Effects of HCM cTnI Mutation R145G on Troponin Structure and Modulation by PKA Phosphorylation Elucidated by Molecular Dynamics Simulations”, *Biophysical Journal*, vol. 108, no. 2. Elsevier BV, pp. 395–407, Jan. 2015. doi: 10.1016/j.bpj.2014.11.3461.  
  
Y. Miao, V. A. Feherand J. A. McCammon, “Gaussian Accelerated Molecular Dynamics: Unconstrained Enhanced Sampling and Free Energy Calculation”, *Journal of Chemical Theory and Computation*, vol. 11, no. 8. American Chemical Society (ACS), pp. 3584–3595, Jul. 30, 2015. doi: 10.1021/acs.jctc.5b00436.  
  
Y. Miao, “Accelerated structure-based design of chemically diverse allosteric modulators of a muscarinic G protein-coupled receptor”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 38. Proceedings of the National Academy of Sciences, Sep. 06, 2016. doi: 10.1073/pnas.1612353113.  
  
Y. Miao and J. A. McCammon, “G-protein coupled receptors: advances in simulation and drug discovery”, *Current Opinion in Structural Biology*, vol. 41. Elsevier BV, pp. 83–89, Dec. 2016. doi: 10.1016/j.sbi.2016.06.008.  
  
Y. Miao and J. A. McCammon, “Unconstrained enhanced sampling for free energy calculations of biomolecules: a review”, *Molecular Simulation*, vol. 42, no. 13. Informa UK Limited, pp. 1046–1055, Jul. 05, 2016. doi: 10.1080/08927022.2015.1121541.  
  
N. Tanaka, “Canine CNGA3 Gene Mutations Provide Novel Insights into Human Achromatopsia-Associated Channelopathies and Treatment”, *PLOS ONE*, vol. 10, no. 9. Public Library of Science (PLoS), p. e0138943, Sep. 25, 2015. doi: 10.1371/journal.pone.0138943.  
  
A. M. Barragan, A. R. Crofts, K. Schultenand I. A. Solov’yov, “Identification of Ubiquinol Binding Motifs at the Q*o*-Site of the Cytochrome*bc*1Complex”, *The Journal of Physical Chemistry B*, vol. 119, no. 2. American Chemical Society (ACS), pp. 433–447, Nov. 24, 2014. doi: 10.1021/jp510022w.  
  
R. C. Bernardi, I. Cannand K. Schulten, “Molecular dynamics study of enhanced Man5B enzymatic activity”, *Biotechnology for Biofuels*, vol. 7, no. 1. Springer Science and Business Media LLC, Jun. 05, 2014. doi: 10.1186/1754-6834-7-83.  
  
E. Cai, “Stable Small Quantum Dots for Synaptic Receptor Tracking on Live Neurons”, *Angewandte Chemie International Edition*. Wiley, p. n/a–n/a, Sep. 26, 2014. doi: 10.1002/anie.201405735.  
  
P. L. Freddolino, C. B. Harrison, Y. Liuand K. Schulten, “Challenges in protein-folding simulations”, *Nature Physics*, vol. 6, no. 10. Springer Science and Business Media LLC, pp. 751–758, Oct. 2010. doi: 10.1038/nphys1713.  
  
A. Girdhar, C. Sathe, K. Schultenand J.-P. Leburton, “Gate-modulated graphene quantum point contact device for DNA sensing”, *Journal of Computational Electronics*, vol. 13, no. 4. Springer Science and Business Media LLC, pp. 839–846, Aug. 08, 2014. doi: 10.1007/s10825-014-0596-6.  
  
A. Girdhar, C. Sathe, K. Schultenand J.-P. Leburton, “Tunable graphene quantum point contact transistor for DNA detection and characterization”, *Nanotechnology*, vol. 26, no. 13. IOP Publishing, p. 134005, Mar. 13, 2015. doi: 10.1088/0957-4484/26/13/134005.  
  
B. C. Goh, “Molecular Mechanisms of Inhibition of Influenza by Surfactant Protein D Revealed by Large-Scale Molecular Dynamics Simulation”, *Biochemistry*, vol. 52, no. 47. American Chemical Society (ACS), pp. 8527–8538, Nov. 13, 2013. doi: 10.1021/bi4010683.  
  
W. Han and K. Schulten, “Fibril Elongation by Aβ17–42: Kinetic Network Analysis of Hybrid-Resolution Molecular Dynamics Simulations”, *Journal of the American Chemical Society*, vol. 136, no. 35. American Chemical Society (ACS), pp. 12450–12460, Aug. 25, 2014. doi: 10.1021/ja507002p.  
  
D. J. Hardy, Z. Wu, J. C. Phillips, J. E. Stone, R. D. Skeeland K. Schulten, “Multilevel Summation Method for Electrostatic Force Evaluation”, *Journal of Chemical Theory and Computation*, vol. 11, no. 2. American Chemical Society (ACS), pp. 766–779, Jan. 08, 2015. doi: 10.1021/ct5009075.  
  
H. Kim, J. Hsin, Y. Liu, P. R. Selvinand K. Schulten, “Formation of Salt Bridges Mediates Internal Dimerization of Myosin VI Medial Tail Domain”, *Structure*, vol. 18, no. 11. Elsevier BV, pp. 1443–1449, Nov. 2010. doi: 10.1016/j.str.2010.09.011.  
  
Y. Lai, “Fusion pore formation and expansion induced by Ca 2+ and synaptotagmin 1”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 4. Proceedings of the National Academy of Sciences, pp. 1333–1338, Jan. 08, 2013. doi: 10.1073/pnas.1218818110.  
  
M. P. Landry, “Comparative Dynamics and Sequence Dependence of DNA and RNA Binding to Single Walled Carbon Nanotubes”, *The Journal of Physical Chemistry C*, vol. 119, no. 18. American Chemical Society (ACS), pp. 10048–10058, Apr. 27, 2015. doi: 10.1021/jp511448e.  
  
Q. Li, “Structural mechanism of voltage-dependent gating in an isolated voltage-sensing domain”, *Nature Structural & Molecular Biology*, vol. 21, no. 3. Springer Science and Business Media LLC, pp. 244–252, Feb. 02, 2014. doi: 10.1038/nsmb.2768.  
  
Y. Liu, J. Hsin, H. Kim, P. R. Selvinand K. Schulten, “Extension of a Three-Helix Bundle Domain of Myosin VI and Key Role of Calmodulins”, *Biophysical Journal*, vol. 100, no. 12. Elsevier BV, pp. 2964–2973, Jun. 2011. doi: 10.1016/j.bpj.2011.05.010.  
  
Y. Liu, M. B. Prigozhin, K. Schultenand M. Gruebele, “Observation of Complete Pressure-Jump Protein Refolding in Molecular Dynamics Simulation and Experiment”, *Journal of the American Chemical Society*, vol. 136, no. 11. American Chemical Society (ACS), pp. 4265–4272, Feb. 03, 2014. doi: 10.1021/ja412639u.  
  
Y. Liu, J. Strümpfer, P. L. Freddolino, M. Gruebeleand K. Schulten, “Structural Characterization of λ-Repressor Folding from All-Atom Molecular Dynamics Simulations”, *The Journal of Physical Chemistry Letters*, vol. 3, no. 9. American Chemical Society (ACS), pp. 1117–1123, Apr. 15, 2012. doi: 10.1021/jz300017c.  
  
W. Ma and K. Schulten, “Mechanism of Substrate Translocation by a Ring-Shaped ATPase Motor at Millisecond Resolution”, *Journal of the American Chemical Society*, vol. 137, no. 8. American Chemical Society (ACS), pp. 3031–3040, Feb. 19, 2015. doi: 10.1021/ja512605w.  
  
J. C. Phillips, Y. Sun, N. Jain, E. J. Bohmand L. V. Kale, “Mapping to Irregular Torus Topologies and Other Techniques for Petascale Biomolecular Simulation”, *SC14: International Conference for High Performance Computing, Networking, Storage and Analysis*. IEEE, Nov. 2014. doi: 10.1109/sc.2014.12.  
  
M. B. Prigozhin, “Misplaced helix slows down ultrafast pressure-jump protein folding”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 20. Proceedings of the National Academy of Sciences, pp. 8087–8092, Apr. 25, 2013. doi: 10.1073/pnas.1219163110.  
  
C. Sathe, A. Girdhar, J.-P. Leburtonand K. Schulten, “Electronic detection of dsDNA transition from helical to zipper conformation using graphene nanopores”, *Nanotechnology*, vol. 25, no. 44. IOP Publishing, p. 445105, Oct. 17, 2014. doi: 10.1088/0957-4484/25/44/445105.  
  
C. Schoeler, “Ultrastable cellulosome-adhesion complex tightens under load”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, Dec. 08, 2014. doi: 10.1038/ncomms6635.  
  
X. Wang, “Atomic Model of Rabbit Hemorrhagic Disease Virus by Cryo-Electron Microscopy and Crystallography”, *PLoS Pathogens*, vol. 9, no. 1. Public Library of Science (PLoS), p. e1003132, Jan. 17, 2013. doi: 10.1371/journal.ppat.1003132.  
  
Y. Wang, “Single molecule FRET reveals pore size and opening mechanism of a mechano-sensitive ion channel”, *eLife*, vol. 3. eLife Sciences Publications, Ltd, Feb. 18, 2014. doi: 10.7554/elife.01834.  
  
S. Wickles, “A structural model of the active ribosome-bound membrane protein insertase YidC”, *eLife*, vol. 3. eLife Sciences Publications, Ltd, Jul. 10, 2014. doi: 10.7554/elife.03035.  
  
A. J. Wirth, Y. Liu, M. B. Prigozhin, K. Schultenand M. Gruebele, “Comparing Fast Pressure Jump and Temperature Jump Protein Folding Experiments and Simulations”, *Journal of the American Chemical Society*, vol. 137, no. 22. American Chemical Society (ACS), pp. 7152–7159, Jun. 02, 2015. doi: 10.1021/jacs.5b02474.  
  
Z. Wu and K. Schulten, “Synaptotagmin’s Role in Neurotransmitter Release Likely Involves Ca 2+ -induced Conformational Transition”, *Biophysical Journal*, vol. 107, no. 5. Elsevier BV, pp. 1156–1166, Sep. 2014. doi: 10.1016/j.bpj.2014.07.041.  
  
K. Zhang, “Flexible interwoven termini determine the thermal stability of thermosomes”, *Protein & Cell*, vol. 4, no. 6. Oxford University Press (OUP), pp. 432–444, May 25, 2013. doi: 10.1007/s13238-013-3026-9.  
  
Q. Zhou, “Molecular insights into the membrane-associated phosphatidylinositol 4-kinase IIα”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, Mar. 28, 2014. doi: 10.1038/ncomms4552.  
  
X. Zou, Y. Liu, Z. Chen, G. I. Cárdenas-Jirónand K. Schulten, “Flow-Induced β-Hairpin Folding of the Glycoprotein Ibα β-Switch”, *Biophysical Journal*, vol. 99, no. 4. Elsevier BV, pp. 1182–1191, Aug. 2010. doi: 10.1016/j.bpj.2010.05.035.  
  
T. Zisis, P. L. Freddolino, P. Turunen, M. C. F. van Teeseling, A. E. Rowanand K. G. Blank, “Interfacial Activation of *Candida antarctica* Lipase B: Combined Evidence from Experiment and Simulation”, *Biochemistry*, vol. 54, no. 38. American Chemical Society (ACS), pp. 5969–5979, Sep. 15, 2015. doi: 10.1021/acs.biochem.5b00586.  
  
N. M. Tubman, E. Liberatore, C. Pierleoni, M. Holzmannand D. M. Ceperley, “Molecular-Atomic Transition along the Deuterium Hugoniot Curve with Coupled Electron-Ion Monte Carlo Simulations”, *Physical Review Letters*, vol. 115, no. 4. American Physical Society (APS), Jul. 22, 2015. doi: 10.1103/physrevlett.115.045301.  
  
Y. Yang, I. Kylänpää, N. M. Tubman, J. T. Krogel, S. Hammes-Schifferand D. M. Ceperley, “How large are nonadiabatic effects in atomic and diatomic systems?”, *The Journal of Chemical Physics*, vol. 143, no. 12. AIP Publishing, p. 124308, Sep. 28, 2015. doi: 10.1063/1.4931667.  
  
Y. Zhuang, H. J. Changlani, N. M. Tubmanand T. L. Hughes, “Phase diagram of theparafermionic chain with chiral interactions”, *Physical Review B*, vol. 92, no. 3. American Physical Society (APS), Jul. 31, 2015. doi: 10.1103/physrevb.92.035154.  
  
F. Aydin, N. Courtemanche, T. D. Pollardand G. A. Voth, “Gating mechanisms during actin filament elongation by formins”, *eLife*, vol. 7. eLife Sciences Publications, Ltd, Jul. 23, 2018. doi: 10.7554/elife.37342.  
  
J. L. Baker, N. Courtemanche, D. L. Parton, M. McCullagh, T. D. Pollardand G. A. Voth, “Electrostatic Interactions between the Bni1p Formin FH2 Domain and Actin Influence Actin Filament Nucleation”, *Structure*, vol. 23, no. 1. Elsevier BV, pp. 68–79, Jan. 2015. doi: 10.1016/j.str.2014.10.014.  
  
J. L. Baker and G. A. Voth, “Effects of ATP and Actin-Filament Binding on the Dynamics of the Myosin II S1 Domain”, *Biophysical Journal*, vol. 105, no. 7. Elsevier BV, pp. 1624–1634, Oct. 2013. doi: 10.1016/j.bpj.2013.08.023.  
  
T. C. Bidone, “New Insights into the Conformational Activation of Full-Length Integrin”, *[]*. Cold Spring Harbor Laboratory, Oct. 15, 2017. doi: 10.1101/203661.  
  
R. Biswas, W. Carpenter, J. A. Fournier, G. A. Vothand A. Tokmakoff, “IR spectral assignments for the hydrated excess proton in liquid water”, *The Journal of Chemical Physics*, vol. 146, no. 15. AIP Publishing, p. 154507, Apr. 21, 2017. doi: 10.1063/1.4980121.  
  
Y. Chen, “Loss of the F-BAR protein CIP4 reduces platelet production by impairing membrane-cytoskeleton remodeling”, *Blood*, vol. 122, no. 10. American Society of Hematology, pp. 1695–1706, Sep. 05, 2013. doi: 10.1182/blood-2013-03-484550.  
  
J. F. Dama, G. M. Hocky, R. Sunand G. A. Voth, “Exploring Valleys without Climbing Every Peak: More Efficient and Forgiving Metabasin Metadynamics via Robust On-the-Fly Bias Domain Restriction”, *Journal of Chemical Theory and Computation*, vol. 11, no. 12. American Chemical Society (ACS), pp. 5638–5650, Nov. 20, 2015. doi: 10.1021/acs.jctc.5b00907.  
  
A. Davtyan, J. F. Dama, A. V. Sinitskiyand G. A. Voth, “The Theory of Ultra-Coarse-Graining. 2. Numerical Implementation”, *Journal of Chemical Theory and Computation*, vol. 10, no. 12. American Chemical Society (ACS), pp. 5265–5275, Dec. 01, 2014. doi: 10.1021/ct500834t.  
  
A. Davtyan, M. Simunovicand G. A. Voth, “The mesoscopic membrane with proteins (MesM-P) model”, *The Journal of Chemical Physics*, vol. 147, no. 4. AIP Publishing, p. 044101, Jul. 24, 2017. doi: 10.1063/1.4993514.  
  
A. Davtyan, G. A. Vothand H. C. Andersen, “Dynamic force matching: Construction of dynamic coarse-grained models with realistic short time dynamics and accurate long time dynamics”, *The Journal of Chemical Physics*, vol. 145, no. 22. AIP Publishing, p. 224107, Dec. 14, 2016. doi: 10.1063/1.4971430.  
  
J. Fan, M. G. Saunders, E. J. Haddadian, K. F. Freed, E. M. De La Cruzand G. A. Voth, “Molecular Origins of Cofilin-Linked Changes in Actin Filament Mechanics”, *Journal of Molecular Biology*, vol. 425, no. 7. Elsevier BV, pp. 1225–1240, Apr. 2013. doi: 10.1016/j.jmb.2013.01.020.  
  
N. Guttenberg, J. F. Dama, M. G. Saunders, G. A. Voth, J. Weareand A. R. Dinner, “Minimizing memory as an objective for coarse-graining”, *The Journal of Chemical Physics*, vol. 138, no. 9. AIP Publishing, p. 094111, Mar. 07, 2013. doi: 10.1063/1.4793313.  
  
A. J. Harker, “Ena/VASP processive elongation is modulated by avidity on actin filaments bundled by the filopodia crosslinker fascin”, *[]*. Cold Spring Harbor Laboratory, Aug. 07, 2018. doi: 10.1101/386961.  
  
G. M. Hocky, T. Dannenhoffer-Lafageand G. A. Voth, “Coarse-Grained Directed Simulation”, *Journal of Chemical Theory and Computation*, vol. 13, no. 9. American Chemical Society (ACS), pp. 4593–4603, Aug. 31, 2017. doi: 10.1021/acs.jctc.7b00690.  
  
Z. Jarin, F.-C. Tsai, A. Davtyan, A. J. Pak, P. Bassereauand G. A. Voth, “Unusual Organization of I-BAR Proteins on Tubular and Vesicular Membranes”, *Biophysical Journal*, vol. 117, no. 3. Elsevier BV, pp. 553–562, Aug. 2019. doi: 10.1016/j.bpj.2019.06.025.  
  
H. H. Katkar, “Insights into the Cooperative Nature of ATP Hydrolysis in Actin Filaments”, *Biophysical Journal*, vol. 115, no. 8. Elsevier BV, pp. 1589–1602, Oct. 2018. doi: 10.1016/j.bpj.2018.08.034.  
  
H. H. Katkar, “Insights into the cooperative nature of ATP hydrolysis in actin filaments”, *[]*. Cold Spring Harbor Laboratory, May 10, 2018. doi: 10.1101/319558.  
  
C.-L. Lai, A. Srivastava, C. Pilling, A. R. Chase, J. J. Falkeand G. A. Voth, “Molecular Mechanism of Membrane Binding of the GRP1 PH Domain”, *Journal of Molecular Biology*, vol. 425, no. 17. Elsevier BV, pp. 3073–3090, Sep. 2013. doi: 10.1016/j.jmb.2013.05.026.  
  
L. Larini, L. Luand G. A. Voth, “The multiscale coarse-graining method. VI. Implementation of three-body coarse-grained potentials”, *The Journal of Chemical Physics*, vol. 132, no. 16. AIP Publishing, p. 164107, Apr. 28, 2010. doi: 10.1063/1.3394863.  
  
S. Lee, R. Liang, G. A. Vothand J. M. J. Swanson, “Computationally Efficient Multiscale Reactive Molecular Dynamics to Describe Amino Acid Deprotonation in Proteins”, *Journal of Chemical Theory and Computation*, vol. 12, no. 2. American Chemical Society (ACS), pp. 879–891, Jan. 20, 2016. doi: 10.1021/acs.jctc.5b01109.  
  
S. Lee, H. B. Mayes, J. M. J. Swansonand G. A. Voth, “The Origin of Coupled Chloride and Proton Transport in a Cl–/H+ Antiporter”, *Journal of the American Chemical Society*, vol. 138, no. 45. American Chemical Society (ACS), pp. 14923–14930, Nov. 08, 2016. doi: 10.1021/jacs.6b06683.  
  
S. Lee, J. M. J. Swansonand G. A. Voth, “Multiscale Simulations Reveal Key Aspects of the Proton Transport Mechanism in the ClC-ec1 Antiporter”, *Biophysical Journal*, vol. 110, no. 6. Elsevier BV, pp. 1334–1345, Mar. 2016. doi: 10.1016/j.bpj.2016.02.014.  
  
R. Liang, H. Li, J. M. J. Swansonand G. A. Voth, “Multiscale simulation reveals a multifaceted mechanism of proton permeation through the influenza A M2 proton channel”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 26. Proceedings of the National Academy of Sciences, pp. 9396–9401, Jun. 16, 2014. doi: 10.1073/pnas.1401997111.  
  
R. Liang, J. M. J. Swanson, Y. Peng, M. Wikströmand G. A. Voth, “Multiscale simulations reveal key features of the proton-pumping mechanism in cytochrome *c* oxidase”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 27. Proceedings of the National Academy of Sciences, pp. 7420–7425, Jun. 23, 2016. doi: 10.1073/pnas.1601982113.  
  
R. Liang, J. M. J. Swansonand G. A. Voth, “Benchmark Study of the SCC-DFTB Approach for a Biomolecular Proton Channel”, *Journal of Chemical Theory and Computation*, vol. 10, no. 1. American Chemical Society (ACS), pp. 451–462, Dec. 24, 2013. doi: 10.1021/ct400832r.  
  
C. Li, Z. Yue, L. M. Espinoza-Fonsecaand G. A. Voth, “Multiscale Simulation Reveals Passive Proton Transport Through SERCA on the Microsecond Timescale”, *Biophysical Journal*, vol. 119, no. 5. Elsevier BV, pp. 1033–1040, Sep. 2020. doi: 10.1016/j.bpj.2020.07.027.  
  
J. Li, A. L. Jonsson, T. Beuming, J. C. Shelleyand G. A. Voth, “Ligand-Dependent Activation and Deactivation of the Human Adenosine A2A Receptor”, *Journal of the American Chemical Society*, vol. 135, no. 23. American Chemical Society (ACS), pp. 8749–8759, May 29, 2013. doi: 10.1021/ja404391q.  
  
J. Li, B. P. Ziemba, J. J. Falkeand G. A. Voth, “Interactions of Protein Kinase C-α C1A and C1B Domains with Membranes: A Combined Computational and Experimental Study”, *Journal of the American Chemical Society*, vol. 136, no. 33. American Chemical Society (ACS), pp. 11757–11766, Aug. 11, 2014. doi: 10.1021/ja505369r.  
  
J. J. Madsen, J. M. A. Grime, J. S. Rossmanand G. A. Voth, “Entropic forces drive clustering and spatial localization of influenza A M2 during viral budding”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 37. Proceedings of the National Academy of Sciences, Aug. 27, 2018. doi: 10.1073/pnas.1805443115.  
  
S. Mani, D. J. Cosgroveand G. A. Voth, “Anisotropic Motions of Fibrils Dictated by Their Orientations in the Lamella: A Coarse-Grained Model of a Plant Cell Wall”, *The Journal of Physical Chemistry B*, vol. 124, no. 17. American Chemical Society (ACS), pp. 3527–3539, Apr. 07, 2020. doi: 10.1021/acs.jpcb.0c01697.  
  
H. B. Mayes, S. Lee, A. D. White, G. A. Vothand J. M. J. Swanson, “Multiscale Kinetic Modeling Reveals an Ensemble of Cl–/H+ Exchange Pathways in ClC-ec1 Antiporter”, *Journal of the American Chemical Society*, vol. 140, no. 5. American Chemical Society (ACS), pp. 1793–1804, Jan. 30, 2018. doi: 10.1021/jacs.7b11463.  
  
M. McCullagh, M. G. Saundersand G. A. Voth, “Unraveling the Mystery of ATP Hydrolysis in Actin Filaments”, *Journal of the American Chemical Society*, vol. 136, no. 37. American Chemical Society (ACS), pp. 13053–13058, Sep. 09, 2014. doi: 10.1021/ja507169f.  
  
M. McCullagh and G. A. Voth, “Unraveling the Role of the Protein Environment for [FeFe]-Hydrogenase: A New Application of Coarse-Graining”, *The Journal of Physical Chemistry B*, vol. 117, no. 15. American Chemical Society (ACS), pp. 4062–4071, Apr. 04, 2013. doi: 10.1021/jp402441s.  
  
V. Monje-Galvan and G. A. Voth, “Binding mechanism of the matrix domain of HIV-1 gag on lipid membranes”, *eLife*, vol. 9. eLife Sciences Publications, Ltd, Aug. 18, 2020. doi: 10.7554/elife.58621.  
  
P. W. Oakes, “Lamellipodium is a myosin-independent mechanosensor”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 11. Proceedings of the National Academy of Sciences, pp. 2646–2651, Feb. 27, 2018. doi: 10.1073/pnas.1715869115.  
  
A. J. Pak, T. Dannenhoffer-Lafage, J. J. Madsenand G. A. Voth, “Systematic Coarse-Grained Lipid Force Fields with Semiexplicit Solvation via Virtual Sites”, *Journal of Chemical Theory and Computation*, vol. 15, no. 3. American Chemical Society (ACS), pp. 2087–2100, Jan. 31, 2019. doi: 10.1021/acs.jctc.8b01033.  
  
Y. Peng, J. M. J. Swanson, S.-. gu . Kang, R. Zhouand G. A. Voth, “Hydrated Excess Protons Can Create Their Own Water Wires”, *The Journal of Physical Chemistry B*, vol. 119, no. 29. American Chemical Society (ACS), pp. 9212–9218, Nov. 12, 2014. doi: 10.1021/jp5095118.  
  
C. Prévost, “Mechanism and Determinants of Amphipathic Helix-Containing Protein Targeting to Lipid Droplets”, *Developmental Cell*, vol. 44, no. 1. Elsevier BV, pp. 73–86.e4, Jan. 2018. doi: 10.1016/j.devcel.2017.12.011.  
  
M. G. Saunders, J. Tempkin, J. Weare, A. R. Dinner, B. Rouxand G. A. Voth, “Nucleotide Regulation of the Structure and Dynamics of G-Actin”, *Biophysical Journal*, vol. 106, no. 8. Elsevier BV, pp. 1710–1720, Apr. 2014. doi: 10.1016/j.bpj.2014.03.012.  
  
M. G. Saunders and G. A. Voth, “Coarse-Graining Methods for Computational Biology”, *Annual Review of Biophysics*, vol. 42, no. 1. Annual Reviews, pp. 73–93, May 06, 2013. doi: 10.1146/annurev-biophys-083012-130348.  
  
M. Simunovic, “How curvature-generating proteins build scaffolds on membrane nanotubes”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 40. Proceedings of the National Academy of Sciences, pp. 11226–11231, Sep. 21, 2016. doi: 10.1073/pnas.1606943113.  
  
M. Simunovic, C. Mim, T. C. Marlovits, G. Resch, V. M. Ungerand G. A. Voth, “Protein-Mediated Transformation of Lipid Vesicles into Tubular Networks”, *Biophysical Journal*, vol. 105, no. 3. Elsevier BV, pp. 711–719, Aug. 2013. doi: 10.1016/j.bpj.2013.06.039.  
  
M. Simunovic, A. Srivastavaand G. A. Voth, “Linear aggregation of proteins on the membrane as a prelude to membrane remodeling”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 51. Proceedings of the National Academy of Sciences, pp. 20396–20401, Nov. 27, 2013. doi: 10.1073/pnas.1309819110.  
  
M. Simunovic and G. A. Voth, “Membrane tension controls the assembly of curvature-generating proteins”, *Nature Communications*, vol. 6, no. 1. Springer Science and Business Media LLC, May 26, 2015. doi: 10.1038/ncomms8219.  
  
A. V. Sinitskiy and G. A. Voth, “Coarse-graining of proteins based on elastic network models”, *Chemical Physics*, vol. 422. Elsevier BV, pp. 165–174, Aug. 2013. doi: 10.1016/j.chemphys.2013.01.024.  
  
O. Sode and G. A. Voth, “Electron transfer activation of a second water channel for proton transport in [FeFe]-hydrogenase”, *The Journal of Chemical Physics*, vol. 141, no. 22. AIP Publishing, pp. 22D527, Dec. 14, 2014. doi: 10.1063/1.4902236.  
  
A. Srivastava and G. A. Voth, “Hybrid Approach for Highly Coarse-Grained Lipid Bilayer Models”, *Journal of Chemical Theory and Computation*, vol. 9, no. 1. American Chemical Society (ACS), pp. 750–765, Nov. 21, 2012. doi: 10.1021/ct300751h.  
  
A. Srivastava and G. A. Voth, “Solvent-Free, Highly Coarse-Grained Models for Charged Lipid Systems”, *Journal of Chemical Theory and Computation*, vol. 10, no. 10. American Chemical Society (ACS), pp. 4730–4744, Sep. 24, 2014. doi: 10.1021/ct500474a.  
  
R. Sun, J. F. Dama, J. S. Tan, J. P. Roseand G. A. Voth, “Transition-Tempered Metadynamics Is a Promising Tool for Studying the Permeation of Drug-like Molecules through Membranes”, *Journal of Chemical Theory and Computation*, vol. 12, no. 10. American Chemical Society (ACS), pp. 5157–5169, Sep. 22, 2016. doi: 10.1021/acs.jctc.6b00206.  
  
R. Sun, Y. Han, J. M. J. Swanson, J. S. Tan, J. P. Roseand G. A. Voth, “Molecular transport through membranes: Accurate permeability coefficients from multidimensional potentials of mean force and local diffusion constants”, *The Journal of Chemical Physics*, vol. 149, no. 7. AIP Publishing, p. 072310, Aug. 21, 2018. doi: 10.1063/1.5027004.  
  
D. Tong and G. A. Voth, “Microtubule Simulations Provide Insight into the Molecular Mechanism Underlying Dynamic Instability”, *Biophysical Journal*, vol. 118, no. 12. Elsevier BV, pp. 2938–2951, Jun. 2020. doi: 10.1016/j.bpj.2020.04.028.  
  
F. X. Vázquez, V. M. Ungerand G. A. Voth, “Autoinhibition of Endophilin in Solution via Interdomain Interactions”, *Biophysical Journal*, vol. 104, no. 2. Elsevier BV, pp. 396–403, Jan. 2013. doi: 10.1016/j.bpj.2012.12.009.  
  
Z. Wang, J. M. J. Swansonand G. A. Voth, “Modulating the Chemical Transport Properties of a Transmembrane Antiporter via Alternative Anion Flux”, *Journal of the American Chemical Society*, vol. 140, no. 48. American Chemical Society (ACS), pp. 16535–16543, Nov. 13, 2018. doi: 10.1021/jacs.8b07614.  
  
A. Yu, K. A. Skorupka, A. J. Pak, B. K. Ganser-Pornillos, O. Pornillosand G. A. Voth, “TRIM5α self-assembly and compartmentalization of the HIV-1 viral capsid”, *Nature Communications*, vol. 11, no. 1. Springer Science and Business Media LLC, Mar. 11, 2020. doi: 10.1038/s41467-020-15106-1.  
  
Z. Yue, C. Li, G. A. Vothand J. M. J. Swanson, “Dynamic Protonation Dramatically Affects the Membrane Permeability of Drug-like Molecules”, *Journal of the American Chemical Society*, vol. 141, no. 34. American Chemical Society (ACS), pp. 13421–13433, Aug. 06, 2019. doi: 10.1021/jacs.9b04387.  
  
R. Liang, J. M. J. Swanson, M. Wikströmand G. A. Voth, “Understanding the essential proton-pumping kinetic gates and decoupling mutations in cytochrome *c* oxidase”, *Proceedings of the National Academy of Sciences*, vol. 114, no. 23. Proceedings of the National Academy of Sciences, pp. 5924–5929, May 23, 2017. doi: 10.1073/pnas.1703654114.  
  
A. D. White, C. Knight, G. M. Hockyand G. A. Voth, “Communication: Improved *ab initio* molecular dynamics by minimally biasing with experimental data”, *The Journal of Chemical Physics*, vol. 146, no. 4. AIP Publishing, p. 041102, Jan. 28, 2017. doi: 10.1063/1.4974837.  
  
I. Backus and T. Quinn, “Fragmentation of protoplanetary discs around M-dwarfs”, *Monthly Notices of the Royal Astronomical Society*, vol. 463, no. 3. Oxford University Press (OUP), pp. 2480–2493, Jul. 30, 2016. doi: 10.1093/mnras/stw1825.  
  
I. S. Butsky, J. N. Burchett, D. Nagai, M. Tremmel, T. R. Quinnand J. K. Werk, “Ultraviolet signatures of the multiphase intracluster and circumgalactic media in the romulusc simulation”, *Monthly Notices of the Royal Astronomical Society*, vol. 490, no. 3. Oxford University Press (OUP), pp. 4292–4306, Oct. 12, 2019. doi: 10.1093/mnras/stz2859.  
  
C. R. Christensen, “Simulating disc galaxy bulges that are consistent with observed scaling relations”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 440, no. 1. Oxford University Press (OUP), pp. L51–L55, Feb. 21, 2014. doi: 10.1093/mnrasl/slu020.  
  
C. R. Christensen, “The effect of models of the interstellar media on the central mass distribution of galaxies”, *Monthly Notices of the Royal Astronomical Society*, vol. 440, no. 3. Oxford University Press (OUP), pp. 2843–2859, Apr. 12, 2014. doi: 10.1093/mnras/stu399.  
  
V. P. Debattista, F. C. van den Bosch, R. Roškar, T. Quinn, B. Mooreand D. R. Cole, “Internal alignments of red versus blue discs in dark matter haloes”, *Monthly Notices of the Royal Astronomical Society*, vol. 452, no. 4. Oxford University Press (OUP), pp. 4094–4110, Aug. 10, 2015. doi: 10.1093/mnras/stv1563.  
  
J. Liu, M. Robson, T. Quinnand M. Kulkarni, “Efficient GPU tree walks for effective distributed n-body simulations”, *Proceedings of the ACM International Conference on Supercomputing*. ACM, Jun. 26, 2019. doi: 10.1145/3330345.3330348.  
  
A. Ricarte, M. Tremmel, P. Natarajanand T. Quinn, “Tracing black hole and galaxy co-evolution in the Romulus simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 489, no. 1. Oxford University Press (OUP), pp. 802–819, Aug. 23, 2019. doi: 10.1093/mnras/stz2161.  
  
J. W. Wadsley, B. W. Kellerand T. R. Quinn, “Gasoline2: a modern smoothed particle hydrodynamics code”, *Monthly Notices of the Royal Astronomical Society*, vol. 471, no. 2. Oxford University Press (OUP), pp. 2357–2369, Jun. 30, 2017. doi: 10.1093/mnras/stx1643.  
  
S. C. Wallace and T. R. Quinn, “N-body simulations of terrestrial planet growth with resonant dynamical friction”, *Monthly Notices of the Royal Astronomical Society*, vol. 489, no. 2. Oxford University Press (OUP), pp. 2159–2176, Aug. 19, 2019. doi: 10.1093/mnras/stz2284.  
  
A. Azizi, “Frustration and Atomic Ordering in a Monolayer Semiconductor Alloy”, *Physical Review Letters*, vol. 124, no. 9. American Physical Society (APS), Mar. 05, 2020. doi: 10.1103/physrevlett.124.096101.  
  
H. R. Barzegar, “Electrostatically Driven Nanoballoon Actuator”, *Nano Letters*, vol. 16, no. 11. American Chemical Society (ACS), pp. 6787–6791, Oct. 07, 2016. doi: 10.1021/acs.nanolett.6b02394.  
  
H. R. Barzegar, “Spontaneous twisting of a collapsed carbon nanotube”, *Nano Research*, vol. 10, no. 6. Springer Science and Business Media LLC, pp. 1942–1949, Jan. 25, 2017. doi: 10.1007/s12274-016-1380-7.  
  
T. Cao, Z. Li, D. Y. Qiuand S. G. Louie, “Gate Switchable Transport and Optical Anisotropy in 90° Twisted Bilayer Black Phosphorus”, *Nano Letters*, vol. 16, no. 9. American Chemical Society (ACS), pp. 5542–5546, Sep. 01, 2016. doi: 10.1021/acs.nanolett.6b02084.  
  
Y. Chen, “Strong correlations and orbital texture in single-layer 1T-TaSe2”, *Nature Physics*, vol. 16, no. 2. Springer Science and Business Media LLC, pp. 218–224, Jan. 06, 2020. doi: 10.1038/s41567-019-0744-9.  
  
L. Guo, “Exchange-driven intravalley mixing of excitons in monolayer transition metal dichalcogenides”, *Nature Physics*, vol. 15, no. 3. Springer Science and Business Media LLC, pp. 228–232, Dec. 10, 2018. doi: 10.1038/s41567-018-0362-y.  
  
F. H. da Jornada, L. Xian, A. Rubioand S. G. Louie, “Universal slow plasmons and giant field enhancement in atomically thin quasi-two-dimensional metals”, *Nature Communications*, vol. 11, no. 1. Springer Science and Business Media LLC, Feb. 21, 2020. doi: 10.1038/s41467-020-14826-8.  
  
Y.-L. Lee, F. Zhao, T. Cao, J. Ihmand S. G. Louie, “Topological Phases in Cove-Edged and Chevron Graphene Nanoribbons: Geometric Structures, Z2 Invariants, and Junction States”, *Nano Letters*, vol. 18, no. 11. American Chemical Society (ACS), pp. 7247–7253, Sep. 25, 2018. doi: 10.1021/acs.nanolett.8b03416.  
  
L. Li, “Direct observation of the layer-dependent electronic structure in phosphorene”, *Nature Nanotechnology*, vol. 12, no. 1. Springer Science and Business Media LLC, pp. 21–25, Sep. 19, 2016. doi: 10.1038/nnano.2016.171.  
  
K. Liu, “Systematic determination of absolute absorption cross-section of individual carbon nanotubes”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 21. Proceedings of the National Academy of Sciences, pp. 7564–7569, May 12, 2014. doi: 10.1073/pnas.1318851111.  
  
Z. Li, G. Antonius, M. Wu, F. H. da Jornadaand S. G. Louie, “Electron-Phonon Coupling from *Ab Initio* Linear-Response Theory within the Method: Correlation-Enhanced Interactions and Superconductivity in ”, *Physical Review Letters*, vol. 122, no. 18. American Physical Society (APS), May 10, 2019. doi: 10.1103/physrevlett.122.186402.  
  
Z. Li, T. Cao, M. Wuand S. G. Louie, “Generation of Anisotropic Massless Dirac Fermions and Asymmetric Klein Tunneling in Few-Layer Black Phosphorus Superlattices”, *Nano Letters*, vol. 17, no. 4. American Chemical Society (ACS), pp. 2280–2286, Mar. 02, 2017. doi: 10.1021/acs.nanolett.6b04942.  
  
A. Malashevich and S. Ismail-Beigi, “First-principles study of oxygen-deficientstructures”, *Physical Review B*, vol. 92, no. 14. American Physical Society (APS), Oct. 06, 2015. doi: 10.1103/physrevb.92.144102.  
  
S. Meyer, “Metal-insulator transition in quasi-one-dimensional in the few-chain limit”, *Physical Review B*, vol. 100, no. 4. American Physical Society (APS), Jul. 09, 2019. doi: 10.1103/physrevb.100.041403.  
  
S. Oh, M. F. Crommieand M. L. Cohen, “Simulating the Nanomechanical Response of Cyclooctatetraene Molecules on a Graphene Device”, *ACS Nano*. American Chemical Society (ACS), Feb. 04, 2019. doi: 10.1021/acsnano.8b07781.  
  
T. Pham, “Formation and Dynamics of Electron-Irradiation-Induced Defects in Hexagonal Boron Nitride at Elevated Temperatures”, *Nano Letters*, vol. 16, no. 11. American Chemical Society (ACS), pp. 7142–7147, Oct. 06, 2016. doi: 10.1021/acs.nanolett.6b03442.  
  
T. Pham, “Torsional instability in the single-chain limit of a transition metal trichalcogenide”, *Science*, vol. 361, no. 6399. American Association for the Advancement of Science (AAAS), pp. 263–266, Jul. 20, 2018. doi: 10.1126/science.aat4749.  
  
D. Y. Qiu, F. H. da Jornadaand S. G. Louie, “Screening and many-body effects in two-dimensional crystals: Monolayer”, *Physical Review B*, vol. 93, no. 23. American Physical Society (APS), Jun. 20, 2016. doi: 10.1103/physrevb.93.235435.  
  
S. Refaely-Abramson, D. Y. Qiu, S. G. Louieand J. B. Neaton, “Defect-Induced Modification of Low-Lying Excitons and Valley Selectivity in Monolayer Transition Metal Dichalcogenides”, *Physical Review Letters*, vol. 121, no. 16. American Physical Society (APS), Oct. 16, 2018. doi: 10.1103/physrevlett.121.167402.  
  
A. Riss, “Local Electronic and Chemical Structure of Oligo-acetylene Derivatives Formed Through Radical Cyclizations at a Surface”, *Nano Letters*, vol. 14, no. 5. American Chemical Society (ACS), pp. 2251–2255, Jan. 13, 2014. doi: 10.1021/nl403791q.  
  
A. Riss, “Imaging and Tuning Molecular Levels at the Surface of a Gated Graphene Device”, *ACS Nano*, vol. 8, no. 6. American Chemical Society (ACS), pp. 5395–5401, May 02, 2014. doi: 10.1021/nn501459v.  
  
D. J. Rizzo, “Topological band engineering of graphene nanoribbons”, *Nature*, vol. 560, no. 7717. Springer Science and Business Media LLC, pp. 204–208, Aug. 2018. doi: 10.1038/s41586-018-0376-8.  
  
D. J. Rizzo, “Length-Dependent Evolution of Type II Heterojunctions in Bottom-Up-Synthesized Graphene Nanoribbons”, *Nano Letters*, vol. 19, no. 5. American Chemical Society (ACS), pp. 3221–3228, Apr. 19, 2019. doi: 10.1021/acs.nanolett.9b00758.  
  
G. Samsonidze, M. L. Cohenand S. G. Louie, “First-principles study of quasiparticle energies of a bipolar molecule in a scanning tunneling microscope measurement”, *Computational Materials Science*, vol. 91. Elsevier BV, pp. 187–191, Aug. 2014. doi: 10.1016/j.commatsci.2014.04.049.  
  
M. M. Ugeda, “Giant bandgap renormalization and excitonic effects in a monolayer transition metal dichalcogenide semiconductor”, *Nature Materials*, vol. 13, no. 12. Springer Science and Business Media LLC, pp. 1091–1095, Aug. 31, 2014. doi: 10.1038/nmat4061.  
  
M. I. B. Utama, “A dielectric-defined lateral heterojunction in a monolayer semiconductor”, *Nature Electronics*, vol. 2, no. 2. Springer Science and Business Media LLC, pp. 60–65, Feb. 11, 2019. doi: 10.1038/s41928-019-0207-4.  
  
M. Wu, Z. Li, T. Caoand S. G. Louie, “Physical origin of giant excitonic and magneto-optical responses in two-dimensional ferromagnetic insulators”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, May 30, 2019. doi: 10.1038/s41467-019-10325-7.  
  
C.-K. Yong, “Valley-dependent exciton fine structure and Autler–Townes doublets from Berry phases in monolayer MoSe2”, *Nature Materials*, vol. 18, no. 10. Springer Science and Business Media LLC, pp. 1065–1070, Aug. 05, 2019. doi: 10.1038/s41563-019-0447-8.  
  
G. Antonius, D. Y. Qiuand S. G. Louie, “Orbital Symmetry and the Optical Response of Single-Layer MX Monochalcogenides”, *Nano Letters*, vol. 18, no. 3. American Chemical Society (ACS), pp. 1925–1929, Feb. 21, 2018. doi: 10.1021/acs.nanolett.7b05286.  
  
C. Bronner, “Hierarchical On-Surface Synthesis of Graphene Nanoribbon Heterojunctions”, *ACS Nano*, vol. 12, no. 3. American Chemical Society (ACS), pp. 2193–2200, Jan. 30, 2018. doi: 10.1021/acsnano.7b08658.  
  
T. Cao, M. Wuand S. G. Louie, “Unifying Optical Selection Rules for Excitons in Two Dimensions: Band Topology and Winding Numbers”, *Physical Review Letters*, vol. 120, no. 8. American Physical Society (APS), Feb. 23, 2018. doi: 10.1103/physrevlett.120.087402.  
  
T. Cao, F. Zhaoand S. G. Louie, “Topological Phases in Graphene Nanoribbons: Junction States, Spin Centers, and Quantum Spin Chains”, *Physical Review Letters*, vol. 119, no. 7. American Physical Society (APS), Aug. 16, 2017. doi: 10.1103/physrevlett.119.076401.  
  
R. A. Durr, “Orbitally Matched Edge-Doping in Graphene Nanoribbons”, *Journal of the American Chemical Society*, vol. 140, no. 2. American Chemical Society (ACS), pp. 807–813, Jan. 02, 2018. doi: 10.1021/jacs.7b11886.  
  
K. Gotlieb, “Symmetry rules shaping spin-orbital textures in surface states”, *Physical Review B*, vol. 95, no. 24. American Physical Society (APS), Jun. 30, 2017. doi: 10.1103/physrevb.95.245142.  
  
Y. Li, “Ultrasensitive tunability of the direct bandgap of 2D InSe flakes via strain engineering”, *2D Materials*, vol. 5, no. 2. IOP Publishing, p. 021002, Jan. 29, 2018. doi: 10.1088/2053-1583/aaa6eb.  
  
G. D. Nguyen, “Atomically precise graphene nanoribbon heterojunctions from a single molecular precursor”, *Nature Nanotechnology*, vol. 12, no. 11. Springer Science and Business Media LLC, pp. 1077–1082, Sep. 25, 2017. doi: 10.1038/nnano.2017.155.  
  
C. S. Ong, S. Coh, M. L. Cohenand S. G. Louie, “Real-space study of the optical absorption in alternative phases of silicon”, *Physical Review Materials*, vol. 1, no. 7. American Physical Society (APS), Dec. 27, 2017. doi: 10.1103/physrevmaterials.1.075408.  
  
D. Y. Qiu, F. H. da Jornadaand S. G. Louie, “Environmental Screening Effects in 2D Materials: Renormalization of the Bandgap, Electronic Structure, and Optical Spectra of Few-Layer Black Phosphorus”, *Nano Letters*, vol. 17, no. 8. American Chemical Society (ACS), pp. 4706–4712, Jul. 05, 2017. doi: 10.1021/acs.nanolett.7b01365.  
  
A. Yan, “Dynamics of Symmetry-Breaking Stacking Boundaries in Bilayer MoS2”, *The Journal of Physical Chemistry C*, vol. 121, no. 40. American Chemical Society (ACS), pp. 22559–22566, Sep. 29, 2017. doi: 10.1021/acs.jpcc.7b08398.  
  
X.-X. Zhang, “Magnetic brightening and control of dark excitons in monolayer WSe2”, *Nature Nanotechnology*, vol. 12, no. 9. Springer Science and Business Media LLC, pp. 883–888, Jun. 26, 2017. doi: 10.1038/nnano.2017.105.  
  
J. Bankert, J. H. Krolikand J. Shi, “STRUCTURE OF RETROGRADE CIRCUMBINARY ACCRETION DISKS”, *The Astrophysical Journal*, vol. 801, no. 2. American Astronomical Society, p. 114, Mar. 12, 2015. doi: 10.1088/0004-637x/801/2/114.  
  
J. F. Hawley, C. Fendt, M. Hardcastle, E. Nokhrinaand A. Tchekhovskoy, “Disks and Jets”, *Space Science Reviews*, vol. 191, no. 1–4. Springer Science and Business Media LLC, pp. 441–469, Jun. 19, 2015. doi: 10.1007/s11214-015-0174-7.  
  
J. F. Hawley, X. Guanand J. H. Krolik, “ASSESSING QUANTITATIVE RESULTS IN ACCRETION SIMULATIONS: FROM LOCAL TO GLOBAL”, *The Astrophysical Journal*, vol. 738, no. 1. American Astronomical Society, p. 84, Aug. 16, 2011. doi: 10.1088/0004-637x/738/1/84.  
  
J. H. Krolik and J. F. Hawley, “A STEADY-STATE ALIGNMENT FRONT IN AN ACCRETION DISK SUBJECTED TO LENSE–THIRRING TORQUES”, *The Astrophysical Journal*, vol. 806, no. 1. American Astronomical Society, p. 141, Jun. 12, 2015. doi: 10.1088/0004-637x/806/1/141.  
  
J. H. Krolik, K. Sorathiaand J. F. Hawley, “Alignment physics of disks warped by Lense–Thirring precession”, *Classical and Quantum Gravity*, vol. 31, no. 24. IOP Publishing, p. 244004, Dec. 01, 2014. doi: 10.1088/0264-9381/31/24/244004.  
  
J.-M. Shi and J. H. Krolik, “THREE-DIMENSIONAL MHD SIMULATION OF CIRCUMBINARY ACCRETION DISKS. II. NET ACCRETION RATE”, *The Astrophysical Journal*, vol. 807, no. 2. American Astronomical Society, p. 131, Jul. 07, 2015. doi: 10.1088/0004-637x/807/2/131.  
  
H. Shiokawa, J. H. Krolik, R. M. Cheng, T. Piranand S. C. Noble, “GENERAL RELATIVISTIC HYDRODYNAMIC SIMULATION OF ACCRETION FLOW FROM A STELLAR TIDAL DISRUPTION”, *The Astrophysical Journal*, vol. 804, no. 2. American Astronomical Society, p. 85, May 05, 2015. doi: 10.1088/0004-637x/804/2/85.  
  
J. B. Simon, J. F. Hawleyand K. Beckwith, “RESISTIVITY-DRIVEN STATE CHANGES IN VERTICALLY STRATIFIED ACCRETION DISKS”, *The Astrophysical Journal*, vol. 730, no. 2. American Astronomical Society, p. 94, Mar. 09, 2011. doi: 10.1088/0004-637x/730/2/94.  
  
S. Chen, “Precipitation Spectra Analysis Over China With High-Resolution Measurements From Optimally-Merged Satellite/Gauge Observations—Part II: Diurnal Variability Analysis”, *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 9, no. 7. Institute of Electrical and Electronics Engineers (IEEE), pp. 2979–2988, Jul. 2016. doi: 10.1109/jstars.2016.2529001.  
  
S. Chen, “Mapping the Precipitation Type Distribution Over the Contiguous United States Using NOAA/NSSL National Multi-Sensor Mosaic QPE”, *IEEE Transactions on Geoscience and Remote Sensing*, vol. 53, no. 8. Institute of Electrical and Electronics Engineers (IEEE), pp. 4434–4443, Aug. 2015. doi: 10.1109/tgrs.2015.2399015.  
  
R. Cintineo, J. A. Otkin, M. Xueand F. Kong, “Evaluating the Performance of Planetary Boundary Layer and Cloud Microphysical Parameterization Schemes in Convection-Permitting Ensemble Forecasts Using Synthetic GOES-13 Satellite Observations”, *Monthly Weather Review*, vol. 142, no. 1. American Meteorological Society, pp. 163–182, Jan. 01, 2014. doi: 10.1175/mwr-d-13-00143.1.  
  
A. J. Clark, R. G. Bullock, T. L. Jensen, M. Xueand F. Kong, “Application of Object-Based Time-Domain Diagnostics for Tracking Precipitation Systems in Convection-Allowing Models”, *Weather and Forecasting*, vol. 29, no. 3. American Meteorological Society, pp. 517–542, Jun. 01, 2014. doi: 10.1175/waf-d-13-00098.1.  
  
A. J. Clark, M. C. Coniglio, B. E. Coffer, G. Thompson, M. Xueand F. Kong, “Sensitivity of 24-h Forecast Dryline Position and Structure to Boundary Layer Parameterizations in Convection-Allowing WRF Model Simulations”, *Weather and Forecasting*, vol. 30, no. 3. American Meteorological Society, pp. 613–638, Jun. 01, 2015. doi: 10.1175/waf-d-14-00078.1.  
  
A. J. Clark, “Tornado Pathlength Forecasts from 2010 to 2011 Using Ensemble Updraft Helicity”, *Weather and Forecasting*, vol. 28, no. 2. American Meteorological Society, pp. 387–407, Apr. 01, 2013. doi: 10.1175/waf-d-12-00038.1.  
  
D. T. Dawson II, M. Xue, J. A. Milbrandtand A. Shapiro, “Sensitivity of Real-Data Simulations of the 3 May 1999 Oklahoma City Tornadic Supercell and Associated Tornadoes to Multimoment Microphysics. Part I: Storm- and Tornado-Scale Numerical Forecasts”, *Monthly Weather Review*, vol. 143, no. 6. American Meteorological Society, pp. 2241–2265, May 28, 2015. doi: 10.1175/mwr-d-14-00279.1.  
  
D. T. Dawson II, M. Xue, A. Shapiro, J. A. Milbrandtand A. D. Schenkman, “Sensitivity of Real-Data Simulations of the 3 May 1999 Oklahoma City Tornadic Supercell and Associated Tornadoes to Multimoment Microphysics. Part II: Analysis of Buoyancy and Dynamic Pressure Forces in Simulated Tornado-Like Vortices”, *Journal of the Atmospheric Sciences*, vol. 73, no. 3. American Meteorological Society, pp. 1039–1061, Feb. 09, 2016. doi: 10.1175/jas-d-15-0114.1.  
  
D. Doughty, J. D. Fuentes, R. Sakai, X.-M. Huand K. Sanchez, “Nocturnal isoprene declines in a semi-urban environment”, *Journal of Atmospheric Chemistry*, vol. 72, no. 3–4. Springer Science and Business Media LLC, pp. 215–234, Feb. 16, 2013. doi: 10.1007/s10874-012-9247-0.  
  
J. D. Duda, X. Wang, F. Kongand M. Xue, “Using Varied Microphysics to Account for Uncertainty in Warm-Season QPF in a Convection-Allowing Ensemble”, *Monthly Weather Review*, vol. 142, no. 6. American Meteorological Society, pp. 2198–2219, May 28, 2014. doi: 10.1175/mwr-d-13-00297.1.  
  
G. Ge, J. Gaoand M. Xue, “Impacts of Assimilating Measurements of Different State Variables with a Simulated Supercell Storm and Three-Dimensional Variational Method”, *Monthly Weather Review*, vol. 141, no. 8. American Meteorological Society, pp. 2759–2777, Jul. 25, 2013. doi: 10.1175/mwr-d-12-00193.1.  
  
J. D. Hall, M. Xue, L. Ranand L. M. Leslie, “High-Resolution Modeling of Typhoon Morakot (2009): Vortex Rossby Waves and Their Role in Extreme Precipitation over Taiwan”, *Journal of the Atmospheric Sciences*, vol. 70, no. 1. American Meteorological Society, pp. 163–186, Jan. 01, 2013. doi: 10.1175/jas-d-11-0338.1.  
  
J. Hardy, J. J. Gourley, P.-E. Kirstetter, Y. Hong, F. Kongand Z. L. Flamig, “A method for probabilistic flash flood forecasting”, *Journal of Hydrology*, vol. 541. Elsevier BV, pp. 480–494, Oct. 2016. doi: 10.1016/j.jhydrol.2016.04.007.  
  
X.-M. Hu, J. D. Fuentes, D. Tooheyand D. Wang, “Chemical processing within and above a loblolly pine forest in North Carolina, USA”, *Journal of Atmospheric Chemistry*, vol. 72, no. 3–4. Springer Science and Business Media LLC, pp. 235–259, Nov. 17, 2013. doi: 10.1007/s10874-013-9276-3.  
  
X.-M. Hu, P. M. Kleinand M. Xue, “Evaluation of the updated YSU planetary boundary layer scheme within WRF for wind resource and air quality assessments”, *Journal of Geophysical Research: Atmospheres*, vol. 118, no. 18. American Geophysical Union (AGU), pp. 10, 490–10, 505, Sep. 24, 2013. doi: 10.1002/jgrd.50823.  
  
X.-M. Hu, P. M. Klein, M. Xue, A. Shapiroand A. Nallapareddy, “Enhanced vertical mixing associated with a nocturnal cold front passage and its impact on near-surface temperature and ozone concentration”, *Journal of Geophysical Research: Atmospheres*, vol. 118, no. 7. American Geophysical Union (AGU), pp. 2714–2728, Apr. 03, 2013. doi: 10.1002/jgrd.50309.  
  
X.-M. Hu, “Impact of the vertical mixing induced by low-level jets on boundary layer ozone concentration”, *Atmospheric Environment*, vol. 70. Elsevier BV, pp. 123–130, May 2013. doi: 10.1016/j.atmosenv.2012.12.046.  
  
X.-M. Hu, X. Li, M. Xue, D. Wuand J. D. Fuentes, “The Formation of Barrier Winds East of the Loess Plateau and Their Effects on Dispersion Conditions in the North China Plains”, *Boundary-Layer Meteorology*, vol. 161, no. 1. Springer Science and Business Media LLC, pp. 145–163, Apr. 18, 2016. doi: 10.1007/s10546-016-0159-4.  
  
X.-M. Hu, “Impact of the Loess Plateau on the atmospheric boundary layer structure and air quality in the North China Plain: A case study”, *Science of The Total Environment*, vol. 499. Elsevier BV, pp. 228–237, Nov. 2014. doi: 10.1016/j.scitotenv.2014.08.053.  
  
X.-M. Hu, “Impact of the Loess Plateau on the atmospheric boundary layer structure and air quality in the North China Plain: A case study”, *Science of The Total Environment*, vol. 499. Elsevier BV, pp. 228–237, Nov. 2014. doi: 10.1016/j.scitotenv.2014.08.053.  
  
X.-M. Hu and M. Xue, “Influence of Synoptic Sea-Breeze Fronts on the Urban Heat Island Intensity in Dallas–Fort Worth, Texas”, *Monthly Weather Review*, vol. 144, no. 4. American Meteorological Society, pp. 1487–1507, Mar. 29, 2016. doi: 10.1175/mwr-d-15-0201.1.  
  
X.-M. Hu, M. Xue, P. M. Klein, B. G. Illstonand S. Chen, “Analysis of Urban Effects in Oklahoma City using a Dense Surface Observing Network”, *Journal of Applied Meteorology and Climatology*, vol. 55, no. 3. American Meteorological Society, pp. 723–741, Mar. 2016. doi: 10.1175/jamc-d-15-0206.1.  
  
E. R. Iyer, A. J. Clark, M. Xueand F. Kong, “A Comparison of 36–60-h Precipitation Forecasts from Convection-Allowing and Convection-Parameterizing Ensembles”, *Weather and Forecasting*, vol. 31, no. 2. American Meteorological Society, pp. 647–661, Apr. 01, 2016. doi: 10.1175/waf-d-15-0143.1.  
  
A. Johnson and X. Wang, “Object-Based Evaluation of a Storm-Scale Ensemble during the 2009 NOAA Hazardous Weather Testbed Spring Experiment”, *Monthly Weather Review*, vol. 141, no. 3. American Meteorological Society, pp. 1079–1098, Mar. 01, 2012. doi: 10.1175/mwr-d-12-00140.1.  
  
A. Johnson, X. Wang, F. Kongand M. Xue, “Object-Based Evaluation of the Impact of Horizontal Grid Spacing on Convection-Allowing Forecasts”, *Monthly Weather Review*, vol. 141, no. 10. American Meteorological Society, pp. 3413–3425, Sep. 25, 2013. doi: 10.1175/mwr-d-13-00027.1.  
  
P. M. Klein, X.-M. Huand M. Xue, “Impacts of Mixing Processes in Nocturnal Atmospheric Boundary Layer on Urban Ozone Concentrations”, *Boundary-Layer Meteorology*, vol. 150, no. 1. Springer Science and Business Media LLC, pp. 107–130, Oct. 04, 2013. doi: 10.1007/s10546-013-9864-4.  
  
J. Labriola, N. Snook, Y. Jung, B. Putnamand M. Xue, “Ensemble Hail Prediction for the Storms of 10 May 2010 in South-Central Oklahoma Using Single- and Double-Moment Microphysical Schemes”, *Monthly Weather Review*, vol. 145, no. 12. American Meteorological Society, pp. 4911–4936, Dec. 2017. doi: 10.1175/mwr-d-17-0039.1.  
  
J. Labriola, N. Snook, Y. Jungand M. Xue, “Explicit Ensemble Prediction of Hail in 19 May 2013 Oklahoma City Thunderstorms and Analysis of Hail Growth Processes with Several Multimoment Microphysics Schemes”, *Monthly Weather Review*, vol. 147, no. 4. American Meteorological Society, pp. 1193–1213, Mar. 25, 2019. doi: 10.1175/mwr-d-18-0266.1.  
  
J. Labriola, N. Snook, M. Xueand K. W. Thomas, “Forecasting the 8 May 2017 Severe Hail Storm in Denver, Colorado, at a Convection-Allowing Resolution: Understanding Rimed Ice Treatments in Multimoment Microphysics Schemes and Their Effects on Hail Size Forecasts”, *Monthly Weather Review*, vol. 147, no. 8. American Meteorological Society, pp. 3045–3068, Aug. 01, 2019. doi: 10.1175/mwr-d-18-0319.1.  
  
Y. Ma, Y. Yang, X.-M. Huand R. Gan, “Characteristics and mechanisms of the sudden warming events in the nocturnal atmospheric boundary layer: A case study using WRF”, *Journal of Meteorological Research*, vol. 29, no. 5. Springer Science and Business Media LLC, pp. 747–763, Oct. 2015. doi: 10.1007/s13351-015-4101-3.  
  
Y. Miao, “Seasonal variation of local atmospheric circulations and boundary layer structure in the Beijing-Tianjin-Hebei region and implications for air quality”, *Journal of Advances in Modeling Earth Systems*, vol. 7, no. 4. American Geophysical Union (AGU), pp. 1602–1626, Oct. 26, 2015. doi: 10.1002/2015ms000522.  
  
Oliveira, Xue, Roberts, Wickerand Yussouf, “Horizontal Vortex Tubes near a Simulated Tornado: Three-Dimensional Structure and Kinematics”, *Atmosphere*, vol. 10, no. 11. MDPI AG, p. 716, Nov. 16, 2019. doi: 10.3390/atmos10110716.  
  
B. J. Putnam, M. Xue, Y. Jung, N. Snookand G. Zhang, “The Analysis and Prediction of Microphysical States and Polarimetric Radar Variables in a Mesoscale Convective System Using Double-Moment Microphysics, Multinetwork Radar Data, and the Ensemble Kalman Filter”, *Monthly Weather Review*, vol. 142, no. 1. American Meteorological Society, pp. 141–162, Jan. 01, 2014. doi: 10.1175/mwr-d-13-00042.1.  
  
B. J. Putnam, M. Xue, Y. Jung, N. Snookand G. Zhang, “The Analysis and Prediction of Microphysical States and Polarimetric Radar Variables in a Mesoscale Convective System Using Double-Moment Microphysics, Multinetwork Radar Data, and the Ensemble Kalman Filter”, *Monthly Weather Review*, vol. 142, no. 1. American Meteorological Society, pp. 141–162, Jan. 01, 2014. doi: 10.1175/mwr-d-13-00042.1.  
  
Y. Qi, J. Zhang, Q. Cao, Y. Hongand X.-M. Hu, “Correction of Radar QPE Errors for Nonuniform VPRs in Mesoscale Convective Systems Using TRMM Observations”, *Journal of Hydrometeorology*, vol. 14, no. 5. American Meteorological Society, pp. 1672–1682, Oct. 01, 2013. doi: 10.1175/jhm-d-12-0165.1.  
  
A. D. Schenkman, M. Xueand D. T. Dawson II, “The Cause of Internal Outflow Surges in a High-Resolution Simulation of the 8 May 2003 Oklahoma City Tornadic Supercell”, *Journal of the Atmospheric Sciences*, vol. 73, no. 1. American Meteorological Society, pp. 353–370, Dec. 30, 2015. doi: 10.1175/jas-d-15-0112.1.  
  
A. D. Schenkman, M. Xueand M. Hu, “Tornadogenesis in a High-Resolution Simulation of the 8 May 2003 Oklahoma City Supercell”, *Journal of the Atmospheric Sciences*, vol. 71, no. 1. American Meteorological Society, pp. 130–154, Dec. 27, 2013. doi: 10.1175/jas-d-13-073.1.  
  
N. Snook, Y. Jung, J. Brotzge, B. Putnamand M. Xue, “Prediction and Ensemble Forecast Verification of Hail in the Supercell Storms of 20 May 2013”, *Weather and Forecasting*, vol. 31, no. 3. American Meteorological Society, pp. 811–825, May 20, 2016. doi: 10.1175/waf-d-15-0152.1.  
  
N. Snook, F. Kong, A. Clark, B. Roberts, K. A. Brewsterand M. Xue, “Comparison and Verification of Point‐Wise and Patch‐Wise Localized Probability‐Matched Mean Algorithms for Ensemble Consensus Precipitation Forecasts”, *Geophysical Research Letters*, vol. 47, no. 12. American Geophysical Union (AGU), Jun. 24, 2020. doi: 10.1029/2020gl087839.  
  
N. Snook, M. Xueand Y. Jung, “Multiscale EnKF Assimilation of Radar and Conventional Observations and Ensemble Forecasting for a Tornadic Mesoscale Convective System”, *Monthly Weather Review*, vol. 143, no. 4. American Meteorological Society, pp. 1035–1057, Mar. 31, 2015. doi: 10.1175/mwr-d-13-00262.1.  
  
D. R. Stratman, M. C. Coniglio, S. E. Kochand M. Xue, “Use of Multiple Verification Methods to Evaluate Forecasts of Convection from Hot- and Cold-Start Convection-Allowing Models”, *Weather and Forecasting*, vol. 28, no. 1. American Meteorological Society, pp. 119–138, Feb. 01, 2013. doi: 10.1175/waf-d-12-00022.1.  
  
T. A. Supinie, N. Yussouf, Y. Jung, M. Xue, J. Chengand S. Wang, “Comparison of the Analyses and Forecasts of a Tornadic Supercell Storm from Assimilating Phased-Array Radar and WSR-88D Observations”, *Weather and Forecasting*, vol. 32, no. 4. American Meteorological Society, pp. 1379–1401, Jul. 03, 2017. doi: 10.1175/waf-d-16-0159.1.  
  
A. Tiwary, A. Namdeo, J. Fuentes, A. Dore, X.-M. Huand M. Bell, “Systems scale assessment of the sustainability implications of emerging green initiatives”, *Environmental Pollution*, vol. 183. Elsevier BV, pp. 213–223, Dec. 2013. doi: 10.1016/j.envpol.2013.03.049.  
  
C. E. Wainwright, D. T. Dawson, M. Xueand G. Zhang, “Diagnosing the Intercept Parameters of the Exponential Drop Size Distributions in a Single-Moment Microphysics Scheme and Impact on Supercell Storm Simulations”, *Journal of Applied Meteorology and Climatology*, vol. 53, no. 8. American Meteorological Society, pp. 2072–2090, Aug. 2014. doi: 10.1175/jamc-d-13-0251.1.  
  
M. Xue, M. Huand A. D. Schenkman, “Numerical Prediction of the 8 May 2003 Oklahoma City Tornadic Supercell and Embedded Tornado Using ARPS with the Assimilation of WSR-88D Data”, *Weather and Forecasting*, vol. 29, no. 1. American Meteorological Society, pp. 39–62, Feb. 01, 2014. doi: 10.1175/waf-d-13-00029.1.  
  
M. Xue, “Prediction of Convective Storms at Convection-Resolving 1 km Resolution over Continental United States with Radar Data Assimilation: An Example Case of 26 May 2008 and Precipitation Forecasts from Spring 2009”, *Advances in Meteorology*, vol. 2013. Hindawi Limited, pp. 1–9, 2013. doi: 10.1155/2013/259052.  
  
M. Xue, X. Luo, K. Zhu, Z. Sunand J. Fei, “The Controlling Role of Boundary Layer Inertial Oscillations in Meiyu Frontal Precipitation and Its Diurnal Cycles Over China”, *Journal of Geophysical Research: Atmospheres*, vol. 123, no. 10. American Geophysical Union (AGU), pp. 5090–5115, May 24, 2018. doi: 10.1029/2018jd028368.  
  
M. Xue, X. Luo, K. Zhu, Z. Sunand J. Fei, “The Controlling Role of Boundary Layer Inertial Oscillations in Meiyu Frontal Precipitation and Its Diurnal Cycles Over China”, *Journal of Geophysical Research: Atmospheres*, vol. 123, no. 10. American Geophysical Union (AGU), pp. 5090–5115, May 24, 2018. doi: 10.1029/2018jd028368.  
  
M. Xue, J. Schleif, F. Kong, K. W. Thomas, Y. Wangand K. Zhu, “Track and Intensity Forecasting of Hurricanes: Impact of Convection-Permitting Resolution and Global Ensemble Kalman Filter Analysis on 2010 Atlantic Season Forecasts”, *Weather and Forecasting*, vol. 28, no. 6. American Meteorological Society, pp. 1366–1384, Dec. 01, 2013. doi: 10.1175/waf-d-12-00063.1.  
  
H. Zhang, Y. Wang, J. Hu, Q. Yingand X.-M. Hu, “Relationships between meteorological parameters and criteria air pollutants in three megacities in China”, *Environmental Research*, vol. 140. Elsevier BV, pp. 242–254, Jul. 2015. doi: 10.1016/j.envres.2015.04.004.  
  
M. Zhang, Y. Qiand X.-M. Hu, “Impact of East Asian winter monsoon on the Pacific storm track”, *Meteorological Applications*, vol. 21, no. 4. Wiley, pp. 873–878, Aug. 02, 2013. doi: 10.1002/met.1423.  
  
E. D. Loken, A. J. Clark, M. Xueand F. Kong, “Comparison of Next-Day Probabilistic Severe Weather Forecasts from Coarse- and Fine-Resolution CAMs and a Convection-Allowing Ensemble”, *Weather and Forecasting*, vol. 32, no. 4. American Meteorological Society, pp. 1403–1421, Jul. 03, 2017. doi: 10.1175/waf-d-16-0200.1.  
  
V. N. Mahale, G. Zhangand M. Xue, “Characterization of the 14 June 2011 Norman, Oklahoma, Downburst through Dual-Polarization Radar Observations and Hydrometeor Classification”, *Journal of Applied Meteorology and Climatology*, vol. 55, no. 12. American Meteorological Society, pp. 2635–2655, Dec. 2016. doi: 10.1175/jamc-d-16-0062.1.  
  
B. J. Putnam, M. Xue, Y. Jung, N. A. Snookand G. Zhang, “Ensemble Probabilistic Prediction of a Mesoscale Convective System and Associated Polarimetric Radar Variables Using Single-Moment and Double-Moment Microphysics Schemes and EnKF Radar Data Assimilation”, *Monthly Weather Review*, vol. 145, no. 6. American Meteorological Society, pp. 2257–2279, May 22, 2017. doi: 10.1175/mwr-d-16-0162.1.  
  
J. C. Snyder, H. B. Bluestein, D. T. Dawson IIand Y. Jung, “Simulations of Polarimetric, X-Band Radar Signatures in Supercells. Part II: ZDR Columns and Rings and KDP Columns”, *Journal of Applied Meteorology and Climatology*, vol. 56, no. 7. American Meteorological Society, pp. 2001–2026, Jul. 2017. doi: 10.1175/jamc-d-16-0139.1.  
  
J. C. Snyder, H. B. Bluestein, D. T. Dawson IIand Y. Jung, “Simulations of Polarimetric, X-Band Radar Signatures in Supercells. Part I: Description of Experiment and Simulated ρhv Rings”, *Journal of Applied Meteorology and Climatology*, vol. 56, no. 7. American Meteorological Society, pp. 1977–1999, Jul. 2017. doi: 10.1175/jamc-d-16-0138.1.  
  
D. J. Stensrud, “Progress and challenges with Warn-on-Forecast”, *Atmospheric Research*, vol. 123. Elsevier BV, pp. 2–16, Apr. 2013. doi: 10.1016/j.atmosres.2012.04.004.  
  
P. Greene, J. Eldredge, X. Zhongand J. Kim, “Numerical Study of Hypersonic Flow Over an Isolated Roughness with a High-Order Cut-Cell Method”, *41st AIAA Fluid Dynamics Conference and Exhibit*. American Institute of Aeronautics and Astronautics, Jun. 14, 2011. doi: 10.2514/6.2011-3249.  
  
P. T. Greene, J. Eldredge, X. Zhongand J. Kim, “Numerical Simulation of High-Speed Flows Over Complex Geometries with a High-Order Multi-Zone Cut-Cell Method”, *52nd Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 10, 2014. doi: 10.2514/6.2014-0426.  
  
P. T. Greene, J. D. Eldredge, X. Zhongand J. Kim, “A high-order multi-zone cut-stencil method for numerical simulations of high-speed flows over complex geometries”, *Journal of Computational Physics*, vol. 316. Elsevier BV, pp. 652–681, Jul. 2016. doi: 10.1016/j.jcp.2016.04.032.  
  
T. Jung, H. Choiand J. Kim, “Effects of the air layer of an idealized superhydrophobic surface on the slip length and skin-friction drag”, *Journal of Fluid Mechanics*, vol. 790. Cambridge University Press (CUP), Feb. 01, 2016. doi: 10.1017/jfm.2016.36.  
  
E. Kim, H. Choiand J. Kim, “Optimal disturbances in the near-wall region of turbulent channel flows”, *Physical Review Fluids*, vol. 1, no. 7. American Physical Society (APS), Nov. 17, 2016. doi: 10.1103/physrevfluids.1.074403.  
  
J. Kim, “Physics and control of wall turbulence for drag reduction”, *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 369, no. 1940. The Royal Society, pp. 1396–1411, Apr. 13, 2011. doi: 10.1098/rsta.2010.0360.  
  
M. Lagha, J. Kim, J. D. Eldredgeand X. Zhong, “A numerical study of compressible turbulent boundary layers”, *Physics of Fluids*, vol. 23, no. 1. AIP Publishing, p. 015106, Jan. 2011. doi: 10.1063/1.3541841.  
  
M. Lagha, J. Kim, J. D. Eldredgeand X. Zhong, “Near-wall dynamics of compressible boundary layers”, *Physics of Fluids*, vol. 23, no. 6. AIP Publishing, p. 065109, Jun. 2011. doi: 10.1063/1.3600659.  
  
H. Park, H. Parkand J. Kim, “A numerical study of the effects of superhydrophobic surface on skin-friction drag in turbulent channel flow”, *Physics of Fluids*, vol. 25, no. 11. AIP Publishing, p. 110815, Nov. 2013. doi: 10.1063/1.4819144.  
  
C. Y. Hu and D. Caballero, “Long-Range Correlation in Positron-Hydrogen Scattering System near the Threshold of &lt;i&gt;Ps&lt;/i&gt;(&lt;i&gt;n&lt;/i&gt; = 2) Formation”, *Journal of Modern Physics*, vol. 4, no. 5. Scientific Research Publishing, Inc., pp. 622–627, 2013. doi: 10.4236/jmp.2013.45090.  
  
L. Astudillo, “The Small Molecule IMR-1 Inhibits the Notch Transcriptional Activation Complex to Suppress Tumorigenesis”, *Cancer Research*, vol. 76, no. 12. American Association for Cancer Research (AACR), pp. 3593–3603, Jun. 14, 2016. doi: 10.1158/0008-5472.can-16-0061.  
  
S. M. Baliban, “Development of a glycoconjugate vaccine to prevent invasive Salmonella Typhimurium infections in sub-Saharan Africa”, *PLOS Neglected Tropical Diseases*, vol. 11, no. 4. Public Library of Science (PLoS), p. e0005493, Apr. 07, 2017. doi: 10.1371/journal.pntd.0005493.  
  
M. G. Cardenas, E. Oswald, W. Yu, F. Xue, A. D. MacKerell Jrand A. M. Melnick, “The Expanding Role of the BCL6 Oncoprotein as a Cancer Therapeutic Target”, *Clinical Cancer Research*, vol. 23, no. 4. American Association for Cancer Research (AACR), pp. 885–893, Feb. 14, 2017. doi: 10.1158/1078-0432.ccr-16-2071.  
  
M. G. Cardenas, “Rationally designed BCL6 inhibitors target activated B cell diffuse large B cell lymphoma”, *Journal of Clinical Investigation*, vol. 126, no. 9. American Society for Clinical Investigation, pp. 3351–3362, Aug. 02, 2016. doi: 10.1172/jci85795.  
  
M. C. Cavalier, “Small Molecule Inhibitors of Ca2+-S100B Reveal Two Protein Conformations”, *Journal of Medicinal Chemistry*, vol. 59, no. 2. American Chemical Society (ACS), pp. 592–608, Jan. 13, 2016. doi: 10.1021/acs.jmedchem.5b01369.  
  
M. C. Cavalier, “Novel protein–inhibitor interactions in site 3 of Ca2+-bound S100B as discovered by X-ray crystallography”, *Acta Crystallographica Section D Structural Biology*, vol. 72, no. 6. International Union of Crystallography (IUCr), pp. 753–760, May 25, 2016. doi: 10.1107/s2059798316005532.  
  
J. Chauhan, “Towards Development of Small Molecule Lipid II Inhibitors as Novel Antibiotics”, *PLOS ONE*, vol. 11, no. 10. Public Library of Science (PLoS), p. e0164515, Oct. 24, 2016. doi: 10.1371/journal.pone.0164515.  
  
I. Glassford, “Ribosome-Templated Azide–Alkyne Cycloadditions: Synthesis of Potent Macrolide Antibiotics by In Situ Click Chemistry”, *Journal of the American Chemical Society*, vol. 138, no. 9. American Chemical Society (ACS), pp. 3136–3144, Feb. 26, 2016. doi: 10.1021/jacs.5b13008.  
  
H. Goel, W. Yu, V. D. Ustach, A. H. Aytenfisu, D. Sunand A. D. MacKerell, “Impact of electronic polarizability on protein-functional group interactions”, *Physical Chemistry Chemical Physics*, vol. 22, no. 13. Royal Society of Chemistry (RSC), pp. 6848–6860, 2020. doi: 10.1039/d0cp00088d.  
  
G. A. Heinzl, “Iminoguanidines as Allosteric Inhibitors of the Iron-Regulated Heme Oxygenase (HemO) of *Pseudomonas aeruginosa*”, *Journal of Medicinal Chemistry*, vol. 59, no. 14. American Chemical Society (ACS), pp. 6929–6942, Jul. 11, 2016. doi: 10.1021/acs.jmedchem.6b00757.  
  
J. Huang, P. E. M. Lopes, B. Rouxand A. D. MacKerell Jr., “Recent Advances in Polarizable Force Fields for Macromolecules: Microsecond Simulations of Proteins Using the Classical Drude Oscillator Model”, *The Journal of Physical Chemistry Letters*, vol. 5, no. 18. American Chemical Society (ACS), pp. 3144–3150, Sep. 02, 2014. doi: 10.1021/jz501315h.  
  
J. Huang and A. D. MacKerell Jr, “CHARMM36 all-atom additive protein force field: Validation based on comparison to NMR data”, *Journal of Computational Chemistry*, vol. 34, no. 25. Wiley, pp. 2135–2145, Jul. 06, 2013. doi: 10.1002/jcc.23354.  
  
J. Huang and A. D. MacKerell Jr., “Induction of Peptide Bond Dipoles Drives Cooperative Helix Formation in the (AAQAA)3 Peptide”, *Biophysical Journal*, vol. 107, no. 4. Elsevier BV, pp. 991–997, Aug. 2014. doi: 10.1016/j.bpj.2014.06.038.  
  
J. Huang, “CHARMM36m: an improved force field for folded and intrinsically disordered proteins”, *Nature Methods*, vol. 14, no. 1. Springer Science and Business Media LLC, pp. 71–73, Nov. 07, 2016. doi: 10.1038/nmeth.4067.  
  
A. A. Kognole and A. D. MacKerell Jr., “Mg2+ Impacts the Twister Ribozyme through Push-Pull Stabilization of Nonsequential Phosphate Pairs”, *Biophysical Journal*, vol. 118, no. 6. Elsevier BV, pp. 1424–1437, Mar. 2020. doi: 10.1016/j.bpj.2020.01.021.  
  
A. Kumar, O. Yolukand A. D. MacKerell Jr., “FFParam: Standalone package for CHARMM additive and Drude polarizable force field parametrization of small molecules”, *Journal of Computational Chemistry*, vol. 41, no. 9. Wiley, pp. 958–970, Dec. 30, 2019. doi: 10.1002/jcc.26138.  
  
P. Kumar, “A Comparative Study of Transferable Aspherical Pseudoatom Databank and Classical Force Fields for Predicting Electrostatic Interactions in Molecular Dimers”, *Journal of Chemical Theory and Computation*, vol. 10, no. 4. American Chemical Society (ACS), pp. 1652–1664, Mar. 11, 2014. doi: 10.1021/ct4011129.  
  
S. K. Lakkaraju, J. A. Lemkul, J. Huangand A. D. MacKerell Jr., “DIRECT-ID: An automated method to identify and quantify conformational variations-application to β2-adrenergic GPCR”, *Journal of Computational Chemistry*, vol. 37, no. 4. Wiley, pp. 416–425, Nov. 12, 2015. doi: 10.1002/jcc.24231.  
  
S. K. Lakkaraju, E. P. Raman, W. Yuand A. D. MacKerell Jr., “Sampling of Organic Solutes in Aqueous and Heterogeneous Environments Using Oscillating Excess Chemical Potentials in Grand Canonical-like Monte Carlo-Molecular Dynamics Simulations”, *Journal of Chemical Theory and Computation*, vol. 10, no. 6. American Chemical Society (ACS), pp. 2281–2290, May 15, 2014. doi: 10.1021/ct500201y.  
  
M. E. Lanning, “Structure-based design of N-substituted 1-hydroxy-4-sulfamoyl-2-naphthoates as selective inhibitors of the Mcl-1 oncoprotein”, *European Journal of Medicinal Chemistry*, vol. 113. Elsevier BV, pp. 273–292, May 2016. doi: 10.1016/j.ejmech.2016.02.006.  
  
J. A. Lemkul, J. Huangand A. D. MacKerell Jr., “Induced Dipole–Dipole Interactions Influence the Unfolding Pathways of Wild-Type and Mutant Amyloid β-Peptides”, *The Journal of Physical Chemistry B*, vol. 119, no. 51. American Chemical Society (ACS), pp. 15574–15582, Dec. 15, 2015. doi: 10.1021/acs.jpcb.5b09978.  
  
J. A. Lemkul, J. Huang, B. Rouxand A. D. MacKerell Jr., “An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications”, *Chemical Reviews*, vol. 116, no. 9. American Chemical Society (ACS), pp. 4983–5013, Jan. 27, 2016. doi: 10.1021/acs.chemrev.5b00505.  
  
J. A. Lemkul, S. K. Lakkarajuand A. D. MacKerell Jr., “Characterization of Mg2+ Distributions around RNA in Solution”, *ACS Omega*, vol. 1, no. 4. American Chemical Society (ACS), pp. 680–688, Oct. 26, 2016. doi: 10.1021/acsomega.6b00241.  
  
J. A. Lemkul and A. D. MacKerell Jr., “Balancing the Interactions of Mg2+ in Aqueous Solution and with Nucleic Acid Moieties For a Polarizable Force Field Based on the Classical Drude Oscillator Model”, *The Journal of Physical Chemistry B*, vol. 120, no. 44. American Chemical Society (ACS), pp. 11436–11448, Oct. 27, 2016. doi: 10.1021/acs.jpcb.6b09262.  
  
J. A. Lemkul and A. D. MacKerell Jr., “Polarizable Force Field for DNA Based on the Classical Drude Oscillator: I. Refinement Using Quantum Mechanical Base Stacking and Conformational Energetics”, *Journal of Chemical Theory and Computation*, vol. 13, no. 5. American Chemical Society (ACS), pp. 2053–2071, Apr. 19, 2017. doi: 10.1021/acs.jctc.7b00067.  
  
J. A. Lemkul, A. Savelyevand A. D. MacKerell Jr., “Induced Polarization Influences the Fundamental Forces in DNA Base Flipping”, *The Journal of Physical Chemistry Letters*, vol. 5, no. 12. American Chemical Society (ACS), pp. 2077–2083, May 29, 2014. doi: 10.1021/jz5009517.  
  
H. Li, J. Chowdhary, L. Huang, X. He, A. D. MacKerell Jr.and B. Roux, “Drude Polarizable Force Field for Molecular Dynamics Simulations of Saturated and Unsaturated Zwitterionic Lipids”, *Journal of Chemical Theory and Computation*, vol. 13, no. 9. American Chemical Society (ACS), pp. 4535–4552, Aug. 08, 2017. doi: 10.1021/acs.jctc.7b00262.  
  
F. Lin and A. D. MacKerell Jr, “Improved Modeling of Cation‐π and Anion‐Ring Interactions Using the Drude Polarizable Empirical Force Field for Proteins”, *Journal of Computational Chemistry*, vol. 41, no. 5. Wiley, pp. 439–448, Sep. 13, 2019. doi: 10.1002/jcc.26067.  
  
T. Li, “Novel LRRK2 GTP-binding inhibitors reduced degeneration in Parkinson’s disease cell and mouse models”, *Human Molecular Genetics*, vol. 23, no. 23. Oxford University Press (OUP), pp. 6212–6222, Jul. 03, 2014. doi: 10.1093/hmg/ddu341.  
  
A. D. MacKerell Jr, S. Jo, S. K. Lakkaraju, C. Lindand W. Yu, “Identification and characterization of fragment binding sites for allosteric ligand design using the site identification by ligand competitive saturation hotspots approach (SILCS-Hotspots)”, *Biochimica et Biophysica Acta (BBA) - General Subjects*, vol. 1864, no. 4. Elsevier BV, p. 129519, Apr. 2020. doi: 10.1016/j.bbagen.2020.129519.  
  
D. S. Patel, X. Heand A. D. MacKerell Jr., “Polarizable Empirical Force Field for Hexopyranose Monosaccharides Based on the Classical Drude Oscillator”, *The Journal of Physical Chemistry B*, vol. 119, no. 3. American Chemical Society (ACS), pp. 637–652, Feb. 24, 2014. doi: 10.1021/jp412696m.  
  
D. S. Patel, R. Pendrill, S. S. Mallajosyula, G. Widmalmand A. D. MacKerell Jr., “Conformational Properties of α- or β-(1→6)-Linked Oligosaccharides: Hamiltonian Replica Exchange MD Simulations and NMR Experiments”, *The Journal of Physical Chemistry B*, vol. 118, no. 11. American Chemical Society (ACS), pp. 2851–2871, Mar. 05, 2014. doi: 10.1021/jp412051v.  
  
E. P. Raman, S. K. Lakkaraju, R. A. Dennyand A. D. MacKerell Jr, “Estimation of relative free energies of binding using pre-computed ensembles based on the single-step free energy perturbation and the site-identification by Ligand competitive saturation approaches”, *Journal of Computational Chemistry*, vol. 38, no. 15. Wiley, pp. 1238–1251, Oct. 26, 2016. doi: 10.1002/jcc.24522.  
  
A. Savelyev and A. D. MacKerell Jr., “Differential Deformability of the DNA Minor Groove and Altered BI/BII Backbone Conformational Equilibrium by the Monovalent Ions Li+, Na+, K+, and Rb+ via Water-Mediated Hydrogen Bonding”, *Journal of Chemical Theory and Computation*, vol. 11, no. 9. American Chemical Society (ACS), pp. 4473–4485, Aug. 26, 2015. doi: 10.1021/acs.jctc.5b00508.  
  
A. Savelyev and A. D. MacKerell Jr., “Balancing the Interactions of Ions, Water, and DNA in the Drude Polarizable Force Field”, *The Journal of Physical Chemistry B*, vol. 118, no. 24. American Chemical Society (ACS), pp. 6742–6757, Jun. 09, 2014. doi: 10.1021/jp503469s.  
  
A. Savelyev and A. D. MacKerell Jr., “All-atom polarizable force field for DNA based on the classical drude oscillator model”, *Journal of Computational Chemistry*, vol. 35, no. 16. Wiley, pp. 1219–1239, Apr. 18, 2014. doi: 10.1002/jcc.23611.  
  
A. Savelyev and A. D. MacKerell Jr., “Differential Impact of the Monovalent Ions Li+, Na+, K+, and Rb+ on DNA Conformational Properties”, *The Journal of Physical Chemistry Letters*, vol. 6, no. 1. American Chemical Society (ACS), pp. 212–216, Dec. 24, 2014. doi: 10.1021/jz5024543.  
  
M. C. Small, A. H. Aytenfisu, F.-Y. Lin, X. Heand A. D. MacKerell Jr., “Drude polarizable force field for aliphatic ketones and aldehydes, and their associated acyclic carbohydrates”, *Journal of Computer-Aided Molecular Design*, vol. 31, no. 4. Springer Science and Business Media LLC, pp. 349–363, Feb. 11, 2017. doi: 10.1007/s10822-017-0010-0.  
  
I. Soteras Gutiérrez, “Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligand–protein interactions”, *Bioorganic & Medicinal Chemistry*, vol. 24, no. 20. Elsevier BV, pp. 4812–4825, Oct. 2016. doi: 10.1016/j.bmc.2016.06.034.  
  
X. Sun, R. Rai, J. R. Deschamps, A. D. MacKerell Jr., A. I. Fadenand F. Xue, “Boc-protected 1-(3-oxocycloalkyl)ureas via a one-step Curtius rearrangement: mechanism and scope”, *Tetrahedron Letters*, vol. 55, no. 4. Elsevier BV, pp. 842–844, Jan. 2014. doi: 10.1016/j.tetlet.2013.12.021.  
  
S. S. Mallajosyula, K. Vanommeslaegheand A. D. MacKerell Jr., “Perturbation of Long-Range Water Dynamics as the Mechanism for the Antifreeze Activity of Antifreeze Glycoprotein”, *The Journal of Physical Chemistry B*, vol. 118, no. 40. American Chemical Society (ACS), pp. 11696–11706, Aug. 26, 2014. doi: 10.1021/jp508128d.  
  
M. Turchi, A. A. Kognole, A. Kumar, Q. Cai, G. Lianand A. D. MacKerell Jr., “Predicting Partition Coefficients of Neutral and Charged Solutes in the Mixed SLES–Fatty Acid Micellar System”, *The Journal of Physical Chemistry B*. American Chemical Society (ACS), Feb. 25, 2020. doi: 10.1021/acs.jpcb.9b11199.  
  
V. D. Ustach, S. K. Lakkaraju, S. Jo, W. Yu, W. Jiangand A. D. MacKerell Jr., “Optimization and Evaluation of Site-Identification by Ligand Competitive Saturation (SILCS) as a Tool for Target-Based Ligand Optimization”, *Journal of Chemical Information and Modeling*, vol. 59, no. 6. American Chemical Society (ACS), pp. 3018–3035, Apr. 29, 2019. doi: 10.1021/acs.jcim.9b00210.  
  
K. Vanommeslaeghe and A. D. MacKerell Jr., “CHARMM additive and polarizable force fields for biophysics and computer-aided drug design”, *Biochimica et Biophysica Acta (BBA) - General Subjects*, vol. 1850, no. 5. Elsevier BV, pp. 861–871, May 2015. doi: 10.1016/j.bbagen.2014.08.004.  
  
R. M. Venable, “CHARMM All-Atom Additive Force Field for Sphingomyelin: Elucidation of Hydrogen Bonding and of Positive Curvature”, *Biophysical Journal*, vol. 107, no. 1. Elsevier BV, pp. 134–145, Jul. 2014. doi: 10.1016/j.bpj.2014.05.034.  
  
X. Xu, “Structure of the cell-binding component of the *Clostridium difficile* binary toxin reveals a di-heptamer macromolecular assembly”, *Proceedings of the National Academy of Sciences*, vol. 117, no. 2. Proceedings of the National Academy of Sciences, pp. 1049–1058, Jan. 02, 2020. doi: 10.1073/pnas.1919490117.  
  
Y. Xu, A. D. MacKerell Jr.and L. Nilsson, “Structural effects of modified ribonucleotides and magnesium in transfer RNAs”, *Bioorganic & Medicinal Chemistry*, vol. 24, no. 20. Elsevier BV, pp. 4826–4834, Oct. 2016. doi: 10.1016/j.bmc.2016.06.037.  
  
Y. Xu, K. Vanommeslaeghe, A. Aleksandrov, A. D. MacKerell Jr.and L. Nilsson, “AdditiveCHARMMforce field for naturally occurring modified ribonucleotides”, *Journal of Computational Chemistry*, vol. 37, no. 10. Wiley, pp. 896–912, Feb. 03, 2016. doi: 10.1002/jcc.24307.  
  
M. Yang, T. Angles d’Ortoli, E. Säwén, M. Jana, G. Widmalmand A. D. MacKerell, “Delineating the conformational flexibility of trisaccharides from NMR spectroscopy experiments and computer simulations”, *Physical Chemistry Chemical Physics*, vol. 18, no. 28. Royal Society of Chemistry (RSC), pp. 18776–18794, 2016. doi: 10.1039/c6cp02970a.  
  
M. Yang, J. Huang, R. Simon, L.-X. Wangand A. D. MacKerell Jr., “Conformational Heterogeneity of the HIV Envelope Glycan Shield”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Jun. 30, 2017. doi: 10.1038/s41598-017-04532-9.  
  
M. Yang, R. Simonand A. D. MacKerell Jr., “Conformational Preference of Serogroup B *Salmonella* O Polysaccharide in Presence and Absence of the Monoclonal Antibody Se155–4”, *The Journal of Physical Chemistry B*, vol. 121, no. 15. American Chemical Society (ACS), pp. 3412–3423, Dec. 06, 2016. doi: 10.1021/acs.jpcb.6b08955.  
  
W. Yu, S. K. Lakkaraju, E. P. Ramanand A. D. MacKerell Jr., “Site-Identification by Ligand Competitive Saturation (SILCS) assisted pharmacophore modeling”, *Journal of Computer-Aided Molecular Design*, vol. 28, no. 5. Springer Science and Business Media LLC, pp. 491–507, Mar. 08, 2014. doi: 10.1007/s10822-014-9728-0.  
  
J. H. Wise, T. Abel, M. J. Turk, M. L. Normanand B. D. Smith, “The birth of a galaxy – II. The role of radiation pressure”, *Monthly Notices of the Royal Astronomical Society*, vol. 427, no. 1. Oxford University Press (OUP), pp. 311–326, Oct. 30, 2012. doi: 10.1111/j.1365-2966.2012.21809.x.  
  
H. Xu, M. L. Norman, B. W. O’Sheaand J. H. Wise, “LATE POP III STAR FORMATION DURING THE EPOCH OF REIONIZATION: RESULTS FROM THE RENAISSANCE SIMULATIONS”, *The Astrophysical Journal*, vol. 823, no. 2. American Astronomical Society, p. 140, Jun. 01, 2016. doi: 10.3847/0004-637x/823/2/140.  
  
K. Ahn, H. Xu, M. L. Norman, M. A. Alvarezand J. H. Wise, “SPATIALLY EXTENDED 21 cm SIGNAL FROM STRONGLY CLUSTERED UV AND X-RAY SOURCES IN THE EARLY UNIVERSE”, *The Astrophysical Journal*, vol. 802, no. 1. American Astronomical Society, p. 8, Mar. 13, 2015. doi: 10.1088/0004-637x/802/1/8.  
  
P. G. Garay, O. A. Martin, H. A. Scheragaand J. A. Vila, “Factors affecting the computation of the13C shielding in disaccharides”, *Journal of Computational Chemistry*, vol. 35, no. 25. Wiley, pp. 1854–1864, Jul. 28, 2014. doi: 10.1002/jcc.23697.  
  
E. I. Gołaś, C. Czaplewski, H. A. Scheragaand A. Liwo, “Common functionally important motions of the nucleotide‐binding domain of H sp70”, *Proteins: Structure, Function, and Bioinformatics*, vol. 83, no. 2. Wiley, pp. 282–299, Dec. 18, 2014. doi: 10.1002/prot.24731.  
  
K. Kachlishvili, G. G. Maisuradze, O. A. Martin, A. Liwo, J. A. Vilaand H. A. Scheraga, “Accounting for a mirror-image conformation as a subtle effect in protein folding”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 23. Proceedings of the National Academy of Sciences, pp. 8458–8463, May 27, 2014. doi: 10.1073/pnas.1407837111.  
  
A. Krokhotin, A. Liwo, G. G. Maisuradze, A. J. Niemiand H. A. Scheraga, “Kinks, loops, and protein folding, with protein A as an example”, *The Journal of Chemical Physics*, vol. 140, no. 2. AIP Publishing, p. 025101, Jan. 14, 2014. doi: 10.1063/1.4855735.  
  
A. Liwo, “A unified coarse-grained model of biological macromolecules based on mean-field multipole–multipole interactions”, *Journal of Molecular Modeling*, vol. 20, no. 8. Springer Science and Business Media LLC, Jul. 15, 2014. doi: 10.1007/s00894-014-2306-5.  
  
A. K. Sieradzan, A. Niadzvedtski, H. A. Scheragaand A. Liwo, “Revised Backbone-Virtual-Bond-Angle Potentials to Treat the l- and d-Amino Acid Residues in the Coarse-Grained United Residue (UNRES) Force Field”, *Journal of Chemical Theory and Computation*, vol. 10, no. 5. American Chemical Society (ACS), pp. 2194–2203, Apr. 30, 2014. doi: 10.1021/ct500119r.  
  
J. A. Vila, Y. A. Arnautova, O. A. Martinand H. A. Scheraga, “Are accurate computations of the13C′ shielding feasible at the DFT level of theory?”, *Journal of Computational Chemistry*, vol. 35, no. 4. Wiley, pp. 309–312, Dec. 03, 2013. doi: 10.1002/jcc.23499.  
  
R. Zhou, “Folding kinetics of WW domains with the united residue force field for bridging microscopic motions and experimental measurements”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 51. Proceedings of the National Academy of Sciences, pp. 18243–18248, Dec. 08, 2014. doi: 10.1073/pnas.1420914111.  
  
A. Khan, V. Paschalidis, M. Ruizand S. L. Shapiro, “Disks around merging binary black holes: From GW150914 to supermassive black holes”, *Physical Review D*, vol. 97, no. 4. American Physical Society (APS), Feb. 23, 2018. doi: 10.1103/physrevd.97.044036.  
  
M. Ruiz, R. N. Lang, V. Paschalidisand S. L. Shapiro, “BINARY NEUTRON STAR MERGERS: A JET ENGINE FOR SHORT GAMMA-RAY BURSTS”, *The Astrophysical Journal*, vol. 824, no. 1. American Astronomical Society, p. L6, Jun. 03, 2016. doi: 10.3847/2041-8205/824/1/l6.  
  
M. Ruiz and S. L. Shapiro, “General relativistic magnetohydrodynamics simulations of prompt-collapse neutron star mergers: The absence of jets”, *Physical Review D*, vol. 96, no. 8. American Physical Society (APS), Oct. 30, 2017. doi: 10.1103/physrevd.96.084063.  
  
M. Ruiz, S. L. Shapiroand A. Tsokaros, “GW170817, general relativistic magnetohydrodynamic simulations, and the neutron star maximum mass”, *Physical Review D*, vol. 97, no. 2. American Physical Society (APS), Jan. 11, 2018. doi: 10.1103/physrevd.97.021501.  
  
M. Ruiz, S. L. Shapiroand A. Tsokaros, “Jet launching from binary black hole-neutron star mergers: Dependence on black hole spin, binary mass ratio, and magnetic field orientation”, *Physical Review D*, vol. 98, no. 12. American Physical Society (APS), Dec. 21, 2018. doi: 10.1103/physrevd.98.123017.  
  
M. Ruiz, A. Tsokaros, V. Paschalidisand S. L. Shapiro, “Effects of spin on magnetized binary neutron star mergers and jet launching”, *Physical Review D*, vol. 99, no. 8. American Physical Society (APS), Apr. 17, 2019. doi: 10.1103/physrevd.99.084032.  
  
S. L. Shapiro, “Black holes, disks, and jets following binary mergers and stellar collapse: The narrow range of electromagnetic luminosities and accretion rates”, *Physical Review D*, vol. 95, no. 10. American Physical Society (APS), May 30, 2017. doi: 10.1103/physrevd.95.101303.  
  
L. Sun, V. Paschalidis, M. Ruizand S. L. Shapiro, “Magnetorotational collapse of supermassive stars: Black hole formation, gravitational waves, and jets”, *Physical Review D*, vol. 96, no. 4. American Physical Society (APS), Aug. 15, 2017. doi: 10.1103/physrevd.96.043006.  
  
L. Sun, M. Ruizand S. L. Shapiro, “Simulating the magnetorotational collapse of supermassive stars: Incorporating gas pressure perturbations and different rotation profiles”, *Physical Review D*, vol. 98, no. 10. American Physical Society (APS), Nov. 12, 2018. doi: 10.1103/physrevd.98.103008.  
  
L. Sun, M. Ruizand S. L. Shapiro, “Magnetic braking and damping of differential rotation in massive stars”, *Physical Review D*, vol. 99, no. 6. American Physical Society (APS), Mar. 29, 2019. doi: 10.1103/physrevd.99.064057.  
  
A. Tsokaros, M. Ruiz, V. Paschalidis, S. L. Shapiro, L. Baiottiand K. Uryū, “Gravitational wave content and stability of uniformly, rotating, triaxial neutron stars in general relativity”, *Physical Review D*, vol. 95, no. 12. American Physical Society (APS), Jun. 30, 2017. doi: 10.1103/physrevd.95.124057.  
  
A. Tsokaros, K. Uryū, M. Ruizand S. L. Shapiro, “Constant circulation sequences of binary neutron stars and their spin characterization”, *Physical Review D*, vol. 98, no. 12. American Physical Society (APS), Dec. 18, 2018. doi: 10.1103/physrevd.98.124019.  
  
J. Aasi, “The NINJA-2 project: detecting and characterizing gravitational waveforms modelled using numerical binary black hole simulations”, *Classical and Quantum Gravity*, vol. 31, no. 11. IOP Publishing, p. 115004, May 20, 2014. doi: 10.1088/0264-9381/31/11/115004.  
  
D. Buaria, P. K. Yeungand B. L. Sawford, “A Lagrangian study of turbulent mixing: forward and backward dispersion of molecular trajectories in isotropic turbulence”, *Journal of Fluid Mechanics*, vol. 799. Cambridge University Press (CUP), pp. 352–382, Jun. 23, 2016. doi: 10.1017/jfm.2016.359.  
  
M. P. Clay and P. K. Yeung, “A numerical study of turbulence under temporally evolving axisymmetric contraction and subsequent relaxation”, *Journal of Fluid Mechanics*, vol. 805. Cambridge University Press (CUP), pp. 460–493, Sep. 22, 2016. doi: 10.1017/jfm.2016.566.  
  
D. A. Donzis and S. Jagannathan, “On the Relation between Small-scale Intermittency and Shocks in Turbulent Flows”, *Procedia IUTAM*, vol. 9. Elsevier BV, pp. 3–15, 2013. doi: 10.1016/j.piutam.2013.09.002.  
  
K. P. Iyer, J. Schumacher, K. R. Sreenivasanand P. K. Yeung, “Steep Cliffs and Saturated Exponents in Three-Dimensional Scalar Turbulence”, *Physical Review Letters*, vol. 121, no. 26. American Physical Society (APS), Dec. 28, 2018. doi: 10.1103/physrevlett.121.264501.  
  
K. P. Iyer, J. Schumacher, K. R. Sreenivasanand P. K. Yeung, “Fractal iso-level sets in high-Reynolds-number scalar turbulence”, *Physical Review Fluids*, vol. 5, no. 4. American Physical Society (APS), Apr. 27, 2020. doi: 10.1103/physrevfluids.5.044501.  
  
K. P. Iyer, K. R. Sreenivasanand P. K. Yeung, “Reynolds number scaling of velocity increments in isotropic turbulence”, *Physical Review E*, vol. 95, no. 2. American Physical Society (APS), Feb. 10, 2017. doi: 10.1103/physreve.95.021101.  
  
K. P. Iyer, K. R. Sreenivasanand P. K. Yeung, “Circulation in High Reynolds Number Isotropic Turbulence is a Bifractal”, *Physical Review X*, vol. 9, no. 4. American Physical Society (APS), Oct. 04, 2019. doi: 10.1103/physrevx.9.041006.  
  
K. P. Iyer and P. K. Yeung, “Structure functions and applicability of Yaglom’s relation in passive-scalar turbulent mixing at low Schmidt numbers with uniform mean gradient”, *Physics of Fluids*, vol. 26, no. 8. AIP Publishing, p. 085107, Aug. 2014. doi: 10.1063/1.4892581.  
  
T. A. Oliver, N. Malaya, R. Ulerichand R. D. Moser, “Estimating uncertainties in statistics computed from direct numerical simulation”, *Physics of Fluids*, vol. 26, no. 3. AIP Publishing, p. 035101, Mar. 2014. doi: 10.1063/1.4866813.  
  
B. L. Sawford and P. K. Yeung, “Direct numerical simulation studies of Lagrangian intermittency in turbulence”, *Physics of Fluids*, vol. 27, no. 6. AIP Publishing, p. 065109, Jun. 2015. doi: 10.1063/1.4922205.  
  
P. K. Yeung, D. A. Donzisand K. R. Sreenivasan, “Dissipation, enstrophy and pressure statistics in turbulence simulations at high Reynolds numbers”, *Journal of Fluid Mechanics*, vol. 700. Cambridge University Press (CUP), pp. 5–15, Feb. 08, 2012. doi: 10.1017/jfm.2012.5.  
  
P. K. Yeung, K. R. Sreenivasanand S. B. Pope, “Effects of finite spatial and temporal resolution in direct numerical simulations of incompressible isotropic turbulence”, *Physical Review Fluids*, vol. 3, no. 6. American Physical Society (APS), Jun. 18, 2018. doi: 10.1103/physrevfluids.3.064603.  
  
X. M. Zhai and P. K. Yeung, “Evolution of anisotropy in direct numerical simulations of MHD turbulence in a strong magnetic field on elongated periodic domains”, *Physical Review Fluids*, vol. 3, no. 8. American Physical Society (APS), Aug. 07, 2018. doi: 10.1103/physrevfluids.3.084602.  
  
J. E. Barnes, K. Wood, A. S. Hilland L. M. Haffner, “Photoionization and heating of a supernova-driven turbulent interstellar medium”, *Monthly Notices of the Royal Astronomical Society*, vol. 440, no. 4. Oxford University Press (OUP), pp. 3027–3035, Apr. 17, 2014. doi: 10.1093/mnras/stu521.  
  
E. Bertram, R. S. Klessenand S. C. O. Glover, “Structure analysis of simulated molecular clouds with the Δ-variance”, *Monthly Notices of the Royal Astronomical Society*, vol. 451, no. 1. Oxford University Press (OUP), pp. 196–209, May 27, 2015. doi: 10.1093/mnras/stv948.  
  
E. Bertram, L. Konstandin, R. Shetty, S. C. O. Gloverand R. S. Klessen, “Centroid velocity statistics of molecular clouds”, *Monthly Notices of the Royal Astronomical Society*, vol. 446, no. 4. Oxford University Press (OUP), pp. 3777–3787, Dec. 09, 2014. doi: 10.1093/mnras/stu2372.  
  
E. Bertram, R. Shetty, S. C. O. Glover, R. S. Klessen, J. Roman-Duvaland C. Federrath, “Principal component analysis of molecular clouds: can CO reveal the dynamics?”, *Monthly Notices of the Royal Astronomical Society*, vol. 440, no. 1. Oxford University Press (OUP), pp. 465–475, Mar. 11, 2014. doi: 10.1093/mnras/stu284.  
  
P. C. Clark, S. C. O. Glover, R. S. Klessenand I. A. Bonnell, “How long does it take to form a molecular cloud?”, *Monthly Notices of the Royal Astronomical Society*, vol. 424, no. 4. Oxford University Press (OUP), pp. 2599–2613, Jul. 17, 2012. doi: 10.1111/j.1365-2966.2012.21259.x.  
  
A. Emerick, M.-M. M. Low, J. Grcevichand A. Gatto, “GAS LOSS BY RAM PRESSURE STRIPPING AND INTERNAL FEEDBACK FROM LOW-MASS MILKY WAY SATELLITES”, *The Astrophysical Journal*, vol. 826, no. 2. American Astronomical Society, p. 148, Jul. 27, 2016. doi: 10.3847/0004-637x/826/2/148.  
  
W. Lyra and M. Kuchner, “Formation of sharp eccentric rings in debris disks with gas but without planets”, *Nature*, vol. 499, no. 7457. Springer Science and Business Media LLC, pp. 184–187, Jul. 2013. doi: 10.1038/nature12281.  
  
J. L. Maron, C. P. McNallyand M.-M. Mac Low, “PHURBAS: AN ADAPTIVE, LAGRANGIAN, MESHLESS, MAGNETOHYDRODYNAMICS CODE. I. ALGORITHM”, *The Astrophysical Journal Supplement Series*, vol. 200, no. 1. American Astronomical Society, p. 6, May 01, 2012. doi: 10.1088/0067-0049/200/1/6.  
  
C. P. McNally, W. Lyraand J.-C. Passy, “A WELL-POSED KELVIN-HELMHOLTZ INSTABILITY TEST AND COMPARISON”, *The Astrophysical Journal Supplement Series*, vol. 201, no. 2. American Astronomical Society, p. 18, Jun. 28, 2012. doi: 10.1088/0067-0049/201/2/18.  
  
C. P. McNally, J. L. Maronand M.-M. Mac Low, “PHURBAS: AN ADAPTIVE, LAGRANGIAN, MESHLESS, MAGNETOHYDRODYNAMICS CODE. II. IMPLEMENTATION AND TESTS”, *The Astrophysical Journal Supplement Series*, vol. 200, no. 1. American Astronomical Society, p. 7, May 01, 2012. doi: 10.1088/0067-0049/200/1/7.  
  
J. E. Staff, “Hydrodynamic simulations of the interaction between an AGB star and a main-sequence companion in eccentric orbits”, *Monthly Notices of the Royal Astronomical Society*, vol. 455, no. 4. Oxford University Press (OUP), pp. 3511–3525, Nov. 30, 2015. doi: 10.1093/mnras/stv2548.  
  
K. Czechowski, C. Battaglino, C. McClanahan, K. Iyer, P.-K. Yeungand R. Vuduc, “On the communication complexity of 3D FFTs and its implications for Exascale”, *Proceedings of the 26th ACM international conference on Supercomputing*. ACM, Jun. 25, 2012. doi: 10.1145/2304576.2304604.  
  
K. P. Iyer, J. Schumacher, K. R. Sreenivasanand P. K. Yeung, “Scaling of locally averaged energy dissipation and enstrophy density in isotropic turbulence”, *New Journal of Physics*, vol. 21, no. 3. IOP Publishing, p. 033016, Mar. 19, 2019. doi: 10.1088/1367-2630/ab05e8.  
  
K. P. Iyer, K. R. Sreenivasanand P. K. Yeung, “Scaling exponents saturate in three-dimensional isotropic turbulence”, *Physical Review Fluids*, vol. 5, no. 5. American Physical Society (APS), May 15, 2020. doi: 10.1103/physrevfluids.5.054605.  
  
B. Kadoch, K. Iyer, D. Donzis, K. Schneider, M. Fargeand P. K. Yeung, “On the role of vortical structures for turbulent mixing using direct numerical simulation and wavelet-based coherent vorticity extraction”, *Journal of Turbulence*, vol. 12. Informa UK Limited, p. N20, Jan. 2011. doi: 10.1080/14685248.2011.562511.  
  
J. R. Cendagorta and T. Ichiye, “The Surface Potential of the Water–Vapor Interface from Classical Simulations”, *The Journal of Physical Chemistry B*, vol. 119, no. 29. American Chemical Society (ACS), pp. 9114–9122, Mar. 05, 2015. doi: 10.1021/jp508878v.  
  
M.-L. Tan, J. R. Cendagortaand T. Ichiye, “The molecular charge distribution, the hydration shell, and the unique properties of liquid water”, *The Journal of Chemical Physics*, vol. 141, no. 24. AIP Publishing, p. 244504, Dec. 28, 2014. doi: 10.1063/1.4904263.  
  
M.-L. Tan, B. T. Miller, J. Te, J. R. Cendagorta, B. R. Brooksand T. Ichiye, “Hydrophobic hydration and the anomalous partial molar volumes in ethanol-water mixtures”, *The Journal of Chemical Physics*, vol. 142, no. 6. AIP Publishing, p. 064501, Feb. 14, 2015. doi: 10.1063/1.4906750.  
  
C. C. Dharmawardhana and T. Ichiye, “Building better water models using the shape of the charge distribution of a water molecule”, *The Journal of Chemical Physics*, vol. 147, no. 19. AIP Publishing, p. 194103, Nov. 21, 2017. doi: 10.1063/1.4986070.  
  
Q. Huang, J. M. Rodgers, R. J. Hemleyand T. Ichiye, “Extreme biophysics: Enzymes under pressure”, *Journal of Computational Chemistry*, vol. 38, no. 15. Wiley, pp. 1174–1182, Jan. 19, 2017. doi: 10.1002/jcc.24737.  
  
Q. Huang, J. M. Rodgers, R. J. Hemleyand T. Ichiye, “Quasiharmonic Analysis of the Energy Landscapes of Dihydrofolate Reductase from Piezophiles and Mesophiles”, *The Journal of Physical Chemistry B*, vol. 122, no. 21. American Chemical Society (ACS), pp. 5527–5533, Jan. 25, 2018. doi: 10.1021/acs.jpcb.7b11838.  
  
Q. Huang, J. Rodgers, R. Hemleyand T. Ichiye, “Effects of Pressure and Temperature on the Atomic Fluctuations of Dihydrofolate Reductase from a Psychropiezophile and a Mesophile”, *International Journal of Molecular Sciences*, vol. 20, no. 6. MDPI AG, p. 1452, Mar. 22, 2019. doi: 10.3390/ijms20061452.  
  
Q. Huang, J. M. Rodgers, R. J. Hemleyand T. Ichiye, “Adaptations for pressure and temperature effects on loop motion in *Escherichia coli* and *Moritella profunda* dihydrofolate reductase”, *High Pressure Research*, vol. 39, no. 2. Informa UK Limited, pp. 225–237, Mar. 05, 2019. doi: 10.1080/08957959.2019.1584799.  
  
T. Ichiye, “What makes proteins work: exploring life in*P–T–X*”, *Physical Biology*, vol. 13, no. 6. IOP Publishing, p. 063001, Nov. 15, 2016. doi: 10.1088/1478-3975/13/6/063001.  
  
T. Ichiye, “Enzymes from piezophiles”, *Seminars in Cell & Developmental Biology*, vol. 84. Elsevier BV, pp. 138–146, Dec. 2018. doi: 10.1016/j.semcdb.2018.01.004.  
  
J. M. Rodgers, R. J. Hemleyand T. Ichiye, “Quasiharmonic analysis of protein energy landscapes from pressure-temperature molecular dynamics simulations”, *The Journal of Chemical Physics*, vol. 147, no. 12. AIP Publishing, p. 125103, Sep. 28, 2017. doi: 10.1063/1.5003823.  
  
M.-L. Tan, K. N. Tran, F. C. Pickard IV, A. C. Simmonett, B. R. Brooksand T. Ichiye, “Molecular Multipole Potential Energy Functions for Water”, *The Journal of Physical Chemistry B*, vol. 120, no. 8. American Chemical Society (ACS), pp. 1833–1842, Nov. 24, 2015. doi: 10.1021/acs.jpcb.5b09565.  
  
X. Teng, Q. Huang, C. C. Dharmawardhanaand T. Ichiye, “Diffusion of aqueous solutions of ionic, zwitterionic, and polar solutes”, *The Journal of Chemical Physics*, vol. 148, no. 22. AIP Publishing, p. 222827, Jun. 14, 2018. doi: 10.1063/1.5023004.  
  
X. Teng and T. Ichiye, “Dynamical Effects of Trimethylamine *N*-Oxide on Aqueous Solutions of Urea”, *The Journal of Physical Chemistry B*, vol. 123, no. 5. American Chemical Society (ACS), pp. 1108–1115, Jan. 14, 2019. doi: 10.1021/acs.jpcb.8b09874.  
  
K. N. Tran, M.-L. Tanand T. Ichiye, “A single-site multipole model for liquid water”, *The Journal of Chemical Physics*, vol. 145, no. 3. AIP Publishing, p. 034501, Jul. 21, 2016. doi: 10.1063/1.4958621.  
  
V. Bondarenko, D. Mowrey, L. T. Liu, Y. Xuand P. Tang, “NMR resolved multiple anesthetic binding sites in the TM domains of the α4β2 nAChR”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1828, no. 2. Elsevier BV, pp. 398–404, Feb. 2013. doi: 10.1016/j.bbamem.2012.09.014.  
  
Q. Chen, “Direct Pore Binding as a Mechanism for Isoflurane Inhibition of the Pentameric Ligand-gated Ion Channel ELIC”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, Sep. 08, 2015. doi: 10.1038/srep13833.  
  
M. N. Kinde, “Conformational Changes Underlying Desensitization of the Pentameric Ligand-Gated Ion Channel ELIC”, *Structure*, vol. 23, no. 6. Elsevier BV, pp. 995–1004, Jun. 2015. doi: 10.1016/j.str.2015.03.017.  
  
D. Mowrey, “Asymmetric Ligand Binding Facilitates Conformational Transitions in Pentameric Ligand-Gated Ion Channels”, *Journal of the American Chemical Society*, vol. 135, no. 6. American Chemical Society (ACS), pp. 2172–2180, Feb. 04, 2013. doi: 10.1021/ja307275v.  
  
D. Mowrey, E. J. Haddadian, L. T. Liu, D. Willenbring, Y. Xuand P. Tang, “Unresponsive Correlated Motion in α7 nAChR to Halothane Binding Explains Its Functional Insensitivity to Volatile Anesthetics”, *The Journal of Physical Chemistry B*, vol. 114, no. 22. American Chemical Society (ACS), pp. 7649–7655, May 13, 2010. doi: 10.1021/jp1009675.  
  
D. Mowrey, Q. Chen, Y. Liang, J. Liang, Y. Xuand P. Tang, “Signal Transduction Pathways in the Pentameric Ligand-Gated Ion Channels”, *PLoS ONE*, vol. 8, no. 5. Public Library of Science (PLoS), p. e64326, May 08, 2013. doi: 10.1371/journal.pone.0064326.  
  
M. M. Wells, T. S. Tillman, D. D. Mowrey, T. Sun, Y. Xuand P. Tang, “Ensemble-Based Virtual Screening for Cannabinoid-Like Potentiators of the Human Glycine Receptor α1 for the Treatment of Pain”, *Journal of Medicinal Chemistry*, vol. 58, no. 7. American Chemical Society (ACS), pp. 2958–2966, Mar. 27, 2015. doi: 10.1021/jm501873p.  
  
Q. Chen, “Structural Basis of Alcohol Inhibition of the Pentameric Ligand-Gated Ion Channel ELIC”, *Structure*, vol. 25, no. 1. Elsevier BV, pp. 180–187, Jan. 2017. doi: 10.1016/j.str.2016.11.007.  
  
L.-J. Jia, P. Tang, N. R. Brandon, Y. Luo, B. Yuand Y. Xu, “Effects of Propofol General Anesthesia on Olfactory Relearning”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Sep. 15, 2016. doi: 10.1038/srep33538.  
  
M. N. Kinde, “Fluorine-19 NMR and computational quantification of isoflurane binding to the voltage-gated sodium channel NaChBac”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 48. Proceedings of the National Academy of Sciences, pp. 13762–13767, Nov. 15, 2016. doi: 10.1073/pnas.1609939113.  
  
M. N. Kinde, W. Bu, Q. Chen, Y. Xu, R. G. Eckenhoffand P. Tang, “Common Anesthetic-binding Site for Inhibition of Pentameric Ligand-gated Ion Channels”, *Anesthesiology*, vol. 124, no. 3. Ovid Technologies (Wolters Kluwer Health), pp. 664–673, Mar. 01, 2016. doi: 10.1097/aln.0000000000001005.  
  
L. M. Stollings, L.-J. Jia, P. Tang, H. Dou, B. Luand Y. Xu, “Immune Modulation by Volatile Anesthetics”, *Anesthesiology*, vol. 125, no. 2. Ovid Technologies (Wolters Kluwer Health), pp. 399–411, Aug. 01, 2016. doi: 10.1097/aln.0000000000001195.  
  
T. S. Tillman, “Functional Human α7 Nicotinic Acetylcholine Receptor (nAChR) Generated from Escherichia coli”, *Journal of Biological Chemistry*, vol. 291, no. 35. Elsevier BV, pp. 18276–18282, Aug. 2016. doi: 10.1074/jbc.m116.729970.  
  
J. Wu, “Heteromeric α7β2 Nicotinic Acetylcholine Receptors in the Brain”, *Trends in Pharmacological Sciences*, vol. 37, no. 7. Elsevier BV, pp. 562–574, Jul. 2016. doi: 10.1016/j.tips.2016.03.005.  
  
A. Sarkar, D. M. Eckmann, P. S. Ayyaswamyand R. Radhakrishnan, “Hydrodynamic interactions of deformable polymeric nanocarriers and the effect of crosslinking”, *Soft Matter*, vol. 11, no. 29. Royal Society of Chemistry (RSC), pp. 5955–5969, 2015. doi: 10.1039/c5sm00669d.  
  
D. R. Slochower, Y.-H. Wang, R. Radhakrishnanand P. A. Janmey, “Physical chemistry and membrane properties of two phosphatidylinositol bisphosphate isomers”, *Physical Chemistry Chemical Physics*, vol. 17, no. 19. Royal Society of Chemistry (RSC), pp. 12608–12615, 2015. doi: 10.1039/c5cp00862j.  
  
R. W. Tourdot, N. Ramakrishnan, T. Baumgartand R. Radhakrishnan, “Application of a free-energy-landscape approach to study tension-dependent bilayer tubulation mediated by curvature-inducing proteins”, *Physical Review E*, vol. 92, no. 4. American Physical Society (APS), Oct. 29, 2015. doi: 10.1103/physreve.92.042715.  
  
H.-Y. Yu, D. M. Eckmann, P. S. Ayyaswamyand R. Radhakrishnan, “Composite generalized Langevin equation for Brownian motion in different hydrodynamic and adhesion regimes”, *Physical Review E*, vol. 91, no. 5. American Physical Society (APS), May 12, 2015. doi: 10.1103/physreve.91.052303.  
  
Y. Cai, I. Fu, N. E. Geacintov, Y. Zhangand S. Broyde, “Synergistic effects of H3 and H4 nucleosome tails on structure and dynamics of a lesion-containing DNA: Binding of a displaced lesion partner base to the H3 tail for GG-NER recognition”, *DNA Repair*, vol. 65. Elsevier BV, pp. 73–78, May 2018. doi: 10.1016/j.dnarep.2018.02.009.  
  
Y. Cai, N. E. Geacintovand S. Broyde, “Nucleotide Excision Repair Efficiencies of Bulky Carcinogen–DNA Adducts Are Governed by a Balance between Stabilizing and Destabilizing Interactions”, *Biochemistry*, vol. 51, no. 7. American Chemical Society (ACS), pp. 1486–1499, Feb. 09, 2012. doi: 10.1021/bi201794x.  
  
Y. Cai, N. E. Geacintovand S. Broyde, “Ribonucleotides as nucleotide excision repair substrates”, *DNA Repair*, vol. 13. Elsevier BV, pp. 55–60, Jan. 2014. doi: 10.1016/j.dnarep.2013.10.010.  
  
Y. Cai, “Differences in the Access of Lesions to the Nucleotide Excision Repair Machinery in Nucleosomes”, *Biochemistry*, vol. 54, no. 27. American Chemical Society (ACS), pp. 4181–4185, Jun. 30, 2015. doi: 10.1021/acs.biochem.5b00564.  
  
Y. Cai, “Free Energy Profiles of Base Flipping in Intercalative Polycyclic Aromatic Hydrocarbon-Damaged DNA Duplexes: Energetic and Structural Relationships to Nucleotide Excision Repair Susceptibility”, *Chemical Research in Toxicology*, vol. 26, no. 7. American Chemical Society (ACS), pp. 1115–1125, Jul. 02, 2013. doi: 10.1021/tx400156a.  
  
S. Chakraborty, “Enhanced spontaneous DNA twisting/bending fluctuations unveiled by fluorescence lifetime distributions promote mismatch recognition by the Rad4 nucleotide excision repair complex”, *Nucleic Acids Research*, vol. 46, no. 3. Oxford University Press (OUP), pp. 1240–1255, Dec. 18, 2017. doi: 10.1093/nar/gkx1216.  
  
I. Fu, Y. Cai, N. E. Geacintov, Y. Zhangand S. Broyde, “Nucleosome Histone Tail Conformation and Dynamics: Impacts of Lysine Acetylation and a Nearby Minor Groove Benzo[*a*]pyrene-Derived Lesion”, *Biochemistry*, vol. 56, no. 14. American Chemical Society (ACS), pp. 1963–1973, Mar. 22, 2017. doi: 10.1021/acs.biochem.6b01208.  
  
I. Fu, Y. Cai, Y. Zhang, N. E. Geacintovand S. Broyde, “Entrapment of a Histone Tail by a DNA Lesion in a Nucleosome Suggests the Lesion Impacts Epigenetic Marking: A Molecular Dynamics Study”, *Biochemistry*, vol. 55, no. 2. American Chemical Society (ACS), pp. 239–242, Jan. 06, 2016. doi: 10.1021/acs.biochem.5b01166.  
  
N. E. Geacintov and S. Broyde, “Repair-Resistant DNA Lesions”, *Chemical Research in Toxicology*, vol. 30, no. 8. American Chemical Society (ACS), pp. 1517–1548, Aug. 10, 2017. doi: 10.1021/acs.chemrestox.7b00128.  
  
S. Ji, “5-Formylcytosine mediated DNA–protein cross-links block DNA replication and induce mutations in human cells”, *Nucleic Acids Research*, vol. 46, no. 18. Oxford University Press (OUP), pp. 9892–9892, Sep. 03, 2018. doi: 10.1093/nar/gky809.  
  
K. Kropachev, “Structural basis for the recognition of diastereomeric 5′,8-cyclo-2′-deoxypurine lesions by the human nucleotide excision repair system”, *Nucleic Acids Research*, vol. 42, no. 8. Oxford University Press (OUP), pp. 5020–5032, Mar. 10, 2014. doi: 10.1093/nar/gku162.  
  
Y.-C. Lee, “The relationships between XPC binding to conformationally diverse DNA adducts and their excision by the human NER system: Is there a correlation?”, *DNA Repair*, vol. 19. Elsevier BV, pp. 55–63, Jul. 2014. doi: 10.1016/j.dnarep.2014.03.026.  
  
L. Lior-Hoffmann, S. Ding, N. E. Geacintov, Y. Zhangand S. Broyde, “Structural and Dynamic Characterization of Polymerase κ’s Minor Groove Lesion Processing Reveals How Adduct Topology Impacts Fidelity”, *Biochemistry*, vol. 53, no. 35. American Chemical Society (ACS), pp. 5683–5691, Aug. 22, 2014. doi: 10.1021/bi5007964.  
  
Z. Liu, “Resistance to Nucleotide Excision Repair of Bulky Guanine Adducts Opposite Abasic Sites in DNA Duplexes and Relationships between Structure and Function”, *PLOS ONE*, vol. 10, no. 9. Public Library of Science (PLoS), p. e0137124, Sep. 04, 2015. doi: 10.1371/journal.pone.0137124.  
  
H. Mu, N. E. Geacintov, S. Broyde, J.-E. Yeoand O. D. Schärer, “Molecular basis for damage recognition and verification by XPC-RAD23B and TFIIH in nucleotide excision repair”, *DNA Repair*, vol. 71. Elsevier BV, pp. 33–42, Nov. 2018. doi: 10.1016/j.dnarep.2018.08.005.  
  
H. Mu, N. E. Geacintov, J.-H. Min, Y. Zhangand S. Broyde, “Nucleotide Excision Repair Lesion-Recognition Protein Rad4 Captures a Pre-Flipped Partner Base in a Benzo[*a*]pyrene-Derived DNA Lesion: How Structure Impacts the Binding Pathway”, *Chemical Research in Toxicology*, vol. 30, no. 6. American Chemical Society (ACS), pp. 1344–1354, May 15, 2017. doi: 10.1021/acs.chemrestox.7b00074.  
  
H. Mu, N. E. Geacintov, Y. Zhangand S. Broyde, “Recognition of Damaged DNA for Nucleotide Excision Repair: A Correlated Motion Mechanism with a Mismatched *cis-syn* Thymine Dimer Lesion”, *Biochemistry*, vol. 54, no. 34. American Chemical Society (ACS), pp. 5263–5267, Aug. 18, 2015. doi: 10.1021/acs.biochem.5b00840.  
  
H. Mu, “Role of Structural and Energetic Factors in Regulating Repair of a Bulky DNA Lesion with Different Opposite Partner Bases”, *Biochemistry*, vol. 52, no. 33. American Chemical Society (ACS), pp. 5517–5521, Aug. 05, 2013. doi: 10.1021/bi4009177.  
  
H. Mu, Y. Zhang, N. E. Geacintovand S. Broyde, “Lesion Sensing during Initial Binding by Yeast XPC/Rad4: Toward Predicting Resistance to Nucleotide Excision Repair”, *Chemical Research in Toxicology*, vol. 31, no. 11. American Chemical Society (ACS), pp. 1260–1268, Oct. 04, 2018. doi: 10.1021/acs.chemrestox.8b00231.  
  
F. A. Rodríguez, “Nuclear Magnetic Resonance Studies of an *N*2-Guanine Adduct Derived from the Tumorigen Dibenzo[*a*,*l*]pyrene in DNA: Impact of Adduct Stereochemistry, Size, and Local DNA Sequence on Solution Conformations”, *Biochemistry*, vol. 53, no. 11. American Chemical Society (ACS), pp. 1827–1841, Mar. 11, 2014. doi: 10.1021/bi4017044.  
  
Y. Tang, “Nuclear Magnetic Resonance Solution Structure of an *N*2-Guanine DNA Adduct Derived from the Potent Tumorigen Dibenzo[*a*,*l*]pyrene: Intercalation from the Minor Groove with Ruptured Watson–Crick Base Pairing”, *Biochemistry*, vol. 51, no. 48. American Chemical Society (ACS), pp. 9751–9762, Nov. 15, 2012. doi: 10.1021/bi3013577.  
  
J. Yang, L. Lior-Hoffmann, S. Wang, Y. Zhangand S. Broyde, “DNA Cytosine Methylation: Structural and Thermodynamic Characterization of the Epigenetic Marking Mechanism”, *Biochemistry*, vol. 52, no. 16. American Chemical Society (ACS), pp. 2828–2838, Apr. 12, 2013. doi: 10.1021/bi400163k.  
  
K. P. Devlin, “Polymorphism and second harmonic generation in a novel diamond-like semiconductor: Li2MnSnS4”, *Journal of Solid State Chemistry*, vol. 231. Elsevier BV, pp. 256–266, Nov. 2015. doi: 10.1016/j.jssc.2015.08.011.  
  
P. C. Gedeon, J. R. Thomasand J. D. Madura, “Accelerated Molecular Dynamics and Protein Conformational Change: A Theoretical and Practical Guide Using a Membrane Embedded Model Neurotransmitter Transporter”, *Methods in Molecular Biology*. Springer New York, pp. 253–287, Sep. 03, 2014. doi: 10.1007/978-1-4939-1465-4\_12.  
  
D. Punihaole, R. J. Workman, Z. Hong, J. D. Maduraand S. A. Asher, “Polyglutamine Fibrils: New Insights into Antiparallel β-Sheet Conformational Preference and Side Chain Structure”, *The Journal of Physical Chemistry B*, vol. 120, no. 12. American Chemical Society (ACS), pp. 3012–3026, Mar. 18, 2016. doi: 10.1021/acs.jpcb.5b11380.  
  
K. A. Rosmus, “Optical Nonlinearity in Cu2CdSnS4 and α/β-Cu2ZnSiS4: Diamond-like Semiconductors with High Laser-Damage Thresholds”, *Inorganic Chemistry*, vol. 53, no. 15. American Chemical Society (ACS), pp. 7809–7811, Jul. 25, 2014. doi: 10.1021/ic501310d.  
  
J. N. Talbot, “Rapid and sustained antidepressant properties of an NMDA antagonist/monoamine reuptake inhibitor identified via transporter-based virtual screening”, *Pharmacology Biochemistry and Behavior*, vol. 150–151. Elsevier BV, pp. 22–30, Nov. 2016. doi: 10.1016/j.pbb.2016.08.007.  
  
M. J. Wasko, K. A. Pellegrene, J. D. Maduraand C. K. Surratt, “A Role for Fragment-Based Drug Design in Developing Novel Lead Compounds for Central Nervous System Targets”, *Frontiers in Neurology*, vol. 6. Frontiers Media SA, Sep. 11, 2015. doi: 10.3389/fneur.2015.00197.  
  
A. H. Beaven, “Gramicidin A Channel Formation Induces Local Lipid Redistribution I: Experiment and Simulation”, *Biophysical Journal*, vol. 112, no. 6. Elsevier BV, pp. 1185–1197, Mar. 2017. doi: 10.1016/j.bpj.2017.01.028.  
  
X. Cheng, J.-K. Kim, Y. Kim, J. U. Bowieand W. Im, “Molecular dynamics simulation strategies for protein–micelle complexes”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1858, no. 7. Elsevier BV, pp. 1566–1572, Jul. 2016. doi: 10.1016/j.bbamem.2015.12.012.  
  
C. Dong, “A mechano-reactive coarse-grained model of the blood-clotting agent von Willebrand factor”, *The Journal of Chemical Physics*, vol. 151, no. 12. AIP Publishing, p. 124905, Sep. 28, 2019. doi: 10.1063/1.5117154.  
  
C. Dong, “Long-ranged Protein-glycan Interactions Stabilize von Willebrand Factor A2 Domain from Mechanical Unfolding”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, Oct. 30, 2018. doi: 10.1038/s41598-018-34374-y.  
  
H. Guterres, H. S. Leeand W. Im, “Ligand-Binding-Site Structure Refinement Using Molecular Dynamics with Restraints Derived from Predicted Binding Site Templates”, *Journal of Chemical Theory and Computation*, vol. 15, no. 11. American Chemical Society (ACS), pp. 6524–6535, Sep. 26, 2019. doi: 10.1021/acs.jctc.9b00751.  
  
A. V. Hughes, D. S. Patel, G. Widmalm, J. B. Klauda, L. A. Cliftonand W. Im, “Physical Properties of Bacterial Outer Membrane Models: Neutron Reflectometry & Molecular Simulation”, *Biophysical Journal*, vol. 116, no. 6. Elsevier BV, pp. 1095–1104, Mar. 2019. doi: 10.1016/j.bpj.2019.02.001.  
  
W. Im, J. Liang, A. Olson, H.-X. Zhou, S. Vajdaand I. A. Vakser, “Challenges in structural approaches to cell modeling”, *Journal of Molecular Biology*, vol. 428, no. 15. Elsevier BV, pp. 2943–2964, Jul. 2016. doi: 10.1016/j.jmb.2016.05.024.  
  
J. C. Jeong, “ST-analyzer: A web-based user interface for simulation trajectory analysis”, *Journal of Computational Chemistry*, vol. 35, no. 12. Wiley, pp. 957–963, Mar. 17, 2014. doi: 10.1002/jcc.23584.  
  
S. Jo, “CHARMM-GUI PDB Manipulator for Advanced Modeling and Simulations of Proteins Containing Nonstandard Residues”, *Advances in Protein Chemistry and Structural Biology*. Elsevier, pp. 235–265, 2014. doi: 10.1016/bs.apcsb.2014.06.002.  
  
S. Jo, Y. Qiand W. Im, “Preferred conformations of*N*-glycan core pentasaccharide in solution and in glycoproteins”, *Glycobiology*. Oxford University Press (OUP), p. cwv083, Sep. 24, 2015. doi: 10.1093/glycob/cwv083.  
  
N. R. Kern, “Lipid-Linked Oligosaccharides in Membranes Sample Conformations That Facilitate Binding to Oligosaccharyltransferase”, *Biophysical Journal*, vol. 107, no. 8. Elsevier BV, pp. 1885–1895, Oct. 2014. doi: 10.1016/j.bpj.2014.09.007.  
  
A. Kesireddy, “Modeling of Specific Lipopolysaccharide Binding Sites on a Gram-Negative Porin”, *The Journal of Physical Chemistry B*, vol. 123, no. 27. American Chemical Society (ACS), pp. 5700–5708, Jun. 17, 2019. doi: 10.1021/acs.jpcb.9b03669.  
  
S. Kim, “Bilayer Properties of Lipid A from Various Gram-Negative Bacteria”, *Biophysical Journal*, vol. 111, no. 8. Elsevier BV, pp. 1750–1760, Oct. 2016. doi: 10.1016/j.bpj.2016.09.001.  
  
S. Kim, M. M. Piresand W. Im, “Insight into Elongation Stages of Peptidoglycan Processing in Bacterial Cytoplasmic Membranes”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, Dec. 07, 2018. doi: 10.1038/s41598-018-36075-y.  
  
D. Kong, “L-Met Activates Arabidopsis GLR Ca2+ Channels Upstream of ROS Production and Regulates Stomatal Movement”, *Cell Reports*, vol. 17, no. 10. Elsevier BV, pp. 2553–2561, Dec. 2016. doi: 10.1016/j.celrep.2016.11.015.  
  
L. Krshnan, S. Park, W. Im, M. J. Calland M. E. Call, “A conserved αβ transmembrane interface forms the core of a compact T-cell receptor–CD3 structure within the membrane”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 43. Proceedings of the National Academy of Sciences, Oct. 10, 2016. doi: 10.1073/pnas.1611445113.  
  
R. Kumar, “Replacing Arginine 33 for Alanine in the Hemophore HasA from *Pseudomonas aeruginosa* Causes Closure of the H32 Loop in the Apo-Protein”, *Biochemistry*, vol. 55, no. 18. American Chemical Society (ACS), pp. 2622–2631, Apr. 28, 2016. doi: 10.1021/acs.biochem.6b00239.  
  
H. S. Lee and W. Im, “G-LoSA: An efficient computational tool for local structure-centric biological studies and drug design”, *Protein Science*, vol. 25, no. 4. Wiley, pp. 865–876, Mar. 06, 2016. doi: 10.1002/pro.2890.  
  
H. S. Lee and W. Im, “*Stalis* : A Computational Method for Template‐Based Ab Initio Ligand Design”, *Journal of Computational Chemistry*, vol. 40, no. 17. Wiley, pp. 1622–1632, Mar. 04, 2019. doi: 10.1002/jcc.25813.  
  
H. S. Lee, Y. Oh, M.-J. Kimand W. Im, “Molecular Basis of Aqueous-like Activity of Lipase Treated with Glucose-Headed Surfactant in Organic Solvent”, *The Journal of Physical Chemistry B*, vol. 122, no. 47. American Chemical Society (ACS), pp. 10659–10668, Nov. 06, 2018. doi: 10.1021/acs.jpcb.8b07686.  
  
J. Lee, “CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field”, *Journal of Chemical Theory and Computation*, vol. 12, no. 1. American Chemical Society (ACS), pp. 405–413, Dec. 03, 2015. doi: 10.1021/acs.jctc.5b00935.  
  
J. H. Lee, M. Oh, H. S. Kim, H. Lee, W. Imand H.-S. Lim, “Converting One-Face α-Helix Mimetics into Amphiphilic α-Helix Mimetics as Potent Inhibitors of Protein–Protein Interactions”, *ACS Combinatorial Science*, vol. 18, no. 1. American Chemical Society (ACS), pp. 36–42, Dec. 22, 2015. doi: 10.1021/acscombsci.5b00080.  
  
J. Lee, D. S. Patel, I. Kucharska, L. K. Tammand W. Im, “Refinement of OprH-LPS Interactions by Molecular Simulations”, *Biophysical Journal*, vol. 112, no. 2. Elsevier BV, pp. 346–355, Jan. 2017. doi: 10.1016/j.bpj.2016.12.006.  
  
J. Lee, “CHARMM-GUI *Membrane Builder* for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans”, *Journal of Chemical Theory and Computation*, vol. 15, no. 1. American Chemical Society (ACS), pp. 775–786, Dec. 11, 2018. doi: 10.1021/acs.jctc.8b01066.  
  
K. I. Lee, W. Imand R. W. Pastor, “Langevin dynamics simulations of charged model phosphatidylinositol lipids in the presence of diffusion barriers: toward an atomic level understanding of corralling of PIP2 by protein fences in biological membranes”, *BMC Biophysics*, vol. 7, no. 1. Springer Science and Business Media LLC, Nov. 26, 2014. doi: 10.1186/s13628-014-0013-3.  
  
J. G. McCoy, “The Structure of a Sugar Transporter of the Glucose EIIC Superfamily Provides Insight into the Elevator Mechanism of Membrane Transport”, *Structure*, vol. 24, no. 6. Elsevier BV, pp. 956–964, Jun. 2016. doi: 10.1016/j.str.2016.04.003.  
  
T. Mori, N. Miyashita, W. Im, M. Feigand Y. Sugita, “Molecular dynamics simulations of biological membranes and membrane proteins using enhanced conformational sampling algorithms”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1858, no. 7. Elsevier BV, pp. 1635–1651, Jul. 2016. doi: 10.1016/j.bbamem.2015.12.032.  
  
M. Oh, “Potential pharmacological chaperones targeting cancer-associated MCL-1 and Parkinson disease-associated α-synuclein”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 30. Proceedings of the National Academy of Sciences, pp. 11007–11012, Jul. 14, 2014. doi: 10.1073/pnas.1320556111.  
  
S. Park, K. J. Gloverand W. Im, “U-shaped caveolin-1 conformations are tightly regulated by hydrogen bonds with lipids”, *Journal of Computational Chemistry*, vol. 40, no. 16. Wiley, pp. 1570–1577, Mar. 03, 2019. doi: 10.1002/jcc.25807.  
  
S. Park and W. Im, “Theory of Adaptive Optimization for Umbrella Sampling”, *Journal of Chemical Theory and Computation*, vol. 10, no. 7. American Chemical Society (ACS), pp. 2719–2728, Jun. 19, 2014. doi: 10.1021/ct500504g.  
  
S. Park and W. Im, “Analysis of Lipid Order States and Domains in Lipid Bilayer Simulations”, *Journal of Chemical Theory and Computation*, vol. 15, no. 1. American Chemical Society (ACS), pp. 688–697, Nov. 23, 2018. doi: 10.1021/acs.jctc.8b00828.  
  
S.-J. Park, “CHARMM-GUI*Glycan Modeler*for modeling and simulation of carbohydrates and glycoconjugates”, *Glycobiology*, vol. 29, no. 4. Oxford University Press (OUP), pp. 320–331, Feb. 26, 2019. doi: 10.1093/glycob/cwz003.  
  
S. Park, M. S. Yeom, O. S. Andersen, R. W. Pastorand W. Im, “Quantitative Characterization of Protein–Lipid Interactions by Free Energy Simulation between Binary Bilayers”, *Journal of Chemical Theory and Computation*, vol. 15, no. 11. American Chemical Society (ACS), pp. 6491–6503, Sep. 27, 2019. doi: 10.1021/acs.jctc.9b00815.  
  
D. S. Patel, “Influence of Ganglioside GM1 Concentration on Lipid Clustering and Membrane Properties and Curvature”, *Biophysical Journal*, vol. 111, no. 9. Elsevier BV, pp. 1987–1999, Nov. 2016. doi: 10.1016/j.bpj.2016.09.021.  
  
D. S. Patel, “Dynamics and Interactions of OmpF and LPS: Influence on Pore Accessibility and Ion Permeability”, *Biophysical Journal*, vol. 110, no. 4. Elsevier BV, pp. 930–938, Feb. 2016. doi: 10.1016/j.bpj.2016.01.002.  
  
Y. Qi, X. Cheng, W. Han, S. Jo, K. Schultenand W. Im, “CHARMM-GUI PACE CG Builder for Solution, Micelle, and Bilayer Coarse-Grained Simulations”, *Journal of Chemical Information and Modeling*, vol. 54, no. 3. American Chemical Society (ACS), pp. 1003–1009, Mar. 13, 2014. doi: 10.1021/ci500007n.  
  
Y. Qi, “CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model”, *Biophysical Journal*, vol. 109, no. 10. Elsevier BV, pp. 2012–2022, Nov. 2015. doi: 10.1016/j.bpj.2015.10.008.  
  
Y. Qi, H. I. Ingólfsson, X. Cheng, J. Lee, S. J. Marrinkand W. Im, “CHARMM-GUI Martini Maker for Coarse-Grained Simulations with the Martini Force Field”, *Journal of Chemical Theory and Computation*, vol. 11, no. 9. American Chemical Society (ACS), pp. 4486–4494, Aug. 27, 2015. doi: 10.1021/acs.jctc.5b00513.  
  
Y. Qi, S. Joand W. Im, “Roles of glycans in interactions between gp120 and HIV broadly neutralizing antibodies”, *Glycobiology*. Oxford University Press (OUP), p. cwv101, Nov. 03, 2015. doi: 10.1093/glycob/cwv101.  
  
Y. Qi, J. B. Klaudaand W. Im, “Effects of Spin-Labels on Membrane Burial Depth of MARCKS-ED Residues”, *Biophysical Journal*, vol. 111, no. 8. Elsevier BV, pp. 1600–1603, Oct. 2016. doi: 10.1016/j.bpj.2016.09.013.  
  
Y. Qi, J. Lee, J. B. Klaudaand W. Im, “CHARMM‐GUI *Nanodisc Builder* for modeling and simulation of various nanodisc systems”, *Journal of Computational Chemistry*, vol. 40, no. 7. Wiley, pp. 893–899, Jan. 24, 2019. doi: 10.1002/jcc.25773.  
  
H. Rui, K. T. Root, J. Lee, K. J. Gloverand W. Im, “Probing the U-Shaped Conformation of Caveolin-1 in a Bilayer”, *Biophysical Journal*, vol. 106, no. 6. Elsevier BV, pp. 1371–1380, Mar. 2014. doi: 10.1016/j.bpj.2014.02.005.  
  
E. L. Wu, “CHARMM-GUI*Membrane Builder*toward realistic biological membrane simulations”, *Journal of Computational Chemistry*, vol. 35, no. 27. Wiley, pp. 1997–2004, Aug. 07, 2014. doi: 10.1002/jcc.23702.  
  
E. L. Wu, “E. coli Outer Membrane and Interactions with OmpLA”, *Biophysical Journal*, vol. 106, no. 11. Elsevier BV, pp. 2493–2502, Jun. 2014. doi: 10.1016/j.bpj.2014.04.024.  
  
E. L. Wu, “Insight into Early-Stage Unfolding of GPI-Anchored Human Prion Protein”, *Biophysical Journal*, vol. 109, no. 10. Elsevier BV, pp. 2090–2100, Nov. 2015. doi: 10.1016/j.bpj.2015.10.009.  
  
E. L. Wu, Y. Qi, K. C. Song, J. B. Klaudaand W. Im, “Preferred Orientations of Phosphoinositides in Bilayers and Their Implications in Protein Recognition Mechanisms”, *The Journal of Physical Chemistry B*, vol. 118, no. 16. American Chemical Society (ACS), pp. 4315–4325, Apr. 11, 2014. doi: 10.1021/jp500610t.  
  
H. Yao, “Concerted Motions Networking Pores and Distant Ferroxidase Centers Enable Bacterioferritin Function and Iron Traffic”, *Biochemistry*, vol. 54, no. 8. American Chemical Society (ACS), pp. 1611–1627, Feb. 17, 2015. doi: 10.1021/bi501255r.  
  
X. Zhuang, E. M. Dávila-Contreras, A. H. Beaven, W. Imand J. B. Klauda, “An extensive simulation study of lipid bilayer properties with different head groups, acyl chain lengths, and chain saturations”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1858, no. 12. Elsevier BV, pp. 3093–3104, Dec. 2016. doi: 10.1016/j.bbamem.2016.09.016.  
  
X. Cheng, S. Jo, Y. Qi, F. M. Marassiand W. Im, “Solid-State NMR-Restrained Ensemble Dynamics of a Membrane Protein in Explicit Membranes”, *Biophysical Journal*, vol. 108, no. 8. Elsevier BV, pp. 1954–1962, Apr. 2015. doi: 10.1016/j.bpj.2015.03.012.  
  
K. Knoblich, “Transmembrane Complexes of DAP12 Crystallized in Lipid Membranes Provide Insights into Control of Oligomerization in Immunoreceptor Assembly”, *Cell Reports*, vol. 11, no. 8. Elsevier BV, pp. 1184–1192, May 2015. doi: 10.1016/j.celrep.2015.04.045.  
  
H. S. Lee, “GS-align for glycan structure alignment and similarity measurement”, *Bioinformatics*, vol. 31, no. 16. Oxford University Press (OUP), pp. 2653–2659, Apr. 08, 2015. doi: 10.1093/bioinformatics/btv202.  
  
H. S. Lee, Y. Qiand W. Im, “Effects of N-glycosylation on protein conformation and dynamics: Protein Data Bank analysis and molecular dynamics simulation study”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, Mar. 09, 2015. doi: 10.1038/srep08926.  
  
H. S. Lee, C. Seokand W. Im, “Potential Application of Alchemical Free Energy Simulations to Discriminate GPCR Ligand Efficacy”, *Journal of Chemical Theory and Computation*, vol. 11, no. 3. American Chemical Society (ACS), pp. 1255–1266, Feb. 27, 2015. doi: 10.1021/ct5008907.  
  
S. Park, A. H. Beaven, J. B. Klaudaand W. Im, “How Tolerant are Membrane Simulations with Mismatch in Area per Lipid between Leaflets?”, *Journal of Chemical Theory and Computation*, vol. 11, no. 7. American Chemical Society (ACS), pp. 3466–3477, Jun. 05, 2015. doi: 10.1021/acs.jctc.5b00232.  
  
L. G. AbdulHalim, “Ag29(BDT)12(TPP)4: A Tetravalent Nanocluster”, *Journal of the American Chemical Society*, vol. 137, no. 37. American Chemical Society (ACS), pp. 11970–11975, Jul. 07, 2015. doi: 10.1021/jacs.5b04547.  
  
M. M. Alvarez, “Hidden Components in Aqueous “Gold-144” Fractionated by PAGE: High-Resolution Orbitrap ESI-MS Identifies the Gold-102 and Higher All-Aromatic Au-*p*MBA Cluster Compounds”, *The Journal of Physical Chemistry B*, vol. 120, no. 26. American Chemical Society (ACS), pp. 6430–6438, Jun. 15, 2016. doi: 10.1021/acs.jpcb.6b04525.  
  
S. M. Aly, L. G. AbdulHalim, T. M. D. Besong, G. Soldan, O. M. Bakrand O. F. Mohammed, “Ultrafast static and diffusion-controlled electron transfer at Ag29 nanocluster/molecular acceptor interfaces”, *Nanoscale*, vol. 8, no. 10. Royal Society of Chemistry (RSC), pp. 5412–5416, 2016. doi: 10.1039/c5nr05328e.  
  
B. T. Andrews and C. E. Catalano, “The Enzymology of a Viral Genome Packaging Motor Is Influenced by the Assembly State of the Motor Subunits”, *Biochemistry*, vol. 51, no. 46. American Chemical Society (ACS), pp. 9342–9353, Nov. 07, 2012. doi: 10.1021/bi300890y.  
  
P. Anzini, “Controlling Self-Assembly of a Peptide-Based Material via Metal-Ion Induced Registry Shift”, *Journal of the American Chemical Society*, vol. 135, no. 28. American Chemical Society (ACS), pp. 10278–10281, Jul. 09, 2013. doi: 10.1021/ja404677c.  
  
S. C. Atkinson, L. Hor, C. Dogovski, R. C. J. Dobsonand M. A. Perugini, “Identification of the*bona fide*DHDPS from a common plant pathogen”, *Proteins: Structure, Function, and Bioinformatics*, vol. 82, no. 9. Wiley, pp. 1869–1883, Jun. 11, 2014. doi: 10.1002/prot.24539.  
  
N. M. Baker, S. Weigand, S. Maar-Mathiasand A. Mondragón, “Solution structures of DNA-bound gyrase”, *Nucleic Acids Research*, vol. 39, no. 2. Oxford University Press (OUP), pp. 755–766, Sep. 23, 2010. doi: 10.1093/nar/gkq799.  
  
A. Ballandras-Colas, “Cryo-EM reveals a novel octameric integrase structure for betaretroviral intasome function”, *Nature*, vol. 530, no. 7590. Springer Science and Business Media LLC, pp. 358–361, Feb. 2016. doi: 10.1038/nature16955.  
  
A. Bepperling, “Alternative bacterial two-component small heat shock protein systems”, *Proceedings of the National Academy of Sciences*, vol. 109, no. 50. Proceedings of the National Academy of Sciences, pp. 20407–20412, Nov. 26, 2012. doi: 10.1073/pnas.1209565109.  
  
A. Bhattacharya, “Structural basis of HIV-1 capsid recognition by PF74 and CPSF6”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 52. Proceedings of the National Academy of Sciences, pp. 18625–18630, Dec. 17, 2014. doi: 10.1073/pnas.1419945112.  
  
A. Bhattacharya, “Effects of T592 phosphomimetic mutations on tetramer stability and dNTPase activity of SAMHD1 can not explain the retroviral restriction defect”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Aug. 11, 2016. doi: 10.1038/srep31353.  
  
M. S. Bootharaju, “Reversible Size Control of Silver Nanoclusters via Ligand-Exchange”, *Chemistry of Materials*, vol. 27, no. 12. American Chemical Society (ACS), pp. 4289–4297, Jun. 05, 2015. doi: 10.1021/acs.chemmater.5b00650.  
  
R. C. Boswell-Casteel, J. M. Johnson, K. D. Duggan, Y. Tsutsuiand F. A. Hays, “Overproduction and biophysical characterization of human HSP70 proteins”, *Protein Expression and Purification*, vol. 106. Elsevier BV, pp. 57–65, Feb. 2015. doi: 10.1016/j.pep.2014.09.013.  
  
A. Brandariz-Nuñez, “Contribution of oligomerization to the anti-HIV-1 properties of SAMHD1”, *Retrovirology*, vol. 10, no. 1. Springer Science and Business Media LLC, Nov. 12, 2013. doi: 10.1186/1742-4690-10-131.  
  
E. H. Brookes, N. Anjum, J. E. Curtis, S. Marru, R. Singhand M. Pierce, “GenApp Module Execution and Airavata Integration”, *2014 9th Gateway Computing Environments Workshop*. IEEE, Nov. 2014. doi: 10.1109/gce.2014.12.  
  
E. H. Brookes and B. Demeler, “Performance optimization of large non-negatively constrained least squares problems with an application in biophysics”, *Proceedings of the 2010 TeraGrid Conference*. ACM, Aug. 02, 2010. doi: 10.1145/1838574.1838579.  
  
E. Brookes, B. Demelerand M. Rocco, “Developments in the US-SOMO Bead Modeling Suite: New Features in the Direct Residue-to-Bead Method, Improved Grid Routines, and Influence of Accessible Surface Area Screening”, *Macromolecular Bioscience*, vol. 10, no. 7. Wiley, pp. 746–753, May 17, 2010. doi: 10.1002/mabi.200900474.  
  
E. Brookes, J. Pérez, B. Cardinali, A. Profumo, P. Vachetteand M. Rocco, “Fibrinogen species as resolved by HPLC-SAXS data processing within the*UltraScan Solution Modeler*(*US-SOMO*) enhanced SAS module”, *Journal of Applied Crystallography*, vol. 46, no. 6. International Union of Crystallography (IUCr), pp. 1823–1833, Nov. 15, 2013. doi: 10.1107/s0021889813027751.  
  
E. Brookes, R. Singh, M. Pierce, S. Marru, B. Demelerand M. Rocco, “Ultrascan solution modeler”, *Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment: Bridging from the eXtreme to the campus and beyond*. ACM, Jul. 16, 2012. doi: 10.1145/2335755.2335839.  
  
E. Brookes, R. Singh, M. Pierce, S. Marru, B. Demelerand M. Rocco, “US-SOMO cluster methods”, *Proceedings of the Conference on Extreme Science and Engineering Discovery Environment: Gateway to Discovery*. ACM, Jul. 22, 2013. doi: 10.1145/2484762.2484815.  
  
D. J. Catanese Jr. and K. S. Matthews, “Disconnected Interacting Protein 1 binds with high affinity to pre-tRNA and ADAT”, *Biochemical and Biophysical Research Communications*, vol. 414, no. 3. Elsevier BV, pp. 506–511, Oct. 2011. doi: 10.1016/j.bbrc.2011.09.096.  
  
J. Chen, M. J. Feige, T. M. Franzmann, A. Bepperlingand J. Buchner, “Regions Outside the α-Crystallin Domain of the Small Heat Shock Protein Hsp26 Are Required for Its Dimerization”, *Journal of Molecular Biology*, vol. 398, no. 1. Elsevier BV, pp. 122–131, Apr. 2010. doi: 10.1016/j.jmb.2010.02.022.  
  
B. M. Childers, X. Cao, G. G. Weber, B. Demeler, P. J. Hartand K. E. Klose, “N-terminal Residues of the Vibrio cholerae Virulence Regulatory Protein ToxT Involved in Dimerization and Modulation by Fatty Acids”, *Journal of Biological Chemistry*, vol. 286, no. 32. Elsevier BV, pp. 28644–28655, Aug. 2011. doi: 10.1074/jbc.m111.258780.  
  
J. V. Chodaparambil, “Molecular functions of the TLE tetramerization domain in Wnt target gene repression”, *The EMBO Journal*, vol. 33, no. 7. Wiley, pp. 719–731, Mar. 03, 2014. doi: 10.1002/embj.201387188.  
  
N. J. Clark, M. Kramer, U. M. Muthurajanand K. Luger, “Alternative Modes of Binding of Poly(ADP-ribose) Polymerase 1 to Free DNA and Nucleosomes”, *Journal of Biological Chemistry*, vol. 287, no. 39. Elsevier BV, pp. 32430–32439, Sep. 2012. doi: 10.1074/jbc.m112.397067.  
  
D. W. Cockburn, “Molecular details of a starch utilization pathway in the human gut symbiont*Eubacterium rectale*”, *Molecular Microbiology*, vol. 95, no. 2. Wiley, pp. 209–230, Dec. 19, 2014. doi: 10.1111/mmi.12859.  
  
D. Comoletti, “The Macromolecular Architecture of Extracellular Domain of αNRXN1: Domain Organization, Flexibility, and Insights into Trans-Synaptic Disposition”, *Structure*, vol. 18, no. 8. Elsevier BV, pp. 1044–1053, Aug. 2010. doi: 10.1016/j.str.2010.06.005.  
  
H. Danjo, “Assembly Modulation by Adjusting Countercharges of Heterobimetallic Supramolecular Polymers Composed of Tris(spiroborate) Twin Bowls”, *Journal of the American Chemical Society*, vol. 132, no. 44. American Chemical Society (ACS), pp. 15556–15558, Oct. 20, 2010. doi: 10.1021/ja1084964.  
  
B. Demeler, “Methods for the Design and Analysis of Sedimentation Velocity and Sedimentation Equilibrium Experiments with Proteins”, *Current Protocols in Protein Science*, vol. 60, no. 1. Wiley, Apr. 2010. doi: 10.1002/0471140864.ps0713s60.  
  
B. Demeler, E. Brookes, R. Wang, V. Schirfand C. A. Kim, “Characterization of Reversible Associations by Sedimentation Velocity with UltraScan”, *Macromolecular Bioscience*, vol. 10, no. 7. Wiley, pp. 775–782, Jun. 21, 2010. doi: 10.1002/mabi.200900481.  
  
B. Demeler, “Characterization of Size, Anisotropy, and Density Heterogeneity of Nanoparticles by Sedimentation Velocity”, *Analytical Chemistry*, vol. 86, no. 15. American Chemical Society (ACS), pp. 7688–7695, Jul. 18, 2014. doi: 10.1021/ac501722r.  
  
B. Demeler, R. Singh, M. Pierce, E. H. Brookes, S. Marruand B. Dubbs, “UltraScan gateway enhancements”, *Proceedings of the 2011 TeraGrid Conference: Extreme Digital Discovery*. ACM, Jul. 18, 2011. doi: 10.1145/2016741.2016778.  
  
L. R. English, A. Tischer, A. K. Demeler, B. Demelerand S. T. Whitten, “Sequence Reversal Prevents Chain Collapse and Yields Heat-Sensitive Intrinsic Disorder”, *Biophysical Journal*, vol. 115, no. 2. Elsevier BV, pp. 328–340, Jul. 2018. doi: 10.1016/j.bpj.2018.06.006.  
  
O. S. Fisher, R. Zhang, X. Li, J. W. Murphy, B. Demelerand T. J. Boggon, “Structural studies of cerebral cavernous malformations 2 (CCM2) reveal a folded helical domain at its C-terminus”, *FEBS Letters*, vol. 587, no. 3. Wiley, pp. 272–277, Dec. 22, 2012. doi: 10.1016/j.febslet.2012.12.011.  
  
T. M. Franzmann, A. Czekallaand S. G. Walter, “Regulatory Circuits of the AAA+ Disaggregase Hsp104”, *Journal of Biological Chemistry*, vol. 286, no. 20. Elsevier BV, pp. 17992–18001, May 2011. doi: 10.1074/jbc.m110.216176.  
  
M. Gabrielsen, K. S. H. Beckham, R. J. Cogdell, O. Byronand A. J. Roe, “FolX from*Pseudomonas aeruginosa*is octameric in both crystal and solution”, *FEBS Letters*, vol. 586, no. 8. Wiley, pp. 1160–1165, Mar. 24, 2012. doi: 10.1016/j.febslet.2012.03.031.  
  
R. P. Ghosh, “Unique Physical Properties and Interactions of the Domains of Methylated DNA Binding Protein 2”, *Biochemistry*, vol. 49, no. 20. American Chemical Society (ACS), pp. 4395–4410, Apr. 28, 2010. doi: 10.1021/bi9019753.  
  
J. M. Gilmore, “Determinants of Affinity and Activity of the Anti-Sigma Factor AsiA”, *Biochemistry*, vol. 49, no. 29. American Chemical Society (ACS), pp. 6143–6154, Jun. 30, 2010. doi: 10.1021/bi1002635.  
  
G. Gorbet, “A Parametrically Constrained Optimization Method for Fitting Sedimentation Velocity Experiments”, *Biophysical Journal*, vol. 106, no. 8. Elsevier BV, pp. 1741–1750, Apr. 2014. doi: 10.1016/j.bpj.2014.02.022.  
  
G. E. Gorbet, S. Mohapatraand B. Demeler, “Multi-speed sedimentation velocity implementation in UltraScan-III”, *European Biophysics Journal*, vol. 47, no. 7. Springer Science and Business Media LLC, pp. 825–835, Apr. 02, 2018. doi: 10.1007/s00249-018-1297-z.  
  
G. E. Gorbet, J. Z. Pearson, A. K. Demeler, H. Cölfenand B. Demeler, “Next-Generation AUC”, *Methods in Enzymology*. Elsevier, pp. 27–47, 2015. doi: 10.1016/bs.mie.2015.04.013.  
  
L. Gu, “Tandem Acyl Carrier Proteins in the Curacin Biosynthetic Pathway Promote Consecutive Multienzyme Reactions with a Synergistic Effect”, *Angewandte Chemie International Edition*, vol. 50, no. 12. Wiley, pp. 2795–2798, Mar. 14, 2011. doi: 10.1002/anie.201005280.  
  
D. B. Halling, S. A. Kenrick, A. F. Riggsand R. W. Aldrich, “Calcium-dependent stoichiometries of the KCa2.2 (SK) intracellular domain/calmodulin complex in solution”, *Journal of General Physiology*, vol. 143, no. 2. Rockefeller University Press, pp. 231–252, Jan. 13, 2014. doi: 10.1085/jgp.201311007.  
  
K. M. Harkness, “Ag44(SR)304−: a silver–thiolate superatom complex”, *Nanoscale*, vol. 4, no. 14. Royal Society of Chemistry (RSC), p. 4269, 2012. doi: 10.1039/c2nr30773a.  
  
K. Hochdörffer, “Rational Design of β-Sheet Ligands Against Aβ42-Induced Toxicity”, *Journal of the American Chemical Society*, vol. 133, no. 12. American Chemical Society (ACS), pp. 4348–4358, Mar. 07, 2011. doi: 10.1021/ja107675n.  
  
A. A. Jalan, B. Demelerand J. D. Hartgerink, “Hydroxyproline-Free Single Composition ABC Collagen Heterotrimer”, *Journal of the American Chemical Society*, vol. 135, no. 16. American Chemical Society (ACS), pp. 6014–6017, Apr. 15, 2013. doi: 10.1021/ja402187t.  
  
C. N. Johnson, G. E. Gorbet, H. Ramsower, J. Urquidi, L. Brancaleonand B. Demeler, “Multi-wavelength analytical ultracentrifugation of human serum albumin complexed with porphyrin”, *European Biophysics Journal*, vol. 47, no. 7. Springer Science and Business Media LLC, pp. 789–797, Apr. 19, 2018. doi: 10.1007/s00249-018-1301-7.  
  
S. E. Junco, “Structure of the Polycomb Group Protein PCGF1 in Complex with BCOR Reveals Basis for Binding Selectivity of PCGF Homologs”, *Structure*, vol. 21, no. 4. Elsevier BV, pp. 665–671, Apr. 2013. doi: 10.1016/j.str.2013.02.013.  
  
T. S. Kaoud, “Activated ERK2 Is a Monomer in Vitro with or without Divalent Cations and When Complexed to the Cytoplasmic Scaffold PEA-15”, *Biochemistry*, vol. 50, no. 21. American Chemical Society (ACS), pp. 4568–4578, May 04, 2011. doi: 10.1021/bi200202y.  
  
E. Karabudak, “Simultaneous Identification of Spectral Properties and Sizes of Multiple Particles in Solution with Subnanometer Resolution”, *Angewandte Chemie International Edition*, vol. 55, no. 39. Wiley, pp. 11770–11774, Jul. 27, 2016. doi: 10.1002/anie.201603844.  
  
F. Kateb, “Structural and Functional Analysis of the DEAF-1 and BS69 MYND Domains”, *PLoS ONE*, vol. 8, no. 1. Public Library of Science (PLoS), p. e54715, Jan. 25, 2013. doi: 10.1371/journal.pone.0054715.  
  
H. Kim, E. Brookes, W. Caoand B. Demeler, “Two-dimensional grid optimization for sedimentation velocity analysis in the analytical ultracentrifuge”, *European Biophysics Journal*, vol. 47, no. 7. Springer Science and Business Media LLC, pp. 837–844, May 17, 2018. doi: 10.1007/s00249-018-1309-z.  
  
H. Kim, E. H. Brookesand B. Demeler, “A performance predictor for UltraScan supercomputer calculations”, *Proceedings of the 2015 XSEDE Conference on Scientific Advancements Enabled by Enhanced Cyberinfrastructure - XSEDE ‘15*. ACM Press, 2015. doi: 10.1145/2792745.2792787.  
  
B. J. Klein, “Bivalent interaction of the PZP domain of BRPF1 with the nucleosome impacts chromatin dynamics and acetylation”, *Nucleic Acids Research*, vol. 44, no. 1. Oxford University Press (OUP), pp. 472–484, Nov. 30, 2015. doi: 10.1093/nar/gkv1321.  
  
E. Krayukhina, S. Uchiyamaand K. Fukui, “Effects of rotational speed on the hydrodynamic properties of pharmaceutical antibodies measured by analytical ultracentrifugation sedimentation velocity”, *European Journal of Pharmaceutical Sciences*, vol. 47, no. 2. Elsevier BV, pp. 367–374, Sep. 2012. doi: 10.1016/j.ejps.2012.06.005.  
  
T. Laue and B. Demeler, “A postreductionist framework for protein biochemistry”, *Nature Chemical Biology*, vol. 7, no. 6. Springer Science and Business Media LLC, pp. 331–334, May 17, 2011. doi: 10.1038/nchembio.575.  
  
J. Lee, “Computationally Designed Peptide Inhibitors of the Ubiquitin E3 Ligase SCFFbx4”, *ChemBioChem*, vol. 14, no. 4. Wiley, pp. 445–451, Feb. 11, 2013. doi: 10.1002/cbic.201200777.  
  
S. Lee, “The E2 Domains of APP and APLP1 Share a Conserved Mode of Dimerization”, *Biochemistry*, vol. 50, no. 24. American Chemical Society (ACS), pp. 5453–5464, May 26, 2011. doi: 10.1021/bi101846x.  
  
H. T. Le, R. Buscaglia, W. L. Dean, J. B. Chairesand J. O. Trent, “Calculation of Hydrodynamic Properties for G-Quadruplex Nucleic Acid Structures from in silico Bead Models”, *Topics in Current Chemistry*. Springer Berlin Heidelberg, pp. 179–210, 2012. doi: 10.1007/128\_2012\_351.  
  
H. T. Le, “Not all G-quadruplexes are created equally: an investigation of the structural polymorphism of the c-Myc G-quadruplex-forming sequence and its interaction with the porphyrin TMPyP4”, *Organic & Biomolecular Chemistry*, vol. 10, no. 47. Royal Society of Chemistry (RSC), p. 9393, 2012. doi: 10.1039/c2ob26504d.  
  
J. A. Lemkul, A. Savelyevand A. D. MacKerell Jr, “Towards a Polarizable Force Field for RNA based on the Classical Drude Oscillator”, *Biophysical Journal*, vol. 108, no. 2. Elsevier BV, p. 159a, Jan. 2015. doi: 10.1016/j.bpj.2014.11.875.  
  
J. Li, K. Richterand J. Buchner, “Mixed Hsp90–cochaperone complexes are important for the progression of the reaction cycle”, *Nature Structural & Molecular Biology*, vol. 18, no. 1. Springer Science and Business Media LLC, pp. 61–66, Dec. 19, 2010. doi: 10.1038/nsmb.1965.  
  
A.-P. Lin, “Construction and Analyses of Tetrameric Forms of Yeast NAD+-Specific Isocitrate Dehydrogenase”, *Biochemistry*, vol. 50, no. 2. American Chemical Society (ACS), pp. 230–239, Dec. 22, 2010. doi: 10.1021/bi101401h.  
  
P. E. M. Lopes, “Development of a Polarizable Force Field for Macromolecules Based on the Classical Drude Oscillator”, *Biophysical Journal*, vol. 106, no. 2. Elsevier BV, p. 43a, Jan. 2014. doi: 10.1016/j.bpj.2013.11.318.  
  
E. M. Medina, B. T. Andrews, E. Nakataniand C. E. Catalano, “The Bacteriophage Lambda gpNu3 Scaffolding Protein Is an Intrinsically Disordered and Biologically Functional Procapsid Assembly Catalyst”, *Journal of Molecular Biology*, vol. 412, no. 4. Elsevier BV, pp. 723–736, Sep. 2011. doi: 10.1016/j.jmb.2011.07.045.  
  
M. Merdanovic, “Determinants of structural and functional plasticity of a widely conserved protease chaperone complex”, *Nature Structural & Molecular Biology*, vol. 17, no. 7. Springer Science and Business Media LLC, pp. 837–843, Jun. 27, 2010. doi: 10.1038/nsmb.1839.  
  
U. M. Muthurajan, “Automodification switches PARP-1 function from chromatin architectural protein to histone chaperone”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 35. Proceedings of the National Academy of Sciences, pp. 12752–12757, Aug. 18, 2014. doi: 10.1073/pnas.1405005111.  
  
U. M. Muthurajan, S. J. McBryant, X. Lu, J. C. Hansenand K. Luger, “The Linker Region of MacroH2A Promotes Self-association of Nucleosomal Arrays”, *Journal of Biological Chemistry*, vol. 286, no. 27. Elsevier BV, pp. 23852–23864, Jul. 2011. doi: 10.1074/jbc.m111.244871.  
  
J. Nardozzi, N. Wenta, N. Yasuhara, U. Vinkemeierand G. Cingolani, “Molecular Basis for the Recognition of Phosphorylated STAT1 by Importin α5”, *Journal of Molecular Biology*, vol. 402, no. 1. Elsevier BV, pp. 83–100, Sep. 2010. doi: 10.1016/j.jmb.2010.07.013.  
  
M. Noda, “Assembly states of the nucleosome assembly protein 1 (NAP-1) revealed by sedimentation velocity and non-denaturing MS”, *Biochemical Journal*, vol. 436, no. 1. Portland Press Ltd., pp. 101–112, Apr. 27, 2011. doi: 10.1042/bj20102063.  
  
S. P. Panda, “Intra- and inter-molecular effects of a conserved arginine residue of neuronal and inducible nitric oxide synthases on FMN and calmodulin binding”, *Archives of Biochemistry and Biophysics*, vol. 533, no. 1–2. Elsevier BV, pp. 88–94, May 2013. doi: 10.1016/j.abb.2013.03.004.  
  
G. Panza, “Molecular Interactions between Prions as Seeds and Recombinant Prion Proteins as Substrates Resemble the Biological Interspecies Barrier In Vitro”, *PLoS ONE*, vol. 5, no. 12. Public Library of Science (PLoS), p. e14283, Dec. 09, 2010. doi: 10.1371/journal.pone.0014283.  
  
D. P. Patterson, M. Su, T. M. Franzmann, A. Sciore, G. Skiniotisand E. N. G. Marsh, “Characterization of a highly flexible self-assembling protein system designed to form nanocages”, *Protein Science*, vol. 23, no. 2. Wiley, pp. 190–199, Dec. 16, 2013. doi: 10.1002/pro.2405.  
  
J. Z. Pearson, F. Krause, D. Haffke, B. Demeler, K. Schillingand H. Cölfen, “Next-Generation AUC Adds a Spectral Dimension”, *Methods in Enzymology*. Elsevier, pp. 1–26, 2015. doi: 10.1016/bs.mie.2015.06.033.  
  
J. D. Pham, B. Demelerand J. S. Nowick, “Polymorphism of Oligomers of a Peptide from β-Amyloid”, *Journal of the American Chemical Society*, vol. 136, no. 14. American Chemical Society (ACS), pp. 5432–5442, Mar. 26, 2014. doi: 10.1021/ja500996d.  
  
M. Pierce, S. Marru, B. Demeler, R. Singhand G. Gorbet, “The Apache Airavata Application Programming Interface: Overview and Evaluation with the UltraScan Science Gateway”, *2014 9th Gateway Computing Environments Workshop*. IEEE, Nov. 2014. doi: 10.1109/gce.2014.15.  
  
G. Plascencia-Villa, “Analytical Characterization of Size-Dependent Properties of Larger Aqueous Gold Nanoclusters”, *The Journal of Physical Chemistry C*, vol. 120, no. 16. American Chemical Society (ACS), pp. 8950–8958, Apr. 15, 2016. doi: 10.1021/acs.jpcc.6b00448.  
  
F. M. Ranaivoson, “Structural and Mechanistic Insights into the Latrophilin3-FLRT3 Complex that Mediates Glutamatergic Synapse Development”, *Structure*, vol. 23, no. 9. Elsevier BV, pp. 1665–1677, Sep. 2015. doi: 10.1016/j.str.2015.06.022.  
  
M. S. Rana and A. F. Riggs, “Indefinite noncooperative self-association of chicken deoxy hemoglobin D”, *Proteins: Structure, Function, and Bioinformatics*, vol. 79, no. 5. Wiley, pp. 1499–1512, Feb. 18, 2011. doi: 10.1002/prot.22978.  
  
M. Retzlaff, “The Regulatory Domain Stabilizes the p53 Tetramer by Intersubunit Contacts with the DNA Binding Domain”, *Journal of Molecular Biology*, vol. 425, no. 1. Elsevier BV, pp. 144–155, Jan. 2013. doi: 10.1016/j.jmb.2012.10.015.  
  
A. K. Robinson, “The Growth-Suppressive Function of the Polycomb Group Protein Polyhomeotic Is Mediated by Polymerization of Its Sterile Alpha Motif (SAM) Domain”, *Journal of Biological Chemistry*, vol. 287, no. 12. Elsevier BV, pp. 8702–8713, Mar. 2012. doi: 10.1074/jbc.m111.336115.  
  
A. K. Robinson, “Human Polyhomeotic Homolog 3 (PHC3) Sterile Alpha Motif (SAM) Linker Allows Open-Ended Polymerization of PHC3 SAM”, *Biochemistry*, vol. 51, no. 27. American Chemical Society (ACS), pp. 5379–5386, Jun. 28, 2012. doi: 10.1021/bi3004318.  
  
M. Rocco and E. Brookes, “Dynamical Aspects of Biomacromolecular Multi-resolution Modelling Using the UltraScan Solution Modeler (US-SOMO) Suite”, *NATO Science for Peace and Security Series A: Chemistry and Biology*. Springer Netherlands, pp. 189–199, Dec. 23, 2013. doi: 10.1007/978-94-017-8550-1\_13.  
  
C. Rosano and M. Rocco, “Solution properties of full-length integrin αIIbβ3 refined models suggest environment-dependent induction of alternative bent /extended resting states”, *FEBS Journal*, vol. 277, no. 15. Wiley, pp. 3190–3202, Jun. 24, 2010. doi: 10.1111/j.1742-4658.2010.07724.x.  
  
E. N. Rubio-Marrero, “Structural Characterization of the Extracellular Domain of CASPR2 and Insights into Its Association with the Novel Ligand Contactin1”, *Journal of Biological Chemistry*, vol. 291, no. 11. Elsevier BV, pp. 5788–5802, Mar. 2016. doi: 10.1074/jbc.m115.705681.  
  
Y. Ruff, T. Moyer, C. J. Newcomb, B. Demelerand S. I. Stupp, “Precision Templating with DNA of a Virus-like Particle with Peptide Nanostructures”, *Journal of the American Chemical Society*, vol. 135, no. 16. American Chemical Society (ACS), pp. 6211–6219, Apr. 10, 2013. doi: 10.1021/ja4008003.  
  
P. J. Salveson, “Correction to “Repurposing Triphenylmethane Dyes To Bind to Trimers Derived from Aβ””, *Journal of the American Chemical Society*, vol. 140, no. 45. American Chemical Society (ACS), pp. 15546–15546, Nov. 05, 2018. doi: 10.1021/jacs.8b11195.  
  
P. J. Salveson, “Repurposing Triphenylmethane Dyes to Bind to Trimers Derived from Aβ”, *Journal of the American Chemical Society*, vol. 140, no. 37. American Chemical Society (ACS), pp. 11745–11754, Aug. 20, 2018. doi: 10.1021/jacs.8b06568.  
  
R. Y. Samson, “Specificity and Function of Archaeal DNA Replication Initiator Proteins”, *Cell Reports*, vol. 3, no. 2. Elsevier BV, pp. 485–496, Feb. 2013. doi: 10.1016/j.celrep.2013.01.002.  
  
K. Sathiyamoorthy, E. Mills, T. M. Franzmann, I. Rosenshineand M. A. Saper, “The Crystal Structure of *Escherichia coli* Group 4 Capsule Protein GfcC Reveals a Domain Organization Resembling That of Wza”, *Biochemistry*, vol. 50, no. 24. American Chemical Society (ACS), pp. 5465–5476, May 27, 2011. doi: 10.1021/bi101869h.  
  
A. Savelyev and A. Mackerell, “CHARMM Drude Polarizable MD Simulations Reproduce Solution X-Ray Diffraction Patterns for B-DNA Sequences and Predict Differential Impact of the Li+, Na+, K+ and Rb+ Ions on DNA Conformational Properties”, *Biophysical Journal*, vol. 108, no. 2. Elsevier BV, p. 231a, Jan. 2015. doi: 10.1016/j.bpj.2014.11.1278.  
  
A. Savelyev and A. D. MacKerell Jr., “Competition among Li+, Na+, K+, and Rb+Monovalent Ions for DNA in Molecular Dynamics Simulations Using the Additive CHARMM36 and Drude Polarizable Force Fields”, *The Journal of Physical Chemistry B*, vol. 119, no. 12. American Chemical Society (ACS), pp. 4428–4440, Mar. 18, 2015. doi: 10.1021/acs.jpcb.5b00683.  
  
S. V. Seetharaman, “Disrupted Zinc-Binding Sites in Structures of Pathogenic SOD1 Variants D124V and H80R”, *Biochemistry*, vol. 49, no. 27. American Chemical Society (ACS), pp. 5714–5725, Jun. 17, 2010. doi: 10.1021/bi100314n.  
  
E. Smirnova, “A new mode of SAM domain mediated oligomerization observed in the CASKIN2 neuronal scaffolding protein”, *Cell Communication and Signaling*, vol. 14, no. 1. Springer Science and Business Media LLC, Aug. 22, 2016. doi: 10.1186/s12964-016-0140-3.  
  
O. W. Sterritt, “Structural and functional characterisation of the entry point to pyocyanin biosynthesis in *Pseudomonas aeruginosa* defines a new 3-deoxy-d-arabino-heptulosonate 7-phosphate synthase subclass”, *Bioscience Reports*, vol. 38, no. 5. Portland Press Ltd., Oct. 17, 2018. doi: 10.1042/bsr20181605.  
  
S. G. Swygert, “Solution-state conformation and stoichiometry of yeast Sir3 heterochromatin fibres”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, Aug. 28, 2014. doi: 10.1038/ncomms5751.  
  
H. J. Szerlong, J. E. Prenni, J. K. Nyborgand J. C. Hansen, “Activator-dependent p300 Acetylation of Chromatin in Vitro”, *Journal of Biological Chemistry*, vol. 285, no. 42. Elsevier BV, pp. 31954–31964, Oct. 2010. doi: 10.1074/jbc.m110.148718.  
  
M. Takacs, “The Asymmetric Binding of PGC-1α to the ERRα and ERRγ Nuclear Receptor Homodimers Involves a Similar Recognition Mechanism”, *PLoS ONE*, vol. 8, no. 7. Public Library of Science (PLoS), p. e67810, Jul. 09, 2013. doi: 10.1371/journal.pone.0067810.  
  
Y. Tsutsui, J. M. Johnson, B. Demeler, M. T. Kinterand F. A. Hays, “Conformation-Dependent Human p52Shc Phosphorylation by Human c-Src”, *Biochemistry*, vol. 54, no. 22. American Chemical Society (ACS), pp. 3469–3482, May 26, 2015. doi: 10.1021/acs.biochem.5b00122.  
  
J. L. Urbauer, A. B. Cowley, H. P. Broussard, H. T. Niedermaierand R. J. Bieber Urbauer, “Solution structure and properties of AlgH from*Pseudomonas aeruginosa*”, *Proteins: Structure, Function, and Bioinformatics*, vol. 83, no. 6. Wiley, pp. 1137–1150, Apr. 29, 2015. doi: 10.1002/prot.24811.  
  
O. D. Villarreal, L. Y. Chen, R. L. Whettenand B. Demeler, “Aspheric Solute Ions Modulate Gold Nanoparticle Interactions in an Aqueous Solution: An Optimal Way To Reversibly Concentrate Functionalized Nanoparticles”, *The Journal of Physical Chemistry B*, vol. 119, no. 50. American Chemical Society (ACS), pp. 15502–15508, Dec. 03, 2015. doi: 10.1021/acs.jpcb.5b09864.  
  
J. Walter, G. Gorbet, T. Akdas, D. Segets, B. Demelerand W. Peukert, “2D analysis of polydisperse core–shell nanoparticles using analytical ultracentrifugation”, *The Analyst*, vol. 142, no. 1. Royal Society of Chemistry (RSC), pp. 206–217, 2017. doi: 10.1039/c6an02236g.  
  
R. Wang, “Polycomb Group Targeting through Different Binding Partners of RING1B C-Terminal Domain”, *Structure*, vol. 18, no. 8. Elsevier BV, pp. 966–975, Aug. 2010. doi: 10.1016/j.str.2010.04.013.  
  
W. Wang, C. Damm, J. Walter, T. J. Nackenand W. Peukert, “Photobleaching and stabilization of carbon nanodots produced by solvothermal synthesis”, *Physical Chemistry Chemical Physics*, vol. 18, no. 1. Royal Society of Chemistry (RSC), pp. 466–475, 2016. doi: 10.1039/c5cp04942c.  
  
Z. Wang, “Functionality of Redox-Active Cysteines Is Required for Restriction of Retroviral Replication by SAMHD1”, *Cell Reports*, vol. 24, no. 4. Elsevier BV, pp. 815–823, Jul. 2018. doi: 10.1016/j.celrep.2018.06.090.  
  
S. Watanabe, “Structural characterization of H3K56Q nucleosomes and nucleosomal arrays”, *Biochimica et Biophysica Acta (BBA) - Gene Regulatory Mechanisms*, vol. 1799, no. 5–6. Elsevier BV, pp. 480–486, May 2010. doi: 10.1016/j.bbagrm.2010.01.009.  
  
N. Wenta and U. Vinkemeier, “Characterization of STAT Self-Association by Analytical Ultracentrifugation”, *Methods in Molecular Biology*. Humana Press, pp. 203–224, Nov. 04, 2012. doi: 10.1007/978-1-62703-242-1\_15.  
  
T. L. Williams, G. E. Gorbetand B. Demeler, “Multi-speed sedimentation velocity simulations with UltraScan-III”, *European Biophysics Journal*, vol. 47, no. 7. Springer Science and Business Media LLC, pp. 815–823, May 10, 2018. doi: 10.1007/s00249-018-1308-0.  
  
D. D. Winkler, U. M. Muthurajan, A. R. Hieband K. Luger, “Histone Chaperone FACT Coordinates Nucleosome Interaction through Multiple Synergistic Binding Events”, *Journal of Biological Chemistry*, vol. 286, no. 48. Elsevier BV, pp. 41883–41892, Dec. 2011. doi: 10.1074/jbc.m111.301465.  
  
S. J. Wong, “KDM2B Recruitment of the Polycomb Group Complex, PRC1.1, Requires Cooperation between PCGF1 and BCORL1”, *Structure*, vol. 24, no. 10. Elsevier BV, pp. 1795–1801, Oct. 2016. doi: 10.1016/j.str.2016.07.011.  
  
F. Xiao, B. Demelerand P. Guo, “Assembly Mechanism of the Sixty-Subunit Nanoparticles *via* Interaction of RNA with the Reengineered Protein Connector of phi29 DNA-Packaging Motor”, *ACS Nano*, vol. 4, no. 6. American Chemical Society (ACS), pp. 3293–3301, May 28, 2010. doi: 10.1021/nn100158k.  
  
J. Xue, “The Role of Individual Carbohydrate-Binding Sites in the Function of the Potent Anti-HIV Lectin Griffithsin”, *Molecular Pharmaceutics*, vol. 9, no. 9. American Chemical Society (ACS), pp. 2613–2625, Aug. 21, 2012. doi: 10.1021/mp300194b.  
  
J. Xue, B. Hoorelbeke, I. Kagiampakis, B. Demeler, J. Balzariniand P. J. LiWang, “The Griffithsin Dimer Is Required for High-Potency Inhibition of HIV-1: Evidence for Manipulation of the Structure of gp120 as Part of the Griffithsin Dimer Mechanism”, *Antimicrobial Agents and Chemotherapy*, vol. 57, no. 8. American Society for Microbiology, pp. 3976–3989, Aug. 2013. doi: 10.1128/aac.00332-13.  
  
C. Yang, M. J. van der Woerd, U. M. Muthurajan, J. C. Hansenand K. Luger, “Biophysical analysis and small-angle X-ray scattering-derived structures of MeCP2–nucleosome complexes”, *Nucleic Acids Research*, vol. 39, no. 10. Oxford University Press (OUP), pp. 4122–4135, Jan. 29, 2011. doi: 10.1093/nar/gkr005.  
  
R. Yelagandula, “The Histone Variant H2A.W Defines Heterochromatin and Promotes Chromatin Condensation in Arabidopsis”, *Cell*, vol. 158, no. 1. Elsevier BV, pp. 98–109, Jul. 2014. doi: 10.1016/j.cell.2014.06.006.  
  
Z. Yudina, “RING Dimerization Links Higher-Order Assembly of TRIM5α to Synthesis of K63-Linked Polyubiquitin”, *Cell Reports*, vol. 12, no. 5. Elsevier BV, pp. 788–797, Aug. 2015. doi: 10.1016/j.celrep.2015.06.072.  
  
D. V. Zaytsev, “Nanometer to Millimeter Scale Peptide-Porphyrin Materials”, *Biomacromolecules*, vol. 11, no. 10. American Chemical Society (ACS), pp. 2602–2609, Aug. 30, 2010. doi: 10.1021/bm100540t.  
  
J. Zhang, “Spectral and Hydrodynamic Analysis of West Nile Virus RNA–Protein Interactions by Multiwavelength Sedimentation Velocity in the Analytical Ultracentrifuge”, *Analytical Chemistry*, vol. 89, no. 1. American Chemical Society (ACS), pp. 862–870, Dec. 15, 2016. doi: 10.1021/acs.analchem.6b03926.  
  
N. Zhang, Y. Jiang, Q. Mao, B. Demeler, Y. J. Taoand D. Pati, “Characterization of the Interaction between the Cohesin Subunits Rad21 and SA1/2”, *PLoS ONE*, vol. 8, no. 7. Public Library of Science (PLoS), p. e69458, Jul. 12, 2013. doi: 10.1371/journal.pone.0069458.  
  
S. Zhang, A. P. Hinckand P. F. Fitzpatrick, “The Amino Acid Specificity for Activation of Phenylalanine Hydroxylase Matches the Specificity for Stabilization of Regulatory Domain Dimers”, *Biochemistry*, vol. 54, no. 33. American Chemical Society (ACS), pp. 5167–5174, Aug. 13, 2015. doi: 10.1021/acs.biochem.5b00616.  
  
J. Zheng, C. D. Fage, B. Demeler, D. W. Hoffmanand A. T. Keatinge-Clay, “The Missing Linker: A Dimerization Motif Located within Polyketide Synthase Modules”, *ACS Chemical Biology*, vol. 8, no. 6. American Chemical Society (ACS), pp. 1263–1270, Mar. 25, 2013. doi: 10.1021/cb400047s.  
  
J. Zheng, D. C. Gay, B. Demeler, M. A. Whiteand A. T. Keatinge-Clay, “Divergence of multimodular polyketide synthases revealed by a didomain structure”, *Nature Chemical Biology*, vol. 8, no. 7. Springer Science and Business Media LLC, pp. 615–621, May 27, 2012. doi: 10.1038/nchembio.964.  
  
Y. Zhuo, “Dynamic Interactions between Clathrin and Locally Structured Elements in a Disordered Protein Mediate Clathrin Lattice Assembly”, *Journal of Molecular Biology*, vol. 404, no. 2. Elsevier BV, pp. 274–290, Nov. 2010. doi: 10.1016/j.jmb.2010.09.044.  
  
M. Green, L. Hatter, E. Brookes, P. Soultanasand D. J. Scott, “Defining the Intrinsically Disordered C-Terminal Domain of SSB Reveals DNA-Mediated Compaction”, *Journal of Molecular Biology*, vol. 428, no. 2. Elsevier BV, pp. 357–364, Jan. 2016. doi: 10.1016/j.jmb.2015.12.007.  
  
M. B. Hamaneh, L. Zhangand M. Buck, “A Direct Coupling between Global and Internal Motions in a Single Domain Protein? MD Investigation of Extreme Scenarios”, *Biophysical Journal*, vol. 101, no. 1. Elsevier BV, pp. 196–204, Jul. 2011. doi: 10.1016/j.bpj.2011.05.041.  
  
S. R. Ribone, M. A. Quevedo, M. Madridand M. C. Briñón, “Rational Approaches for the Design of Effective Human Immunodeficiency Virus Type 1 Nonnucleoside Reverse Transcriptase Inhibitors”, *Journal of Chemical Information and Modeling*, vol. 51, no. 1. American Chemical Society (ACS), pp. 130–138, Dec. 06, 2010. doi: 10.1021/ci1001636.  
  
S. R. Ribone, E. M. Schenfeld, M. Madrid, A. B. Pieriniand M. A. Quevedo, “Evaluation and synthesis of AZT prodrugs with optimized chemical stabilities: experimental and theoretical analyses”, *New J. Chem.*, vol. 40, no. 3. Royal Society of Chemistry (RSC), pp. 2383–2392, 2016. doi: 10.1039/c5nj03002a.  
  
E. Wierzbinski, “Effect of Backbone Flexibility on Charge Transfer Rates in Peptide Nucleic Acid Duplexes”, *Journal of the American Chemical Society*, vol. 134, no. 22. American Chemical Society (ACS), pp. 9335–9342, May 21, 2012. doi: 10.1021/ja301677z.  
  
C. F. Abrams and E. Vanden-Eijnden, “Large-scale conformational sampling of proteins using temperature-accelerated molecular dynamics”, *Proceedings of the National Academy of Sciences*, vol. 107, no. 11. Proceedings of the National Academy of Sciences, pp. 4961–4966, Mar. 2010. doi: 10.1073/pnas.0914540107.  
  
C. F. Abrams and E. Vanden-Eijnden, “On-the-fly free energy parameterization via temperature accelerated molecular dynamics”, *Chemical Physics Letters*, vol. 547. Elsevier BV, pp. 114–119, Sep. 2012. doi: 10.1016/j.cplett.2012.07.064.  
  
K. Acharya, “Recognition of HIV-inactivating peptide triazoles by the recombinant soluble Env trimer, BG505 SOSIP.664”, *Proteins: Structure, Function, and Bioinformatics*, vol. 85, no. 5. Wiley, pp. 843–851, Mar. 11, 2017. doi: 10.1002/prot.25238.  
  
M. K. Baker and C. F. Abrams, “Dynamics of Lipids, Cholesterol, and Transmembrane α-Helices from Microsecond Molecular Dynamics Simulations”, *The Journal of Physical Chemistry B*, vol. 118, no. 47. American Chemical Society (ACS), pp. 13590–13600, Nov. 18, 2014. doi: 10.1021/jp507027t.  
  
A. Bhaduri, J. Gardner, C. F. Abramsand L. Graham-Brady, “Free energy calculation using space filled design and weighted reconstruction: a modified single sweep approach”, *Molecular Simulation*, vol. 46, no. 3. Informa UK Limited, pp. 193–206, Nov. 18, 2019. doi: 10.1080/08927022.2019.1688325.  
  
A. Bucci and C. F. Abrams, “Oxygen Pathways and Allostery in Monomeric Sarcosine Oxidase via Single-Sweep Free-Energy Reconstruction”, *Journal of Chemical Theory and Computation*, vol. 10, no. 7. American Chemical Society (ACS), pp. 2668–2676, Apr. 10, 2014. doi: 10.1021/ct500088z.  
  
A. Bucci, T.-Q. Yu, E. Vanden-Eijndenand C. F. Abrams, “Kinetics of O2 Entry and Exit in Monomeric Sarcosine Oxidase via Markovian Milestoning Molecular Dynamics”, *Journal of Chemical Theory and Computation*, vol. 12, no. 6. American Chemical Society (ACS), pp. 2964–2972, May 19, 2016. doi: 10.1021/acs.jctc.6b00071.  
  
A. Emileh and C. F. Abrams, “A mechanism by which binding of the broadly neutralizing antibody b12 unfolds the inner domain α1 helix in an engineered HIV-1 gp120”, *Proteins: Structure, Function, and Bioinformatics*, vol. 79, no. 2. Wiley, pp. 537–546, Nov. 29, 2010. doi: 10.1002/prot.22901.  
  
A. Emileh, “Covalent Conjugation of a Peptide Triazole to HIV-1 gp120 Enables Intramolecular Binding Site Occupancy”, *Biochemistry*, vol. 53, no. 21. American Chemical Society (ACS), pp. 3403–3414, May 19, 2014. doi: 10.1021/bi500136f.  
  
A. Emileh, “A Model of Peptide Triazole Entry Inhibitor Binding to HIV-1 gp120 and the Mechanism of Bridging Sheet Disruption”, *Biochemistry*, vol. 52, no. 13. American Chemical Society (ACS), pp. 2245–2261, Mar. 22, 2013. doi: 10.1021/bi400166b.  
  
V. K. Gangupomu and C. F. Abrams, “All-Atom Models of the Membrane-Spanning Domain of HIV-1 gp41 from Metadynamics”, *Biophysical Journal*, vol. 99, no. 10. Elsevier BV, pp. 3438–3444, Nov. 2010. doi: 10.1016/j.bpj.2010.09.054.  
  
J. M. Gardner and C. F. Abrams, “Rate of hemifusion diaphragm dissipation and ability to form three-junction bound HD determined by lipid composition”, *The Journal of Chemical Physics*, vol. 147, no. 13. AIP Publishing, p. 134903, Oct. 07, 2017. doi: 10.1063/1.4994320.  
  
J. M. Gardner and C. F. Abrams, “Lipid flip-flop vs. lateral diffusion in the relaxation of hemifusion diaphragms”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1860, no. 7. Elsevier BV, pp. 1452–1459, Jul. 2018. doi: 10.1016/j.bbamem.2018.04.007.  
  
J. M. Gardner and C. F. Abrams, “Energetics of Flap Opening in HIV-1 Protease: String Method Calculations”, *The Journal of Physical Chemistry B*, vol. 123, no. 45. American Chemical Society (ACS), pp. 9584–9591, Oct. 22, 2019. doi: 10.1021/acs.jpcb.9b08348.  
  
J. M. Gardner, M. Desernoand C. F. Abrams, “Effect of intrinsic curvature and edge tension on the stability of binary mixed-membrane three-junctions”, *The Journal of Chemical Physics*, vol. 145, no. 7. AIP Publishing, p. 074901, Aug. 21, 2016. doi: 10.1063/1.4960433.  
  
R. Gordon, S. T. Stoberand C. F. Abrams, “Effects of Optical Purity and Finite System Size on Self-Assembly of 12-Hydroxystearic Acid in Hexane: Molecular Dynamics Simulations”, *The Journal of Physical Chemistry B*, vol. 121, no. 39. American Chemical Society (ACS), pp. 9223–9233, Sep. 21, 2017. doi: 10.1021/acs.jpcb.7b05246.  
  
S. T. Gossert, B. Parajuli, I. Chaikenand C. F. Abrams, “Roles of conserved tryptophans in trimerization of HIV‐1 membrane‐proximal external regions: Implications for virucidal design via alchemical free‐energy molecular simulations”, *Proteins: Structure, Function, and Bioinformatics*, vol. 86, no. 7. Wiley, pp. 707–711, Apr. 19, 2018. doi: 10.1002/prot.25504.  
  
S. T. Gossert, B. Parajuli, I. Chaikenand C. F. Abrams, “Roles of variable linker length in dual acting virucidal entry inhibitors on HIV ‐1 potency via on‐the‐fly free energy molecular simulations”, *Protein Science*, vol. 29, no. 11. Wiley, pp. 2304–2310, Sep. 29, 2020. doi: 10.1002/pro.3949.  
  
A. Herschhorn, “The β20–β21 of gp120 is a regulatory switch for HIV-1 Env conformational transitions”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Oct. 19, 2017. doi: 10.1038/s41467-017-01119-w.  
  
M. Huang and C. Abrams, “Effects of Reactivity Ratios on Network Topology and Thermomechanical Properties in Vinyl Ester/Styrene Thermosets: Molecular Dynamics Simulations”, *Macromolecular Theory and Simulations*, vol. 28, no. 6. Wiley, p. 1900030, Aug. 20, 2019. doi: 10.1002/mats.201900030.  
  
C. Jang, M. Sharifi, G. R. Palmeseand C. F. Abrams, “Crosslink network rearrangement via reactive encapsulation of solvent in epoxy curing: A combined molecular simulation and experimental study”, *Polymer*, vol. 55, no. 16. Elsevier BV, pp. 3859–3868, Aug. 2014. doi: 10.1016/j.polymer.2014.06.022.  
  
C. Jang, M. Sharifi, G. R. Palmeseand C. F. Abrams, “Toughness enhancement of thermosetting polymers using a novel partially reacted substructure curing protocol: A combined molecular simulation and experimental study”, *Polymer*, vol. 90. Elsevier BV, pp. 249–255, May 2016. doi: 10.1016/j.polymer.2016.03.023.  
  
C. Jang, T. W. Sirk, J. W. Andzelmand C. F. Abrams, “Comparison of Crosslinking Algorithms in Molecular Dynamics Simulation of Thermosetting Polymers”, *Macromolecular Theory and Simulations*, vol. 24, no. 3. Wiley, pp. 260–270, Jan. 29, 2015. doi: 10.1002/mats.201400094.  
  
M. Lapelosa and C. F. Abrams, “A Computational Study of Water and CO Migration Sites and Channels Inside Myoglobin”, *Journal of Chemical Theory and Computation*, vol. 9, no. 2. American Chemical Society (ACS), pp. 1265–1271, Jan. 30, 2013. doi: 10.1021/ct300862j.  
  
M. Lu, “Associating HIV-1 envelope glycoprotein structures with states on the virus observed by smFRET”, *Nature*, vol. 568, no. 7752. Springer Science and Business Media LLC, pp. 415–419, Apr. 10, 2019. doi: 10.1038/s41586-019-1101-y.  
  
F. Moraca, K. Acharya, B. Melillo, A. B. Smith III, I. Chaikenand C. F. Abrams, “Computational Evaluation of HIV-1 gp120 Conformations of Soluble Trimeric gp140 Structures as Targets for de Novo Docking of First- and Second-Generation Small-Molecule CD4 Mimics”, *Journal of Chemical Information and Modeling*, vol. 56, no. 10. American Chemical Society (ACS), pp. 2069–2079, Sep. 26, 2016. doi: 10.1021/acs.jcim.6b00393.  
  
F. Moraca, D. Rinaldo, A. B. Smith IIIand C. F. Abrams, “Specific Noncovalent Interactions Determine Optimal Structure of a Buried Ligand Moiety: QM/MM and Pure QM Modeling of Complexes of the Small-Molecule CD4 Mimetics and HIV-1 gp120”, *ChemMedChem*, vol. 13, no. 6. Wiley, pp. 627–633, Feb. 09, 2018. doi: 10.1002/cmdc.201700728.  
  
B. Parajuli, “Restricted HIV-1 Env glycan engagement by lectin-reengineered DAVEI protein chimera is sufficient for lytic inactivation of the virus”, *Biochemical Journal*, vol. 475, no. 5. Portland Press Ltd., pp. 931–957, Mar. 09, 2018. doi: 10.1042/bcj20170662.  
  
B. Parajuli, “Lytic Inactivation of Human Immunodeficiency Virus by Dual Engagement of gp120 and gp41 Domains in the Virus Env Protein Trimer”, *Biochemistry*, vol. 55, no. 44. American Chemical Society (ACS), pp. 6100–6114, Oct. 27, 2016. doi: 10.1021/acs.biochem.6b00570.  
  
S. A. Paz and C. F. Abrams, “Free Energy and Hidden Barriers of the β-Sheet Structure of Prion Protein”, *Journal of Chemical Theory and Computation*, vol. 11, no. 10. American Chemical Society (ACS), pp. 5024–5034, Sep. 16, 2015. doi: 10.1021/acs.jctc.5b00576.  
  
S. A. Paz, L. Maraglianoand C. F. Abrams, “Effect of Intercalated Water on Potassium Ion Transport through Kv1.2 Channels Studied via On-the-Fly Free-Energy Parametrization”, *Journal of Chemical Theory and Computation*, vol. 14, no. 5. American Chemical Society (ACS), pp. 2743–2750, Mar. 23, 2018. doi: 10.1021/acs.jctc.8b00024.  
  
S. A. Paz, E. Vanden-Eijndenand C. F. Abrams, “Polymorphism at 129 dictates metastable conformations of the human prion protein N-terminal β-sheet”, *Chemical Science*, vol. 8, no. 2. Royal Society of Chemistry (RSC), pp. 1225–1232, 2017. doi: 10.1039/c6sc03275c.  
  
J. Prévost, “The HIV-1 Env gp120 Inner Domain Shapes the Phe43 Cavity and the CD4 Binding Site”, *mBio*, vol. 11, no. 3. American Society for Microbiology, Jun. 30, 2020. doi: 10.1128/mbio.00280-20.  
  
M. Sharifi, C. Jang, C. F. Abramsand G. R. Palmese, “Epoxy Polymer Networks with Improved Thermal and Mechanical Properties via Controlled Dispersion of Reactive Toughening Agents”, *Macromolecules*, vol. 48, no. 20. American Chemical Society (ACS), pp. 7495–7502, Oct. 06, 2015. doi: 10.1021/acs.macromol.5b00677.  
  
G. Shrivastav, E. Vanden-Eijndenand C. F. Abrams, “Mapping saddles and minima on free energy surfaces using multiple climbing strings”, *The Journal of Chemical Physics*, vol. 151, no. 12. AIP Publishing, p. 124112, Sep. 28, 2019. doi: 10.1063/1.5120372.  
  
A. S. Sridhar and C. F. Abrams, “Yield and Post-yield Behavior of Fatty-Acid-Functionalized Amidoamine–Epoxy Systems: A Molecular Simulation Study”, *Journal of Dynamic Behavior of Materials*, vol. 5, no. 2. Springer Science and Business Media LLC, pp. 143–149, Mar. 19, 2019. doi: 10.1007/s40870-019-00193-z.  
  
A. Srikanth and C. F. Abrams, “Effect of molecular packing and hydrogen bonding on the properties of epoxy-amido amine systems”, *Computational Materials Science*, vol. 169. Elsevier BV, p. 109082, Nov. 2019. doi: 10.1016/j.commatsci.2019.109082.  
  
A. Srikanth, E. Kinaci, J. Vergara, G. Palmeseand C. F. Abrams, “The effect of alkyl chain length on mechanical properties of fatty-acid-functionalized amidoamine-epoxy systems”, *Computational Materials Science*, vol. 150. Elsevier BV, pp. 70–76, Jul. 2018. doi: 10.1016/j.commatsci.2018.03.073.  
  
A. Srikanth, J. Vergara, G. Palmeseand C. F. Abrams, “The effect of alkyl chain length on material properties of fatty-acid-functionalized amidoamine-epoxy systems”, *European Polymer Journal*, vol. 89. Elsevier BV, pp. 1–12, Apr. 2017. doi: 10.1016/j.eurpolymj.2017.01.037.  
  
S. T. Stober and C. F. Abrams, “Energetics and Mechanism of the Normal-to-Amyloidogenic Isomerization of β2-Microglobulin: On-the-Fly String Method Calculations”, *The Journal of Physical Chemistry B*, vol. 116, no. 31. American Chemical Society (ACS), pp. 9371–9375, Jul. 31, 2012. doi: 10.1021/jp304805v.  
  
S. T. Stober and C. F. Abrams, “Enhanced meta-analysis of acetylcholine binding protein structures reveals conformational signatures of agonism in nicotinic receptors”, *Protein Science*, vol. 21, no. 3. Wiley, pp. 307–317, Jan. 20, 2012. doi: 10.1002/pro.2016.  
  
H. Vashisth and C. F. Abrams, “All-Atom Structural Models for Complexes of Insulin-Like Growth Factors IGF1 and IGF2 with Their Cognate Receptor”, *Journal of Molecular Biology*, vol. 400, no. 3. Elsevier BV, pp. 645–658, Jul. 2010. doi: 10.1016/j.jmb.2010.05.025.  
  
H. Vashisth and C. F. Abrams, “All-atom structural models of insulin binding to the insulin receptor in the presence of a tandem hormone-binding element”, *Proteins: Structure, Function, and Bioinformatics*, vol. 81, no. 6. Wiley, pp. 1017–1030, Feb. 27, 2013. doi: 10.1002/prot.24255.  
  
H. Vashisth, L. Maraglianoand C. F. Abrams, ““DFG-Flip” in the Insulin Receptor Kinase Is Facilitated by a Helical Intermediate State of the Activation Loop”, *Biophysical Journal*, vol. 102, no. 8. Elsevier BV, pp. 1979–1987, Apr. 2012. doi: 10.1016/j.bpj.2012.03.031.  
  
J. H. Yang, A. Srikanth, C. Jangand C. F. Abrams, “Relationships between molecular structure and thermomechanical properties of bio-based thermosetting polymers”, *Journal of Polymer Science Part B: Polymer Physics*, vol. 55, no. 3. Wiley, pp. 285–292, Nov. 22, 2016. doi: 10.1002/polb.24270.  
  
T.-Q. Yu, M. Lapelosa, E. Vanden-Eijndenand C. F. Abrams, “Full Kinetics of CO Entry, Internal Diffusion, and Exit in Myoglobin from Transition-Path Theory Simulations”, *Journal of the American Chemical Society*, vol. 137, no. 8. American Chemical Society (ACS), pp. 3041–3050, Feb. 23, 2015. doi: 10.1021/ja512484q.  
  
M. Zhang, “Structural Basis for Calmodulin as a Dynamic Calcium Sensor”, *Structure*, vol. 20, no. 5. Elsevier BV, pp. 911–923, May 2012. doi: 10.1016/j.str.2012.03.019.  
  
L. Zhang, A. J. Sodt, R. M. Venable, R. W. Pastorand M. Buck, “Prediction, refinement, and persistency of transmembrane helix dimers in lipid bilayers using implicit and explicit solvent/lipid representations: Microsecond molecular dynamics simulations of ErbB1/B2 and EphA1”, *Proteins: Structure, Function, and Bioinformatics*, vol. 81, no. 3. Wiley, pp. 365–376, Nov. 05, 2012. doi: 10.1002/prot.24192.  
  
L. Mereuta, “Slowing down single-molecule trafficking through a protein nanopore reveals intermediates for peptide translocation”, *Scientific Reports*, vol. 4, no. 1. Springer Science and Business Media LLC, Jan. 27, 2014. doi: 10.1038/srep03885.  
  
J. L. Adelman and M. Grabe, “Simulating Current–Voltage Relationships for a Narrow Ion Channel Using the Weighted Ensemble Method”, *Journal of Chemical Theory and Computation*, vol. 11, no. 4. American Chemical Society (ACS), pp. 1907–1918, Mar. 04, 2015. doi: 10.1021/ct501134s.  
  
J. L. Adelman, “Structural Determinants of Water Permeation through the Sodium-Galactose Transporter vSGLT”, *Biophysical Journal*, vol. 106, no. 6. Elsevier BV, pp. 1280–1289, Mar. 2014. doi: 10.1016/j.bpj.2014.01.006.  
  
S. Choe, J. M. Rosenberg, J. Abramson, E. M. Wrightand M. Grabe, “Water Permeation through the Sodium-Dependent Galactose Cotransporter vSGLT”, *Biophysical Journal*, vol. 99, no. 7. Elsevier BV, pp. L56–L58, Oct. 2010. doi: 10.1016/j.bpj.2010.08.055.  
  
O. P. Choudhary, A. Paz, J. L. Adelman, J.-P. Colletier, J. Abramsonand M. Grabe, “Structure-guided simulations illuminate the mechanism of ATP transport through VDAC1”, *Nature Structural & Molecular Biology*, vol. 21, no. 7. Springer Science and Business Media LLC, pp. 626–632, Jun. 08, 2014. doi: 10.1038/nsmb.2841.  
  
N. H. Joh, “De novo design of a transmembrane Zn 2+ -transporting four-helix bundle”, *Science*, vol. 346, no. 6216. American Association for the Advancement of Science (AAAS), pp. 1520–1524, Dec. 19, 2014. doi: 10.1126/science.1261172.  
  
G. Ulas, T. Lemmin, Y. Wu, G. T. Gassnerand W. F. DeGrado, “Designed metalloprotein stabilizes a semiquinone radical”, *Nature Chemistry*, vol. 8, no. 4. Springer Science and Business Media LLC, pp. 354–359, Feb. 15, 2016. doi: 10.1038/nchem.2453.  
  
A. Watanabe, “The mechanism of sodium and substrate release from the binding pocket of vSGLT”, *Nature*, vol. 468, no. 7326. Springer Science and Business Media LLC, pp. 988–991, Dec. 2010. doi: 10.1038/nature09580.  
  
J.-Y. Shim, J. Ruddand T. T. Ding, “Distinct second extracellular loop structures of the brain cannabinoid CB1 receptor: Implication in ligand binding and receptor function”, *Proteins: Structure, Function, and Bioinformatics*, vol. 79, no. 2. Wiley, pp. 581–597, Nov. 30, 2010. doi: 10.1002/prot.22907.  
  
Q. Wang, “Protein recognition and selection through conformational and mutually induced fit”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 51. Proceedings of the National Academy of Sciences, pp. 20545–20550, Dec. 02, 2013. doi: 10.1073/pnas.1312788110.  
  
P. Bisignano, “Ligand-Based Discovery of a New Scaffold for Allosteric Modulation of the μ-Opioid Receptor”, *Journal of Chemical Information and Modeling*, vol. 55, no. 9. American Chemical Society (ACS), pp. 1836–1843, Sep. 15, 2015. doi: 10.1021/acs.jcim.5b00388.  
  
N. T. Burford, “Discovery, Synthesis, and Molecular Pharmacology of Selective Positive Allosteric Modulators of the δ-Opioid Receptor”, *Journal of Medicinal Chemistry*, vol. 58, no. 10. American Chemical Society (ACS), pp. 4220–4229, May 07, 2015. doi: 10.1021/acs.jmedchem.5b00007.  
  
N. Coudray, “Inward-facing conformation of the zinc transporter YiiP revealed by cryoelectron microscopy”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 6. Proceedings of the National Academy of Sciences, pp. 2140–2145, Jan. 22, 2013. doi: 10.1073/pnas.1215455110.  
  
R. S. Crowley, “Synthetic Studies of Neoclerodane Diterpenes from *Salvia divinorum:* Identification of a Potent and Centrally Acting μ Opioid Analgesic with Reduced Abuse Liability”, *Journal of Medicinal Chemistry*, vol. 59, no. 24. American Chemical Society (ACS), pp. 11027–11038, Dec. 13, 2016. doi: 10.1021/acs.jmedchem.6b01235.  
  
M. Filizola, “Insights from molecular dynamics simulations to exploit new trends for the development of improved opioid drugs”, *Neuroscience Letters*, vol. 700. Elsevier BV, pp. 50–55, May 2019. doi: 10.1016/j.neulet.2018.02.037.  
  
M. Fribourg, “Decoding the Signaling of a GPCR Heteromeric Complex Reveals a Unifying Mechanism of Action of Antipsychotic Drugs”, *Cell*, vol. 147, no. 5. Elsevier BV, pp. 1011–1023, Nov. 2011. doi: 10.1016/j.cell.2011.09.055.  
  
T. E. Hughes, “Structure-based characterization of novel TRPV5 inhibitors”, *eLife*, vol. 8. eLife Sciences Publications, Ltd, Oct. 25, 2019. doi: 10.7554/elife.49572.  
  
T. E. T. Hughes, “Structural basis of TRPV5 channel inhibition by econazole revealed by cryo-EM”, *Nature Structural & Molecular Biology*, vol. 25, no. 1. Springer Science and Business Media LLC, pp. 53–60, Jan. 2018. doi: 10.1038/s41594-017-0009-1.  
  
X. Hu, D. Provasi, S. Ramseyand M. Filizola, “Mechanism of μ-Opioid Receptor-Magnesium Interaction and Positive Allosteric Modulation”, *Biophysical Journal*, vol. 118, no. 4. Elsevier BV, pp. 909–921, Feb. 2020. doi: 10.1016/j.bpj.2019.10.007.  
  
J.-. kang . Jiang, “A novel class of ion displacement ligands as antagonists of the αIIbβ3 receptor that limit conformational reorganization of the receptor”, *Bioorganic & Medicinal Chemistry Letters*, vol. 24, no. 4. Elsevier BV, pp. 1148–1153, Feb. 2014. doi: 10.1016/j.bmcl.2013.12.122.  
  
J. M. Johnston, “Making Structural Sense of Dimerization Interfaces of Delta Opioid Receptor Homodimers”, *Biochemistry*, vol. 50, no. 10. American Chemical Society (ACS), pp. 1682–1690, Feb. 09, 2011. doi: 10.1021/bi101474v.  
  
J. M. Johnston and M. Filizola, “Differential Stability of the Crystallographic Interfaces of Mu- and Kappa-Opioid Receptors”, *PLoS ONE*, vol. 9, no. 2. Public Library of Science (PLoS), p. e90694, Feb. 28, 2014. doi: 10.1371/journal.pone.0090694.  
  
J. M. Johnston, H. Wang, D. Provasiand M. Filizola, “Assessing the Relative Stability of Dimer Interfaces in G Protein-Coupled Receptors”, *PLoS Computational Biology*, vol. 8, no. 8. Public Library of Science (PLoS), p. e1002649, Aug. 16, 2012. doi: 10.1371/journal.pcbi.1002649.  
  
A. Kapoor, G. Martinez-Rosell, D. Provasi, G. de Fabritiisand M. Filizola, “Dynamic and Kinetic Elements of µ-Opioid Receptor Functional Selectivity”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Sep. 12, 2017. doi: 10.1038/s41598-017-11483-8.  
  
A. C. Kruegel, “Synthetic and Receptor Signaling Explorations of the*Mitragyna*Alkaloids: Mitragynine as an Atypical Molecular Framework for Opioid Receptor Modulators”, *Journal of the American Chemical Society*, vol. 138, no. 21. American Chemical Society (ACS), pp. 6754–6764, May 18, 2016. doi: 10.1021/jacs.6b00360.  
  
J. Li, “RUC-4”, *Arteriosclerosis, Thrombosis, and Vascular Biology*, vol. 34, no. 10. Ovid Technologies (Wolters Kluwer Health), pp. 2321–2329, Oct. 2014. doi: 10.1161/atvbaha.114.303724.  
  
K. A. Marino and M. Filizola, “Investigating Small-Molecule Ligand Binding to G Protein-Coupled Receptors with Biased or Unbiased Molecular Dynamics Simulations”, *Methods in Molecular Biology*. Springer New York, pp. 351–364, Nov. 30, 2017. doi: 10.1007/978-1-4939-7465-8\_17.  
  
K. A. Marino, D. Prada-Gracia, D. Provasiand M. Filizola, “Impact of Lipid Composition and Receptor Conformation on the Spatio-temporal Organization of μ-Opioid Receptors in a Multi-component Plasma Membrane Model”, *PLOS Computational Biology*, vol. 12, no. 12. Public Library of Science (PLoS), p. e1005240, Dec. 13, 2016. doi: 10.1371/journal.pcbi.1005240.  
  
K. A. Marino, Y. Shangand M. Filizola, “Insights into the function of opioid receptors from molecular dynamics simulations of available crystal structures”, *British Journal of Pharmacology*, vol. 175, no. 14. Wiley, pp. 2834–2845, Apr. 12, 2017. doi: 10.1111/bph.13774.  
  
D. Meral, “Molecular details of dimerization kinetics reveal negligible populations of transient µ-opioid receptor homodimers at physiological concentrations”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, May 16, 2018. doi: 10.1038/s41598-018-26070-8.  
  
S. Mondal, J. M. Johnston, H. Wang, G. Khelashvili, M. Filizolaand H. Weinstein, “Membrane Driven Spatial Organization of GPCRs”, *Scientific Reports*, vol. 3, no. 1. Springer Science and Business Media LLC, Oct. 09, 2013. doi: 10.1038/srep02909.  
  
D. Provasi, M. C. Artacho, A. Negri, J. C. Mobarecand M. Filizola, “Ligand-Induced Modulation of the Free-Energy Landscape of G Protein-Coupled Receptors Explored by Adaptive Biasing Techniques”, *PLoS Computational Biology*, vol. 7, no. 10. Public Library of Science (PLoS), p. e1002193, Oct. 13, 2011. doi: 10.1371/journal.pcbi.1002193.  
  
D. Provasi, M. B. Boz, J. M. Johnstonand M. Filizola, “Preferred Supramolecular Organization and Dimer Interfaces of Opioid Receptors from Simulated Self-Association”, *PLOS Computational Biology*, vol. 11, no. 3. Public Library of Science (PLoS), p. e1004148, Mar. 30, 2015. doi: 10.1371/journal.pcbi.1004148.  
  
D. Provasi and M. Filizola, “Putative Active States of a Prototypic G-Protein-Coupled Receptor from Biased Molecular Dynamics”, *Biophysical Journal*, vol. 98, no. 10. Elsevier BV, pp. 2347–2355, May 2010. doi: 10.1016/j.bpj.2010.01.047.  
  
D. Provasi, J. M. Johnstonand M. Filizola, “Lessons from Free Energy Simulations of δ-Opioid Receptor Homodimers Involving the Fourth Transmembrane Helix”, *Biochemistry*, vol. 49, no. 31. American Chemical Society (ACS), pp. 6771–6776, Jul. 19, 2010. doi: 10.1021/bi100686t.  
  
D. Provasi, A. Negri, B. S. Collerand M. Filizola, “Talin-driven inside-out activation mechanism of platelet αIIbβ3 integrin probed by multimicrosecond, all-atom molecular dynamics simulations”, *Proteins: Structure, Function, and Bioinformatics*, vol. 82, no. 12. Wiley, pp. 3231–3240, Sep. 25, 2014. doi: 10.1002/prot.24540.  
  
G. Scarabelli, D. Provasi, A. Negriand M. Filizola, “Bioactive conformations of two seminal delta opioid receptor penta-peptides inferred from free-energy profiles”, *Biopolymers*, vol. 101, no. 1. Wiley, pp. 21–27, Oct. 25, 2013. doi: 10.1002/bip.22251.  
  
S. Schneider, D. Provasiand M. Filizola, “The Dynamic Process of Drug–GPCR Binding at Either Orthosteric or Allosteric Sites Evaluated by Metadynamics”, *Methods in Molecular Biology*. Springer New York, pp. 277–294, 2015. doi: 10.1007/978-1-4939-2914-6\_18.  
  
S. Schneider, D. Provasiand M. Filizola, “How Oliceridine (TRV-130) Binds and Stabilizes a μ-Opioid Receptor Conformational State That Selectively Triggers G Protein Signaling Pathways”, *Biochemistry*, vol. 55, no. 46. American Chemical Society (ACS), pp. 6456–6466, Nov. 07, 2016. doi: 10.1021/acs.biochem.6b00948.  
  
Y. Shang and M. Filizola, “Opioid receptors: Structural and mechanistic insights into pharmacology and signaling”, *European Journal of Pharmacology*, vol. 763. Elsevier BV, pp. 206–213, Sep. 2015. doi: 10.1016/j.ejphar.2015.05.012.  
  
Y. Shang, V. LeRouzic, S. Schneider, P. Bisignano, G. W. Pasternakand M. Filizola, “Mechanistic Insights into the Allosteric Modulation of Opioid Receptors by Sodium Ions”, *Biochemistry*, vol. 53, no. 31. American Chemical Society (ACS), pp. 5140–5149, Jul. 29, 2014. doi: 10.1021/bi5006915.  
  
Y. Shang, “Proposed Mode of Binding and Action of Positive Allosteric Modulators at Opioid Receptors”, *ACS Chemical Biology*, vol. 11, no. 5. American Chemical Society (ACS), pp. 1220–1229, Feb. 17, 2016. doi: 10.1021/acschembio.5b00712.  
  
H. Wang, “Molecular Determinants and Thermodynamics of the Amyloid Precursor Protein Transmembrane Domain Implicated in Alzheimer’s Disease”, *Journal of Molecular Biology*, vol. 408, no. 5. Elsevier BV, pp. 879–895, May 2011. doi: 10.1016/j.jmb.2011.03.028.  
  
J. H. Wardman, “Identification of a small-molecule ligand that activates the neuropeptide receptor GPR171 and increases food intake”, *Science Signaling*, vol. 9, no. 430. American Association for the Advancement of Science (AAAS), May 31, 2016. doi: 10.1126/scisignal.aac8035.  
  
H. Yano, D. Provasi, N. S. Cai, M. Filizola, S. Ferréand J. A. Javitch, “Development of novel biosensors to study receptor-mediated activation of the G-protein α subunits Gs and Golf”, *Journal of Biological Chemistry*, vol. 292, no. 49. Elsevier BV, pp. 19989–19998, Dec. 2017. doi: 10.1074/jbc.m117.800698.  
  
J. Zhu, “Structure-Guided Design of a High-Affinity Platelet Integrin α IIb β 3 Receptor Antagonist That Disrupts Mg 2+ Binding to the MIDAS”, *Science Translational Medicine*, vol. 4, no. 125. American Association for the Advancement of Science (AAAS), Mar. 14, 2012. doi: 10.1126/scitranslmed.3003576.  
  
J. Zhu, “Closed headpiece of integrin αIIbβ3 and its complex with an αIIbβ3-specific antagonist that does not induce opening”, *Blood*, vol. 116, no. 23. American Society of Hematology, pp. 5050–5059, Dec. 02, 2010. doi: 10.1182/blood-2010-04-281154.  
  
J. J. Virtanen, L. Makowski, T. R. Sosnickand K. F. Freed, “Modeling the Hydration Layer around Proteins: HyPred”, *Biophysical Journal*, vol. 99, no. 5. Elsevier BV, pp. 1611–1619, Sep. 2010. doi: 10.1016/j.bpj.2010.06.027.  
  
J. J. Virtanen, L. Makowski, T. R. Sosnickand K. F. Freed, “Modeling the Hydration Layer around Proteins: Applications to Small- and Wide-Angle X-Ray Scattering”, *Biophysical Journal*, vol. 101, no. 8. Elsevier BV, pp. 2061–2069, Oct. 2011. doi: 10.1016/j.bpj.2011.09.021.  
  
J. J. Virtanen, T. R. Sosnickand K. F. Freed, “Ionic strength independence of charge distributions in solvation of biomolecules”, *The Journal of Chemical Physics*, vol. 141, no. 22. AIP Publishing, pp. 22D503, Dec. 14, 2014. doi: 10.1063/1.4895522.  
  
R. B. Crochet, “Investigating combinatorial approaches in virtual screening on human inducible 6-phosphofructo-2-kinase/fructose-2,6-bisphosphatase (PFKFB3): A case study for small molecule kinases”, *Analytical Biochemistry*, vol. 418, no. 1. Elsevier BV, pp. 143–148, Nov. 2011. doi: 10.1016/j.ab.2011.06.035.  
  
M. Dinpajooh, D. R. Martinand D. V. Matyushov, “Polarizability of the active site of cytochrome c reduces the activation barrier for electron transfer”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Jun. 16, 2016. doi: 10.1038/srep28152.  
  
M. Dinpajooh and D. V. Matyushov, “Non-Gaussian Lineshapes and Dynamics of Time-Resolved Linear and Nonlinear (Correlation) Spectra”, *The Journal of Physical Chemistry B*, vol. 118, no. 28. American Chemical Society (ACS), pp. 7925–7936, Apr. 18, 2014. doi: 10.1021/jp500733s.  
  
M. Dinpajooh and D. V. Matyushov, “Interfacial Structural Transition in Hydration Shells of a Polarizable Solute”, *Physical Review Letters*, vol. 114, no. 20. American Physical Society (APS), May 22, 2015. doi: 10.1103/physrevlett.114.207801.  
  
M. Dinpajooh and D. V. Matyushov, “Free energy of ion hydration: Interface susceptibility and scaling with the ion size”, *The Journal of Chemical Physics*, vol. 143, no. 4. AIP Publishing, p. 044511, Jul. 28, 2015. doi: 10.1063/1.4927570.  
  
M. Dinpajooh and D. V. Matyushov, “Dielectric constant of water in the interface”, *The Journal of Chemical Physics*, vol. 145, no. 1. AIP Publishing, p. 014504, Jul. 07, 2016. doi: 10.1063/1.4955203.  
  
M. Dinpajooh and D. V. Matyushov, “Mobility of nanometer-size solutes in water driven by electric field”, *Physica A: Statistical Mechanics and its Applications*, vol. 463. Elsevier BV, pp. 366–375, Dec. 2016. doi: 10.1016/j.physa.2016.07.054.  
  
M. Dinpajooh, M. D. Newtonand D. V. Matyushov, “Free energy functionals for polarization fluctuations: Pekar factor revisited”, *The Journal of Chemical Physics*, vol. 146, no. 6. AIP Publishing, p. 064504, Feb. 14, 2017. doi: 10.1063/1.4975625.  
  
D. R. Martin, D. Fiorettoand D. V. Matyushov, “Depolarized light scattering and dielectric response of a peptide dissolved in water”, *The Journal of Chemical Physics*, vol. 140, no. 3. AIP Publishing, p. 035101, Jan. 21, 2014. doi: 10.1063/1.4861965.  
  
D. R. Martin and D. V. Matyushov, “Photosynthetic diode: electron transport rectification by wetting the quinone cofactor”, *Physical Chemistry Chemical Physics*, vol. 17, no. 35. Royal Society of Chemistry (RSC), pp. 22523–22528, 2015. doi: 10.1039/c5cp03397g.  
  
D. R. Martin and D. V. Matyushov, “Communication: Microsecond dynamics of the protein and water affect electron transfer in a bacterial *bc*1 complex”, *The Journal of Chemical Physics*, vol. 142, no. 16. AIP Publishing, p. 161101, Apr. 28, 2015. doi: 10.1063/1.4919222.  
  
D. R. Martin and D. V. Matyushov, “Terahertz absorption of lysozyme in solution”, *The Journal of Chemical Physics*, vol. 147, no. 8. AIP Publishing, p. 084502, Aug. 28, 2017. doi: 10.1063/1.4989641.  
  
D. R. Martin and D. V. Matyushov, “Electron-transfer chain in respiratory complex I”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Jul. 14, 2017. doi: 10.1038/s41598-017-05779-y.  
  
D. V. Matyushov, “Electrostatics of liquid interfaces”, *The Journal of Chemical Physics*, vol. 140, no. 22. AIP Publishing, p. 224506, Jun. 14, 2014. doi: 10.1063/1.4882284.  
  
D. V. Matyushov, “Nonlinear dielectric response of polar liquids”, *The Journal of Chemical Physics*, vol. 142, no. 24. AIP Publishing, p. 244502, Jun. 28, 2015. doi: 10.1063/1.4922933.  
  
S. Seyedi, D. R. Martinand D. V. Matyushov, “Dynamical and orientational structural crossovers in low-temperature glycerol”, *Physical Review E*, vol. 94, no. 1. American Physical Society (APS), Jul. 22, 2016. doi: 10.1103/physreve.94.012616.  
  
S. Seyedi and D. V. Matyushov, “Termination of Biological Function at Low Temperatures: Glass or Structural Transition?”, *The Journal of Physical Chemistry Letters*, vol. 9, no. 9. American Chemical Society (ACS), pp. 2359–2366, Apr. 19, 2018. doi: 10.1021/acs.jpclett.8b00537.  
  
S. S. Seyedi, M. M. Waskasiand D. V. Matyushov, “Theory and Electrochemistry of Cytochrome *c*”, *The Journal of Physical Chemistry B*, vol. 121, no. 19. American Chemical Society (ACS), pp. 4958–4967, May 09, 2017. doi: 10.1021/acs.jpcb.7b00917.  
  
M. M. Waskasi, G. Kodis, A. L. Moore, T. A. Moore, D. Gustand D. V. Matyushov, “Marcus Bell-Shaped Electron Transfer Kinetics Observed in an Arrhenius Plot”, *Journal of the American Chemical Society*, vol. 138, no. 29. American Chemical Society (ACS), pp. 9251–9257, Jul. 14, 2016. doi: 10.1021/jacs.6b04777.  
  
M. M. Waskasi, M. D. Newtonand D. V. Matyushov, “Impact of Temperature and Non-Gaussian Statistics on Electron Transfer in Donor–Bridge–Acceptor Molecules”, *The Journal of Physical Chemistry B*, vol. 121, no. 12. American Chemical Society (ACS), pp. 2665–2676, Mar. 06, 2017. doi: 10.1021/acs.jpcb.7b00140.  
  
D. Barr, “Importance of Domain Closure for the Autoactivation of ERK2”, *Biochemistry*, vol. 50, no. 37. American Chemical Society (ACS), pp. 8038–8048, Aug. 25, 2011. doi: 10.1021/bi200503a.  
  
J. C. Phillips, “What You Should Know About NAMD and Charm++ But Were Hoping to Ignore”, *Proceedings of the Practice and Experience on Advanced Research Computing*. ACM, Jul. 22, 2018. doi: 10.1145/3219104.3219134.  
  
H. Cho, “Molecular Mechanism by Which Palmitate Inhibits PKR Autophosphorylation”, *Biochemistry*, vol. 50, no. 6. American Chemical Society (ACS), pp. 1110–1119, Feb. 15, 2011. doi: 10.1021/bi101923r.  
  
B. Dutagaci and M. Feig, “Determination of Hydrophobic Lengths of Membrane Proteins with the HDGB Implicit Membrane Model”, *Journal of Chemical Information and Modeling*, vol. 57, no. 12. American Chemical Society (ACS), pp. 3032–3042, Dec. 01, 2017. doi: 10.1021/acs.jcim.7b00510.  
  
B. Dutagaci, L. Heoand M. Feig, “Structure refinement of membrane proteins via molecular dynamics simulations”, *Proteins: Structure, Function, and Bioinformatics*, vol. 86, no. 7. Wiley, pp. 738–750, May 06, 2018. doi: 10.1002/prot.25508.  
  
B. Dutagaci, M. Sayadiand M. Feig, “Heterogeneous dielectric generalized Born model with a van der Waals term provides improved association energetics of membrane-embedded transmembrane helices”, *Journal of Computational Chemistry*, vol. 38, no. 16. Wiley, pp. 1308–1320, Feb. 04, 2017. doi: 10.1002/jcc.24691.  
  
B. Dutagaci, K. Wittayanarakul, T. Moriand M. Feig, “Discrimination of Native-like States of Membrane Proteins with Implicit Membrane-based Scoring Functions”, *Journal of Chemical Theory and Computation*, vol. 13, no. 6. American Chemical Society (ACS), pp. 3049–3059, May 11, 2017. doi: 10.1021/acs.jctc.7b00254.  
  
L. Fang, H. J. Cho, C. Chanand M. Feig, “Binding site multiplicity with fatty acid ligands: Implications for the regulation of PKR kinase autophosphorylation with palmitate”, *Proteins: Structure, Function, and Bioinformatics*, vol. 82, no. 10. Wiley, pp. 2429–2442, Jun. 03, 2014. doi: 10.1002/prot.24607.  
  
M. A. Farrugia, B. Wang, M. Feigand R. P. Hausinger, “Mutational and Computational Evidence That a Nickel-Transfer Tunnel in UreD Is Used for Activation of *Klebsiella aerogenes* Urease”, *Biochemistry*, vol. 54, no. 41. American Chemical Society (ACS), pp. 6392–6401, Oct. 05, 2015. doi: 10.1021/acs.biochem.5b00942.  
  
M. Feig, “Local Protein Structure Refinement via Molecular Dynamics Simulations with locPREFMD”, *Journal of Chemical Information and Modeling*, vol. 56, no. 7. American Chemical Society (ACS), pp. 1304–1312, Jul. 13, 2016. doi: 10.1021/acs.jcim.6b00222.  
  
M. Feig, “Computational protein structure refinement: almost there, yet still so far to go”, *Wiley Interdisciplinary Reviews: Computational Molecular Science*, vol. 7, no. 3. Wiley, p. e1307, Mar. 28, 2017. doi: 10.1002/wcms.1307.  
  
M. Feig, R. Harada, T. Mori, I. Yu, K. Takahashiand Y. Sugita, “Complete atomistic model of a bacterial cytoplasm for integrating physics, biochemistry, and systems biology”, *Journal of Molecular Graphics and Modelling*, vol. 58. Elsevier BV, pp. 1–9, May 2015. doi: 10.1016/j.jmgm.2015.02.004.  
  
M. Feig and V. Mirjalili, “Protein structure refinement via molecular-dynamics simulations: What works and what does not?”, *Proteins: Structure, Function, and Bioinformatics*, vol. 84. Wiley, pp. 282–292, Aug. 17, 2015. doi: 10.1002/prot.24871.  
  
M. Feig, G. Nawrocki, I. Yu, P.-. hung . Wangand Y. Sugita, “Challenges and opportunities in connecting simulations with experiments via molecular dynamics of cellular environments”, *Journal of Physics: Conference Series*, vol. 1036. IOP Publishing, p. 012010, Jun. 2018. doi: 10.1088/1742-6596/1036/1/012010.  
  
M. Feig and Y. Sugita, “Reaching new levels of realism in modeling biological macromolecules in cellular environments”, *Journal of Molecular Graphics and Modelling*, vol. 45. Elsevier BV, pp. 144–156, Sep. 2013. doi: 10.1016/j.jmgm.2013.08.017.  
  
M. Feig and Y. Sugita, “Whole-Cell Models and Simulations in Molecular Detail”, *Annual Review of Cell and Developmental Biology*, vol. 35, no. 1. Annual Reviews, pp. 191–211, Oct. 06, 2019. doi: 10.1146/annurev-cellbio-100617-062542.  
  
M. Feig, I. Yu, P.-. hung . Wang, G. Nawrockiand Y. Sugita, “Crowding in Cellular Environments at an Atomistic Level from Computer Simulations”, *The Journal of Physical Chemistry B*, vol. 121, no. 34. American Chemical Society (ACS), pp. 8009–8025, Jul. 12, 2017. doi: 10.1021/acs.jpcb.7b03570.  
  
L. Heo, C. F. Arbourand M. Feig, “Driven to near‐experimental accuracy by refinement via molecular dynamics simulations”, *Proteins: Structure, Function, and Bioinformatics*, vol. 87, no. 12. Wiley, pp. 1263–1275, Jun. 24, 2019. doi: 10.1002/prot.25759.  
  
L. Heo and M. Feig, “What makes it difficult to refine protein models further via molecular dynamics simulations?”, *Proteins: Structure, Function, and Bioinformatics*, vol. 86, no. S1. Wiley, pp. 177–188, Oct. 16, 2017. doi: 10.1002/prot.25393.  
  
L. Heo and M. Feig, “PREFMD: a web server for protein structure refinement via molecular dynamics simulations”, *Bioinformatics*, vol. 34, no. 6. Oxford University Press (OUP), pp. 1063–1065, Nov. 08, 2017. doi: 10.1093/bioinformatics/btx726.  
  
L. Heo and M. Feig, “Experimental accuracy in protein structure refinement via molecular dynamics simulations”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 52. Proceedings of the National Academy of Sciences, pp. 13276–13281, Dec. 10, 2018. doi: 10.1073/pnas.1811364115.  
  
L. Heo and M. Feig, “Modeling of Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) Proteins by Machine Learning and Physics-Based Refinement”, *[]*. Cold Spring Harbor Laboratory, Mar. 28, 2020. doi: 10.1101/2020.03.25.008904.  
  
L. Heo and M. Feig, “High‐accuracy protein structures by combining machine‐learning with physics‐based refinement”, *Proteins: Structure, Function, and Bioinformatics*, vol. 88, no. 5. Wiley, pp. 637–642, Nov. 15, 2019. doi: 10.1002/prot.25847.  
  
P. Kar and M. Feig, “Recent Advances in Transferable Coarse-Grained Modeling of Proteins”, *Advances in Protein Chemistry and Structural Biology*. Elsevier, pp. 143–180, 2014. doi: 10.1016/bs.apcsb.2014.06.005.  
  
P. Kar and M. Feig, “Hybrid All-Atom/Coarse-Grained Simulations of Proteins by Direct Coupling of CHARMM and PRIMO Force Fields”, *Journal of Chemical Theory and Computation*, vol. 13, no. 11. American Chemical Society (ACS), pp. 5753–5765, Oct. 19, 2017. doi: 10.1021/acs.jctc.7b00840.  
  
P. Kar, S. M. Gopal, Y.-M. Cheng, A. Panahiand M. Feig, “Transferring the PRIMO Coarse-Grained Force Field to the Membrane Environment: Simulations of Membrane Proteins and Helix–Helix Association”, *Journal of Chemical Theory and Computation*, vol. 10, no. 8. American Chemical Society (ACS), pp. 3459–3472, Jun. 26, 2014. doi: 10.1021/ct500443v.  
  
P. Kar, S. M. Gopal, Y.-M. Cheng, A. Predeusand M. Feig, “PRIMO: A Transferable Coarse-Grained Force Field for Proteins”, *Journal of Chemical Theory and Computation*, vol. 9, no. 8. American Chemical Society (ACS), pp. 3769–3788, Jul. 12, 2013. doi: 10.1021/ct400230y.  
  
V. Mirjalili and M. Feig, “Protein Structure Refinement through Structure Selection and Averaging from Molecular Dynamics Ensembles”, *Journal of Chemical Theory and Computation*, vol. 9, no. 2. American Chemical Society (ACS), pp. 1294–1303, Jan. 24, 2013. doi: 10.1021/ct300962x.  
  
V. Mirjalili and M. Feig, “Interactions of Amino Acid Side-Chain Analogs within Membrane Environments”, *The Journal of Physical Chemistry B*, vol. 119, no. 7. American Chemical Society (ACS), pp. 2877–2885, Feb. 06, 2015. doi: 10.1021/jp511712u.  
  
V. Mirjalili and M. Feig, “Density-Biased Sampling: A Robust Computational Method for Studying Pore Formation in Membranes”, *Journal of Chemical Theory and Computation*, vol. 11, no. 1. American Chemical Society (ACS), pp. 343–350, Dec. 24, 2014. doi: 10.1021/ct5009153.  
  
V. Mirjalili, K. Noyesand M. Feig, “Physics-based protein structure refinement through multiple molecular dynamics trajectories and structure averaging”, *Proteins: Structure, Function, and Bioinformatics*, vol. 82. Wiley, pp. 196–207, Aug. 19, 2013. doi: 10.1002/prot.24336.  
  
G. Nawrocki, W. Im, Y. Sugitaand M. Feig, “Clustering and dynamics of crowded proteins near membranes and their influence on membrane bending”, *Proceedings of the National Academy of Sciences*, vol. 116, no. 49. Proceedings of the National Academy of Sciences, pp. 24562–24567, Nov. 18, 2019. doi: 10.1073/pnas.1910771116.  
  
G. Nawrocki, A. Karaboga, Y. Sugitaand M. Feig, “Effect of protein–protein interactions and solvent viscosity on the rotational diffusion of proteins in crowded environments”, *Physical Chemistry Chemical Physics*, vol. 21, no. 2. Royal Society of Chemistry (RSC), pp. 876–883, 2019. doi: 10.1039/c8cp06142d.  
  
G. Nawrocki, P.-. hung . Wang, I. Yu, Y. Sugitaand M. Feig, “Slow-Down in Diffusion in Crowded Protein Solutions Correlates with Transient Cluster Formation”, *The Journal of Physical Chemistry B*, vol. 121, no. 49. American Chemical Society (ACS), pp. 11072–11084, Nov. 30, 2017. doi: 10.1021/acs.jpcb.7b08785.  
  
P. O. Ochieng, N. A. White, M. Feigand C. G. Hoogstraten, “Intrinsic Base-Pair Rearrangement in the Hairpin Ribozyme Directs RNA Conformational Sampling and Tertiary Interface Formation”, *The Journal of Physical Chemistry B*, vol. 120, no. 42. American Chemical Society (ACS), pp. 10885–10898, Oct. 14, 2016. doi: 10.1021/acs.jpcb.6b05606.  
  
A. Panahi and M. Feig, “Dynamic Heterogeneous Dielectric Generalized Born (DHDGB): An Implicit Membrane Model with a Dynamically Varying Bilayer Thickness”, *Journal of Chemical Theory and Computation*, vol. 9, no. 3. American Chemical Society (ACS), pp. 1709–1719, Mar. 01, 2013. doi: 10.1021/ct300975k.  
  
M. Sayadi and M. Feig, “Role of conformational sampling of Ser16 and Thr17-phosphorylated phospholamban in interactions with SERCA”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1828, no. 2. Elsevier BV, pp. 577–585, Feb. 2013. doi: 10.1016/j.bbamem.2012.08.017.  
  
M. Sharma, A. V. Predeus, N. Kovacsand M. Feig, “Differential Mismatch Recognition Specificities of Eukaryotic MutS Homologs, MutSα and MutSβ”, *Biophysical Journal*, vol. 106, no. 11. Elsevier BV, pp. 2483–2492, Jun. 2014. doi: 10.1016/j.bpj.2014.04.026.  
  
M. Sharma, A. V. Predeus, S. Mukherjeeand M. Feig, “DNA Bending Propensity in the Presence of Base Mismatches: Implications for DNA Repair”, *The Journal of Physical Chemistry B*, vol. 117, no. 20. American Chemical Society (ACS), pp. 6194–6205, May 10, 2013. doi: 10.1021/jp403127a.  
  
Y. Sugita and M. Feig, “Chapter 14. All-atom Molecular Dynamics Simulation of Proteins in Crowded Environments”, *New Developments in NMR*. Royal Society of Chemistry, pp. 228–248, 2019. doi: 10.1039/9781788013079-00228.  
  
Y. Sugita, I. Yuand M. Feig, “Molecular Dynamics Simulations of Biomolecules in Cellular Environments”, *Molecular Science*, vol. 11, no. 1. Japan Society for Molecular Science, p. A0094, 2017. doi: 10.3175/molsci.11.a0094.  
  
B. Wang, M. Feig, R. I. Cukierand Z. F. Burton, “Computational Simulation Strategies for Analysis of Multisubunit RNA Polymerases”, *Chemical Reviews*, vol. 113, no. 11. American Chemical Society (ACS), pp. 8546–8566, Aug. 29, 2013. doi: 10.1021/cr400046x.  
  
B. Wang, J. Francis, M. Sharma, S. M. Law, A. V. Predeusand M. Feig, “Long-Range Signaling in MutS and MSH Homologs via Switching of Dynamic Communication Pathways”, *PLOS Computational Biology*, vol. 12, no. 10. Public Library of Science (PLoS), p. e1005159, Oct. 21, 2016. doi: 10.1371/journal.pcbi.1005159.  
  
B. Wang, A. V. Predeus, Z. F. Burtonand M. Feig, “Energetic and Structural Details of the Trigger-Loop Closing Transition in RNA Polymerase II”, *Biophysical Journal*, vol. 105, no. 3. Elsevier BV, pp. 767–775, Aug. 2013. doi: 10.1016/j.bpj.2013.05.060.  
  
B. Wang, R. E. Sextonand M. Feig, “Kinetics of nucleotide entry into RNA polymerase active site provides mechanism for efficiency and fidelity”, *Biochimica et Biophysica Acta (BBA) - Gene Regulatory Mechanisms*, vol. 1860, no. 4. Elsevier BV, pp. 482–490, Apr. 2017. doi: 10.1016/j.bbagrm.2017.02.008.  
  
A. Yildirim, N. Brenner, R. Sutherlandand M. Feig, “Role of protein interactions in stabilizing canonical DNA features in simulations of DNA in crowded environments”, *BMC Biophysics*, vol. 11, no. 1. Springer Science and Business Media LLC, Dec. 2018. doi: 10.1186/s13628-018-0048-y.  
  
A. Yildirim and M. Feig, “High-resolution 3D models of Caulobacter crescentus chromosome reveal genome structural variability and organization”, *Nucleic Acids Research*, vol. 46, no. 8. Oxford University Press (OUP), pp. 3937–3952, Feb. 26, 2018. doi: 10.1093/nar/gky141.  
  
A. Yildirim, M. Sharma, B. M. Varner, L. Fangand M. Feig, “Conformational Preferences of DNA in Reduced Dielectric Environments”, *The Journal of Physical Chemistry B*, vol. 118, no. 37. American Chemical Society (ACS), pp. 10874–10881, Sep. 10, 2014. doi: 10.1021/jp505727w.  
  
I. Yu, M. Feigand Y. Sugita, “High-Performance Data Analysis on the Big Trajectory Data of Cellular Scale All-atom Molecular Dynamics Simulations”, *Journal of Physics: Conference Series*, vol. 1036. IOP Publishing, p. 012009, Jun. 2018. doi: 10.1088/1742-6596/1036/1/012009.  
  
I. Yu, “Biomolecular interactions modulate macromolecular structure and dynamics in atomistic model of a bacterial cytoplasm”, *eLife*, vol. 5. eLife Sciences Publications, Ltd, Nov. 01, 2016. doi: 10.7554/elife.19274.  
  
M. Andersson, A.-N. Bondar, J. A. Freites, D. J. Tobias, H. R. Kabackand S. H. White, “Proton-Coupled Dynamics in Lactose Permease”, *Structure*, vol. 20, no. 11. Elsevier BV, pp. 1893–1904, Nov. 2012. doi: 10.1016/j.str.2012.08.021.  
  
M. Andersson, J. A. Freites, D. J. Tobiasand S. H. White, “Structural Dynamics of the S4 Voltage-Sensor Helix in Lipid Bilayers Lacking Phosphate Groups”, *The Journal of Physical Chemistry B*, vol. 115, no. 27. American Chemical Society (ACS), pp. 8732–8738, Jun. 22, 2011. doi: 10.1021/jp2001964.  
  
A.-N. Bondar, C. del Val, J. A. Freites, D. J. Tobiasand S. H. White, “Dynamics of SecY Translocons with Translocation-Defective Mutations”, *Structure*, vol. 18, no. 7. Elsevier BV, pp. 847–857, Jul. 2010. doi: 10.1016/j.str.2010.04.010.  
  
J. A. Freites, E. V. Schow, S. H. Whiteand D. J. Tobias, “Microscopic Origin of Gating Current Fluctuations in a Potassium Channel Voltage Sensor”, *Biophysical Journal*, vol. 102, no. 11. Elsevier BV, pp. L44–L46, Jun. 2012. doi: 10.1016/j.bpj.2012.04.021.  
  
M. Heyden, J. A. Freites, M. B. Ulmschneider, S. H. Whiteand D. J. Tobias, “Assembly and stability of α-helical membrane proteins”, *Soft Matter*, vol. 8, no. 30. Royal Society of Chemistry (RSC), p. 7742, 2012. doi: 10.1039/c2sm25402f.  
  
J. B. Klauda, “Update of the CHARMM All-Atom Additive Force Field for Lipids: Validation on Six Lipid Types”, *The Journal of Physical Chemistry B*, vol. 114, no. 23. American Chemical Society (ACS), pp. 7830–7843, May 24, 2010. doi: 10.1021/jp101759q.  
  
M. Mihailescu, “Acyl-Chain Methyl Distributions of Liquid-Ordered and -Disordered Membranes”, *Biophysical Journal*, vol. 100, no. 6. Elsevier BV, pp. 1455–1462, Mar. 2011. doi: 10.1016/j.bpj.2011.01.035.  
  
E. V. Schow, “Arginine in Membranes: The Connection Between Molecular Dynamics Simulations and Translocon-Mediated Insertion Experiments”, *The Journal of Membrane Biology*, vol. 239, no. 1–2. Springer Science and Business Media LLC, pp. 35–48, Dec. 03, 2010. doi: 10.1007/s00232-010-9330-x.  
  
E. V. Schow, J. A. Freites, K. Gogna, S. H. Whiteand D. J. Tobias, “Down-State Model of the Voltage-Sensing Domain of a Potassium Channel”, *Biophysical Journal*, vol. 98, no. 12. Elsevier BV, pp. 2857–2866, Jun. 2010. doi: 10.1016/j.bpj.2010.03.031.  
  
E. V. Schow, J. A. Freites, A. Nizkorodov, S. H. Whiteand D. J. Tobias, “Coupling between the voltage-sensing and pore domains in a voltage-gated potassium channel”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1818, no. 7. Elsevier BV, pp. 1726–1736, Jul. 2012. doi: 10.1016/j.bbamem.2012.02.029.  
  
M. L. Wood, E. V. Schow, J. A. Freites, S. H. White, F. Tombolaand D. J. Tobias, “Water wires in atomistic models of the Hv1 proton channel”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1818, no. 2. Elsevier BV, pp. 286–293, Feb. 2012. doi: 10.1016/j.bbamem.2011.07.045.  
  
S. Gupta, J. A. Dura, J. A. Freites, D. J. Tobiasand J. K. Blasie, “Structural Characterization of the Voltage-Sensor Domain and Voltage-Gated K+-Channel Proteins Vectorially Oriented within a Single Bilayer Membrane at the Solid/Vapor and Solid/Liquid Interfaces via Neutron Interferometry”, *Langmuir*, vol. 28, no. 28. American Chemical Society (ACS), pp. 10504–10520, Jun. 29, 2012. doi: 10.1021/la301219z.  
  
A. W. Götz, M. J. Williamson, D. Xu, D. Poole, S. Le Grandand R. C. Walker, “Routine Microsecond Molecular Dynamics Simulations with AMBER on GPUs. 1. Generalized Born”, *Journal of Chemical Theory and Computation*, vol. 8, no. 5. American Chemical Society (ACS), pp. 1542–1555, Apr. 15, 2012. doi: 10.1021/ct200909j.  
  
C. M. Isborn, A. W. Götz, M. A. Clark, R. C. Walkerand T. J. Martínez, “Electronic Absorption Spectra from MM and *ab Initio* QM/MM Molecular Dynamics: Environmental Effects on the Absorption Spectrum of Photoactive Yellow Protein”, *Journal of Chemical Theory and Computation*, vol. 8, no. 12. American Chemical Society (ACS), pp. 5092–5106, Oct. 17, 2012. doi: 10.1021/ct3006826.  
  
S. Le Grand, A. W. Götzand R. C. Walker, “SPFP: Speed without compromise—A mixed precision model for GPU accelerated molecular dynamics simulations”, *Computer Physics Communications*, vol. 184, no. 2. Elsevier BV, pp. 374–380, Feb. 2013. doi: 10.1016/j.cpc.2012.09.022.  
  
K. Park, A. W. Götz, R. C. Walkerand F. Paesani, “Application of Adaptive QM/MM Methods to Molecular Dynamics Simulations of Aqueous Systems”, *Journal of Chemical Theory and Computation*, vol. 8, no. 8. American Chemical Society (ACS), pp. 2868–2877, Jul. 11, 2012. doi: 10.1021/ct300331f.  
  
R. Salomon-Ferrer, A. W. Götz, D. Poole, S. Le Grandand R. C. Walker, “Routine Microsecond Molecular Dynamics Simulations with AMBER on GPUs. 2. Explicit Solvent Particle Mesh Ewald”, *Journal of Chemical Theory and Computation*, vol. 9, no. 9. American Chemical Society (ACS), pp. 3878–3888, Aug. 20, 2013. doi: 10.1021/ct400314y.  
  
S. A. Yao, K. M. Lancaster, A. W. Götz, S. DeBeerand J. F. Berry, “X-ray Absorption Spectroscopic, Crystallographic, Theoretical (DFT) and Chemical Evidence for a Chalcogen-Chalcogen Two-Center/Three-Electron Half Bond in an Unprecedented “Subselenide” Se23− Ligand”, *Chemistry - A European Journal*, vol. 18, no. 30. Wiley, pp. 9179–9183, Jun. 21, 2012. doi: 10.1002/chem.201201291.  
  
N. Bhatnagar, G. Kamath, I. Chelstand J. J. Potoff, “Direct calculation of 1-octanol–water partition coefficients from adaptive biasing force molecular dynamics simulations”, *The Journal of Chemical Physics*, vol. 137, no. 1. AIP Publishing, p. 014502, Jul. 07, 2012. doi: 10.1063/1.4730040.  
  
N. Bhatnagar, G. Kamathand J. J. Potoff, “Biomolecular Simulations with the Transferable Potentials for Phase Equilibria: Extension to Phospholipids”, *The Journal of Physical Chemistry B*, vol. 117, no. 34. American Chemical Society (ACS), pp. 9910–9921, Aug. 16, 2013. doi: 10.1021/jp404314k.  
  
G. Kamath, N. Bhatnagar, G. A. Baker, S. N. Bakerand J. J. Potoff, “Computational prediction of ionic liquid 1-octanol/water partition coefficients”, *Physical Chemistry Chemical Physics*, vol. 14, no. 13. Royal Society of Chemistry (RSC), p. 4339, 2012. doi: 10.1039/c2cp40122c.  
  
M. V. LeVine, M. A. Cuendet, G. Khelashviliand H. Weinstein, “Allosteric Mechanisms of Molecular Machines at the Membrane: Transport by Sodium-Coupled Symporters”, *Chemical Reviews*, vol. 116, no. 11. American Chemical Society (ACS), pp. 6552–6587, Feb. 19, 2016. doi: 10.1021/acs.chemrev.5b00627.  
  
J. Wereszczynski and J. A. McCammon, “Simulations of the p97 complex suggest novel conformational states of hydrolysis intermediates”, *Protein Science*, vol. 21, no. 4. Wiley, pp. 475–486, Mar. 02, 2012. doi: 10.1002/pro.2024.  
  
W. M. Berhanu and A. E. Masunov, “Controlling the aggregation and rate of release in order to improve insulin formulation: molecular dynamics study of full-length insulin amyloid oligomer models”, *Journal of Molecular Modeling*, vol. 18, no. 3. Springer Science and Business Media LLC, pp. 1129–1142, Jun. 15, 2011. doi: 10.1007/s00894-011-1123-3.  
  
W. M. Berhanu and A. E. Masunov, “Full length amylin oligomer aggregation: insights from molecular dynamics simulations and implications for design of aggregation inhibitors”, *Journal of Biomolecular Structure and Dynamics*, vol. 32, no. 10. Informa UK Limited, pp. 1651–1669, Sep. 13, 2013. doi: 10.1080/07391102.2013.832635.  
  
G. T. Beckham, “Harnessing glycosylation to improve cellulase activity”, *Current Opinion in Biotechnology*, vol. 23, no. 3. Elsevier BV, pp. 338–345, Jun. 2012. doi: 10.1016/j.copbio.2011.11.030.  
  
G. T. Beckham, “Towards a molecular-level theory of carbohydrate processivity in glycoside hydrolases”, *Current Opinion in Biotechnology*, vol. 27. Elsevier BV, pp. 96–106, Jun. 2014. doi: 10.1016/j.copbio.2013.12.002.  
  
L. Berstis, G. T. Beckhamand M. F. Crowley, “Electronic coupling through natural amino acids”, *The Journal of Chemical Physics*, vol. 143, no. 22. AIP Publishing, p. 225102, Dec. 08, 2015. doi: 10.1063/1.4936588.  
  
L. Berstis, T. Elder, M. Crowleyand G. T. Beckham, “Radical Nature of C-Lignin”, *ACS Sustainable Chemistry & Engineering*, vol. 4, no. 10. American Chemical Society (ACS), pp. 5327–5335, May 31, 2016. doi: 10.1021/acssuschemeng.6b00520.  
  
A. S. Borisova, “Sequencing, biochemical characterization, crystal structure and molecular dynamics of cellobiohydrolase Cel7A from *Geotrichum candidum* 3C”, *The FEBS Journal*, vol. 282, no. 23. Wiley, pp. 4515–4537, Oct. 08, 2015. doi: 10.1111/febs.13509.  
  
A. S. Borisova, “Structural and Functional Characterization of a Lytic Polysaccharide Monooxygenase with Broad Substrate Specificity”, *Journal of Biological Chemistry*, vol. 290, no. 38. Elsevier BV, pp. 22955–22969, Sep. 2015. doi: 10.1074/jbc.m115.660183.  
  
L. Bu, “Understanding Trends in Autoignition of Biofuels: Homologous Series of Oxygenated C5 Molecules”, *The Journal of Physical Chemistry A*, vol. 121, no. 29. American Chemical Society (ACS), pp. 5475–5486, Jul. 17, 2017. doi: 10.1021/acs.jpca.7b04000.  
  
T. Elder, L. Berstis, G. T. Beckhamand M. F. Crowley, “Coupling and Reactions of 5-Hydroxyconiferyl Alcohol in Lignin Formation”, *Journal of Agricultural and Food Chemistry*, vol. 64, no. 23. American Chemical Society (ACS), pp. 4742–4750, Jun. 03, 2016. doi: 10.1021/acs.jafc.6b02234.  
  
T. Elder, L. Berstis, G. T. Beckhamand M. F. Crowley, “Density Functional Theory Study of Spirodienone Stereoisomers in Lignin”, *ACS Sustainable Chemistry & Engineering*, vol. 5, no. 8. American Chemical Society (ACS), pp. 7188–7194, Jul. 10, 2017. doi: 10.1021/acssuschemeng.7b01373.  
  
G. A. Ferguson, “Carbocation Stability in H-ZSM5 at High Temperature”, *The Journal of Physical Chemistry A*, vol. 119, no. 46. American Chemical Society (ACS), pp. 11397–11405, Nov. 04, 2015. doi: 10.1021/acs.jpca.5b07025.  
  
G. A. Ferguson, “Ab Initio Surface Phase Diagrams for Coadsorption of Aromatics and Hydrogen on the Pt(111) Surface”, *The Journal of Physical Chemistry C*, vol. 120, no. 46. American Chemical Society (ACS), pp. 26249–26258, Nov. 10, 2016. doi: 10.1021/acs.jpcc.6b07057.  
  
I. Geronimo, “Effect of Mutation and Substrate Binding on the Stability of Cytochrome P450BM3 Variants”, *Biochemistry*, vol. 55, no. 25. American Chemical Society (ACS), pp. 3594–3606, Jun. 16, 2016. doi: 10.1021/acs.biochem.6b00183.  
  
I. Geronimo, S. R. Nigamand C. M. Payne, “Desulfination by 2′-hydroxybiphenyl-2-sulfinate desulfinase proceeds via electrophilic aromatic substitution by the cysteine-27 proton”, *Chemical Science*, vol. 8, no. 7. Royal Society of Chemistry (RSC), pp. 5078–5086, 2017. doi: 10.1039/c7sc00496f.  
  
M. B. Griffin, G. A. Ferguson, D. A. Ruddy, M. J. Biddy, G. T. Beckhamand J. A. Schaidle, “Role of the Support and Reaction Conditions on the Vapor-Phase Deoxygenation of *m*-Cresol over Pt/C and Pt/TiO2 Catalysts”, *ACS Catalysis*, vol. 6, no. 4. American Chemical Society (ACS), pp. 2715–2727, Mar. 23, 2016. doi: 10.1021/acscatal.5b02868.  
  
A. G. Hamre, “Thermodynamic Relationships with Processivity in *Serratia marcescens* Family 18 Chitinases”, *The Journal of Physical Chemistry B*, vol. 119, no. 30. American Chemical Society (ACS), pp. 9601–9613, Jul. 22, 2015. doi: 10.1021/acs.jpcb.5b03817.  
  
A. G. Hamre, S. Jana, N. K. Reppert, C. M. Payneand M. Sørlie, “Processivity, Substrate Positioning, and Binding: The Role of Polar Residues in a Family 18 Glycoside Hydrolase”, *Biochemistry*, vol. 54, no. 49. American Chemical Society (ACS), pp. 7292–7306, Dec. 02, 2015. doi: 10.1021/acs.biochem.5b00830.  
  
R. M. Happs, “O‐glycosylation effects on family 1 carbohydrate‐binding module solution structures”, *The FEBS Journal*, vol. 282, no. 22. Wiley, pp. 4341–4356, Sep. 21, 2015. doi: 10.1111/febs.13500.  
  
S. Jana, “Aromatic-Mediated Carbohydrate Recognition in Processive *Serratia marcescens* Chitinases”, *The Journal of Physical Chemistry B*, vol. 120, no. 7. American Chemical Society (ACS), pp. 1236–1249, Feb. 15, 2016. doi: 10.1021/acs.jpcb.5b12610.  
  
M. Kern, “Structural characterization of a unique marine animal family 7 cellobiohydrolase suggests a mechanism of cellulase salt tolerance”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 25. Proceedings of the National Academy of Sciences, pp. 10189–10194, Jun. 03, 2013. doi: 10.1073/pnas.1301502110.  
  
S. Kim, “Furan Production from Glycoaldehyde over HZSM-5”, *ACS Sustainable Chemistry & Engineering*, vol. 4, no. 5. American Chemical Society (ACS), pp. 2615–2623, Apr. 15, 2016. doi: 10.1021/acssuschemeng.6b00101.  
  
S. Kim, D. J. Robichaud, G. T. Beckham, R. S. Patonand M. R. Nimlos, “Ethanol Dehydration in HZSM-5 Studied by Density Functional Theory: Evidence for a Concerted Process”, *The Journal of Physical Chemistry A*, vol. 119, no. 15. American Chemical Society (ACS), pp. 3604–3614, Apr. 06, 2015. doi: 10.1021/jp513024z.  
  
B. C. Knott, M. F. Crowley, M. E. Himmel, J. Zimmerand G. T. Beckham, “Simulations of cellulose translocation in the bacterial cellulose synthase suggest a regulatory mechanism for the dimeric structure of cellulose”, *Chemical Science*, vol. 7, no. 5. Royal Society of Chemistry (RSC), pp. 3108–3116, 2016. doi: 10.1039/c5sc04558d.  
  
A. A. Kognole and C. M. Payne, “Cello-oligomer-binding dynamics and directionality in family 4 carbohydrate-binding modules”, *Glycobiology*, vol. 25, no. 10. Oxford University Press (OUP), pp. 1100–1111, Jul. 07, 2015. doi: 10.1093/glycob/cwv048.  
  
A. A. Kognole and C. M. Payne, “Inhibition of Mammalian Glycoprotein YKL-40”, *Journal of Biological Chemistry*, vol. 292, no. 7. Elsevier BV, pp. 2624–2636, Feb. 2017. doi: 10.1074/jbc.m116.764985.  
  
R. Kushwaha, A. B. Downieand C. M. Payne, “Uses of Phage Display in Agriculture: Sequence Analysis and Comparative Modeling of Late Embryogenesis Abundant Client Proteins Suggest Protein-Nucleic Acid Binding Functionality”, *Computational and Mathematical Methods in Medicine*, vol. 2013. Hindawi Limited, pp. 1–11, 2013. doi: 10.1155/2013/470390.  
  
H. B. Mayes, B. C. Knott, M. F. Crowley, L. J. Broadbelt, J. Ståhlbergand G. T. Beckham, “Who’s on base? Revealing the catalytic mechanism of inverting family 6 glycoside hydrolases”, *Chemical Science*, vol. 7, no. 9. Royal Society of Chemistry (RSC), pp. 5955–5968, 2016. doi: 10.1039/c6sc00571c.  
  
H. B. Mayes, M. W. Nolte, G. T. Beckham, B. H. Shanksand L. J. Broadbelt, “The Alpha–Bet(a) of Salty Glucose Pyrolysis: Computational Investigations Reveal Carbohydrate Pyrolysis Catalytic Action by Sodium Ions”, *ACS Catalysis*, vol. 5, no. 1. American Chemical Society (ACS), pp. 192–202, Dec. 01, 2014. doi: 10.1021/cs501125n.  
  
M. H. Momeni, “Structural, Biochemical, and Computational Characterization of the Glycoside Hydrolase Family 7 Cellobiohydrolase of the Tree-killing Fungus Heterobasidion irregulare*”, Journal of Biological Chemistry, vol. 288, no. 8. Elsevier BV, pp. 5861–5872, Feb. 2013. doi: 10.1074/jbc.m112.440891.*  
  
*C. M. Payne, “Hallmarks of Processivity in Glycoside Hydrolases from Crystallographic and Computational Studies of the Serratia marcescens Chitinases”, Journal of Biological Chemistry, vol. 287, no. 43. Elsevier BV, pp. 36322–36330, Oct. 2012. doi: 10.1074/jbc.m112.402149.*  
  
*C. M. Payne, “Multiple Functions of Aromatic-Carbohydrate Interactions in a Processive Cellulase Examined with Molecular Simulation”, Journal of Biological Chemistry, vol. 286, no. 47. Elsevier BV, pp. 41028–41035, Nov. 2011. doi: 10.1074/jbc.m111.297713.*  
  
*C. M. Payne, M. E. Himmel, M. F. Crowleyand G. T. Beckham, “Decrystallization of Oligosaccharides from the Cellulose Iβ Surface with Molecular Simulation”, The Journal of Physical Chemistry Letters, vol. 2, no. 13. American Chemical Society (ACS), pp. 1546–1550, Jun. 08, 2011. doi: 10.1021/jz2005122.*  
  
*C. M. Payne, W. Jiang, M. R. Shirts, M. E. Himmel, M. F. Crowleyand G. T. Beckham, “Glycoside Hydrolase Processivity Is Directly Related to Oligosaccharide Binding Free Energy”, Journal of the American Chemical Society, vol. 135, no. 50. American Chemical Society (ACS), pp. 18831–18839, Dec. 05, 2013. doi: 10.1021/ja407287f.*  
  
*C. M. Payne, “Fungal Cellulases”, Chemical Reviews, vol. 115, no. 3. American Chemical Society (ACS), pp. 1308–1448, Jan. 28, 2015. doi: 10.1021/cr500351c.*  
  
*C. M. Payne, “Glycosylated linkers in multimodular lignocellulose-degrading enzymes dynamically bind to cellulose”, Proceedings of the National Academy of Sciences, vol. 110, no. 36. Proceedings of the National Academy of Sciences, pp. 14646–14651, Aug. 19, 2013. doi: 10.1073/pnas.1309106110.*  
  
*A. Robinson, “Enhanced Hydrodeoxygenation of m-Cresol over Bimetallic Pt–Mo Catalysts through an Oxophilic Metal-Induced Tautomerization Pathway”, ACS Catalysis, vol. 6, no. 7. American Chemical Society (ACS), pp. 4356–4368, Jun. 10, 2016. doi: 10.1021/acscatal.6b01131.*  
  
*D. W. Sammond, C. M. Payne, R. Brunecky, M. E. Himmel, M. F. Crowleyand G. T. Beckham, “Cellulase Linkers Are Optimized Based on Domain Type and Function: Insights from Sequence Analysis, Biophysical Measurements, and Molecular Simulation”, PLoS ONE, vol. 7, no. 11. Public Library of Science (PLoS), p. e48615, Nov. 06, 2012. doi: 10.1371/journal.pone.0048615.*  
  
*C. B. Taylor, C. M. Payne, M. E. Himmel, M. F. Crowley, C. McCabeand G. T. Beckham, “Binding Site Dynamics and Aromatic–Carbohydrate Interactions in Processive and Non-Processive Family 7 Glycoside Hydrolases”, The Journal of Physical Chemistry B, vol. 117, no. 17. American Chemical Society (ACS), pp. 4924–4933, Apr. 10, 2013. doi: 10.1021/jp401410h.*  
  
*J. V. Vermaas, M. F. Crowley, G. T. Beckhamand C. M. Payne, “Effects of Lytic Polysaccharide Monooxygenase Oxidation on Cellulose Structure and Binding of Oxidized Cellulose Oligomers to Cellulases”, The Journal of Physical Chemistry B, vol. 119, no. 20. American Chemical Society (ACS), pp. 6129–6143, Apr. 02, 2015. doi: 10.1021/acs.jpcb.5b00778.*  
  
*C. Wilkens, “Plant α‐glucan phosphatases SEX4 and LSF2 display different affinity for amylopectin and amylose”, FEBS Letters, vol. 590, no. 1. Wiley, pp. 118–128, Jan. 2016. doi: 10.1002/1873-3468.12027.*  
  
*M. Wu, “Crystal Structure and Computational Characterization of the Lytic Polysaccharide Monooxygenase GH61D from the Basidiomycota Fungus Phanerochaete chrysosporium”, Journal of Biological Chemistry, vol. 288, no. 18. Elsevier BV, pp. 12828–12839, May 2013. doi: 10.1074/jbc.m113.459396.*  
  
*Y. Yu, I. A. Fursule, L. C. Mills, D. L. Englert, B. J. Berronand C. M. Payne, “CHARMM force field parameters for 2′-hydroxybiphenyl-2-sulfinate, 2-hydroxybiphenyl, and related analogs”, Journal of Molecular Graphics and Modelling, vol. 72. Elsevier BV, pp. 32–42, Mar. 2017. doi: 10.1016/j.jmgm.2016.12.005.*  
  
*M. Chen, M. E. Himmel, D. B. Wilsonand J. W. Brady, “Simulation studies of substrate recognition by the exocellulase CelF from Clostridium cellulolyticum”, Biotechnology and Bioengineering, vol. 113, no. 7. Wiley, pp. 1433–1440, Jan. 28, 2016. doi: 10.1002/bit.25909.*  
  
*P. R. Burney and J. Pfaendtner, “Structural and Dynamic Features of Candida rugosa Lipase 1 in Water, Octane, Toluene, and Ionic Liquids BMIM-PF6 and BMIM-NO3”, The Journal of Physical Chemistry B, vol. 117, no. 9. American Chemical Society (ACS), pp. 2662–2670, Feb. 27, 2013. doi: 10.1021/jp312299d.*  
  
*R. Chelakkot, A. Gopinath, L. Mahadevanand M. F. Hagan, “Flagellar dynamics of a connected chain of active, polar, Brownian particles”, Journal of The Royal Society Interface, vol. 11, no. 92. The Royal Society, p. 20130884, Mar. 06, 2014. doi: 10.1098/rsif.2013.0884.*  
  
*G. Duclos, “Topological structure and dynamics of three-dimensional active nematics”, Science, vol. 367, no. 6482. American Association for the Advancement of Science (AAAS), pp. 1120–1124, Mar. 06, 2020. doi: 10.1126/science.aaz4547.*  
  
*Y. Fily, A. Baskaranand M. F. Hagan, “Dynamics and density distribution of strongly confined noninteracting nonaligning self-propelled particles in a nonconvex boundary”, Physical Review E, vol. 91, no. 1. American Physical Society (APS), Jan. 14, 2015. doi: 10.1103/physreve.91.012125.*  
  
*Y. Fily, A. Baskaranand M. F. Hagan, “Equilibrium mappings in polar-isotropic confined active particles”, The European Physical Journal E, vol. 40, no. 6. Springer Science and Business Media LLC, Jun. 2017. doi: 10.1140/epje/i2017-11551-3.*  
  
*Y. Fily, Y. Kafri, A. P. Solon, J. Tailleurand A. Turner, “Mechanical pressure and momentum conservation in dry active matter”, Journal of Physics A: Mathematical and Theoretical, vol. 51, no. 4. IOP Publishing, p. 044003, Dec. 19, 2017. doi: 10.1088/1751-8121/aa99b6.*  
  
*M. F. HAGAN, “Modeling Viral Capsid Assembly”, Advances in Chemical Physics. John Wiley & Sons, Inc., pp. 1–68, Apr. 04, 2014. doi: 10.1002/9781118755815.ch01.*  
  
*S. Dharmavaram, B. She, G. Lázaro, M. F. Haganand R. Bruinsma, “Gaussian curvature and the budding kinetics of enveloped viruses”, []. Cold Spring Harbor Laboratory, Oct. 30, 2018. doi: 10.1101/457135.*  
  
*M. F. Hagan, O. M. Elradand R. L. Jack, “Mechanisms of kinetic trapping in self-assembly and phase transformation”, The Journal of Chemical Physics, vol. 135, no. 10. AIP Publishing, p. 104115, Sep. 14, 2011. doi: 10.1063/1.3635775.*  
  
*A. Joshi, E. Putzig, A. Baskaranand M. F. Hagan, “The interplay between activity and filament flexibility determines the emergent properties of active nematics”, Soft Matter, vol. 15, no. 1. Royal Society of Chemistry (RSC), pp. 94–101, 2019. doi: 10.1039/c8sm02202j.*  
  
*S. J. Kerns, “The energy landscape of adenylate kinase during catalysis”, Nature Structural & Molecular Biology, vol. 22, no. 2. Springer Science and Business Media LLC, pp. 124–131, Jan. 12, 2015. doi: 10.1038/nsmb.2941.*  
  
*G. R. Lazaro and M. F. Hagan, “Allosteric Control of Icosahedral Capsid Assembly”, The Journal of Physical Chemistry B, vol. 120, no. 26. American Chemical Society (ACS), pp. 6306–6318, May 09, 2016. doi: 10.1021/acs.jpcb.6b02768.*  
  
*G. R. Lázaro, S. Mukhopadhyayand M. F. Hagan, “Why Enveloped Viruses Need Cores—The Contribution of a Nucleocapsid Core to Viral Budding”, Biophysical Journal, vol. 114, no. 3. Elsevier BV, pp. 619–630, Feb. 2018. doi: 10.1016/j.bpj.2017.11.3782.*  
  
*J. M. Miller, “All twist and no bend makes raft edges splay: Spontaneous curvature of domain edges in colloidal membranes”, Science Advances, vol. 6, no. 31. American Association for the Advancement of Science (AAAS), Jul. 31, 2020. doi: 10.1126/sciadv.aba2331.*  
  
*J. M. Miller, “Conformational switching of chiral colloidal rafts regulates raft–raft attractions and repulsions”, Proceedings of the National Academy of Sciences, vol. 116, no. 32. Proceedings of the National Academy of Sciences, pp. 15792–15801, Jul. 18, 2019. doi: 10.1073/pnas.1900615116.*  
  
*F. Mohajerani and M. F. Hagan, “The role of the encapsulated cargo in microcompartment assembly”, PLOS Computational Biology, vol. 14, no. 7. Public Library of Science (PLoS), p. e1006351, Jul. 31, 2018. doi: 10.1371/journal.pcbi.1006351.*  
  
*F. Mohajerani, E. Sayer, C. Neil, K. Inlowand M. F. Hagan, “Mechanisms of Scaffold-Mediated Microcompartment Assembly and Size Control”, ACS Nano, vol. 15, no. 3. American Chemical Society (ACS), pp. 4197–4212, Mar. 08, 2021. doi: 10.1021/acsnano.0c05715.*  
  
*M. M. Norton, “Insensitivity of active nematic liquid crystal dynamics to topological constraints”, Physical Review E, vol. 97, no. 1. American Physical Society (APS), Jan. 10, 2018. doi: 10.1103/physreve.97.012702.*  
  
*M. R. Perkett and M. F. Hagan, “Using Markov state models to study self-assembly”, The Journal of Chemical Physics, vol. 140, no. 21. AIP Publishing, p. 214101, Jun. 07, 2014. doi: 10.1063/1.4878494.*  
  
*M. R. Perkett, D. T. Mirijanianand M. F. Hagan, “The allosteric switching mechanism in bacteriophage MS2”, The Journal of Chemical Physics, vol. 145, no. 3. AIP Publishing, p. 035101, Jul. 21, 2016. doi: 10.1063/1.4955187.*  
  
*J. D. Perlmutter and M. F. Hagan, “The Role of Packaging Sites in Efficient and Specific Virus Assembly”, Journal of Molecular Biology, vol. 427, no. 15. Elsevier BV, pp. 2451–2467, Jul. 2015. doi: 10.1016/j.jmb.2015.05.008.*  
  
*J. D. Perlmutter, F. Mohajeraniand M. F. Hagan, “Many-molecule encapsulation by an icosahedral shell”, eLife, vol. 5. eLife Sciences Publications, Ltd, May 11, 2016. doi: 10.7554/elife.14078.*  
  
*M. S. E. Peterson, M. F. Haganand A. Baskaran, “Statistical properties of a tangentially driven active filament”, Journal of Statistical Mechanics: Theory and Experiment, vol. 2020, no. 1. IOP Publishing, p. 013216, Jan. 22, 2020. doi: 10.1088/1742-5468/ab6097.*  
  
*F. Pontiggia, “Free energy landscape of activation in a signalling protein at atomic resolution”, Nature Communications, vol. 6, no. 1. Springer Science and Business Media LLC, Jun. 15, 2015. doi: 10.1038/ncomms8284.*  
  
*G. S. Redner, M. F. Haganand A. Baskaran, “Structure and Dynamics of a Phase-Separating Active Colloidal Fluid”, Physical Review Letters, vol. 110, no. 5. American Physical Society (APS), Jan. 31, 2013. doi: 10.1103/physrevlett.110.055701.*  
  
*G. S. Redner, C. G. Wagner, A. Baskaranand M. F. Hagan, “Classical Nucleation Theory Description of Active Colloid Assembly”, Physical Review Letters, vol. 117, no. 14. American Physical Society (APS), Sep. 30, 2016. doi: 10.1103/physrevlett.117.148002.*  
  
*G. R. Lázaro, B. Dragneaand M. F. Hagan, “Self-assembly of convex particles on spherocylindrical surfaces”, Soft Matter, vol. 14, no. 28. Royal Society of Chemistry (RSC), pp. 5728–5740, 2018. doi: 10.1039/c8sm00129d.*  
  
*T. Ruiz-Herrero, E. Velascoand M. F. Hagan, “Mechanisms of Budding of Nanoscale Particles through Lipid Bilayers”, The Journal of Physical Chemistry B, vol. 116, no. 32. American Chemical Society (ACS), pp. 9595–9603, Aug. 03, 2012. doi: 10.1021/jp301601g.*  
  
*A. P. Solon, “Pressure is not a state function for generic active fluids”, Nature Physics, vol. 11, no. 8. Springer Science and Business Media LLC, pp. 673–678, Jun. 29, 2015. doi: 10.1038/nphys3377.*  
  
*J. B. Stiller, “Probing the transition state in enzyme catalysis by high-pressure NMR dynamics”, Nature Catalysis, vol. 2, no. 8. Springer Science and Business Media LLC, pp. 726–734, Jun. 24, 2019. doi: 10.1038/s41929-019-0307-6.*  
  
*J. Villali, F. Pontiggia, M. W. Clarkson, M. F. Haganand D. Kern, “Evidence Against the “Y–T Coupling” Mechanism of Activation in the Response Regulator NtrC”, Journal of Molecular Biology, vol. 426, no. 7. Elsevier BV, pp. 1554–1567, Apr. 2014. doi: 10.1016/j.jmb.2013.12.027.*  
  
*C. G. Wagner, M. F. Haganand A. Baskaran, “Response of active Brownian particles to boundary driving”, Physical Review E, vol. 100, no. 4. American Physical Society (APS), Oct. 18, 2019. doi: 10.1103/physreve.100.042610.*  
  
*S. Xie, M. F. Haganand R. A. Pelcovits, “Interaction of chiral rafts in self-assembled colloidal membranes”, Physical Review E, vol. 93, no. 3. American Physical Society (APS), Mar. 31, 2016. doi: 10.1103/physreve.93.032706.*  
  
*S. Xie, R. A. Pelcovitsand M. F. Hagan, “Probing a self-assembledvirus membrane with a microtubule”, Physical Review E, vol. 93, no. 6. American Physical Society (APS), Jun. 13, 2016. doi: 10.1103/physreve.93.062608.*  
  
*N. Yu, A. Ghoshand M. F. Hagan, “Faceted particles formed by the frustrated packing of anisotropic colloids on curved surfaces”, Soft Matter, vol. 12, no. 44. Royal Society of Chemistry (RSC), pp. 8990–8998, 2016. doi: 10.1039/c6sm01498d.*  
  
*N. Yu and M. F. Hagan, “Simulations of HIV Capsid Protein Dimerization Reveal the Effect of Chemistry and Topography on the Mechanism of Hydrophobic Protein Association”, Biophysical Journal, vol. 103, no. 6. Elsevier BV, pp. 1363–1369, Sep. 2012. doi: 10.1016/j.bpj.2012.08.016.*  
  
*C. Zeng, G. Rodriguez Lázaro, I. B. Tsvetkova, M. F. Haganand B. Dragnea, “Defects and Chirality in the Nanoparticle-Directed Assembly of Spherocylindrical Shells of Virus Coat Proteins”, ACS Nano, vol. 12, no. 6. American Chemical Society (ACS), pp. 5323–5332, Apr. 25, 2018. doi: 10.1021/acsnano.8b00069.*  
  
*T. Zhu, “Fragment-Based Drug Discovery Using a Multidomain, Parallel MD-MM/PBSA Screening Protocol”, Journal of Chemical Information and Modeling, vol. 53, no. 3. American Chemical Society (ACS), pp. 560–572, Mar. 14, 2013. doi: 10.1021/ci300502h.*  
  
*J. DeBartolo, G. Hocky, M. Wilde, J. Xu, K. F. Freedand T. R. Sosnick, “Protein structure prediction enhanced with evolutionary diversity: SPEED”, Protein Science, vol. 19, no. 3. Wiley, pp. 520–534, Jan. 11, 2010. doi: 10.1002/pro.330.*  
  
*N. S. Abraham and M. R. Shirts, “Thermal Gradient Approach for the Quasi-harmonic Approximation and Its Application to Improved Treatment of Anisotropic Expansion”, Journal of Chemical Theory and Computation, vol. 14, no. 11. American Chemical Society (ACS), pp. 5904–5919, Oct. 03, 2018. doi: 10.1021/acs.jctc.8b00460.*  
  
*B. J. Coscia and M. R. Shirts, “Chemically Selective Transport in a Cross-Linked HII Phase Lyotropic Liquid Crystal Membrane”, The Journal of Physical Chemistry B, vol. 123, no. 29. American Chemical Society (ACS), pp. 6314–6330, Jun. 27, 2019. doi: 10.1021/acs.jpcb.9b04472.*  
  
*B. J. Coscia, J. Yelk, M. A. Glaser, D. L. Gin, X. Fengand M. R. Shirts, “Understanding the Nanoscale Structure of Inverted Hexagonal Phase Lyotropic Liquid Crystal Polymer Membranes”, The Journal of Physical Chemistry B, vol. 123, no. 1. American Chemical Society (ACS), pp. 289–309, Dec. 06, 2018. doi: 10.1021/acs.jpcb.8b09944.*  
  
*B. A. Hall, D. W. Wright, S. Jhaand P. V. Coveney, “Quantized Water Access to the HIV-1 Protease Active Site as a Proposed Mechanism for Cooperative Mutations in Drug Affinity”, Biochemistry, vol. 51, no. 33. American Chemical Society (ACS), pp. 6487–6489, Aug. 08, 2012. doi: 10.1021/bi300432u.*  
  
*S. Jha, J. Qiu, A. Luckow, P. Manthaand G. C. Fox, “A Tale of Two Data-Intensive Paradigms: Applications, Abstractions, and Architectures”, 2014 IEEE International Congress on Big Data. IEEE, Jun. 2014. doi: 10.1109/bigdata.congress.2014.137.*  
  
*A. Luckow, M. Santcroos, A. Zebrowskiand S. Jha, “Pilot-Data: An abstraction for distributed data”, Journal of Parallel and Distributed Computing, vol. 79–80. Elsevier BV, pp. 16–30, May 2015. doi: 10.1016/j.jpdc.2014.09.009.*  
  
*H. S. C. Martin, S. Jhaand P. V. Coveney, “Comparative analysis of nucleotide translocation through protein nanopores using steered molecular dynamics and an adaptive biasing force”, Journal of Computational Chemistry, vol. 35, no. 9. Wiley, pp. 692–702, Jan. 09, 2014. doi: 10.1002/jcc.23525.*  
  
*H. S. C. Martin, S. Jhaand P. V. Coveney, “Comparative analysis of nucleotide translocation through protein nanopores using steered molecular dynamics and an adaptive biasing force”, Journal of Computational Chemistry, vol. 35, no. 9. Wiley, pp. 692–702, Jan. 09, 2014. doi: 10.1002/jcc.23525.*  
  
*A. Merzky, O. Weidnerand S. Jha, “SAGA: A standardized access layer to heterogeneous Distributed Computing Infrastructure”, SoftwareX, vol. 1–2. Elsevier BV, pp. 3–8, Sep. 2015. doi: 10.1016/j.softx.2015.03.001.*  
  
*A. Ragothaman, “Developing eThread Pipeline Using SAGA-Pilot Abstraction for Large-Scale Structural Bioinformatics”, BioMed Research International, vol. 2014. Hindawi Limited, pp. 1–12, 2014. doi: 10.1155/2014/348725.*  
  
*N. P. Schieber and M. R. Shirts, “Configurational mapping significantly increases the efficiency of solid-solid phase coexistence calculations via molecular dynamics: Determining the FCC-HCP coexistence line of Lennard-Jones particles”, The Journal of Chemical Physics, vol. 150, no. 16. AIP Publishing, p. 164112, Apr. 28, 2019. doi: 10.1063/1.5080431.*  
  
*D. W. Wright, B. A. Hall, P. Kellamand P. V. Coveney, “Global Conformational Dynamics of HIV-1 Reverse Transcriptase Bound to Non-Nucleoside Inhibitors”, Biology, vol. 1, no. 2. MDPI AG, pp. 222–244, Jul. 26, 2012. doi: 10.3390/biology1020222.*  
  
*D. W. Wright, B. A. Hall, O. A. Kenway, S. Jhaand P. V. Coveney, “Computing Clinically Relevant Binding Free Energies of HIV-1 Protease Inhibitors”, Journal of Chemical Theory and Computation, vol. 10, no. 3. American Chemical Society (ACS), pp. 1228–1241, Feb. 14, 2014. doi: 10.1021/ct4007037.*  
  
*D. W. Wright, S. K. Sadiq, G. De Fabritiisand P. V. Coveney, “Thumbs Down for HIV: Domain Level Rearrangements Do Occur in the NNRTI-Bound HIV-1 Reverse Transcriptase”, Journal of the American Chemical Society, vol. 134, no. 31. American Chemical Society (ACS), pp. 12885–12888, Jul. 30, 2012. doi: 10.1021/ja301565k.*  
  
*M. Khoshlessan, I. Paraskevakos, S. Jhaand O. Beckstein, “Parallel Analysis in MDAnalysis using the Dask Parallel Computing Library”, Proceedings of the 16th Python in Science Conference. SciPy, 2017. doi: 10.25080/shinma-7f4c6e7-00a.*  
  
*A. Biesso, J. Xu, P. L. Muíño, P. R. Callisand J. R. Knutson, “Charge Invariant Protein–Water Relaxation in GB1 via Ultrafast Tryptophan Fluorescence”, Journal of the American Chemical Society, vol. 136, no. 7. American Chemical Society (ACS), pp. 2739–2747, Feb. 06, 2014. doi: 10.1021/ja406126a.*  
  
*P. R. Callis, “Simulating electrostatic effects on electronic transitions in proteins”, Molecular Simulation, vol. 41, no. 1–3. Informa UK Limited, pp. 190–204, Jun. 13, 2014. doi: 10.1080/08927022.2014.923571.*  
  
*M. Drobizhev, “Unified Description of Optical Properties and Photostability of Fluorescent Proteins by Means of the Chromophore-Protein Electrostatic Interactions”, Biophysical Journal, vol. 102, no. 3. Elsevier BV, pp. 403a–404a, Jan. 2012. doi: 10.1016/j.bpj.2011.11.2204.*  
  
*M. Drobizhev, “Primary Role of the Chromophore Bond Length Alternation in Reversible Photoconversion of Red Fluorescence Proteins”, Scientific Reports, vol. 2, no. 1. Springer Science and Business Media LLC, Sep. 24, 2012. doi: 10.1038/srep00688.*  
  
*M. Drobizhev, J. N. Scott, P. R. Callisand A. Rebane, “All-Optical Sensing of the Components of the Internal Local Electric Field in Proteins”, IEEE Photonics Journal, vol. 4, no. 5. Institute of Electrical and Electronics Engineers (IEEE), pp. 1996–2001, Oct. 2012. doi: 10.1109/jphot.2012.2221124.*  
  
*A. Mikhaylov, S. de Reguardati, J. Pahapill, P. R. Callis, B. Kohlerand A. Rebane, “Two-photon absorption spectra of fluorescent isomorphic DNA base analogs”, Biomedical Optics Express, vol. 9, no. 2. Optica Publishing Group, p. 447, Jan. 05, 2018. doi: 10.1364/boe.9.000447.*  
  
*P. L. Muíño, J. N. Scottand P. R. Callis, “Fine-Grained Spatial and Temporal Resolution of Water and Protein Contributions to Ultra-Fast and Slower Fluorescence Shifts from MD + QM Simulations”, Biophysical Journal, vol. 106, no. 2. Elsevier BV, p. 205a, Jan. 2014. doi: 10.1016/j.bpj.2013.11.1206.*  
  
*J. N. Scott and P. R. Callis, “MD Simulations Reveal Ultrafast Dielectric Compensation by Water of Large Stokes Shifts from Charged Groups in Staphylococcal Nuclease”, Biophysical Journal, vol. 102, no. 3. Elsevier BV, p. 734a, Jan. 2012. doi: 10.1016/j.bpj.2011.11.3982.*  
  
*J. N. Scott and P. R. Callis, “Md+Qm Calculations Explore the Origins of Differences amongst the Red Fluorescent Proteins”, Biophysical Journal, vol. 104, no. 2. Elsevier BV, p. 684a, Jan. 2013. doi: 10.1016/j.bpj.2012.11.3774.*  
  
*J. N. Scott and P. R. Callis, “Insensitivity of Tryptophan Fluorescence to Local Charge Mutations”, The Journal of Physical Chemistry B, vol. 117, no. 33. American Chemical Society (ACS), pp. 9598–9605, Aug. 09, 2013. doi: 10.1021/jp4041716.*  
  
*J. N. Scott and P. R. Callis, “MD+QM Investigations of the Length Scale and Forcefield Dependence of the Time Dependent Fluorescent Stokes Shift of Wild Type Staphylococcal Nuclease and Charge Mutants”, Biophysical Journal, vol. 108, no. 2. Elsevier BV, p. 622a, Jan. 2015. doi: 10.1016/j.bpj.2014.11.3382.*  
  
*P. R. Callis and J. R. Tusell, “MD + QM Correlations with Tryptophan Fluorescence Spectral Shifts and Lifetimes”, Methods in Molecular Biology. Humana Press, pp. 171–214, Aug. 30, 2013. doi: 10.1007/978-1-62703-649-8\_8.*  
  
*J. R. Tusell and P. R. Callis, “Simulations of Tryptophan Fluorescence Dynamics during Folding of the Villin Headpiece”, The Journal of Physical Chemistry B, vol. 116, no. 8. American Chemical Society (ACS), pp. 2586–2594, Feb. 16, 2012. doi: 10.1021/jp211217w.*  
  
*K. R. Bradnam, “Assemblathon 2: evaluating de novo methods of genome assembly in three vertebrate species”, GigaScience, vol. 2, no. 1. Oxford University Press (OUP), Jul. 22, 2013. doi: 10.1186/2047-217x-2-10.*  
  
*R. M. Calisi and M. D. MacManes, “RNAseq-ing a more integrative understanding of animal behavior”, Current Opinion in Behavioral Sciences, vol. 6. Elsevier BV, pp. 65–68, Dec. 2015. doi: 10.1016/j.cobeha.2015.09.007.*  
  
*B. J. Haas, “De novo transcript sequence reconstruction from RNA-seq using the Trinity platform for reference generation and analysis”, Nature Protocols, vol. 8, no. 8. Springer Science and Business Media LLC, pp. 1494–1512, Jul. 11, 2013. doi: 10.1038/nprot.2013.084.*  
  
*M. p . Lesser and M. MacManes, “Transcriptomic Resources for the Rocky Intertidal Blue MusselMytilus edulisfrom the Gulf of Maine”, Journal of Shellfish Research, vol. 35, no. 2. National Shellfisheries Association, pp. 435–465, Aug. 2016. doi: 10.2983/035.035.0218.*  
  
*M. D. MacManes, “On the optimal trimming of high-throughput mRNA sequence data”, Frontiers in Genetics, vol. 5. Frontiers Media SA, 2014. doi: 10.3389/fgene.2014.00013.*  
  
*M. D. MacManes and M. B. Eisen, “Improving transcriptome assembly through error correction of high-throughput sequence reads”, PeerJ, vol. 1. PeerJ, p. e113, Jul. 23, 2013. doi: 10.7717/peerj.113.*  
  
*M. D. MacManes and M. B. Eisen, “Characterization of the transcriptome, nucleotide sequence polymorphism, and natural selection in the desert adapted mousePeromyscus eremicus”, PeerJ, vol. 2. PeerJ, p. e642, Oct. 28, 2014. doi: 10.7717/peerj.642.*  
  
*T. A. Schuelke, A. Westbrook, K. Broders, K. Woesteand M. D. MacManes, “De novogenome assembly ofGeosmithia morbida, the causal agent of thousand cankers disease”, PeerJ, vol. 4. PeerJ, p. e1952, May 02, 2016. doi: 10.7717/peerj.1952.*  
  
*J. D. Chodera and M. R. Shirts, “Replica exchange and expanded ensemble simulations as Gibbs sampling: Simple improvements for enhanced mixing”, The Journal of Chemical Physics, vol. 135, no. 19. AIP Publishing, p. 194110, Nov. 21, 2011. doi: 10.1063/1.3660669.*  
  
*J. P. Nilmeier, G. E. Crooks, D. D. L. Minhand J. D. Chodera, “Nonequilibrium candidate Monte Carlo is an efficient tool for equilibrium simulation”, Proceedings of the National Academy of Sciences, vol. 108, no. 45. Proceedings of the National Academy of Sciences, Oct. 24, 2011. doi: 10.1073/pnas.1106094108.*  
  
*J. A. Brown and I. F. Thorpe, “Dual Allosteric Inhibitors Jointly Modulate Protein Structure and Dynamics in the Hepatitis C Virus Polymerase”, Biochemistry, vol. 54, no. 26. American Chemical Society (ACS), pp. 4131–4141, Jun. 26, 2015. doi: 10.1021/acs.biochem.5b00411.*  
  
*B. C. Davis, J. A. Brownand I. F. Thorpe, “Allosteric Inhibitors Have Distinct Effects, but Also Common Modes of Action, in the HCV Polymerase”, Biophysical Journal, vol. 108, no. 7. Elsevier BV, pp. 1785–1795, Apr. 2015. doi: 10.1016/j.bpj.2015.03.005.*  
  
*M. Bykhovskaia, A. Jagota, A. Gonzalez, A. Vasinand J. T. Littleton, “Interaction of the Complexin Accessory Helix with the C-Terminus of the SNARE Complex: Molecular-Dynamics Model of the Fusion Clamp”, Biophysical Journal, vol. 105, no. 3. Elsevier BV, pp. 679–690, Aug. 2013. doi: 10.1016/j.bpj.2013.06.018.*  
  
*D. Roxbury, A. Jagotaand J. Mittal, “Sequence-Specific Self-Stitching Motif of Short Single-Stranded DNA on a Single-Walled Carbon Nanotube”, Journal of the American Chemical Society, vol. 133, no. 34. American Chemical Society (ACS), pp. 13545–13550, Aug. 10, 2011. doi: 10.1021/ja204413v.*  
  
*S. Iliafar, J. Mittal, D. Vezenovand A. Jagota, “Interaction of Single-Stranded DNA with Curved Carbon Nanotube Is Much Stronger Than with Flat Graphite”, Journal of the American Chemical Society, vol. 136, no. 37. American Chemical Society (ACS), pp. 12947–12957, Sep. 08, 2014. doi: 10.1021/ja5055498.*  
  
*W. H. Lee, Z.-D. Deng, T.-S. Kim, A. F. Laine, S. H. Lisanbyand A. V. Peterchev, “Regional electric field induced by electroconvulsive therapy in a realistic finite element head model: Influence of white matter anisotropic conductivity”, NeuroImage, vol. 59, no. 3. Elsevier BV, pp. 2110–2123, Feb. 2012. doi: 10.1016/j.neuroimage.2011.10.029.*  
  
*L. T. Braiterman, “Distinct phenotype of a Wilson disease mutation reveals a novel trafficking determinant in the copper transporter ATP7B”, Proceedings of the National Academy of Sciences, vol. 111, no. 14. Proceedings of the National Academy of Sciences, Mar. 24, 2014. doi: 10.1073/pnas.1314161111.*  
  
*K. T. Debiec, D. S. Cerutti, L. R. Baker, A. M. Gronenborn, D. A. Caseand L. T. Chong, “Further along the Road Less Traveled: AMBER ff15ipq, an Original Protein Force Field Built on a Self-Consistent Physical Model”, Journal of Chemical Theory and Computation, vol. 12, no. 8. American Chemical Society (ACS), pp. 3926–3947, Jul. 22, 2016. doi: 10.1021/acs.jctc.6b00567.*  
  
*K. M. Oshaben, R. Salari, D. R. McCaslin, L. T. Chongand W. S. Horne, “The Native GCN4 Leucine-Zipper Domain Does Not Uniquely Specify a Dimeric Oligomerization State”, Biochemistry, vol. 51, no. 47. American Chemical Society (ACS), pp. 9581–9591, Nov. 13, 2012. doi: 10.1021/bi301132k.*  
  
*M. T. Panteva, R. Salari, M. Bhattacharjeeand L. T. Chong, “Direct Observations of Shifts in the β-Sheet Register of a Protein-Peptide Complex Using Explicit Solvent Simulations”, Biophysical Journal, vol. 100, no. 9. Elsevier BV, pp. L50–L52, May 2011. doi: 10.1016/j.bpj.2011.03.035.*  
  
*R. Salari and L. T. Chong, “Desolvation Costs of Salt Bridges across Protein Binding Interfaces: Similarities and Differences between Implicit and Explicit Solvent Models”, The Journal of Physical Chemistry Letters, vol. 1, no. 19. American Chemical Society (ACS), pp. 2844–2848, Sep. 13, 2010. doi: 10.1021/jz1010863.*  
  
*R. Salari and L. T. Chong, “Effects of High Temperature on Desolvation Costs of Salt Bridges Across Protein Binding Interfaces: Similarities and Differences between Implicit and Explicit Solvent Models”, The Journal of Physical Chemistry B, vol. 116, no. 8. American Chemical Society (ACS), pp. 2561–2567, Feb. 21, 2012. doi: 10.1021/jp210172b.*  
  
*E. Suárez, “Simultaneous Computation of Dynamical and Equilibrium Information Using a Weighted Ensemble of Trajectories”, Journal of Chemical Theory and Computation, vol. 10, no. 7. American Chemical Society (ACS), pp. 2658–2667, Mar. 24, 2014. doi: 10.1021/ct401065r.*  
  
*E. Suárez, A. J. Pratt, L. T. Chongand D. M. Zuckerman, “Estimating first-passage time distributions from weighted ensemble simulations and non-Markovian analyses”, Protein Science, vol. 25, no. 1. Wiley, pp. 67–78, Sep. 09, 2015. doi: 10.1002/pro.2738.*  
  
*M. C. Zwier, “WESTPA: An Interoperable, Highly Scalable Software Package for Weighted Ensemble Simulation and Analysis”, Journal of Chemical Theory and Computation, vol. 11, no. 2. American Chemical Society (ACS), pp. 800–809, Jan. 29, 2015. doi: 10.1021/ct5010615.*  
  
*M. C. Zwier, A. J. Pratt, J. L. Adelman, J. W. Kaus, D. M. Zuckermanand L. T. Chong, “Efficient Atomistic Simulation of Pathways and Calculation of Rate Constants for a Protein–Peptide Binding Process: Application to the MDM2 Protein and an Intrinsically Disordered p53 Peptide”, The Journal of Physical Chemistry Letters, vol. 7, no. 17. American Chemical Society (ACS), pp. 3440–3445, Aug. 22, 2016. doi: 10.1021/acs.jpclett.6b01502.*  
  
*J. A. Smith, M. Romanus, P. K. Mantha, Y. El Khamra, T. C. Bishopand S. Jha, “Scalable online comparative genomics of mononucleosomes”, Proceedings of the Conference on Extreme Science and Engineering Discovery Environment: Gateway to Discovery. ACM, Jul. 22, 2013. doi: 10.1145/2484762.2484819.*  
  
*M. Palla, C.-P. Chen, Y. Zhang, J. Li, J. Juand J.-C. Liao, “Mechanism of flexibility control for ATP access of hepatitis C virus NS3 helicase”, Journal of Biomolecular Structure and Dynamics, vol. 31, no. 2. Informa UK Limited, pp. 129–141, Feb. 2013. doi: 10.1080/07391102.2012.698236.*  
  
*Y. Zhang and J.-C. Liao, “Identifying Highly Conserved and Unique Structural Elements in Myosin VI”, Cellular and Molecular Bioengineering, vol. 5, no. 4. Springer Science and Business Media LLC, pp. 375–389, Oct. 02, 2012. doi: 10.1007/s12195-012-0254-7.*  
  
*M. Adams, E. Wang, X. Zhuangand J. B. Klauda, “Simulations of simple Bovine and Homo sapiens outer cortex ocular lens membrane models with a majority concentration of cholesterol”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1860, no. 10. Elsevier BV, pp. 2134–2144, Oct. 2018. doi: 10.1016/j.bbamem.2017.11.010.*  
  
*M. Ghorbani, E. Wang, A. Krämerand J. B. Klauda, “Molecular dynamics simulations of ethanol permeation through single and double-lipid bilayers”, The Journal of Chemical Physics, vol. 153, no. 12. AIP Publishing, p. 125101, Sep. 28, 2020. doi: 10.1063/5.0013430.*  
  
*N. B. Guros, A. Balijepalliand J. B. Klauda, “The Role of Lipid Interactions in Simulations of the α-Hemolysin Ion-Channel-Forming Toxin”, Biophysical Journal, vol. 115, no. 9. Elsevier BV, pp. 1720–1730, Nov. 2018. doi: 10.1016/j.bpj.2018.09.009.*  
  
*N. B. Guros, A. Balijepalliand J. B. Klauda, “Microsecond-timescale simulations suggest 5-HT–mediated preactivation of the 5-HT 3A serotonin receptor”, Proceedings of the National Academy of Sciences, vol. 117, no. 1. Proceedings of the National Academy of Sciences, pp. 405–414, Dec. 23, 2019. doi: 10.1073/pnas.1908848117.*  
  
*J. B. Klauda, V. Monje, T. Kimand W. Im, “Improving the CHARMM Force Field for Polyunsaturated Fatty Acid Chains”, The Journal of Physical Chemistry B, vol. 116, no. 31. American Chemical Society (ACS), pp. 9424–9431, Jul. 03, 2012. doi: 10.1021/jp304056p.*  
  
*A. Krämer, “Membrane permeability of small molecules from unbiased molecular dynamics simulations”, The Journal of Chemical Physics, vol. 153, no. 12. AIP Publishing, p. 124107, Sep. 28, 2020. doi: 10.1063/5.0013429.*  
  
*V. Monje-Galvan and J. B. Klauda, “Peripheral membrane proteins: Tying the knot between experiment and computation”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1858, no. 7. Elsevier BV, pp. 1584–1593, Jul. 2016. doi: 10.1016/j.bbamem.2016.02.018.*  
  
*V. Monje-Galvan and J. B. Klauda, “Two sterols, two bilayers: insights on membrane structure from molecular dynamics”, Molecular Simulation, vol. 43, no. 13–16. Informa UK Limited, pp. 1179–1188, Jul. 19, 2017. doi: 10.1080/08927022.2017.1353690.*  
  
*V. Monje-Galvan and J. B. Klauda, “Preferred Binding Mechanism of Osh4’s Amphipathic Lipid-Packing Sensor Motif, Insights from Molecular Dynamics”, The Journal of Physical Chemistry B, vol. 122, no. 42. American Chemical Society (ACS), pp. 9713–9723, Oct. 03, 2018. doi: 10.1021/acs.jpcb.8b07067.*  
  
*V. Monje-Galvan and J. B. Klauda, “Interfacial properties of aqueous solutions of butanol isomers and cyclohexane”, Fluid Phase Equilibria, vol. 513. Elsevier BV, p. 112551, Jun. 2020. doi: 10.1016/j.fluid.2020.112551.*  
  
*J. W. O’Connor and J. B. Klauda, “Lipid Membranes with a Majority of Cholesterol: Applications to the Ocular Lens and Aquaporin 0”, The Journal of Physical Chemistry B, vol. 115, no. 20. American Chemical Society (ACS), pp. 6455–6464, May 03, 2011. doi: 10.1021/jp108650u.*  
  
*K. R. Pandit and J. B. Klauda, “Membrane models of E. coli containing cyclic moieties in the aliphatic lipid chain”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1818, no. 5. Elsevier BV, pp. 1205–1210, May 2012. doi: 10.1016/j.bbamem.2012.01.009.*  
  
*B. Rogaski and J. B. Klauda, “Membrane-Binding Mechanism of a Peripheral Membrane Protein through Microsecond Molecular Dynamics Simulations”, Journal of Molecular Biology, vol. 423, no. 5. Elsevier BV, pp. 847–861, Nov. 2012. doi: 10.1016/j.jmb.2012.08.015.*  
  
*D. Subramanian, C. T. Boughter, J. B. Klauda, B. Hammoudaand M. A. Anisimov, “Mesoscale inhomogeneities in aqueous solutions of small amphiphilic molecules”, Faraday Discussions, vol. 167. Royal Society of Chemistry (RSC), p. 217, 2013. doi: 10.1039/c3fd00070b.*  
  
*D. Subramanian, J. B. Klauda, P. J. Collingsand M. A. Anisimov, “Mesoscale Phenomena in Ternary Solutions of Tertiary Butyl Alcohol, Water, and Propylene Oxide”, The Journal of Physical Chemistry B, vol. 118, no. 22. American Chemical Society (ACS), pp. 5994–6006, May 21, 2014. doi: 10.1021/jp4125183.*  
  
*E. Wang and J. B. Klauda, “Molecular Dynamics Simulations of Ceramide and Ceramide-Phosphatidylcholine Bilayers”, The Journal of Physical Chemistry B, vol. 121, no. 43. American Chemical Society (ACS), pp. 10091–10104, Oct. 20, 2017. doi: 10.1021/acs.jpcb.7b08967.*  
  
*E. Wang and J. B. Klauda, “Examination of Mixtures Containing Sphingomyelin and Cholesterol by Molecular Dynamics Simulations”, The Journal of Physical Chemistry B, vol. 121, no. 18. American Chemical Society (ACS), pp. 4833–4844, Apr. 26, 2017. doi: 10.1021/acs.jpcb.7b01832.*  
  
*E. Wang and J. B. Klauda, “Models for the Stratum Corneum Lipid Matrix: Effects of Ceramide Concentration, Ceramide Hydroxylation, and Free Fatty Acid Protonation”, The Journal of Physical Chemistry B, vol. 122, no. 50. American Chemical Society (ACS), pp. 11996–12008, Nov. 28, 2018. doi: 10.1021/acs.jpcb.8b06188.*  
  
*E. Wang and J. B. Klauda, “Simulations of Pure Ceramide and Ternary Lipid Mixtures as Simple Interior Stratum Corneum Models”, The Journal of Physical Chemistry B, vol. 122, no. 10. American Chemical Society (ACS), pp. 2757–2768, Feb. 21, 2018. doi: 10.1021/acs.jpcb.8b00348.*  
  
*E. Wang and J. B. Klauda, “Structure and Permeability of Ceramide Bilayers and Multilayers”, The Journal of Physical Chemistry B, vol. 123, no. 11. American Chemical Society (ACS), pp. 2525–2535, Feb. 22, 2019. doi: 10.1021/acs.jpcb.9b00037.*  
  
*E. Wang and J. B. Klauda, “Molecular Structure of the Long Periodicity Phase in the Stratum Corneum”, Journal of the American Chemical Society, vol. 141, no. 42. American Chemical Society (ACS), pp. 16930–16943, Sep. 24, 2019. doi: 10.1021/jacs.9b08995.*  
  
*A. West, “How Do Ethanolamine Plasmalogens Contribute to Order and Structure of Neurological Membranes?”, The Journal of Physical Chemistry B, vol. 124, no. 5. American Chemical Society (ACS), pp. 828–839, Jan. 09, 2020. doi: 10.1021/acs.jpcb.9b08850.*  
  
*K. D. Wildermuth, V. Monje-Galvan, L. M. Warburtonand J. B. Klauda, “Effect of Membrane Lipid Packing on Stable Binding of the ALPS Peptide”, Journal of Chemical Theory and Computation, vol. 15, no. 2. American Chemical Society (ACS), pp. 1418–1429, Jan. 11, 2019. doi: 10.1021/acs.jctc.8b00945.*  
  
*X. Zhuang, A. Ouand J. B. Klauda, “Simulations of simple linoleic acid-containing lipid membranes and models for the soybean plasma membranes”, The Journal of Chemical Physics, vol. 146, no. 21. AIP Publishing, p. 215103, Jun. 06, 2017. doi: 10.1063/1.4983655.*  
  
*L. Gavrilenko and J. B. Klauda, “Aggregation of modified hexabenzocoronenes as models for early stage asphaltene self-assembly”, Molecular Simulation, vol. 44, no. 12. Informa UK Limited, pp. 992–1003, May 09, 2018. doi: 10.1080/08927022.2018.1469752.*  
  
*D. J. Beltran-Villegas and A. Jayaraman, “Assembly of Amphiphilic Block Copolymers and Nanoparticles in Solution: Coarse-Grained Molecular Simulation Study”, Journal of Chemical & Engineering Data, vol. 63, no. 7. American Chemical Society (ACS), pp. 2351–2367, Feb. 05, 2018. doi: 10.1021/acs.jced.7b00925.*  
  
*D. J. Beltran-Villegas, I. Lyubimovand A. Jayaraman, “Molecular dynamics simulations and PRISM theory study of solutions of nanoparticles and triblock copolymers with solvophobic end blocks”, Molecular Systems Design & Engineering, vol. 3, no. 3. Royal Society of Chemistry (RSC), pp. 453–472, 2018. doi: 10.1039/c7me00128b.*  
  
*R. M. Elder, T. Emrickand A. Jayaraman, “Understanding the Effect of Polylysine Architecture on DNA Binding Using Molecular Dynamics Simulations”, Biomacromolecules, vol. 12, no. 11. American Chemical Society (ACS), pp. 3870–3879, Sep. 27, 2011. doi: 10.1021/bm201113y.*  
  
*R. M. Elder and A. Jayaraman, “Sequence-Specific Recognition of Cancer Drug-DNA Adducts by HMGB1a Repair Protein”, Biophysical Journal, vol. 102, no. 10. Elsevier BV, pp. 2331–2338, May 2012. doi: 10.1016/j.bpj.2012.04.013.*  
  
*R. M. Elder and A. Jayaraman, “Molecular Simulations of Polycation–DNA Binding Exploring the Effect of Peptide Chemistry and Sequence in Nuclear Localization Sequence Based Polycations”, The Journal of Physical Chemistry B, vol. 117, no. 40. American Chemical Society (ACS), pp. 11988–11999, Sep. 25, 2013. doi: 10.1021/jp406875a.*  
  
*R. M. Elder and A. Jayaraman, “Simulation study of the effects of surface chemistry and temperature on the conformations of ssDNA oligomers near hydrophilic and hydrophobic surfaces”, The Journal of Chemical Physics, vol. 140, no. 15. AIP Publishing, p. 155103, Apr. 21, 2014. doi: 10.1063/1.4870776.*  
  
*R. M. Elder, J. Pfaendtnerand A. Jayaraman, “Effect of Hydrophobic and Hydrophilic Surfaces on the Stability of Double-Stranded DNA”, Biomacromolecules, vol. 16, no. 6. American Chemical Society (ACS), pp. 1862–1869, May 21, 2015. doi: 10.1021/acs.biomac.5b00469.*  
  
*J. J. Roberts, R. M. Elder, A. J. Neumann, A. Jayaramanand S. J. Bryant, “Interaction of Hyaluronan Binding Peptides with Glycosaminoglycans in Poly(ethylene glycol) Hydrogels”, Biomacromolecules, vol. 15, no. 4. American Chemical Society (ACS), pp. 1132–1141, Mar. 20, 2014. doi: 10.1021/bm401524h.*  
  
*F. Stanzione and A. Jayaraman, “Computational Design of Oligopeptide Containing Poly(ethylene glycol) Brushes for Stimuli-Responsive Drug Delivery”, The Journal of Physical Chemistry B, vol. 119, no. 42. American Chemical Society (ACS), pp. 13309–13320, Oct. 13, 2015. doi: 10.1021/acs.jpcb.5b06838.*  
  
*F. Stanzione and A. Jayaraman, “Hybrid Atomistic and Coarse-Grained Molecular Dynamics Simulations of Polyethylene Glycol (PEG) in Explicit Water”, The Journal of Physical Chemistry B, vol. 120, no. 17. American Chemical Society (ACS), pp. 4160–4173, Apr. 25, 2016. doi: 10.1021/acs.jpcb.6b02327.*  
  
*D. Cui, B. W. Zhang, N. Matubayasiand R. M. Levy, “The Role of Interfacial Water in Protein–Ligand Binding: Insights from the Indirect Solvent Mediated Potential of Mean Force”, Journal of Chemical Theory and Computation, vol. 14, no. 2. American Chemical Society (ACS), pp. 512–526, Jan. 12, 2018. doi: 10.1021/acs.jctc.7b01076.*  
  
*W. Dai, A. M. Senguptaand R. M. Levy, “First Passage Times, Lifetimes, and Relaxation Times of Unfolded Proteins”, Physical Review Letters, vol. 115, no. 4. American Physical Society (APS), Jul. 21, 2015. doi: 10.1103/physrevlett.115.048101.*  
  
*N. Deng, D. Cui, B. W. Zhang, J. Xia, J. Cruzand R. Levy, “Comparing alchemical and physical pathway methods for computing the absolute binding free energy of charged ligands”, Physical Chemistry Chemical Physics, vol. 20, no. 25. Royal Society of Chemistry (RSC), pp. 17081–17092, 2018. doi: 10.1039/c8cp01524d.*  
  
*N. Deng, “Large scale free energy calculations for blind predictions of protein–ligand binding: the D3R Grand Challenge 2015”, Journal of Computer-Aided Molecular Design, vol. 30, no. 9. Springer Science and Business Media LLC, pp. 743–751, Aug. 25, 2016. doi: 10.1007/s10822-016-9952-x.*  
  
*N. Deng, “Distinguishing Binders from False Positives by Free Energy Calculations: Fragment Screening Against the Flap Site of HIV Protease”, The Journal of Physical Chemistry B, vol. 119, no. 3. American Chemical Society (ACS), pp. 976–988, Sep. 17, 2014. doi: 10.1021/jp506376z.*  
  
*N. Deng, “Allosteric HIV-1 integrase inhibitors promote aberrant protein multimerization by directly mediating inter-subunit interactions: Structural and thermodynamic modeling studies”, Protein Science, vol. 25, no. 11. Wiley, pp. 1911–1917, Aug. 17, 2016. doi: 10.1002/pro.2997.*  
  
*N. Deng, B. W. Zhangand R. M. Levy, “Connecting Free Energy Surfaces in Implicit and Explicit Solvent: An Efficient Method To Compute Conformational and Solvation Free Energies”, Journal of Chemical Theory and Computation, vol. 11, no. 6. American Chemical Society (ACS), pp. 2868–2878, May 05, 2015. doi: 10.1021/acs.jctc.5b00264.*  
  
*W. F. Flynn, “Deep Sequencing of Protease Inhibitor Resistant HIV Patient Isolates Reveals Patterns of Correlated Mutations in Gag and Protease”, PLOS Computational Biology, vol. 11, no. 4. Public Library of Science (PLoS), p. e1004249, Apr. 20, 2015. doi: 10.1371/journal.pcbi.1004249.*  
  
*W. F. Flynn, A. Haldane, B. E. Torbettand R. M. Levy, “Inference of epistatic effects leading to entrenchment and drug resistance in HIV-1 protease”, []. Cold Spring Harbor Laboratory, Jul. 13, 2016. doi: 10.1101/063750.*  
  
*W. F. Flynn, A. Haldane, B. E. Torbettand R. M. Levy, “Inference of Epistatic Effects Leading to Entrenchment and Drug Resistance in HIV-1 Protease”, Molecular Biology and Evolution, vol. 34, no. 6. Oxford University Press (OUP), pp. 1291–1306, Mar. 20, 2017. doi: 10.1093/molbev/msx095.*  
  
*E. Gallicchio, “Role of Ligand Reorganization and Conformational Restraints on the Binding Free Energies of DAPY Non-Nucleoside Inhibitors to HIV Reverse Transcriptase”, Computational Molecular Bioscience, vol. 2, no. 1. Scientific Research Publishing, Inc., pp. 7–22, 2012. doi: 10.4236/cmb.2012.21002.*  
  
*E. Gallicchio, “BEDAM binding free energy predictions for the SAMPL4 octa-acid host challenge”, Journal of Computer-Aided Molecular Design, vol. 29, no. 4. Springer Science and Business Media LLC, pp. 315–325, Mar. 01, 2015. doi: 10.1007/s10822-014-9795-2.*  
  
*E. Gallicchio, “Virtual screening of integrase inhibitors by large scale binding free energy calculations: the SAMPL4 challenge”, Journal of Computer-Aided Molecular Design, vol. 28, no. 4. Springer Science and Business Media LLC, pp. 475–490, Feb. 07, 2014. doi: 10.1007/s10822-014-9711-9.*  
  
*E. Gallicchio and R. M. Levy, “Prediction of SAMPL3 host-guest affinities with the binding energy distribution analysis method (BEDAM)”, Journal of Computer-Aided Molecular Design, vol. 26, no. 5. Springer Science and Business Media LLC, pp. 505–516, Feb. 22, 2012. doi: 10.1007/s10822-012-9552-3.*  
  
*E. Gallicchio, “Asynchronous replica exchange software for grid and heterogeneous computing”, Computer Physics Communications, vol. 196. Elsevier BV, pp. 236–246, Nov. 2015. doi: 10.1016/j.cpc.2015.06.010.*  
  
*A. Haldane, W. F. Flynn, P. Heand R. M. Levy, “Coevolutionary Landscape of Kinase Family Proteins: Sequence Probabilities and Functional Motifs”, Biophysical Journal, vol. 114, no. 1. Elsevier BV, pp. 21–31, Jan. 2018. doi: 10.1016/j.bpj.2017.10.028.*  
  
*A. Haldane, W. F. Flynn, P. He, R. S. K. Vijayanand R. M. Levy, “Structural propensities of kinase family proteins from a Potts model of residue co-variation”, Protein Science, vol. 25, no. 8. Wiley, pp. 1378–1384, Jun. 26, 2016. doi: 10.1002/pro.2954.*  
  
*R. C. Harris, N. Deng, R. M. Levy, R. Ishizukaand N. Matubayasi, “Computing conformational free energy differences in explicit solvent: An efficient thermodynamic cycle using an auxiliary potential and a free energy functional constructed from the end points”, Journal of Computational Chemistry, vol. 38, no. 15. Wiley, pp. 1198–1208, Dec. 23, 2016. doi: 10.1002/jcc.24668.*  
  
*P. He, B. W. Zhang, S. Arasteh, L. Wang, R. Abeland R. M. Levy, “Conformational Free Energy Changes via an Alchemical Path without Reaction Coordinates”, The Journal of Physical Chemistry Letters, vol. 9, no. 15. American Chemical Society (ACS), pp. 4428–4435, Jul. 19, 2018. doi: 10.1021/acs.jpclett.8b01851.*  
  
*R. M. Levy, “Recollection”, Protein Science, vol. 25, no. 1. Wiley, pp. 9–11, Dec. 09, 2015. doi: 10.1002/pro.2844.*  
  
*R. M. Levy, D. Cui, B. W. Zhangand N. Matubayasi, “Relationship between Solvation Thermodynamics from IST and DFT Perspectives”, The Journal of Physical Chemistry B, vol. 121, no. 15. American Chemical Society (ACS), pp. 3825–3841, Feb. 28, 2017. doi: 10.1021/acs.jpcb.6b12889.*  
  
*R. M. Levy, W. Dai, N.-J. Dengand D. E. Makarov, “How long does it take to equilibrate the unfolded state of a protein?”, Protein Science, vol. 22, no. 11. Wiley, pp. 1459–1465, Sep. 17, 2013. doi: 10.1002/pro.2335.*  
  
*R. M. Levy, A. Haldaneand W. F. Flynn, “Potts Hamiltonian models of protein co-variation, free energy landscapes, and evolutionary fitness”, Current Opinion in Structural Biology, vol. 43. Elsevier BV, pp. 55–62, Apr. 2017. doi: 10.1016/j.sbi.2016.11.004.*  
  
*A. Mentes, N.-J. Deng, R. S. K. Vijayan, J. Xia, E. Gallicchioand R. M. Levy, “Binding Energy Distribution Analysis Method: Hamiltonian Replica Exchange with Torsional Flattening for Binding Mode Prediction and Binding Free Energy Estimation”, Journal of Chemical Theory and Computation, vol. 12, no. 5. American Chemical Society (ACS), pp. 2459–2470, Apr. 26, 2016. doi: 10.1021/acs.jctc.6b00134.*  
  
*D. Patel, “A New Class of Allosteric HIV-1 Integrase Inhibitors Identified by Crystallographic Fragment Screening of the Catalytic Core Domain”, Journal of Biological Chemistry, vol. 291, no. 45. Elsevier BV, pp. 23569–23577, Nov. 2016. doi: 10.1074/jbc.m116.753384.*  
  
*A. Slaughter, “The mechanism of H171T resistance reveals the importance of Nδ-protonated His171 for the binding of allosteric inhibitor BI-D to HIV-1 integrase”, Retrovirology, vol. 11, no. 1. Springer Science and Business Media LLC, Nov. 25, 2014. doi: 10.1186/s12977-014-0100-1.*  
  
*Z. Tan, J. Xia, B. W. Zhangand R. M. Levy, “Locally weighted histogram analysis and stochastic solution for large-scale multi-state free energy estimation”, The Journal of Chemical Physics, vol. 144, no. 3. AIP Publishing, p. 034107, Jan. 21, 2016. doi: 10.1063/1.4939768.*  
  
*R. S. K. Vijayan, “Conformational Analysis of the DFG-Out Kinase Motif and Biochemical Profiling of Structurally Validated Type II Inhibitors”, Journal of Medicinal Chemistry, vol. 58, no. 1. American Chemical Society (ACS), pp. 466–479, Dec. 12, 2014. doi: 10.1021/jm501603h.*  
  
*L. Wickstrom, “Parameterization of an effective potential for protein-ligand binding from host-guest affinity data”, Journal of Molecular Recognition, vol. 29, no. 1. Wiley, pp. 10–21, Aug. 10, 2015. doi: 10.1002/jmr.2489.*  
  
*J. Xia, N.-. jie . Dengand R. M. Levy, “NMR Relaxation in Proteins with Fast Internal Motions and Slow Conformational Exchange: Model-Free Framework and Markov State Simulations”, The Journal of Physical Chemistry B, vol. 117, no. 22. American Chemical Society (ACS), pp. 6625–6634, May 28, 2013. doi: 10.1021/jp400797y.*  
  
*J. Xia, “Large-scale asynchronous and distributed multidimensional replica exchange molecular simulations and efficiency analysis”, Journal of Computational Chemistry, vol. 36, no. 23. Wiley, pp. 1772–1785, Jul. 07, 2015. doi: 10.1002/jcc.23996.*  
  
*J. Xia, W. Flynnand R. M. Levy, “Improving Prediction Accuracy of Binding Free Energies and Poses of HIV Integrase Complexes Using the Binding Energy Distribution Analysis Method with Flattening Potentials”, Journal of Chemical Information and Modeling, vol. 58, no. 7. American Chemical Society (ACS), pp. 1356–1371, Jun. 21, 2018. doi: 10.1021/acs.jcim.8b00194.*  
  
*J. Xia and R. M. Levy, “Molecular Dynamics of the Proline Switch and Its Role in Crk Signaling”, The Journal of Physical Chemistry B, vol. 118, no. 17. American Chemical Society (ACS), pp. 4535–4545, Apr. 16, 2014. doi: 10.1021/jp5013297.*  
  
*B. W. Zhang, D. Cui, N. Matubayasiand R. M. Levy, “The Excess Chemical Potential of Water at the Interface with a Protein from End Point Simulations”, The Journal of Physical Chemistry B, vol. 122, no. 17. American Chemical Society (ACS), pp. 4700–4707, Apr. 10, 2018. doi: 10.1021/acs.jpcb.8b02666.*  
  
*B. W. Zhang, “Simulating Replica Exchange: Markov State Models, Proposal Schemes, and the Infinite Swapping Limit”, The Journal of Physical Chemistry B, vol. 120, no. 33. American Chemical Society (ACS), pp. 8289–8301, Apr. 29, 2016. doi: 10.1021/acs.jpcb.6b02015.*  
  
*B. W. Zhang, N. Deng, Z. Tanand R. M. Levy, “Stratified UWHAM and Its Stochastic Approximation for Multicanonical Simulations Which Are Far from Equilibrium”, Journal of Chemical Theory and Computation, vol. 13, no. 10. American Chemical Society (ACS), pp. 4660–4674, Sep. 28, 2017. doi: 10.1021/acs.jctc.7b00651.*  
  
*B. W. Zhang, J. Xia, Z. Tanand R. M. Levy, “A Stochastic Solution to the Unbinned WHAM Equations”, The Journal of Physical Chemistry Letters, vol. 6, no. 19. American Chemical Society (ACS), pp. 3834–3840, Sep. 14, 2015. doi: 10.1021/acs.jpclett.5b01771.*  
  
*E. Asgari and M. R. K. Mofrad, “Continuous Distributed Representation of Biological Sequences for Deep Proteomics and Genomics”, PLOS ONE, vol. 10, no. 11. Public Library of Science (PLoS), p. e0141287, Nov. 10, 2015. doi: 10.1371/journal.pone.0141287.*  
  
*P. D. Boyer, H. Shams, S. L. Baker, M. R. K. Mofrad, M. F. Islamand K. N. Dahl, “Enhanced intracellular delivery of small molecules and drugs via non-covalent ternary dispersions of single-wall carbon nanotubes”, Journal of Materials Chemistry B, vol. 4, no. 7. Royal Society of Chemistry (RSC), pp. 1324–1330, 2016. doi: 10.1039/c5tb02016f.*  
  
*J. Golji and M. R. K. Mofrad, “The Talin Dimer Structure Orientation Is Mechanically Regulated”, Biophysical Journal, vol. 107, no. 8. Elsevier BV, pp. 1802–1809, Oct. 2014. doi: 10.1016/j.bpj.2014.08.038.*  
  
*Z. Jahed, H. Shamsand M. R. K. Mofrad, “A Disulfide Bond Is Required for the Transmission of Forces through SUN-KASH Complexes”, Biophysical Journal, vol. 109, no. 3. Elsevier BV, pp. 501–509, Aug. 2015. doi: 10.1016/j.bpj.2015.06.057.*  
  
*C. Lazarus, M. Soheilypourand M. R. K. Mofrad, “Torsional Behavior of Axonal Microtubule Bundles”, Biophysical Journal, vol. 109, no. 2. Elsevier BV, pp. 231–239, Jul. 2015. doi: 10.1016/j.bpj.2015.06.029.*  
  
*C. L. Zhao, S. H. Mahboobi, R. Moussavi-Baygiand M. R. K. Mofrad, “The Interaction of CRM1 and the Nuclear Pore Protein Tpr”, PLoS ONE, vol. 9, no. 4. Public Library of Science (PLoS), p. e93709, Apr. 10, 2014. doi: 10.1371/journal.pone.0093709.*  
  
*R. Moussavi-Baygi and M. R. K. Mofrad, “Rapid Brownian Motion Primes Ultrafast Reconstruction of Intrinsically Disordered Phe-Gly Repeats Inside the Nuclear Pore Complex”, Scientific Reports, vol. 6, no. 1. Springer Science and Business Media LLC, Jul. 29, 2016. doi: 10.1038/srep29991.*  
  
*M. Peyro, M. Soheilypour, A. Ghavamiand M. R. K. Mofrad, “Nucleoporin’s Like Charge Regions Are Major Regulators of FG Coverage and Dynamics Inside the Nuclear Pore Complex”, PLOS ONE, vol. 10, no. 12. Public Library of Science (PLoS), p. e0143745, Dec. 11, 2015. doi: 10.1371/journal.pone.0143745.*  
  
*A. Shamloo, M. Heibatollahiand M. R. K. Mofrad, “Directional migration and differentiation of neural stem cells within three-dimensional microenvironments”, Integrative Biology, vol. 7, no. 3. Oxford University Press (OUP), pp. 335–344, 2015. doi: 10.1039/c4ib00144c.*  
  
*H. Shams, “Actin Reorganization through Dynamic Interactions with Single-Wall Carbon Nanotubes”, ACS Nano, vol. 8, no. 1. American Chemical Society (ACS), pp. 188–197, Dec. 24, 2013. doi: 10.1021/nn402865e.*  
  
*M. Soheilypour, M. Peyro, Z. Jahedand M. R. K. Mofrad, “On the Nuclear Pore Complex and Its Roles in Nucleo-Cytoskeletal Coupling and Mechanobiology”, Cellular and Molecular Bioengineering, vol. 9, no. 2. Springer Science and Business Media LLC, pp. 217–226, May 11, 2016. doi: 10.1007/s12195-016-0443-x.*  
  
*M. Soheilypour, M. Peyro, S. J. Peterand M. R. K. Mofrad, “Buckling Behavior of Individual and Bundled Microtubules”, Biophysical Journal, vol. 108, no. 7. Elsevier BV, pp. 1718–1726, Apr. 2015. doi: 10.1016/j.bpj.2015.01.030.*  
  
*J. K. Colbourne, “The Ecoresponsive Genome of Daphnia pulex”, Science, vol. 331, no. 6017. American Association for the Advancement of Science (AAAS), pp. 555–561, Feb. 04, 2011. doi: 10.1126/science.1197761.*  
  
*D. G. Gilbert, “Genes of the Pig, Sus scrofa, reconstructed with EvidentialGene”, []. Cold Spring Harbor Laboratory, Sep. 09, 2018. doi: 10.1101/412130.*  
  
*D. G. Gilbert, “Longest protein, longest transcript or most expression, for accurate gene reconstruction of transcriptomes?”, []. Cold Spring Harbor Laboratory, Nov. 02, 2019. doi: 10.1101/829184.*  
  
*M. Gulia-Nuss, “Genomic insights into the Ixodes scapularis tick vector of Lyme disease”, Nature Communications, vol. 7, no. 1. Springer Science and Business Media LLC, Feb. 09, 2016. doi: 10.1038/ncomms10507.*  
  
*J. C. Motamayor, “The genome sequence of the most widely cultivated cacao type and its use to identify candidate genes regulating pod color”, Genome Biology, vol. 14, no. 6. Springer Science and Business Media LLC, Jun. 2013. doi: 10.1186/gb-2013-14-6-r53.*  
  
*D. B. Neale, “Decoding the massive genome of loblolly pine using haploid DNA and novel assembly strategies”, Genome Biology, vol. 15, no. 3. Springer Science and Business Media LLC, p. R59, 2014. doi: 10.1186/gb-2014-15-3-r59.*  
  
*L. Orsini, “Daphnia magna transcriptome by RNA-Seq across 12 environmental stressors”, Scientific Data, vol. 3, no. 1. Springer Science and Business Media LLC, May 10, 2016. doi: 10.1038/sdata.2016.30.*  
  
*N. M. Reid, “The Landscape of Extreme Genomic Variation in the Highly Adaptable Atlantic Killifish”, Genome Biology and Evolution, vol. 9, no. 3. Oxford University Press (OUP), pp. 659–676, Mar. 01, 2017. doi: 10.1093/gbe/evx023.*  
  
*R. B. Best, D. de Sanchoand J. Mittal, “Residue-Specific α-Helix Propensities from Molecular Simulation”, Biophysical Journal, vol. 102, no. 6. Elsevier BV, pp. 1462–1467, Mar. 2012. doi: 10.1016/j.bpj.2012.02.024.*  
  
*J. Mittal and R. B. Best, “Dependence of Protein Folding Stability and Dynamics on the Density and Composition of Macromolecular Crowders”, Biophysical Journal, vol. 98, no. 2. Elsevier BV, pp. 315–320, Jan. 2010. doi: 10.1016/j.bpj.2009.10.009.*  
  
*A. K. Sangha, J. M. Parks, R. F. Standaert, A. Ziebell, M. Davisand J. C. Smith, “Radical Coupling Reactions in Lignin Synthesis: A Density Functional Theory Study”, The Journal of Physical Chemistry B, vol. 116, no. 16. American Chemical Society (ACS), pp. 4760–4768, Apr. 13, 2012. doi: 10.1021/jp2122449.*  
  
*H. Bai, “Different states of synaptotagmin regulate evoked versus spontaneous release”, Nature Communications, vol. 7, no. 1. Springer Science and Business Media LLC, Mar. 22, 2016. doi: 10.1038/ncomms10971.*  
  
*H. Bao, “Dynamics and number of trans-SNARE complexes determine nascent fusion pore properties”, Nature, vol. 554, no. 7691. Springer Science and Business Media LLC, pp. 260–263, Jan. 31, 2018. doi: 10.1038/nature25481.*  
  
*X. Cai, “Network analysis of a proposed exit pathway for protons to the P-side of cytochrome c oxidase”, Biochimica et Biophysica Acta (BBA) - Bioenergetics, vol. 1859, no. 10. Elsevier BV, pp. 997–1005, Oct. 2018. doi: 10.1016/j.bbabio.2018.05.010.*  
  
*H. Chen, “NMR Structural Analysis of Isolated Shaker Voltage-Sensing Domain in LPPG Micelles”, Biophysical Journal, vol. 117, no. 2. Elsevier BV, pp. 388–398, Jul. 2019. doi: 10.1016/j.bpj.2019.06.020.*  
  
*A. S. Christensen, M. Elstnerand Q. Cui, “Improving intermolecular interactions in DFTB3 using extended polarization from chemical-potential equalization”, The Journal of Chemical Physics, vol. 143, no. 8. AIP Publishing, p. 084123, Aug. 28, 2015. doi: 10.1063/1.4929335.*  
  
*A. S. Christensen, J. C. Kromann, J. H. Jensenand Q. Cui, “Intermolecular interactions in the condensed phase: Evaluation of semi-empirical quantum mechanical methods”, The Journal of Chemical Physics, vol. 147, no. 16. AIP Publishing, p. 161704, Oct. 28, 2017. doi: 10.1063/1.4985605.*  
  
*S. G. F. Condon, “The FtsLB subcomplex of the bacterial divisome is a tetramer with an uninterrupted FtsL helix linking the transmembrane and periplasmic regions”, Journal of Biological Chemistry, vol. 293, no. 5. Elsevier BV, pp. 1623–1641, Feb. 2018. doi: 10.1074/jbc.ra117.000426.*  
  
*N. Dalchand, Q. Cuiand F. M. Geiger, “Electrostatics, Hydrogen Bonding, and Molecular Structure at Polycation and Peptide:Lipid Membrane Interfaces”, ACS Applied Materials & Interfaces, vol. 12, no. 19. American Chemical Society (ACS), pp. 21149–21158, Dec. 31, 2019. doi: 10.1021/acsami.9b17431.*  
  
*M. Das, U. Dahal, O. Mesele, D. Liangand Q. Cui, “Molecular Dynamics Simulation of Interaction between Functionalized Nanoparticles with Lipid Membranes: Analysis of Coarse-Grained Models”, The Journal of Physical Chemistry B, vol. 123, no. 49. American Chemical Society (ACS), pp. 10547–10561, Nov. 01, 2019. doi: 10.1021/acs.jpcb.9b08259.*  
  
*M. Doǧangün, “Hydrogen-Bond Networks near Supported Lipid Bilayers from Vibrational Sum Frequency Generation Experiments and Atomistic Simulations”, The Journal of Physical Chemistry B, vol. 122, no. 18. American Chemical Society (ACS), pp. 4870–4879, Apr. 24, 2018. doi: 10.1021/acs.jpcb.8b02138.*  
  
*M. Gaus, Q. Cuiand M. Elstner, “Density functional tight binding: application to organic and biological molecules”, WIREs Computational Molecular Science, vol. 4, no. 1. Wiley, pp. 49–61, Jun. 13, 2013. doi: 10.1002/wcms.1156.*  
  
*M. Gaus, “DFTB3 Parametrization for Copper: The Importance of Orbital Angular Momentum Dependence of Hubbard Parameters”, Journal of Chemical Theory and Computation, vol. 11, no. 9. American Chemical Society (ACS), pp. 4205–4219, Aug. 24, 2015. doi: 10.1021/acs.jctc.5b00600.*  
  
*M. Gaus, X. Lu, M. Elstnerand Q. Cui, “Parameterization of DFTB3/3OB for Sulfur and Phosphorus for Chemical and Biological Applications”, Journal of Chemical Theory and Computation, vol. 10, no. 4. American Chemical Society (ACS), pp. 1518–1537, Mar. 27, 2014. doi: 10.1021/ct401002w.*  
  
*M. P. Goldschen-Ohm, “Structure and dynamics underlying elementary ligand binding events in human pacemaking channels”, eLife, vol. 5. eLife Sciences Publications, Ltd, Nov. 18, 2016. doi: 10.7554/elife.20797.*  
  
*P. Goyal, “Molecular Simulation of Water and Hydration Effects in Different Environments: Challenges and Developments for DFTB Based Models”, The Journal of Physical Chemistry B, vol. 118, no. 38. American Chemical Society (ACS), pp. 11007–11027, Sep. 16, 2014. doi: 10.1021/jp503372v.*  
  
*M. Gruden, “Benchmarking density functional tight binding models for barrier heights and reaction energetics of organic molecules”, Journal of Computational Chemistry, vol. 38, no. 25. Wiley, pp. 2171–2185, Jul. 24, 2017. doi: 10.1002/jcc.24866.*  
  
*J. Hong, R. J. Hamers, J. A. Pedersenand Q. Cui, “A Hybrid Molecular Dynamics/Multiconformer Continuum Electrostatics (MD/MCCE) Approach for the Determination of Surface Charge of Nanomaterials”, The Journal of Physical Chemistry C, vol. 121, no. 6. American Chemical Society (ACS), pp. 3584–3596, Feb. 06, 2017. doi: 10.1021/acs.jpcc.6b11537.*  
  
*H. Jin, P. Goyal, A. K. Das, M. Gaus, M. Meuwlyand Q. Cui, “Copper Oxidation/Reduction in Water and Protein: Studies with DFTB3/MM and VALBOND Molecular Dynamics Simulations”, The Journal of Physical Chemistry B, vol. 120, no. 8. American Chemical Society (ACS), pp. 1894–1910, Dec. 17, 2015. doi: 10.1021/acs.jpcb.5b09656.*  
  
*E. N. Korkmaz, “A composite approach towards a complete model of the myosin rod”, Proteins: Structure, Function, and Bioinformatics, vol. 84, no. 1. Wiley, pp. 172–189, Dec. 09, 2015. doi: 10.1002/prot.24964.*  
  
*E. N. Korkmaz, B. F. Volkmanand Q. Cui, “Interplay of Electrostatics and Hydrophobic Effects in the Metamorphic Protein Human Lymphotactin”, The Journal of Physical Chemistry B, vol. 119, no. 30. American Chemical Society (ACS), pp. 9547–9558, Jul. 16, 2015. doi: 10.1021/acs.jpcb.5b02810.*  
  
*J. C. Kromann, A. S. Christensen, Q. Cuiand J. H. Jensen, “Towards a barrier height benchmark set for biologically relevant systems”, PeerJ, vol. 4. PeerJ, p. e1994, May 03, 2016. doi: 10.7717/peerj.1994.*  
  
*M. Leander, Y. Yuan, A. Meger, Q. Cuiand S. Raman, “Functional Plasticity and Evolutionary Adaptation of Allosteric Regulation”, []. Cold Spring Harbor Laboratory, Feb. 11, 2020. doi: 10.1101/2020.02.10.942417.*  
  
*D. Liang, “Analysis of the conformational properties of amine ligands at the gold/water interface with QM, MM and QM/MM simulations”, Physical Chemistry Chemical Physics, vol. 20, no. 5. Royal Society of Chemistry (RSC), pp. 3349–3362, 2018. doi: 10.1039/c7cp06709g.*  
  
*C. B. Lietz, Z. Chen, C. Yun Son, X. Pang, Q. Cuiand L. Li, “Multiple gas-phase conformations of proline-containing peptides: is it always cis/trans isomerization?”, The Analyst, vol. 141, no. 16. Royal Society of Chemistry (RSC), pp. 4863–4869, 2016. doi: 10.1039/c5an00835b.*  
  
*X. Lu, J. Duchimaza-Herediaand Q. Cui, “Analysis of Density Functional Tight Binding with Natural Bonding Orbitals”, The Journal of Physical Chemistry A, vol. 123, no. 34. American Chemical Society (ACS), pp. 7439–7453, Aug. 02, 2019. doi: 10.1021/acs.jpca.9b05072.*  
  
*X. Lu, M. Gaus, M. Elstnerand Q. Cui, “Parametrization of DFTB3/3OB for Magnesium and Zinc for Chemical and Biological Applications”, The Journal of Physical Chemistry B, vol. 119, no. 3. American Chemical Society (ACS), pp. 1062–1082, Sep. 16, 2014. doi: 10.1021/jp506557r.*  
  
*X. Lu, V. Ovchinnikov, D. Demapan, D. Rostonand Q. Cui, “Regulation and Plasticity of Catalysis in Enzymes: Insights from Analysis of Mechanochemical Coupling in Myosin”, Biochemistry, vol. 56, no. 10. American Chemical Society (ACS), pp. 1482–1497, Mar. 01, 2017. doi: 10.1021/acs.biochem.7b00016.*  
  
*T. Mandal, W. Lough, S. E. Spagnolie, A. Audhyaand Q. Cui, “Molecular Simulation of Mechanical Properties and Membrane Activities of the ESCRT-III Complexes”, Biophysical Journal, vol. 118, no. 6. Elsevier BV, pp. 1333–1343, Mar. 2020. doi: 10.1016/j.bpj.2020.01.033.*  
  
*A. C. McGeachy, E. R. Caudill, D. Liang, Q. Cui, J. A. Pedersenand F. M. Geiger, “Counting charges on membrane-bound peptides”, Chemical Science, vol. 9, no. 18. Royal Society of Chemistry (RSC), pp. 4285–4298, 2018. doi: 10.1039/c8sc00804c.*  
  
*T. Mori, R. J. Hamers, J. A. Pedersenand Q. Cui, “Integrated Hamiltonian Sampling: A Simple and Versatile Method for Free Energy Simulations and Conformational Sampling”, The Journal of Physical Chemistry B, vol. 118, no. 28. American Chemical Society (ACS), pp. 8210–8220, Mar. 27, 2014. doi: 10.1021/jp501339t.*  
  
*V. Ngo, “Quantum Effects in Cation Interactions with First and Second Coordination Shell Ligands in Metalloproteins”, Journal of Chemical Theory and Computation, vol. 11, no. 10. American Chemical Society (ACS), pp. 4992–5001, Oct. 05, 2015. doi: 10.1021/acs.jctc.5b00524.*  
  
*Y. Nomura, D. Roston, E. J. Montemayor, Q. Cuiand S. E. Butcher, “Structural and mechanistic basis for preferential deadenylation of U6 snRNA by Usb1”, Nucleic Acids Research, vol. 46, no. 21. Oxford University Press (OUP), pp. 11488–11501, Sep. 12, 2018. doi: 10.1093/nar/gky812.*  
  
*G. H. Pham, A. S. J. B. Rana, E. N. Korkmaz, V. H. Trang, Q. Cuiand E. R. Strieter, “Comparison of native and non-native ubiquitin oligomers reveals analogous structures and reactivities”, Protein Science, vol. 25, no. 2. Wiley, pp. 456–471, Jan. 12, 2016. doi: 10.1002/pro.2834.*  
  
*D. Roston and Q. Cui, “QM/MM Analysis of Transition States and Transition State Analogues in Metalloenzymes”, Methods in Enzymology. Elsevier, pp. 213–250, 2016. doi: 10.1016/bs.mie.2016.05.016.*  
  
*D. Roston and Q. Cui, “Substrate and Transition State Binding in Alkaline Phosphatase Analyzed by Computation of Oxygen Isotope Effects”, Journal of the American Chemical Society, vol. 138, no. 36. American Chemical Society (ACS), pp. 11946–11957, Aug. 31, 2016. doi: 10.1021/jacs.6b07347.*  
  
*D. Roston, D. Demapanand Q. Cui, “Leaving Group Ability Observably Affects Transition State Structure in a Single Enzyme Active Site”, Journal of the American Chemical Society, vol. 138, no. 23. American Chemical Society (ACS), pp. 7386–7394, Jun. 02, 2016. doi: 10.1021/jacs.6b03156.*  
  
*D. Roston, D. Demapanand Q. Cui, “Extensive free-energy simulations identify water as the base in nucleotide addition by DNA polymerase”, Proceedings of the National Academy of Sciences, vol. 116, no. 50. Proceedings of the National Academy of Sciences, pp. 25048–25056, Nov. 22, 2019. doi: 10.1073/pnas.1914613116.*  
  
*T. M. A. Santos, “Small Molecule Chelators Reveal That Iron Starvation Inhibits Late Stages of Bacterial Cytokinesis”, ACS Chemical Biology, vol. 13, no. 1. American Chemical Society (ACS), pp. 235–246, Dec. 20, 2017. doi: 10.1021/acschembio.7b00560.*  
  
*Q.-T. Shen, “Structural analysis and modeling reveals new mechanisms governing ESCRT-III spiral filament assembly”, Journal of Cell Biology, vol. 206, no. 6. Rockefeller University Press, pp. 763–777, Sep. 08, 2014. doi: 10.1083/jcb.201403108.*  
  
*C. Y. Son, J. G. McDaniel, Q. Cuiand A. Yethiraj, “Conformational and Dynamic Properties of Poly(ethylene oxide) in BMIM+BF4–: A Microsecond Computer Simulation Study Using ab Initio Force Fields”, Macromolecules, vol. 51, no. 14. American Chemical Society (ACS), pp. 5336–5345, Jul. 11, 2018. doi: 10.1021/acs.macromol.8b01002.*  
  
*C. Y. Son, J. G. McDaniel, Q. Cuiand A. Yethiraj, “Proper Thermal Equilibration of Simulations with Drude Polarizable Models: Temperature-Grouped Dual-Nosé–Hoover Thermostat”, The Journal of Physical Chemistry Letters, vol. 10, no. 23. American Chemical Society (ACS), pp. 7523–7530, Nov. 14, 2019. doi: 10.1021/acs.jpclett.9b02983.*  
  
*C. Y. Son, J. G. McDaniel, J. R. Schmidt, Q. Cuiand A. Yethiraj, “First-Principles United Atom Force Field for the Ionic Liquid BMIM+BF4–: An Alternative to Charge Scaling”, The Journal of Physical Chemistry B, vol. 120, no. 14. American Chemical Society (ACS), pp. 3560–3568, Apr. 01, 2016. doi: 10.1021/acs.jpcb.5b12371.*  
  
*K. C. Taylor, “Skip residues modulate the structural properties of the myosin rod and guide thick filament assembly”, Proceedings of the National Academy of Sciences, vol. 112, no. 29. Proceedings of the National Academy of Sciences, Jul. 06, 2015. doi: 10.1073/pnas.1505813112.*  
  
*J. M. Troiano, “Quantifying the Electrostatics of Polycation–Lipid Bilayer Interactions”, Journal of the American Chemical Society, vol. 139, no. 16. American Chemical Society (ACS), pp. 5808–5816, Apr. 14, 2017. doi: 10.1021/jacs.6b12887.*  
  
*M. Vujović, “Exploring the applicability of density functional tight binding to transition metal ions. Parameterization for nickel with the spin‐polarized DFTB3 model”, Journal of Computational Chemistry, vol. 40, no. 2. Wiley, pp. 400–413, Oct. 09, 2018. doi: 10.1002/jcc.25614.*  
  
*H. C. Watanabe and Q. Cui, “Quantitative Analysis of QM/MM Boundary Artifacts and Correction in Adaptive QM/MM Simulations”, Journal of Chemical Theory and Computation, vol. 15, no. 7. American Chemical Society (ACS), pp. 3917–3928, May 16, 2019. doi: 10.1021/acs.jctc.9b00180.*  
  
*Z. Xu, “Small molecule-mediated control of hydroxyapatite growth: Free energy calculations benchmarked to density functional theory”, Journal of Computational Chemistry, vol. 35, no. 1. Wiley, pp. 70–81, Oct. 28, 2013. doi: 10.1002/jcc.23474.*  
  
*Z. Xu, “Molecular mechanisms for intrafibrillar collagen mineralization in skeletal tissues”, Biomaterials, vol. 39. Elsevier BV, pp. 59–66, Jan. 2015. doi: 10.1016/j.biomaterials.2014.10.048.*  
  
*L. Zhang, M. Rajendram, D. B. Weibel, A. Yethirajand Q. Cui, “Ionic Hydrogen Bonds and Lipid Packing Defects Determine the Binding Orientation and Insertion Depth of RecA on Multicomponent Lipid Bilayers”, The Journal of Physical Chemistry B, vol. 120, no. 33. American Chemical Society (ACS), pp. 8424–8437, May 02, 2016. doi: 10.1021/acs.jpcb.6b02164.*  
  
*L. Zhang, A. Yethirajand Q. Cui, “Free Energy Calculations for the Peripheral Binding of Proteins/Peptides to an Anionic Membrane. 1. Implicit Membrane Models”, Journal of Chemical Theory and Computation, vol. 10, no. 7. American Chemical Society (ACS), pp. 2845–2859, May 29, 2014. doi: 10.1021/ct500218p.*  
  
*W. Zhao, Z. Xu, Q. Cuiand N. Sahai, “Predicting the Structure–Activity Relationship of Hydroxyapatite-Binding Peptides by Enhanced-Sampling Molecular Simulation”, Langmuir, vol. 32, no. 27. American Chemical Society (ACS), pp. 7009–7022, Jun. 29, 2016. doi: 10.1021/acs.langmuir.6b01582.*  
  
*Y. Zheng and Q. Cui, “The histone H3 N-terminal tail: a computational analysis of the free energy landscape and kinetics”, Physical Chemistry Chemical Physics, vol. 17, no. 20. Royal Society of Chemistry (RSC), pp. 13689–13698, 2015. doi: 10.1039/c5cp01858g.*  
  
*Y. Zheng and Q. Cui, “Microscopic mechanisms that govern the titration response and p K a values of buried residues in staphylococcal nuclease mutants”, Proteins: Structure, Function, and Bioinformatics, vol. 85, no. 2. Wiley, pp. 268–281, Dec. 14, 2016. doi: 10.1002/prot.25213.*  
  
*Y. Zheng and Q. Cui, “Multiple Pathways and Time Scales for Conformational Transitions in apo-Adenylate Kinase”, Journal of Chemical Theory and Computation, vol. 14, no. 3. American Chemical Society (ACS), pp. 1716–1726, Jan. 29, 2018. doi: 10.1021/acs.jctc.7b01064.*  
  
*J. K. Noel, P. C. Whitford, K. Y. Sanbonmatsuand J. N. Onuchic, “SMOG@ctbp: simplified deployment of structure-based models in GROMACS”, Nucleic Acids Research, vol. 38, no. suppl\_2. Oxford University Press (OUP), pp. W657–W661, Jun. 04, 2010. doi: 10.1093/nar/gkq498.*  
  
*P. C. Whitford, S. C. Blanchard, J. H. D. Cateand K. Y. Sanbonmatsu, “Connecting the Kinetics and Energy Landscape of tRNA Translocation on the Ribosome”, PLoS Computational Biology, vol. 9, no. 3. Public Library of Science (PLoS), p. e1003003, Mar. 21, 2013. doi: 10.1371/journal.pcbi.1003003.*  
  
*T. Mamonova, M. Kurnikovaand P. A. Friedman, “Structural Basis for NHERF1 PDZ Domain Binding”, Biochemistry, vol. 51, no. 14. American Chemical Society (ACS), pp. 3110–3120, Mar. 27, 2012. doi: 10.1021/bi201213w.*  
  
*T. Mamonova, Q. Zhang, J. A. Khajeh, Z. Bu, A. Biselloand P. A. Friedman, “Canonical and Noncanonical Sites Determine NPT2A Binding Selectivity to NHERF1 PDZ1”, PLOS ONE, vol. 10, no. 6. Public Library of Science (PLoS), p. e0129554, Jun. 12, 2015. doi: 10.1371/journal.pone.0129554.*  
  
*R. E. Trager, P. Giblock, S. Soltani, A. A. Upadhyay, B. Rekapalliand Y. K. Peterson, “Docking optimization, variance and promiscuity for large-scale drug-like chemical space using high performance computing architectures”, Drug Discovery Today, vol. 21, no. 10. Elsevier BV, pp. 1672–1680, Oct. 2016. doi: 10.1016/j.drudis.2016.06.023.*  
  
*M. J. M. Niesen, S. Bhattacharyaand N. Vaidehi, “The Role of Conformational Ensembles in Ligand Recognition in G-Protein Coupled Receptors”, Journal of the American Chemical Society, vol. 133, no. 33. American Chemical Society (ACS), pp. 13197–13204, Jul. 29, 2011. doi: 10.1021/ja205313h.*  
  
*G. A. Khoury, P. Tamamis, N. Pinnaduwage, J. Smadbeck, C. A. Kieslichand C. A. Floudas, “Princeton\_TIGRESS: Protein geometry refinement using simulations and support vector machines”, Proteins: Structure, Function, and Bioinformatics, vol. 82, no. 5. Wiley, pp. 794–814, Nov. 22, 2013. doi: 10.1002/prot.24459.*  
  
*G. A. Khoury, J. P. Thompson, J. Smadbeck, C. A. Kieslichand C. A. Floudas, “Forcefield\_PTM: Ab Initio Charge and AMBER Forcefield Parameters for Frequently Occurring Post-Translational Modifications”, Journal of Chemical Theory and Computation, vol. 9, no. 12. American Chemical Society (ACS), pp. 5653–5674, Dec. 02, 2013. doi: 10.1021/ct400556v.*  
  
*A. Colavin, J. Hsinand K. C. Huang, “Effects of polymerization and nucleotide identity on the conformational dynamics of the bacterial actin homolog MreB”, Proceedings of the National Academy of Sciences, vol. 111, no. 9. Proceedings of the National Academy of Sciences, pp. 3585–3590, Feb. 18, 2014. doi: 10.1073/pnas.1317061111.*  
  
*A. Colavin, H. Shiand K. C. Huang, “RodZ modulates geometric localization of the bacterial actin MreB to regulate cell shape”, Nature Communications, vol. 9, no. 1. Springer Science and Business Media LLC, Mar. 29, 2018. doi: 10.1038/s41467-018-03633-x.*  
  
*R. L. Gill Jr., “Structural basis for the geometry-driven localization of a small protein”, Proceedings of the National Academy of Sciences, vol. 112, no. 15. Proceedings of the National Academy of Sciences, Mar. 30, 2015. doi: 10.1073/pnas.1423868112.*  
  
*J. Hsin, R. Fuand K. C. Huang, “Dimer Dynamics and Filament Organization of the Bacterial Cell Division Protein FtsA”, Journal of Molecular Biology, vol. 425, no. 22. Elsevier BV, pp. 4415–4426, Nov. 2013. doi: 10.1016/j.jmb.2013.07.016.*  
  
*Y. Li, “FtsZ Protofilaments Use a Hinge-Opening Mechanism for Constrictive Force Generation”, Science, vol. 341, no. 6144. American Association for the Advancement of Science (AAAS), pp. 392–395, Jul. 26, 2013. doi: 10.1126/science.1239248.*  
  
*A. Miguel, J. Hsin, T. Liu, G. Tang, R. B. Altmanand K. C. Huang, “Variations in the Binding Pocket of an Inhibitor of the Bacterial Division Protein FtsZ across Genotypes and Species”, PLOS Computational Biology, vol. 11, no. 3. Public Library of Science (PLoS), p. e1004117, Mar. 26, 2015. doi: 10.1371/journal.pcbi.1004117.*  
  
*A. R. Pereira, “FtsZ-Dependent Elongation of a Coccoid Bacterium”, mBio, vol. 7, no. 5. American Society for Microbiology, Nov. 02, 2016. doi: 10.1128/mbio.00908-16.*  
  
*J. Y. Lee and E. Lyman, “Predictions for Cholesterol Interaction Sites on the A2A Adenosine Receptor”, Journal of the American Chemical Society, vol. 134, no. 40. American Chemical Society (ACS), pp. 16512–16515, Sep. 26, 2012. doi: 10.1021/ja307532d.*  
  
*J. Y. Lee and E. Lyman, “Agonist Dynamics and Conformational Selection during Microsecond Simulations of the A2A Adenosine Receptor”, Biophysical Journal, vol. 102, no. 9. Elsevier BV, pp. 2114–2120, May 2012. doi: 10.1016/j.bpj.2012.03.061.*  
  
*A. J. Sodt, R. W. Pastorand E. Lyman, “Hexagonal Substructure and Hydrogen Bonding in Liquid-Ordered Phases Containing Palmitoyl Sphingomyelin”, Biophysical Journal, vol. 109, no. 5. Elsevier BV, pp. 948–955, Sep. 2015. doi: 10.1016/j.bpj.2015.07.036.*  
  
*A. J. Sodt, M. L. Sandar, K. Gawrisch, R. W. Pastorand E. Lyman, “The Molecular Structure of the Liquid-Ordered Phase of Lipid Bilayers”, Journal of the American Chemical Society, vol. 136, no. 2. American Chemical Society (ACS), pp. 725–732, Jan. 03, 2014. doi: 10.1021/ja4105667.*  
  
*N. Coudray, “Structure of the SLC4 transporter Bor1p in an inward‐facing conformation”, Protein Science, vol. 26, no. 1. Wiley, pp. 130–145, Oct. 21, 2016. doi: 10.1002/pro.3061.*  
  
*S. Lin, J. Zhang, M. S. Stranoand D. Blankschtein, “Understanding selective molecular recognition in integrated carbon nanotube–polymer sensors by simulating physical analyte binding on carbon nanotube–polymer scaffolds”, Soft Matter, vol. 10, no. 32. Royal Society of Chemistry (RSC), pp. 5991–6004, 2014. doi: 10.1039/c4sm00974f.*  
  
*J. Zhang, “Molecular recognition using corona phase complexes made of synthetic polymers adsorbed on carbon nanotubes”, Nature Nanotechnology, vol. 8, no. 12. Springer Science and Business Media LLC, pp. 959–968, Nov. 24, 2013. doi: 10.1038/nnano.2013.236.*  
  
*H. Moon, “Design, Solid-Phase Synthesis, and Evaluation of a Phenyl-Piperazine-Triazine Scaffold as α-Helix Mimetics”, ACS Combinatorial Science, vol. 16, no. 12. American Chemical Society (ACS), pp. 695–701, Nov. 03, 2014. doi: 10.1021/co500114f.*  
  
*P. Das and S. Matysiak, “Direct Characterization of Hydrophobic Hydration during Cold and Pressure Denaturation”, The Journal of Physical Chemistry B, vol. 116, no. 18. American Chemical Society (ACS), pp. 5342–5348, May 02, 2012. doi: 10.1021/jp211832c.*  
  
*S. Matysiak, P. G. Debenedettiand P. J. Rossky, “Dissecting the Energetics of Hydrophobic Hydration of Polypeptides”, The Journal of Physical Chemistry B, vol. 115, no. 49. American Chemical Society (ACS), pp. 14859–14865, Nov. 16, 2011. doi: 10.1021/jp2079633.*  
  
*S. Matysiak, P. G. Debenedettiand P. J. Rossky, “Role of Hydrophobic Hydration in Protein Stability: A 3D Water-Explicit Protein Model Exhibiting Cold and Heat Denaturation”, The Journal of Physical Chemistry B, vol. 116, no. 28. American Chemical Society (ACS), pp. 8095–8104, Jul. 10, 2012. doi: 10.1021/jp3039175.*  
  
*S. Romero-Vargas Castrillón, S. Matysiak, F. H. Stillinger, P. J. Rosskyand P. G. Debenedetti, “Phase Behavior of a Lattice Hydrophobic Oligomer in Explicit Water”, The Journal of Physical Chemistry B, vol. 116, no. 31. American Chemical Society (ACS), pp. 9540–9548, Jul. 23, 2012. doi: 10.1021/jp3039237.*  
  
*S. Romero-Vargas Castrillón, S. Matysiak, F. H. Stillinger, P. J. Rosskyand P. G. Debenedetti, “Thermal Stability of Hydrophobic Helical Oligomers: A Lattice Simulation Study in Explicit Water”, The Journal of Physical Chemistry B, vol. 116, no. 33. American Chemical Society (ACS), pp. 9963–9970, Aug. 10, 2012. doi: 10.1021/jp305134w.*  
  
*P. J. Fleming, J. A. Freites, C. P. Moon, D. J. Tobiasand K. G. Fleming, “Outer membrane phospholipase A in phospholipid bilayers: A model system for concerted computational and experimental investigations of amino acid side chain partitioning into lipid bilayers”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1818, no. 2. Elsevier BV, pp. 126–134, Feb. 2012. doi: 10.1016/j.bbamem.2011.07.016.*  
  
*C. P. Moon, N. R. Zaccai, P. J. Fleming, D. Gessmannand K. G. Fleming, “Membrane protein thermodynamic stability may serve as the energy sink for sorting in the periplasm”, Proceedings of the National Academy of Sciences, vol. 110, no. 11. Proceedings of the National Academy of Sciences, pp. 4285–4290, Feb. 25, 2013. doi: 10.1073/pnas.1212527110.*  
  
*K. W. Lexa and H. A. Carlson, “Improving Protocols for Protein Mapping through Proper Comparison to Crystallography Data”, Journal of Chemical Information and Modeling, vol. 53, no. 2. American Chemical Society (ACS), pp. 391–402, Feb. 13, 2013. doi: 10.1021/ci300430v.*  
  
*P. M. U. Ung, P. Ghanakota, S. E. Graham, K. W. Lexaand H. A. Carlson, “Identifying binding hot spots on protein surfaces by mixed‐solvent molecular dynamics: HIV‐1 protease as a test case”, Biopolymers, vol. 105, no. 1. Wiley, pp. 21–34, Oct. 26, 2015. doi: 10.1002/bip.22742.*  
  
*P. D. Adams, “Outcome of the First wwPDB/CCDC/D3R Ligand Validation Workshop”, Structure, vol. 24, no. 4. Elsevier BV, pp. 502–508, Apr. 2016. doi: 10.1016/j.str.2016.02.017.*  
  
*W. J. Allen, “DOCK 6: Impact of new features and current docking performance”, Journal of Computational Chemistry, vol. 36, no. 15. Wiley, pp. 1132–1156, Apr. 27, 2015. doi: 10.1002/jcc.23905.*  
  
*D. A. Case, “149 The distribution of water and ions around nucleic acids”, Journal of Biomolecular Structure and Dynamics, vol. 33, no. sup1. Informa UK Limited, pp. 97–97, May 18, 2015. doi: 10.1080/07391102.2015.1032782.*  
  
*H. Chen, T. J. Giese, B. L. Goldenand D. M. York, “Divalent Metal Ion Activation of a Guanine General Base in the Hammerhead Ribozyme: Insights from Molecular Simulations”, Biochemistry, vol. 56, no. 24. American Chemical Society (ACS), pp. 2985–2994, Jun. 12, 2017. doi: 10.1021/acs.biochem.6b01192.*  
  
*I. Fu, D. A. Caseand J. Baum, “Dynamic Water-Mediated Hydrogen Bonding in a Collagen Model Peptide”, Biochemistry, vol. 54, no. 39. American Chemical Society (ACS), pp. 6029–6037, Sep. 23, 2015. doi: 10.1021/acs.biochem.5b00622.*  
  
*C. S. Gaines and D. M. York, “Ribozyme Catalysis with a Twist: Active State of the Twister Ribozyme in Solution Predicted from Molecular Simulation”, Journal of the American Chemical Society, vol. 138, no. 9. American Chemical Society (ACS), pp. 3058–3065, Feb. 25, 2016. doi: 10.1021/jacs.5b12061.*  
  
*C. S. Gaines and D. M. York, “Model for the Functional Active State of the TS Ribozyme from Molecular Simulation”, Angewandte Chemie International Edition, vol. 56, no. 43. Wiley, pp. 13392–13395, Sep. 08, 2017. doi: 10.1002/anie.201705608.*  
  
*M. Gebala, “Cation–Anion Interactions within the Nucleic Acid Ion Atmosphere Revealed by Ion Counting”, Journal of the American Chemical Society, vol. 137, no. 46. American Chemical Society (ACS), pp. 14705–14715, Nov. 12, 2015. doi: 10.1021/jacs.5b08395.*  
  
*G. M. Giambaşu, D. A. Caseand D. M. York, “Predicting Site-Binding Modes of Ions and Water to Nucleic Acids Using Molecular Solvation Theory”, Journal of the American Chemical Society, vol. 141, no. 6. American Chemical Society (ACS), pp. 2435–2445, Jan. 11, 2019. doi: 10.1021/jacs.8b11474.*  
  
*G. M. Giambaşu, M. K. Gebala, M. T. Panteva, T. Luchko, D. A. Caseand D. M. York, “Competitive interaction of monovalent cations with DNA from 3D-RISM”, Nucleic Acids Research, vol. 43, no. 17. Oxford University Press (OUP), pp. 8405–8415, Aug. 24, 2015. doi: 10.1093/nar/gkv830.*  
  
*T. J. Giese and D. M. York, “Ambient-Potential Composite Ewald Method for ab Initio Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation”, Journal of Chemical Theory and Computation, vol. 12, no. 6. American Chemical Society (ACS), pp. 2611–2632, May 26, 2016. doi: 10.1021/acs.jctc.6b00198.*  
  
*T. J. Giese and D. M. York, “Quantum mechanical force fields for condensed phase molecular simulations”, Journal of Physics: Condensed Matter, vol. 29, no. 38. IOP Publishing, p. 383002, Aug. 17, 2017. doi: 10.1088/1361-648x/aa7c5c.*  
  
*T. J. Giese and D. M. York, “A GPU-Accelerated Parameter Interpolation Thermodynamic Integration Free Energy Method”, Journal of Chemical Theory and Computation, vol. 14, no. 3. American Chemical Society (ACS), pp. 1564–1582, Jan. 22, 2018. doi: 10.1021/acs.jctc.7b01175.*  
  
*A. Gutmanas, “NMR Exchange Format: a unified and open standard for representation of NMR restraint data”, Nature Structural & Molecular Biology, vol. 22, no. 6. Springer Science and Business Media LLC, pp. 433–434, Jun. 2015. doi: 10.1038/nsmb.3041.*  
  
*M. E. Harris, J. A. Piccirilliand D. M. York, “Enzyme transition states from theory and experiment”, Biochimica et Biophysica Acta (BBA) - Proteins and Proteomics, vol. 1854, no. 11. Elsevier BV, pp. 1727–1728, Nov. 2015. doi: 10.1016/j.bbapap.2015.08.006.*  
  
*M. E. Harris, J. A. Piccirilliand D. M. York, “Integration of kinetic isotope effect analyses to elucidate ribonuclease mechanism”, Biochimica et Biophysica Acta (BBA) - Proteins and Proteomics, vol. 1854, no. 11. Elsevier BV, pp. 1801–1808, Nov. 2015. doi: 10.1016/j.bbapap.2015.04.022.*  
  
*M. E. Harris, D. M. York, J. A. Piccirilliand V. E. Anderson, “Kinetic Isotope Effect Analysis of RNA 2′- O -Transphosphorylation”, Measurement and Analysis of Kinetic Isotope Effects. Elsevier, pp. 433–457, 2017. doi: 10.1016/bs.mie.2017.07.017.*  
  
*C.-H. Hsu, “The Dependence of Carbohydrate–Aromatic Interaction Strengths on the Structure of the Carbohydrate”, Journal of the American Chemical Society, vol. 138, no. 24. American Chemical Society (ACS), pp. 7636–7648, Jun. 14, 2016. doi: 10.1021/jacs.6b02879.*  
  
*M. Huang, “A Multidimensional B-Spline Correction for Accurate Modeling Sugar Puckering in QM/MM Simulations”, Journal of Chemical Theory and Computation, vol. 13, no. 9. American Chemical Society (ACS), pp. 3975–3984, Aug. 17, 2017. doi: 10.1021/acs.jctc.7b00161.*  
  
*M. Huang, T. J. Gieseand D. M. York, “Nucleic acid reactivity: Challenges for next-generation semiempirical quantum models”, Journal of Computational Chemistry, vol. 36, no. 18. Wiley, pp. 1370–1389, May 06, 2015. doi: 10.1002/jcc.23933.*  
  
*I. Ivani, “Parmbsc1: a refined force field for DNA simulations”, Nature Methods, vol. 13, no. 1. Springer Science and Business Media LLC, pp. 55–58, Nov. 16, 2015. doi: 10.1038/nmeth.3658.*  
  
*P. A. Janowski, C. Liu, J. Deckmanand D. A. Case, “Molecular dynamics simulation of triclinic lysozyme in a crystal lattice”, Protein Science, vol. 25, no. 1. Wiley, pp. 87–102, Jun. 11, 2015. doi: 10.1002/pro.2713.*  
  
*J. Johnson, D. A. Case, T. Yamazaki, S. Gusarov, A. Kovalenkoand T. Luchko, “Small molecule hydration energy and entropy from 3D-RISM”, Journal of Physics: Condensed Matter, vol. 28, no. 34. IOP Publishing, p. 344002, Jul. 01, 2016. doi: 10.1088/0953-8984/28/34/344002.*  
  
*S. C. Keane, “Structure of the HIV-1 RNA packaging signal”, Science, vol. 348, no. 6237. American Association for the Advancement of Science (AAAS), pp. 917–921, May 22, 2015. doi: 10.1126/science.aaa9266.*  
  
*D. L. Kellerman, K. S. Simmons, M. Pedraza, J. A. Piccirilli, D. M. Yorkand M. E. Harris, “Determination of hepatitis delta virus ribozyme N(–1) nucleobase and functional group specificity using internal competition kinetics”, Analytical Biochemistry, vol. 483. Elsevier BV, pp. 12–20, Aug. 2015. doi: 10.1016/j.ab.2015.04.024.*  
  
*G. König, B. R. Brooks, W. Thieland D. M. York, “On the convergence of multi-scale free energy simulations”, Molecular Simulation, vol. 44, no. 13–14. Informa UK Limited, pp. 1062–1081, May 30, 2018. doi: 10.1080/08927022.2018.1475741.*  
  
*G. König, “A Comparison of QM/MM Simulations with and without the Drude Oscillator Model Based on Hydration Free Energies of Simple Solutes”, Molecules, vol. 23, no. 10. MDPI AG, p. 2695, Oct. 19, 2018. doi: 10.3390/molecules23102695.*  
  
*E. R. Kuechler, T. J. Gieseand D. M. York, “Charge-dependent many-body exchange and dispersion interactions in combined QM/MM simulations”, The Journal of Chemical Physics, vol. 143, no. 23. AIP Publishing, p. 234111, Dec. 21, 2015. doi: 10.1063/1.4937166.*  
  
*E. R. Kuechler, T. J. Gieseand D. M. York, “VR-SCOSMO: A smooth conductor-like screening model with charge-dependent radii for modeling chemical reactions”, The Journal of Chemical Physics, vol. 144, no. 16. AIP Publishing, p. 164115, Apr. 28, 2016. doi: 10.1063/1.4946779.*  
  
*T.-S. Lee, “GPU-Accelerated Molecular Dynamics and Free Energy Methods in Amber18: Performance Enhancements and New Features”, Journal of Chemical Information and Modeling, vol. 58, no. 10. American Chemical Society (ACS), pp. 2043–2050, Sep. 10, 2018. doi: 10.1021/acs.jcim.8b00462.*  
  
*T.-S. Lee, Y. Hu, B. Sherborne, Z. Guoand D. M. York, “Toward Fast and Accurate Binding Affinity Prediction with pmemdGTI: An Efficient Implementation of GPU-Accelerated Thermodynamic Integration”, Journal of Chemical Theory and Computation, vol. 13, no. 7. American Chemical Society (ACS), pp. 3077–3084, Jun. 23, 2017. doi: 10.1021/acs.jctc.7b00102.*  
  
*T.-S. Lee, B. K. Radak, M. E. Harrisand D. M. York, “A Two-Metal-Ion-Mediated Conformational Switching Pathway for HDV Ribozyme Activation”, ACS Catalysis, vol. 6, no. 3. American Chemical Society (ACS), pp. 1853–1869, Feb. 18, 2016. doi: 10.1021/acscatal.5b02158.*  
  
*H. T. Nguyen, S. A. Pabit, S. P. Meisburger, L. Pollackand D. A. Case, “Accurate small and wide angle x-ray scattering profiles from atomic models of proteins and nucleic acids”, The Journal of Chemical Physics, vol. 141, no. 22. AIP Publishing, pp. 22D508, Dec. 14, 2014. doi: 10.1063/1.4896220.*  
  
*H. T. Nguyen, S. A. Pabit, L. Pollackand D. A. Case, “Extracting water and ion distributions from solution x-ray scattering experiments”, The Journal of Chemical Physics, vol. 144, no. 21. AIP Publishing, p. 214105, Jun. 07, 2016. doi: 10.1063/1.4953037.*  
  
*M. T. Panteva, G. M. Giambaşuand D. M. York, “Force Field for Mg2+, Mn2+, Zn2+, and Cd2+ Ions That Have Balanced Interactions with Nucleic Acids”, The Journal of Physical Chemistry B, vol. 119, no. 50. American Chemical Society (ACS), pp. 15460–15470, Dec. 03, 2015. doi: 10.1021/acs.jpcb.5b10423.*  
  
*B. K. Radak, T.-S. Lee, M. E. Harrisand D. M. York, “Assessment of metal-assisted nucleophile activation in the hepatitis delta virus ribozyme from molecular simulation and 3D-RISM”, RNA, vol. 21, no. 9. Cold Spring Harbor Laboratory, pp. 1566–1577, Jul. 13, 2015. doi: 10.1261/rna.051466.115.*  
  
*L. Salmon, “Modulating RNA Alignment Using Directional Dynamic Kinks: Application in Determining an Atomic-Resolution Ensemble for a Hairpin using NMR Residual Dipolar Couplings”, Journal of the American Chemical Society, vol. 137, no. 40. American Chemical Society (ACS), pp. 12954–12965, Sep. 29, 2015. doi: 10.1021/jacs.5b07229.*  
  
*J. Swails, T. Zhu, X. Heand D. A. Case, “AFNMR: automated fragmentation quantum mechanical calculation of NMR chemical shifts for biomolecules”, Journal of Biomolecular NMR, vol. 63, no. 2. Springer Science and Business Media LLC, pp. 125–139, Aug. 02, 2015. doi: 10.1007/s10858-015-9970-3.*  
  
*S. Zhang, “Isotope effect analyses provide evidence for an altered transition state for RNA 2′-O-transphosphorylation catalyzed by Zn2+”, Chemical Communications, vol. 52, no. 24. Royal Society of Chemistry (RSC), pp. 4462–4465, 2016. doi: 10.1039/c5cc10212j.*  
  
*A. Albaugh, “Advanced Potential Energy Surfaces for Molecular Simulation”, The Journal of Physical Chemistry B, vol. 120, no. 37. American Chemical Society (ACS), pp. 9811–9832, Aug. 11, 2016. doi: 10.1021/acs.jpcb.6b06414.*  
  
*Y. Hu, B. Sherborne, T.-S. Lee, D. A. Case, D. M. Yorkand Z. Guo, “The importance of protonation and tautomerization in relative binding affinity prediction: a comparison of AMBER TI and Schrödinger FEP”, Journal of Computer-Aided Molecular Design, vol. 30, no. 7. Springer Science and Business Media LLC, pp. 533–539, Jul. 2016. doi: 10.1007/s10822-016-9920-5.*  
  
*P. A. Janowski, “Improved ligand geometries in crystallographic refinement usingAFITTinPHENIX”, Acta Crystallographica Section D Structural Biology, vol. 72, no. 9. International Union of Crystallography (IUCr), pp. 1062–1072, Aug. 31, 2016. doi: 10.1107/s2059798316012225.*  
  
*M. R. Shirts, “Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset”, Journal of Computer-Aided Molecular Design, vol. 31, no. 1. Springer Science and Business Media LLC, pp. 147–161, Oct. 27, 2016. doi: 10.1007/s10822-016-9977-1.*  
  
*M. R. Shirts, “Erratum to: Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset”, Journal of Computer-Aided Molecular Design, vol. 31, no. 8. Springer Science and Business Media LLC, pp. 777–777, Jul. 27, 2017. doi: 10.1007/s10822-017-0043-4.*  
  
*H. Zhang, “HIV-1 Capsid Function Is Regulated by Dynamics: Quantitative Atomic-Resolution Insights by Integrating Magic-Angle-Spinning NMR, QM/MM, and MD”, Journal of the American Chemical Society, vol. 138, no. 42. American Chemical Society (ACS), pp. 14066–14075, Oct. 18, 2016. doi: 10.1021/jacs.6b08744.*  
  
*Y. Chu, J. Yaoand H. Guo, “QM/MM MD and Free Energy Simulations of G9a-Like Protein (GLP) and Its Mutants: Understanding the Factors that Determine the Product Specificity”, PLoS ONE, vol. 7, no. 5. Public Library of Science (PLoS), p. e37674, May 18, 2012. doi: 10.1371/journal.pone.0037674.*  
  
*J. Yao, Y. Chu, R. Anand H. Guo, “Understanding Product Specificity of Protein Lysine Methyltransferases from QM/MM Molecular Dynamics and Free Energy Simulations: The Effects of Mutation on SET7/9 beyond the Tyr/Phe Switch”, Journal of Chemical Information and Modeling, vol. 52, no. 2. American Chemical Society (ACS), pp. 449–456, Feb. 16, 2012. doi: 10.1021/ci200364m.*  
  
*J. Yao, A. Wlodawerand H. Guo, “Understanding the Autocatalytic Process of Pro-kumamolisin Activation from Molecular Dynamics and Quantum Mechanical/Molecular Mechanical (QM/MM) Free-Energy Simulations”, Chemistry - A European Journal, vol. 19, no. 33. Wiley, pp. 10849–10852, Jul. 02, 2013. doi: 10.1002/chem.201301310.*  
  
*J. Yao, Q. Xuand H. Guo, “QM/MM and free-energy simulations of deacylation reaction catalysed by sedolisin, a serine-carboxyl peptidase”, Molecular Simulation, vol. 39, no. 3. Informa UK Limited, pp. 206–213, Mar. 2013. doi: 10.1080/08927022.2012.714467.*  
  
*I. Garitaonandia, “Increased Risk of Genetic and Epigenetic Instability in Human Embryonic Stem Cells Associated with Specific Culture Conditions”, PLOS ONE, vol. 10, no. 2. Public Library of Science (PLoS), p. e0118307, Feb. 25, 2015. doi: 10.1371/journal.pone.0118307.*  
  
*X. Liao, “Matched miRNA and mRNA signatures from a hESC-based in vitro model of pancreatic differentiation reveal novel regulatory interactions”, Journal of Cell Science. The Company of Biologists, Jan. 01, 2013. doi: 10.1242/jcs.123570.*  
  
*H. Ma, “Incompatibility between Nuclear and Mitochondrial Genomes Contributes to an Interspecies Reproductive Barrier”, Cell Metabolism, vol. 24, no. 2. Elsevier BV, pp. 283–294, Aug. 2016. doi: 10.1016/j.cmet.2016.06.012.*  
  
*D. Ramsköld, “Full-length mRNA-Seq from single-cell levels of RNA and individual circulating tumor cells”, Nature Biotechnology, vol. 30, no. 8. Springer Science and Business Media LLC, pp. 777–782, Jul. 22, 2012. doi: 10.1038/nbt.2282.*  
  
*I. Sancho-Martinez, “Establishment of human iPSC-based models for the study and targeting of glioma initiating cells”, Nature Communications, vol. 7, no. 1. Springer Science and Business Media LLC, Feb. 22, 2016. doi: 10.1038/ncomms10743.*  
  
*J. Yang, “Genome-Wide RNAi Screening Identifies Genes Inhibiting the Migration of Glioblastoma Cells”, PLoS ONE, vol. 8, no. 4. Public Library of Science (PLoS), p. e61915, Apr. 12, 2013. doi: 10.1371/journal.pone.0061915.*  
  
*S. Khumsubdee, Y. Fanand K. Burgess, “A Comparison between Oxazoline-imidazolinylidene, -imidazolylidine, -benzimidazolylidene Hydrogenation Catalysts”, The Journal of Organic Chemistry, vol. 78, no. 19. American Chemical Society (ACS), pp. 9969–9974, Sep. 19, 2013. doi: 10.1021/jo4013783.*  
  
*Y.-S. Kim, “Multivalency of Non-Peptide Integrin αVβ3 Antagonist Slows Tumor Growth”, Molecular Pharmaceutics, vol. 10, no. 10. American Chemical Society (ACS), pp. 3603–3611, Sep. 05, 2013. doi: 10.1021/mp400096z.*  
  
*Q. Shao, Y. Fan, L. Yangand Y. Qin Gao, “From protein denaturant to protectant: Comparative molecular dynamics study of alcohol/protein interactions”, The Journal of Chemical Physics, vol. 136, no. 11. AIP Publishing, p. 115101, Mar. 21, 2012. doi: 10.1063/1.3692801.*  
  
*L. Yang, Y. Fanand Y. Q. Gao, “Differences of Cations and Anions: Their Hydration, Surface Adsorption, and Impact on Water Dynamics”, The Journal of Physical Chemistry B, vol. 115, no. 43. American Chemical Society (ACS), pp. 12456–12465, Oct. 11, 2011. doi: 10.1021/jp207652h.*  
  
*J. K. Jarett, M. D. MacManes, K. M. Morrow, M. S. Pankeyand M. P. Lesser, “Comparative Genomics of Color Morphs In the Coral Montastraea cavernosa”, Scientific Reports, vol. 7, no. 1. Springer Science and Business Media LLC, Nov. 22, 2017. doi: 10.1038/s41598-017-16371-9.*  
  
*L. Kordonowy and M. MacManes, “Characterizing the reproductive transcriptomic correlates of acute dehydration in males in the desert-adapted rodent, Peromyscus eremicus”, BMC Genomics, vol. 18, no. 1. Springer Science and Business Media LLC, Jun. 23, 2017. doi: 10.1186/s12864-017-3840-1.*  
  
*A. Lang, L. Kordonowy, E. Laceyand M. MacManes, “Transcriptomic analyses reveal tissue-specific selection on genes related to apoptotic processes in the subterranean rodent,Ctenomys sociabilis”, []. Cold Spring Harbor Laboratory, Jan. 30, 2018. doi: 10.1101/256875.*  
  
*M. D. MacManes, “Severe acute dehydration in a desert rodent elicits a transcriptional response that effectively prevents kidney injury”, American Journal of Physiology-Renal Physiology, vol. 313, no. 2. American Physiological Society, pp. F262–F272, Aug. 01, 2017. doi: 10.1152/ajprenal.00067.2017.*  
  
*M. D. MacManes, S. H. Austin, A. S. Lang, A. Booth, V. Farrarand R. M. Calisi, “Widespread patterns of sexually dimorphic gene expression in an avian hypothalamic–pituitary–gonadal (HPG) axis”, Scientific Reports, vol. 7, no. 1. Springer Science and Business Media LLC, Apr. 18, 2017. doi: 10.1038/srep45125.*  
  
*T. A. Schuelke, “Comparative Genomics of Pathogenic and Nonpathogenic Beetle-Vectored Fungi in the Genus Geosmithia”, Genome Biology and Evolution, vol. 9, no. 12. Oxford University Press (OUP), pp. 3312–3327, Nov. 23, 2017. doi: 10.1093/gbe/evx242.*  
  
*G. Rendon, R. J. Mashl, S. Saladiand E. Jakobsson, “Bacterial Roots and Branches of the HCN/CNG Family of Ion Channels: Phylogeny, Structure, and Implications for Eukaryotic HCN/CNG Structure and Function”, Biophysical Journal, vol. 104, no. 2. Elsevier BV, p. 278a, Jan. 2013. doi: 10.1016/j.bpj.2012.11.1560.*  
  
*R. Laghaei, D. G. Evansand R. D. Coalson, “Metal binding sites of human H-chain ferritin and iron transport mechanism to the ferroxidase sites: A molecular dynamics simulation study”, Proteins: Structure, Function, and Bioinformatics, vol. 81, no. 6. Wiley, pp. 1042–1050, Apr. 01, 2013. doi: 10.1002/prot.24251.*  
  
*R. Laghaei, W. Kowallis, D. G. Evansand R. D. Coalson, “Calculation of Iron Transport through Human H-chain Ferritin”, The Journal of Physical Chemistry A, vol. 118, no. 35. American Chemical Society (ACS), pp. 7442–7453, Mar. 07, 2014. doi: 10.1021/jp500198u.*  
  
*C. L. Carswell, “Role of the Fourth Transmembrane α Helix in the Allosteric Modulation of Pentameric Ligand-Gated Ion Channels”, Structure, vol. 23, no. 9. Elsevier BV, pp. 1655–1664, Sep. 2015. doi: 10.1016/j.str.2015.06.020.*  
  
*Z. Cournia, “Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory”, The Journal of Membrane Biology, vol. 248, no. 4. Springer Science and Business Media LLC, pp. 611–640, Jun. 11, 2015. doi: 10.1007/s00232-015-9802-0.*  
  
*J. Hénin, R. Salari, S. Murlidaranand G. Brannigan, “A Predicted Binding Site for Cholesterol on the GABAA Receptor”, Biophysical Journal, vol. 106, no. 9. Elsevier BV, pp. 1938–1949, May 2014. doi: 10.1016/j.bpj.2014.03.024.*  
  
*D. N. LeBard, J. Hénin, R. G. Eckenhoff, M. L. Kleinand G. Brannigan, “General Anesthetics Predicted to Block the GLIC Pore with Micromolar Affinity”, PLoS Computational Biology, vol. 8, no. 5. Public Library of Science (PLoS), p. e1002532, May 31, 2012. doi: 10.1371/journal.pcbi.1002532.*  
  
*R. Salari, S. Murlidaranand G. Brannigan, “Pentameric ligand-gated ion channels: insights from computation”, Molecular Simulation, vol. 40, no. 10–11. Informa UK Limited, pp. 821–829, Apr. 17, 2014. doi: 10.1080/08927022.2014.896462.*  
  
*B. P. Weiser, R. Salari, R. G. Eckenhoffand G. Brannigan, “Computational Investigation of Cholesterol Binding Sites on Mitochondrial VDAC”, The Journal of Physical Chemistry B, vol. 118, no. 33. American Chemical Society (ACS), pp. 9852–9860, Aug. 11, 2014. doi: 10.1021/jp504516a.*  
  
*T. Westergard, R. Salari, J. V. Martinand G. Brannigan, “Interactions of L-3,5,3’-Triiodothyronine, Allopregnanolone, and Ivermectin with the GABAA Receptor: Evidence for Overlapping Intersubunit Binding Modes”, PLOS ONE, vol. 10, no. 9. Public Library of Science (PLoS), p. e0139072, Sep. 30, 2015. doi: 10.1371/journal.pone.0139072.*  
  
*K. A. Woll, W. P. Dailey, G. Branniganand R. G. Eckenhoff, “Shedding Light on Anesthetic Mechanisms”, Anesthesia & Analgesia, vol. 123, no. 5. Ovid Technologies (Wolters Kluwer Health), pp. 1253–1262, Nov. 2016. doi: 10.1213/ane.0000000000001365.*  
  
*K. A. Woll, “A Novel Bifunctional Alkylphenol Anesthetic Allows Characterization of γ-Aminobutyric Acid, Type A (GABAA), Receptor Subunit Binding Selectivity in Synaptosomes”, Journal of Biological Chemistry, vol. 291, no. 39. Elsevier BV, pp. 20473–20486, Sep. 2016. doi: 10.1074/jbc.m116.736975.*  
  
*J. S. Rao and L. Cruz, “Effects of Confinement on the Structure and Dynamics of an Intrinsically Disordered Peptide: A Molecular-Dynamics Study”, The Journal of Physical Chemistry B, vol. 117, no. 14. American Chemical Society (ACS), pp. 3707–3719, Mar. 28, 2013. doi: 10.1021/jp310623x.*  
  
*L. Cruz, J. S. Rao, D. B. Teplowand B. Urbanc, “Dynamics of Metastable β-Hairpin Structures in the Folding Nucleus of Amyloid β-Protein”, The Journal of Physical Chemistry B, vol. 116, no. 22. American Chemical Society (ACS), pp. 6311–6325, May 24, 2012. doi: 10.1021/jp301619v.*  
  
*M. D. Smith and L. Cruz, “Effect of Ionic Aqueous Environments on the Structure and Dynamics of the Aβ21–30 Fragment: A Molecular-Dynamics Study”, The Journal of Physical Chemistry B, vol. 117, no. 22. American Chemical Society (ACS), pp. 6614–6624, May 29, 2013. doi: 10.1021/jp312653h.*  
  
*J. T. Kindt, “Simulations of grain boundaries between ordered hard sphere monolayer domains: Orientation-dependent stiffness and its correlation with grain coarsening dynamics”, The Journal of Chemical Physics, vol. 149, no. 4. AIP Publishing, p. 044503, Jul. 28, 2018. doi: 10.1063/1.5029813.*  
  
*Z. Guo and J. T. Kindt, “Gibbs ensemble Monte Carlo with solvent repacking: phase coexistence of size–asymmetrical binary Lennard-Jones mixtures”, Molecular Simulation, vol. 44, no. 4. Informa UK Limited, pp. 300–308, Sep. 11, 2017. doi: 10.1080/08927022.2017.1373192.*  
  
*Z. Guo and J. T. Kindt, “Partitioning of Size-Mismatched Impurities to Grain Boundaries in 2d Solid Hard-Sphere Monolayers”, Langmuir, vol. 34, no. 43. American Chemical Society (ACS), pp. 12947–12956, Oct. 08, 2018. doi: 10.1021/acs.langmuir.8b02633.*  
  
*Z. Guo, P. Wuand J. T. Kindt, “Ordering of colloidal hard spheres under gravity: from monolayer to multilayer”, Soft Matter, vol. 15, no. 5. Royal Society of Chemistry (RSC), pp. 1027–1037, 2019. doi: 10.1039/c8sm02243g.*  
  
*J. T. Kindt, “Grand canonical Monte Carlo using solvent repacking: Application to phase behavior of hard disk mixtures”, The Journal of Chemical Physics, vol. 143, no. 12. AIP Publishing, p. 124109, Sep. 28, 2015. doi: 10.1063/1.4931731.*  
  
*J. T. Kindt, “Competing factors in grain boundary loop shrinkage: Two-dimensional hard sphere colloidal crystals”, The Journal of Chemical Physics, vol. 151, no. 8. AIP Publishing, p. 084505, Aug. 28, 2019. doi: 10.1063/1.5110394.*  
  
*J. T. Kindt, “Size-asymmetrical Lennard-Jones solid solutions: Interstitials and substitutions”, The Journal of Chemical Physics, vol. 148, no. 16. AIP Publishing, p. 164504, Apr. 28, 2018. doi: 10.1063/1.5024230.*  
  
*L. A. Patel and J. T. Kindt, “Coarse-grained molecular simulations of the melting kinetics of small unilamellar vesicles”, Soft Matter, vol. 12, no. 6. Royal Society of Chemistry (RSC), pp. 1765–1777, 2016. doi: 10.1039/c5sm02560e.*  
  
*K. A. Reid, C. M. Davis, R. B. Dyerand J. T. Kindt, “Binding, folding and insertion of a β-hairpin peptide at a lipid bilayer surface: Influence of electrostatics and lipid tail packing”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1860, no. 3. Elsevier BV, pp. 792–800, Mar. 2018. doi: 10.1016/j.bbamem.2017.12.019.*  
  
*A. West, K. Ma, J. L. Chungand J. T. Kindt, “Simulation Studies of Structure and Edge Tension of Lipid Bilayer Edges: Effects of Tail Structure and Force-Field”, The Journal of Physical Chemistry A, vol. 117, no. 32. American Chemical Society (ACS), pp. 7114–7123, Apr. 18, 2013. doi: 10.1021/jp400371k.*  
  
*L. Yang and J. T. Kindt, “Line Tension Assists Membrane Permeation at the Transition Temperature in Mixed-Phase Lipid Bilayers”, The Journal of Physical Chemistry B, vol. 120, no. 45. American Chemical Society (ACS), pp. 11740–11750, Nov. 04, 2016. doi: 10.1021/acs.jpcb.6b06690.*  
  
*F. Yin and J. T. Kindt, “Hydrophobic Mismatch and Lipid Sorting Near OmpA in Mixed Bilayers: Atomistic and Coarse-Grained Simulations”, Biophysical Journal, vol. 102, no. 10. Elsevier BV, pp. 2279–2287, May 2012. doi: 10.1016/j.bpj.2012.04.005.*  
  
*X. Zhang, J. G. Arce Nunezand J. T. Kindt, “Derivation of micelle size-dependent free energies of aggregation for octyl phosphocholine from molecular dynamics simulation”, Fluid Phase Equilibria, vol. 485. Elsevier BV, pp. 83–93, Apr. 2019. doi: 10.1016/j.fluid.2018.12.001.*  
  
*W. Zheng, “Quantum Dots Encapsulated within Phospholipid Membranes: Phase-Dependent Structure, Photostability, and Site-Selective Functionalization”, Journal of the American Chemical Society, vol. 136, no. 5. American Chemical Society (ACS), pp. 1992–1999, Jan. 24, 2014. doi: 10.1021/ja411339f.*  
  
*P. Larsson and P. M. Kasson, “Lipid Tail Protrusion in Simulations Predicts Fusogenic Activity of Influenza Fusion Peptide Mutants and Conformational Models”, PLoS Computational Biology, vol. 9, no. 3. Public Library of Science (PLoS), p. e1002950, Mar. 07, 2013. doi: 10.1371/journal.pcbi.1002950.*  
  
*Y. Liu, “Identification of a Novel De Novo Mutation Associated with PRKAG2 Cardiac Syndrome and Early Onset of Heart Failure”, PLoS ONE, vol. 8, no. 5. Public Library of Science (PLoS), p. e64603, May 31, 2013. doi: 10.1371/journal.pone.0064603.*  
  
*T. G. Bartholow, “Strictly Conserved Lysine of Prolyl-tRNA Synthetase Editing Domain Facilitates Binding and Positioning of Misacylated tRNAPro”, Biochemistry, vol. 53, no. 6. American Chemical Society (ACS), pp. 1059–1068, Feb. 03, 2014. doi: 10.1021/bi401279r.*  
  
*Q. H. Hu, “Editing Domain Motions Preorganize the Synthetic Active Site of Prolyl-tRNA Synthetase”, ACS Catalysis, vol. 10, no. 17. American Chemical Society (ACS), pp. 10229–10242, Aug. 14, 2020. doi: 10.1021/acscatal.0c02381.*  
  
*J. M. Johnson, “Multiple Pathways Promote Dynamical Coupling between Catalytic Domains in Escherichia coli Prolyl-tRNA Synthetase”, Biochemistry, vol. 52, no. 25. American Chemical Society (ACS), pp. 4399–4412, Jun. 17, 2013. doi: 10.1021/bi400079h.*  
  
*B. Sanford, “Role of Coupled Dynamics in the Catalytic Activity of Prokaryotic-like Prolyl-tRNA Synthetases”, Biochemistry, vol. 51, no. 10. American Chemical Society (ACS), pp. 2146–2156, Mar. 01, 2012. doi: 10.1021/bi300097g.*  
  
*A. M. Strom, S. C. Fehling, S. Bhattacharyyaand S. Hati, “Probing the global and local dynamics of aminoacyl-tRNA synthetases using all-atom and coarse-grained simulations”, Journal of Molecular Modeling, vol. 20, no. 5. Springer Science and Business Media LLC, May 2014. doi: 10.1007/s00894-014-2245-1.*  
  
*N. Warren, “Comparison of the Intrinsic Dynamics of Aminoacyl-tRNA Synthetases”, The Protein Journal, vol. 33, no. 2. Springer Science and Business Media LLC, pp. 184–198, Mar. 04, 2014. doi: 10.1007/s10930-014-9548-z.*  
  
*T. J. Tschaplinski, “Down-regulation of the caffeic acid O-methyltransferase gene in switchgrass reveals a novel monolignol analog”, Biotechnology for Biofuels, vol. 5, no. 1. Springer Science and Business Media LLC, p. 71, 2012. doi: 10.1186/1754-6834-5-71.*  
  
*G. Kodali, K. A. Kistler, M. Narayanan, S. Matsikaand R. J. Stanley, “Change in Electronic Structure upon Optical Excitation of 8-Vinyladenosine: An Experimental and Theoretical Study”, The Journal of Physical Chemistry A, vol. 114, no. 1. American Chemical Society (ACS), pp. 256–267, Nov. 25, 2009. doi: 10.1021/jp908055h.*  
  
*G. Kodali, M. Narayananand R. J. Stanley, “Excited-State Electronic Properties of 6-Methylisoxanthopterin (6-MI): An Experimental and Theoretical Study”, The Journal of Physical Chemistry B, vol. 116, no. 9. American Chemical Society (ACS), pp. 2981–2989, Feb. 28, 2012. doi: 10.1021/jp2110083.*  
  
*G. Kodali, M. Narayananand R. J. Stanley, “Excited-State Electronic Properties of 6-Methylisoxanthopterin (6-MI): An Experimental and Theoretical Study”, The Journal of Physical Chemistry B, vol. 116, no. 9. American Chemical Society (ACS), pp. 2981–2989, Feb. 28, 2012. doi: 10.1021/jp2110083.*  
  
*M. Narayanan, G. Kodali, V. R. Singh, V. Velvadapuand R. J. Stanley, “Oxidation and reduction potentials of 8-vinyladenosine measured by cyclic voltammetry: Implications for photoinduced electron transfer quenching of a fluorescent adenine analog”, Journal of Photochemistry and Photobiology A: Chemistry, vol. 249. Elsevier BV, pp. 9–14, Dec. 2012. doi: 10.1016/j.jphotochem.2012.08.018.*  
  
*M. Narayanan, G. Kodali, V. R. Singh, V. Velvadapuand R. J. Stanley, “Oxidation and reduction potentials of 8-vinyladenosine measured by cyclic voltammetry: Implications for photoinduced electron transfer quenching of a fluorescent adenine analog”, Journal of Photochemistry and Photobiology A: Chemistry, vol. 249. Elsevier BV, pp. 9–14, Dec. 2012. doi: 10.1016/j.jphotochem.2012.08.018.*  
  
*M. Narayanan, G. Kodali, Y. Xing, M. E. Hawkinsand R. J. Stanley, “Differential Fluorescence Quenching of Fluorescent Nucleic Acid Base Analogues by Native Nucleic Acid Monophosphates”, The Journal of Physical Chemistry B, vol. 114, no. 17. American Chemical Society (ACS), pp. 5953–5963, Apr. 13, 2010. doi: 10.1021/jp1011507.*  
  
*M. Narayanan, G. Kodali, Y. Xingand R. J. Stanley, “Photoinduced Electron Transfer Occurs between 2-Aminopurine and the DNA Nucleic Acid Monophosphates: Results from Cyclic Voltammetry and Fluorescence Quenching”, The Journal of Physical Chemistry B, vol. 114, no. 32. American Chemical Society (ACS), pp. 10573–10580, Jul. 27, 2010. doi: 10.1021/jp102355v.*  
  
*M. L. Kireeva, “Molecular dynamics and mutational analysis of the catalytic and translocation cycle of RNA polymerase”, BMC Biophysics, vol. 5, no. 1. Springer Science and Business Media LLC, Jun. 07, 2012. doi: 10.1186/2046-1682-5-11.*  
  
*Y. A. Nedialkov, “The RNA polymerase bridge helix YFI motif in catalysis, fidelity and translocation”, Biochimica et Biophysica Acta (BBA) - Gene Regulatory Mechanisms, vol. 1829, no. 2. Elsevier BV, pp. 187–198, Feb. 2013. doi: 10.1016/j.bbagrm.2012.11.005.*  
  
*B. Wang, K. Opron, Z. F. Burton, R. I. Cukierand M. Feig, “Five checkpoints maintaining the fidelity of transcription by RNA polymerases in structural and energetic details”, Nucleic Acids Research, vol. 43, no. 2. Oxford University Press (OUP), pp. 1133–1146, Dec. 30, 2014. doi: 10.1093/nar/gku1370.*  
  
*X. Du, “Supramolecular Assemblies of a Conjugate of Nucleobase, Amino Acids, and Saccharide Act as Agonists for Proliferation of Embryonic Stem Cells and Development of Zygotes”, Bioconjugate Chemistry, vol. 25, no. 6. American Chemical Society (ACS), pp. 1031–1035, May 18, 2014. doi: 10.1021/bc500187m.*  
  
*C. E. Faller and O. Guvench, “Terminal sialic acids on CD44 N-glycans can block hyaluronan binding by forming competing intramolecular contacts with arginine sidechains”, Proteins: Structure, Function, and Bioinformatics, vol. 82, no. 11. Wiley, pp. 3079–3089, Sep. 29, 2014. doi: 10.1002/prot.24668.*  
  
*G. G. Gregorio, “Single-molecule analysis of ligand efficacy in β2AR–G-protein activation”, Nature, vol. 547, no. 7661. Springer Science and Business Media LLC, pp. 68–73, Jun. 07, 2017. doi: 10.1038/nature22354.*  
  
*G. Khelashvili, M. Doktorova, M. A. Sahai, N. Johner, L. Shiand H. Weinstein, “Computational modeling of the N-terminus of the human dopamine transporter and its interaction with PIP2 -containing membranes”, Proteins: Structure, Function, and Bioinformatics, vol. 83, no. 5. Wiley, pp. 952–969, Mar. 25, 2015. doi: 10.1002/prot.24792.*  
  
*G. Khelashvili, “Spontaneous Inward Opening of the Dopamine Transporter Is Triggered by PIP2-Regulated Dynamics of the N-Terminus”, ACS Chemical Neuroscience, vol. 6, no. 11. American Chemical Society (ACS), pp. 1825–1837, Aug. 17, 2015. doi: 10.1021/acschemneuro.5b00179.*  
  
*M. V. LeVine, G. Khelashvili, L. Shi, M. Quick, J. A. Javitchand H. Weinstein, “Role of Annular Lipids in the Functional Properties of Leucine Transporter LeuT Proteomicelles”, Biochemistry, vol. 55, no. 6. American Chemical Society (ACS), pp. 850–859, Feb. 05, 2016. doi: 10.1021/acs.biochem.5b01268.*  
  
*M. V. LeVine and H. Weinstein, “NbIT - A New Information Theory-Based Analysis of Allosteric Mechanisms Reveals Residues that Underlie Function in the Leucine Transporter LeuT”, PLoS Computational Biology, vol. 10, no. 5. Public Library of Science (PLoS), p. e1003603, May 01, 2014. doi: 10.1371/journal.pcbi.1003603.*  
  
*X. Li, “Structural modeling defines transmembrane residues in ADAM17 that are crucial for Rhbdf2/ADAM17-dependent proteolysis”, Journal of Cell Science. The Company of Biologists, Jan. 01, 2017. doi: 10.1242/jcs.196436.*  
  
*S. Stolzenberg, M. Michino, M. V. LeVine, H. Weinsteinand L. Shi, “Computational approaches to detect allosteric pathways in transmembrane molecular machines”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1858, no. 7. Elsevier BV, pp. 1652–1662, Jul. 2016. doi: 10.1016/j.bbamem.2016.01.010.*  
  
*S. Stolzenberg, “Mechanism of the Association between Na+ Binding and Conformations at the Intracellular Gate in Neurotransmitter:Sodium Symporters”, Journal of Biological Chemistry, vol. 290, no. 22. Elsevier BV, pp. 13992–14003, May 2015. doi: 10.1074/jbc.m114.625343.*  
  
*R. T. Wragg, “Evolutionary Divergence of the C-terminal Domain of Complexin Accounts for Functional Disparities between Vertebrate and Invertebrate Complexins”, Frontiers in Molecular Neuroscience, vol. 10. Frontiers Media SA, May 26, 2017. doi: 10.3389/fnmol.2017.00146.*  
  
*A. K. Clark, “The Promiscuity of Allosteric Regulation of Nuclear Receptors by Retinoid X Receptor”, The Journal of Physical Chemistry B, vol. 120, no. 33. American Chemical Society (ACS), pp. 8338–8345, Apr. 25, 2016. doi: 10.1021/acs.jpcb.6b02057.*  
  
*Q. R. Johnson, R. J. Lindsay, R. B. Nellas, E. J. Fernandezand T. Shen, “Mapping Allostery through Computational Glycine Scanning and Correlation Analysis of Residue–Residue Contacts”, Biochemistry, vol. 54, no. 7. American Chemical Society (ACS), pp. 1534–1541, Feb. 06, 2015. doi: 10.1021/bi501152d.*  
  
*Q. Johnson, R. Lindsay, L. Petridisand T. Shen, “Investigation of Carbohydrate Recognition via Computer Simulation”, Molecules, vol. 20, no. 5. MDPI AG, pp. 7700–7718, Apr. 28, 2015. doi: 10.3390/molecules20057700.*  
  
*Q. R. Johnson, R. J. Lindsay, S. R. Raval, J. S. Dobbs, R. B. Nellasand T. Shen, “Effects of Branched O-Glycosylation on a Semiflexible Peptide Linker”, The Journal of Physical Chemistry B, vol. 118, no. 8. American Chemical Society (ACS), pp. 2050–2057, Feb. 18, 2014. doi: 10.1021/jp410788r.*  
  
*Q. R. Johnson, R. J. Lindsayand T. Shen, “CAMERRA: An analysis tool for the computation of conformational dynamics by evaluating residue-residue associations”, Journal of Computational Chemistry, vol. 39, no. 20. Wiley, pp. 1568–1578, Feb. 21, 2018. doi: 10.1002/jcc.25192.*  
  
*Q. R. Johnson, R. B. Nellasand T. Shen, “Solvent-Dependent Gating Motions of an Extremophilic Lipase from Pseudomonas aeruginosa”, Biochemistry, vol. 51, no. 31. American Chemical Society (ACS), pp. 6238–6245, Jul. 25, 2012. doi: 10.1021/bi300557y.*  
  
*R. J. Lindsay, Q. R. Johnson, W. Evangelista, R. B. Nellasand T. Shen, “DMSO enhanced conformational switch of an interfacial enzyme”, Biopolymers, vol. 105, no. 12. Wiley, pp. 864–872, Sep. 22, 2016. doi: 10.1002/bip.22924.*  
  
*R. J. Lindsay, B. Pham, T. Shenand R. P. McCord, “Characterizing the 3D structure and dynamics of chromosomes and proteins in a common contact matrix framework”, Nucleic Acids Research, vol. 46, no. 16. Oxford University Press (OUP), pp. 8143–8152, Jul. 10, 2018. doi: 10.1093/nar/gky604.*  
  
*R. J. Lindsay, “Characterizing protein conformations by correlation analysis of coarse-grained contact matrices”, The Journal of Chemical Physics, vol. 148, no. 2. AIP Publishing, p. 025101, Jan. 14, 2018. doi: 10.1063/1.5004141.*  
  
*R. B. Nellas, Q. R. Johnsonand T. Shen, “Solvent-Induced α- to 310-Helix Transition of an Amphiphilic Peptide”, Biochemistry, vol. 52, no. 40. American Chemical Society (ACS), pp. 7137–7144, Sep. 25, 2013. doi: 10.1021/bi400537z.*  
  
*B. Pham, A. B. Arons, J. G. Vincent, E. J. Fernandezand T. Shen, “Regulatory Mechanics of Constitutive Androstane Receptors: Basal and Ligand-Directed Actions”, Journal of Chemical Information and Modeling, vol. 59, no. 12. American Chemical Society (ACS), pp. 5174–5182, Nov. 12, 2019. doi: 10.1021/acs.jcim.9b00695.*  
  
*B. Pham, R. J. Lindsayand T. Shen, “Effector-Binding-Directed Dimerization and Dynamic Communication between Allosteric Sites of Ribonucleotide Reductase”, Biochemistry, vol. 58, no. 6. American Chemical Society (ACS), pp. 697–705, Dec. 20, 2018. doi: 10.1021/acs.biochem.8b01131.*  
  
*R. B. Best, C. Millerand J. Mittal, “Role of solvation in pressure-induced helix stabilization”, The Journal of Chemical Physics, vol. 141, no. 22. AIP Publishing, pp. 22D522, Dec. 14, 2014. doi: 10.1063/1.4901112.*  
  
*R. B. Best, J. Mittal, M. Feigand A. D. MacKerell Jr., “Inclusion of Many-Body Effects in the Additive CHARMM Protein CMAP Potential Results in Enhanced Cooperativity of α-Helix and β-Hairpin Formation”, Biophysical Journal, vol. 103, no. 5. Elsevier BV, pp. 1045–1051, Sep. 2012. doi: 10.1016/j.bpj.2012.07.042.*  
  
*R. B. Best, W. Zhengand J. Mittal, “Balanced Protein–Water Interactions Improve Properties of Disordered Proteins and Non-Specific Protein Association”, Journal of Chemical Theory and Computation, vol. 10, no. 11. American Chemical Society (ACS), pp. 5113–5124, Oct. 16, 2014. doi: 10.1021/ct500569b.*  
  
*R. B. Best, W. Zhengand J. Mittal, “Correction to Balanced Protein–Water Interactions Improve Properties of Disordered Proteins and Non-Specific Protein Association”, Journal of Chemical Theory and Computation, vol. 11, no. 4. American Chemical Society (ACS), pp. 1978–1978, Mar. 18, 2015. doi: 10.1021/acs.jctc.5b00219.*  
  
*A. Bhattacharya, R. B. Bestand J. Mittal, “Smoothing of the GB1 Hairpin Folding Landscape by Interfacial Confinement”, Biophysical Journal, vol. 103, no. 3. Elsevier BV, pp. 596–600, Aug. 2012. doi: 10.1016/j.bpj.2012.07.005.*  
  
*A. Bhattacharya, Y. C. Kimand J. Mittal, “Protein–protein interactions in a crowded environment”, Biophysical Reviews, vol. 5, no. 2. Springer Science and Business Media LLC, pp. 99–108, Apr. 16, 2013. doi: 10.1007/s12551-013-0111-5.*  
  
*A. E. Conicella, “TDP-43 α-helical structure tunes liquid-liquid phase separation and function”, []. Cold Spring Harbor Laboratory, May 18, 2019. doi: 10.1101/640615.*  
  
*A. E. Conicella, “TDP-43 α-helical structure tunes liquid–liquid phase separation and function”, Proceedings of the National Academy of Sciences, vol. 117, no. 11. Proceedings of the National Academy of Sciences, pp. 5883–5894, Mar. 04, 2020. doi: 10.1073/pnas.1912055117.*  
  
*A. E. Conicella, G. H. Zerze, J. Mittaland N. L. Fawzi, “ALS Mutations Disrupt Phase Separation Mediated by α-Helical Structure in the TDP-43 Low-Complexity C-Terminal Domain”, Structure, vol. 24, no. 9. Elsevier BV, pp. 1537–1549, Sep. 2016. doi: 10.1016/j.str.2016.07.007.*  
  
*P. Das, S. Matysiakand J. Mittal, “Looking at the Disordered Proteins through the Computational Microscope”, ACS Central Science, vol. 4, no. 5. American Chemical Society (ACS), pp. 534–542, Mar. 22, 2018. doi: 10.1021/acscentsci.7b00626.*  
  
*G. L. Dignon, R. B. Bestand J. Mittal, “Biomolecular Phase Separation: From Molecular Driving Forces to Macroscopic Properties”, Annual Review of Physical Chemistry, vol. 71, no. 1. Annual Reviews, pp. 53–75, Apr. 20, 2020. doi: 10.1146/annurev-physchem-071819-113553.*  
  
*G. L. Dignon, G. H. Zerzeand J. Mittal, “Interplay Between Membrane Composition and Structural Stability of Membrane-Bound hIAPP”, The Journal of Physical Chemistry B, vol. 121, no. 37. American Chemical Society (ACS), pp. 8661–8668, Sep. 08, 2017. doi: 10.1021/acs.jpcb.7b05689.*  
  
*G. L. Dignon, W. Zheng, R. B. Best, Y. C. Kimand J. Mittal, “Relation between single-molecule properties and phase behavior of intrinsically disordered proteins”, Proceedings of the National Academy of Sciences, vol. 115, no. 40. Proceedings of the National Academy of Sciences, pp. 9929–9934, Sep. 14, 2018. doi: 10.1073/pnas.1804177115.*  
  
*G. L. Dignon, W. Zheng, Y. C. Kim, R. B. Bestand J. Mittal, “Sequence determinants of protein phase behavior from a coarse-grained model”, []. Cold Spring Harbor Laboratory, Dec. 21, 2017. doi: 10.1101/238170.*  
  
*G. L. Dignon, W. Zheng, Y. C. Kim, R. B. Bestand J. Mittal, “Sequence determinants of protein phase behavior from a coarse-grained model”, PLOS Computational Biology, vol. 14, no. 1. Public Library of Science (PLoS), p. e1005941, Jan. 24, 2018. doi: 10.1371/journal.pcbi.1005941.*  
  
*G. L. Dignon, W. Zheng, Y. C. Kimand J. Mittal, “Temperature-Controlled Liquid–Liquid Phase Separation of Disordered Proteins”, ACS Central Science, vol. 5, no. 5. American Chemical Society (ACS), pp. 821–830, May 01, 2019. doi: 10.1021/acscentsci.9b00102.*  
  
*G. L. Dignon, W. Zhengand J. Mittal, “Simulation methods for liquid–liquid phase separation of disordered proteins”, Current Opinion in Chemical Engineering, vol. 23. Elsevier BV, pp. 92–98, Mar. 2019. doi: 10.1016/j.coche.2019.03.004.*  
  
*Y. Ding and J. Mittal, “Insights into DNA-mediated interparticle interactions from a coarse-grained model”, The Journal of Chemical Physics, vol. 141, no. 18. AIP Publishing, p. 184901, Nov. 14, 2014. doi: 10.1063/1.4900891.*  
  
*Y. Ding and J. Mittal, “Equilibrium and nonequilibrium dynamics of soft sphere fluids”, Soft Matter, vol. 11, no. 26. Royal Society of Chemistry (RSC), pp. 5274–5281, 2015. doi: 10.1039/c5sm00637f.*  
  
*T. V. Galassi, “An optical nanoreporter of endolysosomal lipid accumulation reveals enduring effects of diet on hepatic macrophages in vivo”, Science Translational Medicine, vol. 10, no. 461. American Association for the Advancement of Science (AAAS), Oct. 03, 2018. doi: 10.1126/scitranslmed.aar2680.*  
  
*J. D. Harvey, “A carbon nanotube reporter of microRNA hybridization events in vivo”, Nature Biomedical Engineering, vol. 1, no. 4. Springer Science and Business Media LLC, Mar. 13, 2017. doi: 10.1038/s41551-017-0041.*  
  
*J. D. Harvey, G. H. Zerze, K. M. Tully, J. Mittaland D. A. Heller, “Electrostatic Screening Modulates Analyte Binding and Emission of Carbon Nanotubes”, The Journal of Physical Chemistry C, vol. 122, no. 19. American Chemical Society (ACS), pp. 10592–10599, May 07, 2018. doi: 10.1021/acs.jpcc.8b01239.*  
  
*H. W. Hatch, J. Mittaland V. K. Shen, “Computational study of trimer self-assembly and fluid phase behavior”, The Journal of Chemical Physics, vol. 142, no. 16. AIP Publishing, p. 164901, Apr. 28, 2015. doi: 10.1063/1.4918557.*  
  
*H. W. Hatch, S.-Y. Yang, J. Mittaland V. K. Shen, “Self-assembly of trimer colloids: effect of shape and interaction range”, Soft Matter, vol. 12, no. 18. Royal Society of Chemistry (RSC), pp. 4170–4179, 2016. doi: 10.1039/c6sm00473c.*  
  
*A. M. Janke, “Lysines in the RNA Polymerase II C-Terminal Domain Contribute to TAF15 Fibril Recruitment”, Biochemistry, vol. 57, no. 17. American Chemical Society (ACS), pp. 2549–2563, Sep. 25, 2017. doi: 10.1021/acs.biochem.7b00310.*  
  
*Y. C. Kim, A. Bhattacharyaand J. Mittal, “Macromolecular Crowding Effects on Coupled Folding and Binding”, The Journal of Physical Chemistry B, vol. 118, no. 44. American Chemical Society (ACS), pp. 12621–12629, Oct. 23, 2014. doi: 10.1021/jp508046y.*  
  
*N. A. Mahynski, R. Mao, E. Pretti, V. K. Shenand J. Mittal, “Grand canonical inverse design of multicomponent colloidal crystals”, Soft Matter, vol. 16, no. 13. Royal Society of Chemistry (RSC), pp. 3187–3194, 2020. doi: 10.1039/c9sm02426c.*  
  
*N. A. Mahynski, E. Pretti, V. K. Shenand J. Mittal, “Using symmetry to elucidate the importance of stoichiometry in colloidal crystal assembly”, Nature Communications, vol. 10, no. 1. Springer Science and Business Media LLC, May 02, 2019. doi: 10.1038/s41467-019-10031-4.*  
  
*N. A. Mahynski, H. Zerze, H. W. Hatch, V. K. Shenand J. Mittal, “Assembly of multi-flavored two-dimensional colloidal crystals”, Soft Matter, vol. 13, no. 32. Royal Society of Chemistry (RSC), pp. 5397–5408, 2017. doi: 10.1039/c7sm01005b.*  
  
*T. A. Maula, H. W. Hatch, V. K. Shen, S. Rangarajanand J. Mittal, “Designing molecular building blocks for the self-assembly of complex porous networks”, Molecular Systems Design & Engineering, vol. 4, no. 3. Royal Society of Chemistry (RSC), pp. 644–653, 2019. doi: 10.1039/c9me00006b.*  
  
*C. M. Miller, A. C. Brownand J. Mittal, “Disorder in Cholesterol-Binding Functionality of CRAC Peptides: A Molecular Dynamics Study”, The Journal of Physical Chemistry B, vol. 118, no. 46. American Chemical Society (ACS), pp. 13169–13174, Nov. 10, 2014. doi: 10.1021/jp5106423.*  
  
*C. M. Miller, Y. C. Kimand J. Mittal, “Protein Composition Determines the Effect of Crowding on the Properties of Disordered Proteins”, Biophysical Journal, vol. 111, no. 1. Elsevier BV, pp. 28–37, Jul. 2016. doi: 10.1016/j.bpj.2016.05.033.*  
  
*Z. Monahan, “Phosphorylation of the FUS low‐complexity domain disrupts phase separation, aggregation, and toxicity”, The EMBO Journal, vol. 36, no. 20. EMBO, pp. 2951–2967, Aug. 08, 2017. doi: 10.15252/embj.201696394.*  
  
*I. Moskowitz, M. A. Snyderand J. Mittal, “Water transport through functionalized nanotubes with tunable hydrophobicity”, The Journal of Chemical Physics, vol. 141, no. 18. AIP Publishing, pp. 18C532, Nov. 14, 2014. doi: 10.1063/1.4897974.*  
  
*A. C. Murthy, “Molecular interactions underlying liquid−liquid phase separation of the FUS low-complexity domain”, Nature Structural & Molecular Biology, vol. 26, no. 7. Springer Science and Business Media LLC, pp. 637–648, Jul. 2019. doi: 10.1038/s41594-019-0250-x.*  
  
*E. Pretti, R. Maoand J. Mittal, “Modelling and simulation of DNA-mediated self-assembly for superlattice design”, Molecular Simulation, vol. 45, no. 14–15. Informa UK Limited, pp. 1203–1210, May 02, 2019. doi: 10.1080/08927022.2019.1610951.*  
  
*E. Pretti and J. Mittal, “Extension of the Einstein molecule method for solid free energy calculation to non-periodic and semi-periodic systems”, The Journal of Chemical Physics, vol. 151, no. 5. AIP Publishing, p. 054105, Aug. 07, 2019. doi: 10.1063/1.5100960.*  
  
*E. Pretti, V. K. Shen, J. Mittaland N. A. Mahynski, “Symmetry-Based Crystal Structure Enumeration in Two Dimensions”, The Journal of Physical Chemistry A, vol. 124, no. 16. American Chemical Society (ACS), pp. 3276–3285, Mar. 16, 2020. doi: 10.1021/acs.jpca.0c00846.*  
  
*E. Pretti, “Assembly of three-dimensional binary superlattices from multi-flavored particles”, Soft Matter, vol. 14, no. 30. Royal Society of Chemistry (RSC), pp. 6303–6312, 2018. doi: 10.1039/c8sm00989a.*  
  
*E. Pretti, H. Zerze, M. Song, Y. Ding, R. Maoand J. Mittal, “Size-dependent thermodynamic structural selection in colloidal crystallization”, Science Advances, vol. 5, no. 9. American Association for the Advancement of Science (AAAS), Sep. 06, 2019. doi: 10.1126/sciadv.aaw5912.*  
  
*L. Rani, J. Mittaland S. S. Mallajosyula, “Effect of Phosphorylation and O-GlcNAcylation on Proline-Rich Domains of Tau”, The Journal of Physical Chemistry B, vol. 124, no. 10. American Chemical Society (ACS), pp. 1909–1918, Feb. 17, 2020. doi: 10.1021/acs.jpcb.9b11720.*  
  
*V. H. Ryan, “Mechanistic View of hnRNPA2 Low-Complexity Domain Structure, Interactions, and Phase Separation Altered by Mutation and Arginine Methylation”, Molecular Cell, vol. 69, no. 3. Elsevier BV, pp. 465–479.e7, Feb. 2018. doi: 10.1016/j.molcel.2017.12.022.*  
  
*T. Sanyal, J. Mittaland M. S. Shell, “A hybrid, bottom-up, structurally accurate, Go¯-like coarse-grained protein model”, The Journal of Chemical Physics, vol. 151, no. 4. AIP Publishing, p. 044111, Jul. 28, 2019. doi: 10.1063/1.5108761.*  
  
*B. S. Schuster, “Identifying Sequence Perturbations to an Intrinsically Disordered Protein that Determine Its Phase Separation Behavior”, []. Cold Spring Harbor Laboratory, Jan. 06, 2020. doi: 10.1101/2020.01.06.894576.*  
  
*B. S. Schuster, “Identifying sequence perturbations to an intrinsically disordered protein that determine its phase-separation behavior”, Proceedings of the National Academy of Sciences, vol. 117, no. 21. Proceedings of the National Academy of Sciences, pp. 11421–11431, May 11, 2020. doi: 10.1073/pnas.2000223117.*  
  
*A. Shankar, A. Jagotaand J. Mittal, “DNA Base Dimers Are Stabilized by Hydrogen-Bonding Interactions Including Non-Watson–Crick Pairing Near Graphite Surfaces”, The Journal of Physical Chemistry B, vol. 116, no. 40. American Chemical Society (ACS), pp. 12088–12094, Sep. 26, 2012. doi: 10.1021/jp304260t.*  
  
*M. Song, Y. Ding, H. Zerze, M. A. Snyderand J. Mittal, “Binary Superlattice Design by Controlling DNA-Mediated Interactions”, Langmuir, vol. 34, no. 3. American Chemical Society (ACS), pp. 991–998, Nov. 20, 2017. doi: 10.1021/acs.langmuir.7b02835.*  
  
*M. Song, M. A. Snyderand J. Mittal, “Effect of molecular structure on fluid transport through carbon nanotubes”, Molecular Physics, vol. 112, no. 20. Informa UK Limited, pp. 2658–2664, Apr. 03, 2014. doi: 10.1080/00268976.2014.903578.*  
  
*R. Wuttke, “Temperature-dependent solvation modulates the dimensions of disordered proteins”, Proceedings of the National Academy of Sciences, vol. 111, no. 14. Proceedings of the National Academy of Sciences, pp. 5213–5218, Mar. 21, 2014. doi: 10.1073/pnas.1313006111.*  
  
*G. H. Zerze, R. B. Bestand J. Mittal, “Modest Influence of FRET Chromophores on the Properties of Unfolded Proteins”, Biophysical Journal, vol. 107, no. 7. Elsevier BV, pp. 1654–1660, Oct. 2014. doi: 10.1016/j.bpj.2014.07.071.*  
  
*G. H. Zerze, R. B. Bestand J. Mittal, “Sequence- and Temperature-Dependent Properties of Unfolded and Disordered Proteins from Atomistic Simulations”, The Journal of Physical Chemistry B, vol. 119, no. 46. American Chemical Society (ACS), pp. 14622–14630, Nov. 10, 2015. doi: 10.1021/acs.jpcb.5b08619.*  
  
*G. H. Zerze, C. M. Miller, D. Granataand J. Mittal, “Free Energy Surface of an Intrinsically Disordered Protein: Comparison between Temperature Replica Exchange Molecular Dynamics and Bias-Exchange Metadynamics”, Journal of Chemical Theory and Computation, vol. 11, no. 6. American Chemical Society (ACS), pp. 2776–2782, May 12, 2015. doi: 10.1021/acs.jctc.5b00047.*  
  
*G. H. Zerze and J. Mittal, “Effect of O-Linked Glycosylation on the Equilibrium Structural Ensemble of Intrinsically Disordered Polypeptides”, The Journal of Physical Chemistry B, vol. 119, no. 51. American Chemical Society (ACS), pp. 15583–15592, Dec. 15, 2015. doi: 10.1021/acs.jpcb.5b10022.*  
  
*G. H. Zerze, J. Mittaland R. B. Best, “Diffusive Dynamics of Contact Formation in Disordered Polypeptides”, Physical Review Letters, vol. 116, no. 6. American Physical Society (APS), Feb. 11, 2016. doi: 10.1103/physrevlett.116.068102.*  
  
*G. H. Zerze, B. Uzand J. Mittal, “Folding thermodynamics ofβ-hairpins studied by replica-exchange molecular dynamics simulations”, Proteins: Structure, Function, and Bioinformatics, vol. 83, no. 7. Wiley, pp. 1307–1315, May 29, 2015. doi: 10.1002/prot.24827.*  
  
*G. H. Zerze, W. Zheng, R. B. Bestand J. Mittal, “Evolution of All-Atom Protein Force Fields to Improve Local and Global Properties”, The Journal of Physical Chemistry Letters, vol. 10, no. 9. American Chemical Society (ACS), pp. 2227–2234, Apr. 16, 2019. doi: 10.1021/acs.jpclett.9b00850.*  
  
*W. Zheng, G. Dignon, M. Brown, Y. C. Kimand J. Mittal, “Hydropathy Patterning Complements Charge Patterning to Describe Conformational Preferences of Disordered Proteins”, The Journal of Physical Chemistry Letters, vol. 11, no. 9. American Chemical Society (ACS), pp. 3408–3415, Mar. 31, 2020. doi: 10.1021/acs.jpclett.0c00288.*  
  
*W. Zheng, G. H. Zerze, A. Borgia, J. Mittal, B. Schulerand R. B. Best, “Inferring properties of disordered chains from FRET transfer efficiencies”, The Journal of Chemical Physics, vol. 148, no. 12. AIP Publishing, p. 123329, Mar. 28, 2018. doi: 10.1063/1.5006954.*  
  
*M. R. Ali, R. Latif, T. F. Daviesand M. Mezei, “Monte Carlo loop refinement and virtual screening of the thyroid-stimulating hormone receptor transmembrane domain”, Journal of Biomolecular Structure and Dynamics, vol. 33, no. 5. Informa UK Limited, pp. 1140–1152, Jul. 11, 2014. doi: 10.1080/07391102.2014.932310.*  
  
*R. Ali, Y. Beasley, T. Skazko, M. Sadoqiand M. Mezei, “Molecular Dynamics and Docking Studies on Neurotensin Receptor”, Biophysical Journal, vol. 112, no. 3. Elsevier BV, p. 352a, Feb. 2017. doi: 10.1016/j.bpj.2016.11.1907.*  
  
*R. Ali, M. Sadoqi, S. Moller, A. Boutajangoutand M. Mezei, “Molecular Dynamics and Docking Studies on Acetylcholinesterase (AChE) Inhibitors”, Biophysical Journal, vol. 114, no. 3. Elsevier BV, p. 340a, Feb. 2018. doi: 10.1016/j.bpj.2017.11.1899.*  
  
*R. Latif, M. R. Ali, M. Mezeiand T. F. Davies, “Transmembrane Domains of Attraction on the TSH Receptor”, Endocrinology, vol. 156, no. 2. The Endocrine Society, pp. 488–498, Nov. 19, 2014. doi: 10.1210/en.2014-1509.*  
  
*W. Zheng, M. A. Rohrdanzand C. Clementi, “Rapid Exploration of Configuration Space with Diffusion-Map-Directed Molecular Dynamics”, The Journal of Physical Chemistry B, vol. 117, no. 42. American Chemical Society (ACS), pp. 12769–12776, Aug. 07, 2013. doi: 10.1021/jp401911h.*  
  
*J. Franco, “A structural comparative approach to identifying novel antimalarial inhibitors”, Computational Biology and Chemistry, vol. 45. Elsevier BV, pp. 42–47, Aug. 2013. doi: 10.1016/j.compbiolchem.2013.04.002.*  
  
*C. Wilsey, J. Gurka, D. Tothand J. Franco, “A large scale virtual screen of DprE1”, Computational Biology and Chemistry, vol. 47. Elsevier BV, pp. 121–125, Dec. 2013. doi: 10.1016/j.compbiolchem.2013.08.006.*  
  
*M. Chaibva, “Acetylation within the First 17 Residues of Huntingtin Exon 1 Alters Aggregation and Lipid Binding”, Biophysical Journal, vol. 111, no. 2. Elsevier BV, pp. 349–362, Jul. 2016. doi: 10.1016/j.bpj.2016.06.018.*  
  
*G. S. Custer, P. Dasand S. Matysiak, “Interplay between Conformational Heterogeneity and Hydration in the Folding Landscape of a Designed Three-Helix Bundle”, The Journal of Physical Chemistry B, vol. 121, no. 13. American Chemical Society (ACS), pp. 2731–2738, Mar. 23, 2017. doi: 10.1021/acs.jpcb.6b12286.*  
  
*S. J. Ganesan and S. Matysiak, “Role of Backbone Dipole Interactions in the Formation of Secondary and Supersecondary Structures of Proteins”, Journal of Chemical Theory and Computation, vol. 10, no. 6. American Chemical Society (ACS), pp. 2569–2576, May 21, 2014. doi: 10.1021/ct401087a.*  
  
*S. J. Ganesan and S. Matysiak, “Interplay between the hydrophobic effect and dipole interactions in peptide aggregation at interfaces”, Physical Chemistry Chemical Physics, vol. 18, no. 4. Royal Society of Chemistry (RSC), pp. 2449–2458, 2016. doi: 10.1039/c5cp05867h.*  
  
*S. J. Ganesan, H. Xuand S. Matysiak, “Influence of Monovalent Cation Size on Nanodomain Formation in Anionic–Zwitterionic Mixed Bilayers”, The Journal of Physical Chemistry B, vol. 121, no. 4. American Chemical Society (ACS), pp. 787–799, Jan. 18, 2017. doi: 10.1021/acs.jpcb.6b10099.*  
  
*M. McCutchen, L. G. Chen, H. Bermudezand S. Matysiak, “Interplay of Dynamical Properties between Ionic Liquids and Ionic Surfactants: Mechanism and Aggregation”, The Journal of Physical Chemistry B, vol. 119, no. 30. American Chemical Society (ACS), pp. 9925–9932, Jul. 10, 2015. doi: 10.1021/acs.jpcb.5b05151.*  
  
*A. Nagarajan, S. Jawaheryand S. Matysiak, “The Effects of Flanking Sequences in the Interaction of Polyglutamine Peptides with a Membrane Bilayer”, The Journal of Physical Chemistry B, vol. 118, no. 24. American Chemical Society (ACS), pp. 6368–6379, Jan. 06, 2014. doi: 10.1021/jp407900c.*  
  
*A. Nagarajan, C. Junghansand S. Matysiak, “Multiscale Simulation of Liquid Water Using a Four-to-One Mapping for Coarse-Graining”, Journal of Chemical Theory and Computation, vol. 9, no. 11. American Chemical Society (ACS), pp. 5168–5175, Oct. 24, 2013. doi: 10.1021/ct400566j.*  
  
*L. Zhang and M. Buck, “Molecular Simulations of a Dynamic Protein Complex: Role of Salt-Bridges and Polar Interactions in Configurational Transitions”, Biophysical Journal, vol. 105, no. 10. Elsevier BV, pp. 2412–2417, Nov. 2013. doi: 10.1016/j.bpj.2013.09.052.*  
  
*L. Zhang and M. Buck, “Molecular Dynamics Simulations Reveal Isoform Specific Contact Dynamics between the Plexin Rho GTPase Binding Domain (RBD) and Small Rho GTPases Rac1 and Rnd1”, The Journal of Physical Chemistry B, vol. 121, no. 7. American Chemical Society (ACS), pp. 1485–1498, Feb. 08, 2017. doi: 10.1021/acs.jpcb.6b11022.*  
  
*L. Zhang, T. Centaand M. Buck, “Structure and Dynamics Analysis on Plexin-B1 Rho GTPase Binding Domain as a Monomer and Dimer”, The Journal of Physical Chemistry B, vol. 118, no. 26. American Chemical Society (ACS), pp. 7302–7311, Jun. 25, 2014. doi: 10.1021/jp503668k.*  
  
*P. J. Fleming, “BamA POTRA Domain Interacts with a Native Lipid Membrane Surface”, Biophysical Journal, vol. 110, no. 12. Elsevier BV, pp. 2698–2709, Jun. 2016. doi: 10.1016/j.bpj.2016.05.010.*  
  
*D. Winogradoff, I. Echeverria, D. A. Potoyanand G. A. Papoian, “The Acetylation Landscape of the H4 Histone Tail: Disentangling the Interplay between the Specific and Cumulative Effects”, Journal of the American Chemical Society, vol. 137, no. 19. American Chemical Society (ACS), pp. 6245–6253, May 08, 2015. doi: 10.1021/jacs.5b00235.*  
  
*J. L. MacCallum, A. Perezand K. A. Dill, “Determining protein structures by combining semireliable data with atomistic physical models by Bayesian inference”, Proceedings of the National Academy of Sciences, vol. 112, no. 22. Proceedings of the National Academy of Sciences, pp. 6985–6990, May 18, 2015. doi: 10.1073/pnas.1506788112.*  
  
*A. Perez, J. L. MacCallum, E. Brini, C. Simmerlingand K. A. Dill, “Grid-Based Backbone Correction to the ff12SB Protein Force Field for Implicit-Solvent Simulations”, Journal of Chemical Theory and Computation, vol. 11, no. 10. American Chemical Society (ACS), pp. 4770–4779, Sep. 17, 2015. doi: 10.1021/acs.jctc.5b00662.*  
  
*A. Perez, J. L. MacCallum, E. A. Coutsiasand K. A. Dill, “Constraint methods that accelerate free-energy simulations of biomolecules”, The Journal of Chemical Physics, vol. 143, no. 24. AIP Publishing, p. 243143, Dec. 28, 2015. doi: 10.1063/1.4936911.*  
  
*A. Perez, J. L. MacCallumand K. A. Dill, “Accelerating molecular simulations of proteins using Bayesian inference on weak information”, Proceedings of the National Academy of Sciences, vol. 112, no. 38. Proceedings of the National Academy of Sciences, pp. 11846–11851, Sep. 08, 2015. doi: 10.1073/pnas.1515561112.*  
  
*A. Perez, J. A. Morrone, C. Simmerlingand K. A. Dill, “Advances in free-energy-based simulations of protein folding and ligand binding”, Current Opinion in Structural Biology, vol. 36. Elsevier BV, pp. 25–31, Feb. 2016. doi: 10.1016/j.sbi.2015.12.002.*  
  
*E.-H. Yap, T. Rosche, S. Almoand A. Fiser, “Functional Clustering of Immunoglobulin Superfamily Proteins with Protein–Protein Interaction Information Calibrated Hidden Markov Model Sequence Profiles”, Journal of Molecular Biology, vol. 426, no. 4. Elsevier BV, pp. 945–961, Feb. 2014. doi: 10.1016/j.jmb.2013.11.009.*  
  
*J. M. Dybas and A. Fiser, “Development of a motif-based topology-independent structure comparison method to identify evolutionarily related folds”, Proteins: Structure, Function, and Bioinformatics, vol. 84, no. 12. Wiley, pp. 1859–1874, Oct. 11, 2016. doi: 10.1002/prot.25169.*  
  
*E.-H. Yap and A. Fiser, “ProtLID, a Residue-Based Pharmacophore Approach to Identify Cognate Protein Ligands in the Immunoglobulin Superfamily”, Structure, vol. 24, no. 12. Elsevier BV, pp. 2217–2226, Dec. 2016. doi: 10.1016/j.str.2016.10.012.*  
  
*V. Ngo, D. Stefanovski, S. Haasand R. A. Farley, “Non-Equilibrium Dynamics Contribute to Ion Selectivity in the KcsA Channel”, PLoS ONE, vol. 9, no. 1. Public Library of Science (PLoS), p. e86079, Jan. 17, 2014. doi: 10.1371/journal.pone.0086079.*  
  
*J. L. Bingaman, S. Zhang, D. R. Stevens, N. H. Yennawar, S. Hammes-Schifferand P. C. Bevilacqua, “The GlcN6P cofactor plays multiple catalytic roles in the glmS ribozyme”, Nature Chemical Biology, vol. 13, no. 4. Springer Science and Business Media LLC, pp. 439–445, Feb. 13, 2017. doi: 10.1038/nchembio.2300.*  
  
*A. Ganguly, P. Thaplyal, E. Rosta, P. C. Bevilacquaand S. Hammes-Schiffer, “Quantum Mechanical/Molecular Mechanical Free Energy Simulations of the Self-Cleavage Reaction in the Hepatitis Delta Virus Ribozyme”, Journal of the American Chemical Society, vol. 136, no. 4. American Chemical Society (ACS), pp. 1483–1496, Jan. 15, 2014. doi: 10.1021/ja4104217.*  
  
*J. J. Goings and S. Hammes-Schiffer, “Early Photocycle of Slr1694 Blue-Light Using Flavin Photoreceptor Unraveled through Adiabatic Excited-State Quantum Mechanical/Molecular Mechanical Dynamics”, Journal of the American Chemical Society, vol. 141, no. 51. American Chemical Society (ACS), pp. 20470–20479, Nov. 19, 2019. doi: 10.1021/jacs.9b11196.*  
  
*M. Horitani, “13C ENDOR Spectroscopy of Lipoxygenase–Substrate Complexes Reveals the Structural Basis for C–H Activation by Tunneling”, Journal of the American Chemical Society, vol. 139, no. 5. American Chemical Society (ACS), pp. 1984–1997, Jan. 25, 2017. doi: 10.1021/jacs.6b11856.*  
  
*S. Hu, A. V. Soudackov, S. Hammes-Schifferand J. P. Klinman, “Enhanced Rigidification within a Double Mutant of Soybean Lipoxygenase Provides Experimental Support for Vibronically Nonadiabatic Proton-Coupled Electron Transfer Models”, ACS Catalysis, vol. 7, no. 5. American Chemical Society (ACS), pp. 3569–3574, Apr. 20, 2017. doi: 10.1021/acscatal.7b00688.*  
  
*P. Li and S. Hammes-Schiffer, “Substrate-to-Product Conversion Facilitates Active Site Loop Opening in Yeast Enolase: A Molecular Dynamics Study”, ACS Catalysis, vol. 9, no. 10. American Chemical Society (ACS), pp. 8985–8990, Aug. 27, 2019. doi: 10.1021/acscatal.9b03249.*  
  
*P. Li, A. Rangadurai, H. M. Al-Hashimiand S. Hammes-Schiffer, “Environmental Effects on Guanine-Thymine Mispair Tautomerization Explored with Quantum Mechanical/Molecular Mechanical Free Energy Simulations”, Journal of the American Chemical Society, vol. 142, no. 25. American Chemical Society (ACS), pp. 11183–11191, May 27, 2020. doi: 10.1021/jacs.0c03774.*  
  
*P. Li, A. V. Soudackovand S. Hammes-Schiffer, “Impact of Mutations on the Binding Pocket of Soybean Lipoxygenase: Implications for Proton-Coupled Electron Transfer”, The Journal of Physical Chemistry Letters, vol. 9, no. 22. American Chemical Society (ACS), pp. 6444–6449, Oct. 25, 2018. doi: 10.1021/acs.jpclett.8b02945.*  
  
*P. Li, A. V. Soudackovand S. Hammes-Schiffer, “Fundamental Insights into Proton-Coupled Electron Transfer in Soybean Lipoxygenase from Quantum Mechanical/Molecular Mechanical Free Energy Simulations”, Journal of the American Chemical Society, vol. 140, no. 8. American Chemical Society (ACS), pp. 3068–3076, Feb. 19, 2018. doi: 10.1021/jacs.7b13642.*  
  
*P. Li, A. V. Soudackov, B. Koronkiewicz, J. M. Mayerand S. Hammes-Schiffer, “Theoretical Study of Shallow Distance Dependence of Proton-Coupled Electron Transfer in Oligoproline Peptides”, Journal of the American Chemical Society, vol. 142, no. 32. American Chemical Society (ACS), pp. 13795–13804, Jul. 15, 2020. doi: 10.1021/jacs.0c04716.*  
  
*E. R. Sayfutyarova, J. J. Goingsand S. Hammes-Schiffer, “Electron-Coupled Double Proton Transfer in the Slr1694 BLUF Photoreceptor: A Multireference Electronic Structure Study”, The Journal of Physical Chemistry B, vol. 123, no. 2. American Chemical Society (ACS), pp. 439–447, Dec. 19, 2018. doi: 10.1021/acs.jpcb.8b10973.*  
  
*E. R. Sayfutyarova and S. Hammes-Schiffer, “Constructing Molecular π-Orbital Active Spaces for Multireference Calculations of Conjugated Systems”, Journal of Chemical Theory and Computation, vol. 15, no. 3. American Chemical Society (ACS), pp. 1679–1689, Jan. 28, 2019. doi: 10.1021/acs.jctc.8b01196.*  
  
*E. R. Sayfutyarova and S. Hammes-Schiffer, “Substituent Effects on Photochemistry of Anthracene–Phenol–Pyridine Triads Revealed by Multireference Calculations”, Journal of the American Chemical Society, vol. 142, no. 1. American Chemical Society (ACS), pp. 487–494, Dec. 17, 2019. doi: 10.1021/jacs.9b11425.*  
  
*E. R. Sayfutyarova and S. Hammes-Schiffer, “Excited State Molecular Dynamics of Photoinduced Proton-Coupled Electron Transfer in Anthracene–Phenol–Pyridine Triads”, The Journal of Physical Chemistry Letters, vol. 11, no. 17. American Chemical Society (ACS), pp. 7109–7115, Aug. 05, 2020. doi: 10.1021/acs.jpclett.0c02012.*  
  
*D. R. Stevens and S. Hammes-Schiffer, “Exploring the Role of the Third Active Site Metal Ion in DNA Polymerase η with QM/MM Free Energy Simulations”, Journal of the American Chemical Society, vol. 140, no. 28. American Chemical Society (ACS), pp. 8965–8969, Jun. 22, 2018. doi: 10.1021/jacs.8b05177.*  
  
*D. R. Stevens and S. Hammes-Schiffer, “Examining the Mechanism of Phosphite Dehydrogenase with Quantum Mechanical/Molecular Mechanical Free Energy Simulations”, Biochemistry, vol. 59, no. 8. American Chemical Society (ACS), pp. 943–954, Feb. 07, 2020. doi: 10.1021/acs.biochem.9b01089.*  
  
*P. Thaplyal, A. Ganguly, S. Hammes-Schifferand P. C. Bevilacqua, “Inverse Thio Effects in the Hepatitis Delta Virus Ribozyme Reveal that the Reaction Pathway Is Controlled by Metal Ion Charge Density”, Biochemistry, vol. 54, no. 12. American Chemical Society (ACS), pp. 2160–2175, Mar. 23, 2015. doi: 10.1021/acs.biochem.5b00190.*  
  
*M. N. Ucisik, P. C. Bevilacquaand S. Hammes-Schiffer, “Molecular Dynamics Study of Twister Ribozyme: Role of Mg2+ Ions and the Hydrogen-Bonding Network in the Active Site”, Biochemistry, vol. 55, no. 27. American Chemical Society (ACS), pp. 3834–3846, Jun. 27, 2016. doi: 10.1021/acs.biochem.6b00203.*  
  
*M. N. Ucisik and S. Hammes-Schiffer, “Comparative Molecular Dynamics Studies of Human DNA Polymerase η”, Journal of Chemical Information and Modeling, vol. 55, no. 12. American Chemical Society (ACS), pp. 2672–2681, Nov. 20, 2015. doi: 10.1021/acs.jcim.5b00606.*  
  
*M. N. Ucisik and S. Hammes-Schiffer, “Relative Binding Free Energies of Adenine and Guanine to Damaged and Undamaged DNA in Human DNA Polymerase η: Clues for Fidelity and Overall Efficiency”, Journal of the American Chemical Society, vol. 137, no. 41. American Chemical Society (ACS), pp. 13240–13243, Oct. 12, 2015. doi: 10.1021/jacs.5b08451.*  
  
*M. N. Ucisik and S. Hammes-Schiffer, “Effects of Active Site Mutations on Specificity of Nucleobase Binding in Human DNA Polymerase η”, The Journal of Physical Chemistry B, vol. 121, no. 15. American Chemical Society (ACS), pp. 3667–3675, Nov. 23, 2016. doi: 10.1021/acs.jpcb.6b09973.*  
  
*S. Zhang, A. Ganguly, P. Goyal, J. L. Bingaman, P. C. Bevilacquaand S. Hammes-Schiffer, “Role of the Active Site Guanine in the glmS Ribozyme Self-Cleavage Mechanism: Quantum Mechanical/Molecular Mechanical Free Energy Simulations”, Journal of the American Chemical Society, vol. 137, no. 2. American Chemical Society (ACS), pp. 784–798, Jan. 12, 2015. doi: 10.1021/ja510387y.*  
  
*S. Zhang, D. R. Stevens, P. Goyal, J. L. Bingaman, P. C. Bevilacquaand S. Hammes-Schiffer, “Assessing the Potential Effects of Active Site Mg2+ Ions in the glmS Ribozyme–Cofactor Complex”, The Journal of Physical Chemistry Letters, vol. 7, no. 19. American Chemical Society (ACS), pp. 3984–3988, Sep. 28, 2016. doi: 10.1021/acs.jpclett.6b01854.*  
  
*S. Sim, P. Wang, B. N. Beyer, K. J. Cutrona, M. L. Radhakrishnanand D. E. Elmore, “Investigating the nucleic acid interactions of histone‐derived antimicrobial peptides”, FEBS Letters, vol. 591, no. 5. Wiley, pp. 706–717, Mar. 2017. doi: 10.1002/1873-3468.12574.*  
  
*K.-Y. M. Chen, J. Sun, J. S. Salvo, D. Bakerand P. Barth, “High-Resolution Modeling of Transmembrane Helical Protein Structures from Distant Homologues”, PLoS Computational Biology, vol. 10, no. 5. Public Library of Science (PLoS), p. e1003636, May 22, 2014. doi: 10.1371/journal.pcbi.1003636.*  
  
*R. A. Aglietti, S. N. Floor, C. L. McClendon, M. P. Jacobsonand J. D. Gross, “Active Site Conformational Dynamics Are Coupled to Catalysis in the mRNA Decapping Enzyme Dcp2”, Structure, vol. 21, no. 9. Elsevier BV, pp. 1571–1580, Sep. 2013. doi: 10.1016/j.str.2013.06.021.*  
  
*L. X. Peng, M. T. Hsu, M. Bonomi, D. A. Agardand M. P. Jacobson, “The Free Energy Profile of Tubulin Straight-Bent Conformational Changes, with Implications for Microtubule Assembly and Drug Discovery”, PLoS Computational Biology, vol. 10, no. 2. Public Library of Science (PLoS), p. e1003464, Feb. 06, 2014. doi: 10.1371/journal.pcbi.1003464.*  
  
*C. L. McClendon, L. Hua, G. Barreiroand M. P. Jacobson, “Comparing Conformational Ensembles Using the Kullback–Leibler Divergence Expansion”, Journal of Chemical Theory and Computation, vol. 8, no. 6. American Chemical Society (ACS), pp. 2115–2126, May 02, 2012. doi: 10.1021/ct300008d.*  
  
*A. Narayanan, L. L. LeClaire, D. L. Barberand M. P. Jacobson, “Phosphorylation of the Arp2 Subunit Relieves Auto-inhibitory Interactions for Arp2/3 Complex Activation”, PLoS Computational Biology, vol. 7, no. 11. Public Library of Science (PLoS), p. e1002226, Nov. 10, 2011. doi: 10.1371/journal.pcbi.1002226.*  
  
*J. D. Sadowsky, M. A. Burlingame, D. W. Wolan, C. L. McClendon, M. P. Jacobsonand J. A. Wells, “Turning a protein kinase on or off from a single allosteric site via disulfide trapping”, Proceedings of the National Academy of Sciences, vol. 108, no. 15. Proceedings of the National Academy of Sciences, pp. 6056–6061, Mar. 23, 2011. doi: 10.1073/pnas.1102376108.*  
  
*M. Chen, “Experimental and Modeling Studies of an Unusual Water-Filled Pore Structure with Possible Mechanistic Implications in Family 48 Cellulases”, The Journal of Physical Chemistry B, vol. 118, no. 9. American Chemical Society (ACS), pp. 2306–2315, Feb. 19, 2014. doi: 10.1021/jp408767j.*  
  
*K. A. Allison, M. U. Kaikkonen, T. Gaasterlandand C. K. Glass, “Vespucci: a system for building annotated databases of nascent transcripts”, Nucleic Acids Research, vol. 42, no. 4. Oxford University Press (OUP), pp. 2433–2447, Dec. 04, 2013. doi: 10.1093/nar/gkt1237.*  
  
*J. C. Davis-Turak, “Considering the kinetics of mRNA synthesis in the analysis of the genome and epigenome reveals determinants of co-transcriptional splicing”, Nucleic Acids Research, vol. 43, no. 2. Oxford University Press (OUP), pp. 699–707, Dec. 24, 2014. doi: 10.1093/nar/gku1338.*  
  
*S. Heinz, “Effect of natural genetic variation on enhancer selection and function”, Nature, vol. 503, no. 7477. Springer Science and Business Media LLC, pp. 487–492, Oct. 13, 2013. doi: 10.1038/nature12615.*  
  
*M. U. Kaikkonen, “Remodeling of the Enhancer Landscape during Macrophage Activation Is Coupled to Enhancer Transcription”, Molecular Cell, vol. 51, no. 3. Elsevier BV, pp. 310–325, Aug. 2013. doi: 10.1016/j.molcel.2013.07.010.*  
  
*P. D. Blood, S. Marcusand M. C. Schatz, “Large-scale Sequencing and Assembly of Cereal Genomes Using Blacklight”, Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616502.*  
  
*N. B. O’Hara, “Metagenomic characterization of ambulances across the USA”, Microbiome, vol. 5, no. 1. Springer Science and Business Media LLC, Sep. 22, 2017. doi: 10.1186/s40168-017-0339-6.*  
  
*W. Xu, Z. Lai, R. J. Oliveira, V. B. P. Leiteand J. Wang, “Configuration-Dependent Diffusion Dynamics of Downhill and Two-State Protein Folding”, The Journal of Physical Chemistry B, vol. 116, no. 17. American Chemical Society (ACS), pp. 5152–5159, Apr. 20, 2012. doi: 10.1021/jp212132v.*  
  
*J.-X. Yue, J.-K. Yu, N. H. Putnamand L. Z. Holland, “The Transcriptome of an Amphioxus, Asymmetron lucayanum, from the Bahamas: A Window into Chordate Evolution”, Genome Biology and Evolution, vol. 6, no. 10. Oxford University Press (OUP), pp. 2681–2696, Sep. 19, 2014. doi: 10.1093/gbe/evu212.*  
  
*B. C. Davis and I. F. Thorpe, “Molecular Simulations Illuminate the Role of Regulatory Components of the RNA Polymerase from the Hepatitis C Virus in Influencing Protein Structure and Dynamics”, Biochemistry, vol. 52, no. 26. American Chemical Society (ACS), pp. 4541–4552, Jun. 21, 2013. doi: 10.1021/bi400251g.*  
  
*E. Sesmero and I. Thorpe, “Using the Hepatitis C Virus RNA-Dependent RNA Polymerase as a Model to Understand Viral Polymerase Structure, Function and Dynamics”, Viruses, vol. 7, no. 7. MDPI AG, pp. 3974–3994, Jul. 17, 2015. doi: 10.3390/v7072808.*  
  
*O. Beckstein, S. L. Seyler, A. Kumarand M. F. Thorpe, “Quantifying Macromolecular Conformational Transition Pathways”, Biophysical Journal, vol. 108, no. 2. Elsevier BV, p. 13a, Jan. 2015. doi: 10.1016/j.bpj.2014.11.096.*  
  
*D. L. Dotson, “Recent Structures and Molecular Dynamics Simulations Offer New Perspective on Na+/H+ Antiporters”, Biophysical Journal, vol. 108, no. 2. Elsevier BV, p. 197a, Jan. 2015. doi: 10.1016/j.bpj.2014.11.1086.*  
  
*C. Lee, “A two-domain elevator mechanism for sodium/proton antiport”, Nature, vol. 501, no. 7468. Springer Science and Business Media LLC, pp. 573–577, Sep. 2013. doi: 10.1038/nature12484.*  
  
*C. Y. Cheng, F.-C. Chouand R. Das, “Modeling Complex RNA Tertiary Folds with Rosetta”, Methods in Enzymology. Elsevier, pp. 35–64, 2015. doi: 10.1016/bs.mie.2014.10.051.*  
  
*R. Das, “Atomic-Accuracy Prediction of Protein Loop Structures through an RNA-Inspired Ansatz”, PLoS ONE, vol. 8, no. 10. Public Library of Science (PLoS), p. e74830, Oct. 21, 2013. doi: 10.1371/journal.pone.0074830.*  
  
*J. Lipfert, “Double-stranded RNA under force and torque: Similarities to and striking differences from double-stranded DNA”, Proceedings of the National Academy of Sciences, vol. 111, no. 43. Proceedings of the National Academy of Sciences, pp. 15408–15413, Oct. 13, 2014. doi: 10.1073/pnas.1407197111.*  
  
*P. Sripakdeevong, “Structure determination of noncanonical RNA motifs guided by 1H NMR chemical shifts”, Nature Methods, vol. 11, no. 4. Springer Science and Business Media LLC, pp. 413–416, Mar. 02, 2014. doi: 10.1038/nmeth.2876.*  
  
*F.-C. Chou, J. Lipfertand R. Das, “Blind Predictions of DNA and RNA Tweezers Experiments with Force and Torque”, PLoS Computational Biology, vol. 10, no. 8. Public Library of Science (PLoS), p. e1003756, Aug. 07, 2014. doi: 10.1371/journal.pcbi.1003756.*  
  
*B. Vallat, C. Madrid-Alisteand A. Fiser, “Modularity of Protein Folds as a Tool for Template-Free Modeling of Structures”, PLOS Computational Biology, vol. 11, no. 8. Public Library of Science (PLoS), p. e1004419, Aug. 07, 2015. doi: 10.1371/journal.pcbi.1004419.*  
  
*M. Pujato, F. Kieken, A. A. Skiles, N. Tapinosand A. Fiser, “Prediction of DNA binding motifs from 3D models of transcription factors; identifying TLX3 regulated genes”, Nucleic Acids Research, vol. 42, no. 22. Oxford University Press (OUP), pp. 13500–13512, Nov. 26, 2014. doi: 10.1093/nar/gku1228.*  
  
*C. E. Darris, “Molecular tools to support metabolic and immune function research in the Guinea Fowl (Numida meleagris)”, BMC Genomics, vol. 16, no. 1. Springer Science and Business Media LLC, May 07, 2015. doi: 10.1186/s12864-015-1520-6.*  
  
*D. R. Martin, D. N. LeBardand D. V. Matyushov, “Coulomb Soup of Bioenergetics: Electron Transfer in a Bacterial bc1 Complex”, The Journal of Physical Chemistry Letters, vol. 4, no. 21. American Chemical Society (ACS), pp. 3602–3606, Oct. 14, 2013. doi: 10.1021/jz401910e.*  
  
*X. Wu, A. K. Singh, X. Wu, Y. Lyu, A. K. Bhuniaand G. Narsimhan, “Characterization of antimicrobial activity against Listeria and cytotoxicity of native melittin and its mutant variants”, Colloids and Surfaces B: Biointerfaces, vol. 143. Elsevier BV, pp. 194–205, Jul. 2016. doi: 10.1016/j.colsurfb.2016.03.037.*  
  
*L. Prieto, Y. Heand T. Lazaridis, “Protein Arcs May Form Stable Pores in Lipid Membranes”, Biophysical Journal, vol. 106, no. 1. Elsevier BV, pp. 154–161, Jan. 2014. doi: 10.1016/j.bpj.2013.11.4490.*  
  
*N. Smolin and S. L. Robia, “A Structural Mechanism for Calcium Transporter Headpiece Closure”, The Journal of Physical Chemistry B, vol. 119, no. 4. American Chemical Society (ACS), pp. 1407–1415, Jan. 09, 2015. doi: 10.1021/jp511433v.*  
  
*D. G. Ackerman, F. A. Heberleand G. W. Feigenson, “Limited Perturbation of a DPPC Bilayer by Fluorescent Lipid Probes: A Molecular Dynamics Study”, The Journal of Physical Chemistry B, vol. 117, no. 17. American Chemical Society (ACS), pp. 4844–4852, Apr. 19, 2013. doi: 10.1021/jp400289d.*  
  
*J. K. Holden, “Structure-Based Design of Bacterial Nitric Oxide Synthase Inhibitors”, Journal of Medicinal Chemistry, vol. 58, no. 2. American Chemical Society (ACS), pp. 994–1004, Jan. 06, 2015. doi: 10.1021/jm501723p.*  
  
*Y. Madrona, S. A. Hollingsworth, B. Khanand T. L. Poulos, “P450cin Active Site Water: Implications for Substrate Binding and Solvent Accessibility”, Biochemistry, vol. 52, no. 30. American Chemical Society (ACS), pp. 5039–5050, Jul. 18, 2013. doi: 10.1021/bi4006946.*  
  
*M. H. Cheng, E. Block, F. Hu, M. C. Cobanoglu, A. Sorkinand I. Bahar, “Insights into the Modulation of Dopamine Transporter Function by Amphetamine, Orphenadrine, and Cocaine Binding”, Frontiers in Neurology, vol. 6. Frontiers Media SA, Jun. 09, 2015. doi: 10.3389/fneur.2015.00134.*  
  
*N. K. Banavali, “The Mechanism of Cholesterol Modification of Hedgehog Ligand”, Journal of Computational Chemistry, vol. 41, no. 6. Wiley, pp. 520–527, Nov. 14, 2019. doi: 10.1002/jcc.26097.*  
  
*S. R. Manjari and N. K. Banavali, “Structural Articulation of Biochemical Reactions Using Restrained Geometries and Topology Switching”, Journal of Chemical Information and Modeling, vol. 58, no. 2. American Chemical Society (ACS), pp. 453–463, Feb. 05, 2018. doi: 10.1021/acs.jcim.7b00699.*  
  
*S. R. Manjari, J. D. Pataand N. K. Banavali, “Cytosine Unstacking and Strand Slippage at an Insertion–Deletion Mutation Sequence in an Overhang-Containing DNA Duplex”, Biochemistry, vol. 53, no. 23. American Chemical Society (ACS), pp. 3807–3816, Jun. 09, 2014. doi: 10.1021/bi500189g.*  
  
*D. G. Ackerman and G. W. Feigenson, “Multiscale Modeling of Four-Component Lipid Mixtures: Domain Composition, Size, Alignment, and Properties of the Phase Interface”, The Journal of Physical Chemistry B, vol. 119, no. 11. American Chemical Society (ACS), pp. 4240–4250, Jan. 22, 2015. doi: 10.1021/jp511083z.*  
  
*M. Doktorova, D. Harriesand G. Khelashvili, “Determination of bending rigidity and tilt modulus of lipid membranes from real-space fluctuation analysis of molecular dynamics simulations”, Physical Chemistry Chemical Physics, vol. 19, no. 25. Royal Society of Chemistry (RSC), pp. 16806–16818, 2017. doi: 10.1039/c7cp01921a.*  
  
*M. Doktorova, “Gramicidin Increases Lipid Flip-Flop in Symmetric and Asymmetric Lipid Vesicles”, Biophysical Journal, vol. 116, no. 5. Elsevier BV, pp. 860–873, Mar. 2019. doi: 10.1016/j.bpj.2019.01.016.*  
  
*M. Doktorova, M. V. LeVine, G. Khelashviliand H. Weinstein, “A New Computational Method for Membrane Compressibility: Bilayer Mechanical Thickness Revisited”, Biophysical Journal, vol. 116, no. 3. Elsevier BV, pp. 487–502, Feb. 2019. doi: 10.1016/j.bpj.2018.12.016.*  
  
*M. Doktorova and H. Weinstein, “Accurate In Silico Modeling of Asymmetric Bilayers Based on Biophysical Principles”, Biophysical Journal, vol. 115, no. 9. Elsevier BV, pp. 1638–1643, Nov. 2018. doi: 10.1016/j.bpj.2018.09.008.*  
  
*M. D. Weiner and G. W. Feigenson, “Presence and Role of Midplane Cholesterol in Lipid Bilayers Containing Registered or Antiregistered Phase Domains”, The Journal of Physical Chemistry B, vol. 122, no. 34. American Chemical Society (ACS), pp. 8193–8200, Aug. 10, 2018. doi: 10.1021/acs.jpcb.8b03949.*  
  
*M. D. Weiner and G. W. Feigenson, “Molecular Dynamics Simulations Reveal Leaflet Coupling in Compositionally Asymmetric Phase-Separated Lipid Membranes”, The Journal of Physical Chemistry B, vol. 123, no. 18. American Chemical Society (ACS), pp. 3968–3975, Apr. 22, 2019. doi: 10.1021/acs.jpcb.9b03488.*  
  
*J. B. Fields, K. L. Németh-Cahalan, J. A. Freites, I. Vorontsova, J. E. Halland D. J. Tobias, “Calmodulin Gates Aquaporin 0 Permeability through a Positively Charged Cytoplasmic Loop”, Journal of Biological Chemistry, vol. 292, no. 1. Elsevier BV, pp. 185–195, Jan. 2017. doi: 10.1074/jbc.m116.743724.*  
  
*D. Khago, E. K. Wong, C. N. Kingsley, J. Alfredo Freites, D. J. Tobiasand R. W. Martin, “Increased hydrophobic surface exposure in the cataract-related G18V variant of human γS-crystallin”, Biochimica et Biophysica Acta (BBA) - General Subjects, vol. 1860, no. 1. Elsevier BV, pp. 325–332, Jan. 2016. doi: 10.1016/j.bbagen.2015.09.022.*  
  
*V. Prytkova, “Multi-Conformation Monte Carlo: A Method for Introducing Flexibility in Efficient Simulations of Many-Protein Systems”, The Journal of Physical Chemistry B, vol. 120, no. 33. American Chemical Society (ACS), pp. 8115–8126, Apr. 21, 2016. doi: 10.1021/acs.jpcb.6b00827.*  
  
*A. Amcheslavsky, “Molecular Biophysics of Orai Store-Operated Ca2+ Channels”, Biophysical Journal, vol. 108, no. 2. Elsevier BV, pp. 237–246, Jan. 2015. doi: 10.1016/j.bpj.2014.11.3473.*  
  
*S. Capponi, J. A. Freites, D. J. Tobiasand S. H. White, “Interleaflet mixing and coupling in liquid-disordered phospholipid bilayers”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1858, no. 2. Elsevier BV, pp. 354–362, Feb. 2016. doi: 10.1016/j.bbamem.2015.11.024.*  
  
*J. A. Freites and D. J. Tobias, “Voltage Sensing in Membranes: From Macroscopic Currents to Molecular Motions”, The Journal of Membrane Biology, vol. 248, no. 3. Springer Science and Business Media LLC, pp. 419–430, May 14, 2015. doi: 10.1007/s00232-015-9805-x.*  
  
*A. Kyrychenko, J. A. Freites, J. He, D. J. Tobias, W. C. Wimleyand A. S. Ladokhin, “Structural Plasticity in the Topology of the Membrane-Interacting Domain of HIV-1 gp41”, Biophysical Journal, vol. 106, no. 3. Elsevier BV, pp. 610–620, Feb. 2014. doi: 10.1016/j.bpj.2013.12.032.*  
  
*G. Starek, J. A. Freites, S. Bernècheand D. J. Tobias, “Gating energetics of a voltage-dependent K+ channel pore domain”, Journal of Computational Chemistry, vol. 38, no. 16. Wiley, pp. 1472–1478, Feb. 16, 2017. doi: 10.1002/jcc.24742.*  
  
*A. Y. Tronin, “Direct Evidence of Conformational Changes Associated with Voltage Gating in a Voltage Sensor Protein by Time-Resolved X-ray/Neutron Interferometry”, Langmuir, vol. 30, no. 16. American Chemical Society (ACS), pp. 4784–4796, Apr. 16, 2014. doi: 10.1021/la500560w.*  
  
*M. L. Wood, J. A. Freites, F. Tombolaand D. J. Tobias, “Atomistic Modeling of Ion Conduction through the Voltage-Sensing Domain of the Shaker K+ Ion Channel”, The Journal of Physical Chemistry B, vol. 121, no. 15. American Chemical Society (ACS), pp. 3804–3812, Jan. 25, 2017. doi: 10.1021/acs.jpcb.6b12639.*  
  
*S. E. Boyken, “A Conserved Isoleucine Maintains the Inactive State of Bruton’s Tyrosine Kinase”, Journal of Molecular Biology, vol. 426, no. 21. Elsevier BV, pp. 3656–3669, Oct. 2014. doi: 10.1016/j.jmb.2014.08.018.*  
  
*J. E. Basconi, G. Cartaand M. R. Shirts, “Multiscale modeling of protein adsorption and transport in macroporous and polymer-grafted ion exchangers”, AIChE Journal, vol. 60, no. 11. Wiley, pp. 3888–3901, Sep. 30, 2014. doi: 10.1002/aic.14621.*  
  
*J. E. Basconi, G. Cartaand M. R. Shirts, “Effects of protein properties on adsorption and transport in polymer‐grafted ion exchangers: A multiscale modeling study”, AIChE Journal, vol. 63, no. 10. Wiley, pp. 4564–4575, May 27, 2017. doi: 10.1002/aic.15798.*  
  
*E. C. Dybeck, N. S. Abraham, N. P. Schieberand M. R. Shirts, “Capturing Entropic Contributions to Temperature-Mediated Polymorphic Transformations Through Molecular Modeling”, Crystal Growth & Design, vol. 17, no. 4. American Chemical Society (ACS), pp. 1775–1787, Mar. 14, 2017. doi: 10.1021/acs.cgd.6b01762.*  
  
*E. C. Dybeck, N. P. Schieberand M. R. Shirts, “Effects of a More Accurate Polarizable Hamiltonian on Polymorph Free Energies Computed Efficiently by Reweighting Point-Charge Potentials”, Journal of Chemical Theory and Computation, vol. 12, no. 8. American Chemical Society (ACS), pp. 3491–3505, Jul. 25, 2016. doi: 10.1021/acs.jctc.6b00397.*  
  
*P. T. Merz and M. R. Shirts, “Testing for Physical Validity in Molecular Simulations”, []. American Chemical Society (ACS), Mar. 21, 2018. doi: 10.26434/chemrxiv.6005279.v1.*  
  
*P. T. Merz and M. R. Shirts, “Testing for physical validity in molecular simulations”, PLOS ONE, vol. 13, no. 9. Public Library of Science (PLoS), p. e0202764, Sep. 06, 2018. doi: 10.1371/journal.pone.0202764.*  
  
*J. I. Monroe and M. R. Shirts, “Converging free energies of binding in cucurbit[7]uril and octa-acid host–guest systems from SAMPL4 using expanded ensemble simulations”, Journal of Computer-Aided Molecular Design, vol. 28, no. 4. Springer Science and Business Media LLC, pp. 401–415, Mar. 08, 2014. doi: 10.1007/s10822-014-9716-4.*  
  
*N. P. Schieber, E. C. Dybeckand M. R. Shirts, “Using reweighting and free energy surface interpolation to predict solid-solid phase diagrams”, The Journal of Chemical Physics, vol. 148, no. 14. AIP Publishing, p. 144104, Apr. 14, 2018. doi: 10.1063/1.5013273.*  
  
*T. J. Harpole and C. Grosman, “Side-chain conformation at the selectivity filter shapes the permeation free-energy landscape of an ion channel”, Proceedings of the National Academy of Sciences, vol. 111, no. 31. Proceedings of the National Academy of Sciences, Jul. 21, 2014. doi: 10.1073/pnas.1408950111.*  
  
*D. B. Sloan, D. A. Triant, N. J. Forrester, L. M. Bergner, M. Wuand D. R. Taylor, “A recurring syndrome of accelerated plastid genome evolution in the angiosperm tribe Sileneae (Caryophyllaceae)”, Molecular Phylogenetics and Evolution, vol. 72. Elsevier BV, pp. 82–89, Mar. 2014. doi: 10.1016/j.ympev.2013.12.004.*  
  
*J. Feng, M. F. Brownand B. Mertz, “Retinal Flip in Rhodopsin Activation?”, Biophysical Journal, vol. 108, no. 12. Elsevier BV, pp. 2767–2770, Jun. 2015. doi: 10.1016/j.bpj.2015.04.040.*  
  
*J. Feng and B. Mertz, “Proteorhodopsin Activation Is Modulated by Dynamic Changes in Internal Hydration”, Biochemistry, vol. 54, no. 48. American Chemical Society (ACS), pp. 7132–7141, Nov. 25, 2015. doi: 10.1021/acs.biochem.5b00932.*  
  
*C. Lee and B. Mertz, “Theoretical Evidence for Multiple Charge Transfer Pathways in Bacteriorhodopsin”, Journal of Chemical Theory and Computation, vol. 12, no. 4. American Chemical Society (ACS), pp. 1639–1646, Mar. 14, 2016. doi: 10.1021/acs.jctc.6b00033.*  
  
*B. Mertz, J. Feng, C. Corcoranand B. Neeley, “Explaining the mobility of retinal in activated rhodopsin and opsin”, Photochemical & Photobiological Sciences, vol. 14, no. 11. Springer Science and Business Media LLC, pp. 1952–1964, Nov. 2015. doi: 10.1039/c5pp00173k.*  
  
*M. Bykhovskaia, “Calcium Binding Promotes Conformational Flexibility of the Neuronal Ca 2+ Sensor Synaptotagmin”, Biophysical Journal, vol. 108, no. 10. Elsevier BV, pp. 2507–2520, May 2015. doi: 10.1016/j.bpj.2015.04.007.*  
  
*L. Michaeli, I. Gottfried, M. Bykhovskaiaand U. Ashery, “Phosphatidylinositol (4, 5)-bisphosphate targets double C2 domain protein B to the plasma membrane”, Traffic, vol. 18, no. 12. Wiley, pp. 825–839, Oct. 23, 2017. doi: 10.1111/tra.12528.*  
  
*A. Vasin, D. Volfson, J. T. Littletonand M. Bykhovskaia, “Interaction of the Complexin Accessory Helix with Synaptobrevin Regulates Spontaneous Fusion”, Biophysical Journal, vol. 111, no. 9. Elsevier BV, pp. 1954–1964, Nov. 2016. doi: 10.1016/j.bpj.2016.09.017.*  
  
*Y. O. Adeshina, E. J. Deedsand J. Karanicolas, “Machine learning classification can reduce false positives in structure-based virtual screening”, Proceedings of the National Academy of Sciences, vol. 117, no. 31. Proceedings of the National Academy of Sciences, pp. 18477–18488, Jul. 15, 2020. doi: 10.1073/pnas.2000585117.*  
  
*A. M. Ali, “Optogenetic Inhibitor of the Transcription Factor CREB”, Chemistry & Biology, vol. 22, no. 11. Elsevier BV, pp. 1531–1539, Nov. 2015. doi: 10.1016/j.chembiol.2015.09.018.*  
  
*A. Bazzoli and J. Karanicolas, ““Solvent hydrogen-bond occlusion”: A new model of polar desolvation for biomolecular energetics”, Journal of Computational Chemistry, vol. 38, no. 16. Wiley, pp. 1321–1331, Mar. 20, 2017. doi: 10.1002/jcc.24740.*  
  
*A. Bazzoli, S. P. Kelowand J. Karanicolas, “Enhancements to the Rosetta Energy Function Enable Improved Identification of Small Molecules that Inhibit Protein-Protein Interactions”, PLOS ONE, vol. 10, no. 10. Public Library of Science (PLoS), p. e0140359, Oct. 20, 2015. doi: 10.1371/journal.pone.0140359.*  
  
*A. Bazzoli, “Using homology modeling to interrogate binding affinity in neutralization of ricin toxin by a family of single domain antibodies”, Proteins: Structure, Function, and Bioinformatics, vol. 85, no. 11. Wiley, pp. 1994–2008, Aug. 04, 2017. doi: 10.1002/prot.25353.*  
  
*S. J. Budiardjo, “Full and Partial Agonism of a Designed Enzyme Switch”, ACS Synthetic Biology, vol. 5, no. 12. American Chemical Society (ACS), pp. 1475–1484, Jul. 22, 2016. doi: 10.1021/acssynbio.6b00097.*  
  
*R. Gowthaman, E. J. Deedsand J. Karanicolas, “Structural Properties of Non-Traditional Drug Targets Present New Challenges for Virtual Screening”, Journal of Chemical Information and Modeling, vol. 53, no. 8. American Chemical Society (ACS), pp. 2073–2081, Aug. 13, 2013. doi: 10.1021/ci4002316.*  
  
*R. Gowthaman, S. Lyskovand J. Karanicolas, “DARC 2.0: Improved Docking and Virtual Screening at Protein Interaction Sites”, PLOS ONE, vol. 10, no. 7. Public Library of Science (PLoS), p. e0131612, Jul. 16, 2015. doi: 10.1371/journal.pone.0131612.*  
  
*R. Gowthaman, “DARC: Mapping Surface Topography by Ray-Casting for Effective Virtual Screening at Protein Interaction Sites”, Journal of Medicinal Chemistry, vol. 59, no. 9. American Chemical Society (ACS), pp. 4152–4170, Jul. 10, 2015. doi: 10.1021/acs.jmedchem.5b00150.*  
  
*D. K. Johnson and J. Karanicolas, “Druggable Protein Interaction Sites Are More Predisposed to Surface Pocket Formation than the Rest of the Protein Surface”, PLoS Computational Biology, vol. 9, no. 3. Public Library of Science (PLoS), p. e1002951, Mar. 07, 2013. doi: 10.1371/journal.pcbi.1002951.*  
  
*D. K. Johnson and J. Karanicolas, “Selectivity by Small-Molecule Inhibitors of Protein Interactions Can Be Driven by Protein Surface Fluctuations”, PLOS Computational Biology, vol. 11, no. 2. Public Library of Science (PLoS), p. e1004081, Feb. 23, 2015. doi: 10.1371/journal.pcbi.1004081.*  
  
*D. K. Johnson and J. Karanicolas, “Ultra-High-Throughput Structure-Based Virtual Screening for Small-Molecule Inhibitors of Protein–Protein Interactions”, Journal of Chemical Information and Modeling, vol. 56, no. 2. American Chemical Society (ACS), pp. 399–411, Jan. 14, 2016. doi: 10.1021/acs.jcim.5b00572.*  
  
*C. E. Keohane, “Promysalin Elicits Species-Selective Inhibition of Pseudomonas aeruginosa by Targeting Succinate Dehydrogenase”, Journal of the American Chemical Society, vol. 140, no. 5. American Chemical Society (ACS), pp. 1774–1782, Jan. 24, 2018. doi: 10.1021/jacs.7b11212.*  
  
*K. R. Khar, L. Goldschmidtand J. Karanicolas, “Fast Docking on Graphics Processing Units via Ray-Casting”, PLoS ONE, vol. 8, no. 8. Public Library of Science (PLoS), p. e70661, Aug. 16, 2013. doi: 10.1371/journal.pone.0070661.*  
  
*J. Khowsathit, A. Bazzoli, H. Chengand J. Karanicolas, “Computational Design of an Allosteric Antibody Switch by Deletion and Rescue of a Complex Structural Constellation”, ACS Central Science, vol. 6, no. 3. American Chemical Society (ACS), pp. 390–403, Mar. 11, 2020. doi: 10.1021/acscentsci.9b01065.*  
  
*S. Malhotra and J. Karanicolas, “When Does Chemical Elaboration Induce a Ligand To Change Its Binding Mode?”, Journal of Medicinal Chemistry, vol. 60, no. 1. American Chemical Society (ACS), pp. 128–145, Dec. 16, 2016. doi: 10.1021/acs.jmedchem.6b00725.*  
  
*Y. Xia, “The Designability of Protein Switches by Chemical Rescue of Structure: Mechanisms of Inactivation and Reactivation”, Journal of the American Chemical Society, vol. 135, no. 50. American Chemical Society (ACS), pp. 18840–18849, Dec. 06, 2013. doi: 10.1021/ja407644b.*  
  
*H. Zhang, “Targeting CDK9 Reactivates Epigenetically Silenced Genes in Cancer”, Cell, vol. 175, no. 5. Elsevier BV, pp. 1244–1258.e26, Nov. 2018. doi: 10.1016/j.cell.2018.09.051.*  
  
*A. Iuga, “Understanding Force-Field Bias in Pin1WW”, Biophysical Journal, vol. 108, no. 2. Elsevier BV, p. 46a, Jan. 2015. doi: 10.1016/j.bpj.2014.11.287.*  
  
*W. M. Jones, A. Davis, I. Sumnerand S. Zamfir, “Computational Analysis of the Mechanism of the Ubiquitin Conjugating Enzyme Ubc13”, Biophysical Journal, vol. 112, no. 3. Elsevier BV, p. 291a, Feb. 2017. doi: 10.1016/j.bpj.2016.11.1579.*  
  
*I. Sumner, R. H. Wilson, W. M. Jones, A. G. Davisand S. Zamfir, “Mechanistic Insights into Ubc13-Catalyzed Ubiquitination”, Biophysical Journal, vol. 112, no. 3. Elsevier BV, p. 65a, Feb. 2017. doi: 10.1016/j.bpj.2016.11.389.*  
  
*R. H. Wilson and I. Sumner, “A Computational Investigation into the Mechanism of the Histone Acetyltransferase, Gcn5”, Biophysical Journal, vol. 112, no. 3. Elsevier BV, p. 65a, Feb. 2017. doi: 10.1016/j.bpj.2016.11.391.*  
  
*R. H. Wilson, S. Zamfirand I. Sumner, “Molecular dynamics simulations reveal a new role for a conserved active site asparagine in a ubiquitin-conjugating enzyme”, Journal of Molecular Graphics and Modelling, vol. 76. Elsevier BV, pp. 403–411, Sep. 2017. doi: 10.1016/j.jmgm.2017.07.006.*  
  
*S. Zamfir, “Molecular Dynamics Studies of the Ubiquitin Conjugation Mechanism”, Biophysical Journal, vol. 108, no. 2. Elsevier BV, p. 532a, Jan. 2015. doi: 10.1016/j.bpj.2014.11.2914.*  
  
*R. P. B, N. V. Plotnikov, J. Lameiraand A. Warshel, “Quantitative exploration of the molecular origin of the activation of GTPase”, Proceedings of the National Academy of Sciences, vol. 110, no. 51. Proceedings of the National Academy of Sciences, pp. 20509–20514, Nov. 26, 2013. doi: 10.1073/pnas.1319854110.*  
  
*N. V. Plotnikov, “Computing the Free Energy Barriers for Less by Sampling with a Coarse Reference Potential while Retaining Accuracy of the Target Fine Model”, Journal of Chemical Theory and Computation, vol. 10, no. 8. American Chemical Society (ACS), pp. 2987–3001, Jun. 06, 2014. doi: 10.1021/ct500109m.*  
  
*N. V. Plotnikov, B. R. Prasad, S. Chakrabarty, Z. T. Chuand A. Warshel, “Quantifying the Mechanism of Phosphate Monoester Hydrolysis in Aqueous Solution by Evaluating the Relevant Ab Initio QM/MM Free-Energy Surfaces”, The Journal of Physical Chemistry B, vol. 117, no. 42. American Chemical Society (ACS), pp. 12807–12819, May 30, 2013. doi: 10.1021/jp4020146.*  
  
*C. T. Harvey, G. A. Moyerbrailean, G. O. Davis, X. Wen, F. Lucaand R. Pique-Regi, “QuASAR: quantitative allele-specific analysis of reads”, Bioinformatics, vol. 31, no. 8. Oxford University Press (OUP), pp. 1235–1242, Dec. 04, 2014. doi: 10.1093/bioinformatics/btu802.*  
  
*X. Wen, F. Lucaand R. Pique-Regi, “Cross-Population Joint Analysis of eQTLs: Fine Mapping and Functional Annotation”, PLOS Genetics, vol. 11, no. 4. Public Library of Science (PLoS), p. e1005176, Apr. 23, 2015. doi: 10.1371/journal.pgen.1005176.*  
  
*S. M. Saladi, N. Javed, A. Müllerand W. M. Clemons, “A Machine Learning Approach to Heterologous Membrane Protein Overexpression”, Biophysical Journal, vol. 110, no. 3. Elsevier BV, p. 39a, Feb. 2016. doi: 10.1016/j.bpj.2015.11.278.*  
  
*C. Balusek and J. C. Gumbart, “Role of the Native Outer-Membrane Environment on the Transporter BtuB”, Biophysical Journal, vol. 111, no. 7. Elsevier BV, pp. 1409–1417, Oct. 2016. doi: 10.1016/j.bpj.2016.08.033.*  
  
*A. V. Dvornikov, N. Smolin, M. Zhang, J. L. Martin, S. L. Robiaand P. P. de Tombe, “Restrictive Cardiomyopathy Troponin I R145W Mutation Does Not Perturb Myofilament Length-dependent Activation in Human Cardiac Sarcomeres”, Journal of Biological Chemistry, vol. 291, no. 41. Elsevier BV, pp. 21817–21828, Oct. 2016. doi: 10.1074/jbc.m116.746172.*  
  
*R. D. Himes, N. Smolin, A. Kukol, J. Bossuyt, D. M. Bersand S. L. Robia, “L30A Mutation of Phospholemman Mimics Effects of Cardiac Glycosides in Isolated Cardiomyocytes”, Biochemistry, vol. 55, no. 44. American Chemical Society (ACS), pp. 6196–6204, Oct. 25, 2016. doi: 10.1021/acs.biochem.6b00633.*  
  
*R. Lamichhane, “Dynamic conformational changes in the rhesus TRIM5α dimer dictate the potency of HIV-1 restriction”, Virology, vol. 500. Elsevier BV, pp. 161–168, Jan. 2017. doi: 10.1016/j.virol.2016.10.003.*  
  
*O. N. Raguimova, “Redistribution of SERCA calcium pump conformers during intracellular calcium signaling”, Journal of Biological Chemistry, vol. 293, no. 28. Elsevier BV, pp. 10843–10856, Jul. 2018. doi: 10.1074/jbc.ra118.002472.*  
  
*K. L. Mack, M. A. Ballinger, M. Phifer-Rixeyand M. W. Nachman, “Gene regulation underlies environmental adaptation in house mice”, Genome Research, vol. 28, no. 11. Cold Spring Harbor Laboratory, pp. 1636–1645, Sep. 07, 2018. doi: 10.1101/gr.238998.118.*  
  
*K. Mack, M. Phifer-Rixey, B. Harrand M. Nachman, “Gene Expression Networks Across Multiple Tissues Are Associated with Rates of Molecular Evolution in Wild House Mice”, Genes, vol. 10, no. 3. MDPI AG, p. 225, Mar. 18, 2019. doi: 10.3390/genes10030225.*  
  
*M. Phifer-Rixey, “The genomic basis of environmental adaptation in house mice”, PLOS Genetics, vol. 14, no. 9. Public Library of Science (PLoS), p. e1007672, Sep. 24, 2018. doi: 10.1371/journal.pgen.1007672.*  
  
*M. Phifer-Rixey, M. Bomhoffand M. W. Nachman, “Genome-Wide Patterns of Differentiation Among House Mouse Subspecies”, Genetics, vol. 198, no. 1. Oxford University Press (OUP), pp. 283–297, Jul. 03, 2014. doi: 10.1534/genetics.114.166827.*  
  
*T. A. Suzuki, “Host genetic determinants of the gut microbiota of wild mice”, Molecular Ecology, vol. 28, no. 13. Wiley, pp. 3197–3207, Jun. 11, 2019. doi: 10.1111/mec.15139.*  
  
*K. L. Mack, P. Campbelland M. W. Nachman, “Gene regulation and speciation in house mice”, Genome Research, vol. 26, no. 4. Cold Spring Harbor Laboratory, pp. 451–461, Feb. 01, 2016. doi: 10.1101/gr.195743.115.*  
  
*V. M. Anisimov, M. J. Hallockand T. V. Pogorelov, “CDD”, Proceedings of the 2015 XSEDE Conference on Scientific Advancements Enabled by Enhanced Cyberinfrastructure - XSEDE ’15. ACM Press, 2015. doi: 10.1145/2792745.2792788.*  
  
*J. L. Baylon, J. V. Vermaas, M. P. Muller, M. J. Arcario, T. V. Pogorelovand E. Tajkhorshid, “Atomic-level description of protein–lipid interactions using an accelerated membrane model”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1858, no. 7. Elsevier BV, pp. 1573–1583, Jul. 2016. doi: 10.1016/j.bbamem.2016.02.027.*  
  
*D. P. Cogan, “Structural insights into enzymatic [4+2] aza -cycloaddition in thiopeptide antibiotic biosynthesis”, Proceedings of the National Academy of Sciences, vol. 114, no. 49. Proceedings of the National Academy of Sciences, pp. 12928–12933, Nov. 20, 2017. doi: 10.1073/pnas.1716035114.*  
  
*S. A. Davis, “C3-OH of Amphotericin B Plays an Important Role in Ion Conductance”, Journal of the American Chemical Society, vol. 137, no. 48. American Chemical Society (ACS), pp. 15102–15104, Nov. 30, 2015. doi: 10.1021/jacs.5b05766.*  
  
*A. M. De Lio, D. Paul, R. Jain, J. H. Morrisseyand T. V. Pogorelov, “Proteins and Ions Compete for Membrane Interaction: the case of Lactadherin”, []. Cold Spring Harbor Laboratory, Apr. 03, 2020. doi: 10.1101/2020.04.03.023838.*  
  
*J. S. Goodman, S.-H. Chao, T. V. Pogorelovand M. Gruebele, “Filling Up the Heme Pocket Stabilizes Apomyoglobin and Speeds Up Its Folding”, The Journal of Physical Chemistry B, vol. 118, no. 24. American Chemical Society (ACS), pp. 6511–6518, Feb. 10, 2014. doi: 10.1021/jp412459z.*  
  
*Y. Z. Ohkubo, T. V. Pogorelov, M. J. Arcario, G. A. Christensenand E. Tajkhorshid, “Accelerating Membrane Insertion of Peripheral Proteins with a Novel Membrane Mimetic Model”, Biophysical Journal, vol. 102, no. 9. Elsevier BV, pp. 2130–2139, May 2012. doi: 10.1016/j.bpj.2012.03.015.*  
  
*T. V. Pogorelov, J. V. Vermaas, M. J. Arcarioand E. Tajkhorshid, “Partitioning of Amino Acids into a Model Membrane: Capturing the Interface”, The Journal of Physical Chemistry B, vol. 118, no. 6. American Chemical Society (ACS), pp. 1481–1492, Jan. 30, 2014. doi: 10.1021/jp4089113.*  
  
*M. B. Prigozhin, S.-H. Chao, S. Sukenik, T. V. Pogorelovand M. Gruebele, “Mapping fast protein folding with multiple-site fluorescent probes”, Proceedings of the National Academy of Sciences, vol. 112, no. 26. Proceedings of the National Academy of Sciences, pp. 7966–7971, Jun. 15, 2015. doi: 10.1073/pnas.1422683112.*  
  
*K. K. Skeby, O. J. Andersen, T. V. Pogorelov, E. Tajkhorshidand B. Schiøtt, “Conformational Dynamics of the Human Islet Amyloid Polypeptide in a Membrane Environment: Toward the Aggregation Prone Form”, Biochemistry, vol. 55, no. 13. American Chemical Society (ACS), pp. 2031–2042, Mar. 22, 2016. doi: 10.1021/acs.biochem.5b00507.*  
  
*J. V. Vermaas, T. V. Pogorelovand E. Tajkhorshid, “Extension of the Highly Mobile Membrane Mimetic to Transmembrane Systems through Customized in Silico Solvents”, The Journal of Physical Chemistry B, vol. 121, no. 15. American Chemical Society (ACS), pp. 3764–3776, Mar. 13, 2017. doi: 10.1021/acs.jpcb.6b11378.*  
  
*M. J. Hallock, “Calcium-Induced Lipid Nanocluster Structures: Sculpturing of the Plasma Membrane”, Biochemistry, vol. 57, no. 50. American Chemical Society (ACS), pp. 6897–6905, Nov. 20, 2018. doi: 10.1021/acs.biochem.8b01069.*  
  
*R. LeDuc, “Leveraging the national cyberinfrastructure for biomedical research”, Journal of the American Medical Informatics Association, vol. 21, no. 2. Oxford University Press (OUP), pp. 195–199, Mar. 2014. doi: 10.1136/amiajnl-2013-002059.*  
  
*Z. Peng, X. Li, I. V. Pivkin, M. Dao, G. E. Karniadakisand S. Suresh, “Lipid bilayer and cytoskeletal interactions in a red blood cell”, Proceedings of the National Academy of Sciences, vol. 110, no. 33. Proceedings of the National Academy of Sciences, pp. 13356–13361, Jul. 29, 2013. doi: 10.1073/pnas.1311827110.*  
  
*D. L. Clemens, P. Ge, B.-Y. Lee, M. A. Horwitzand Z. H. Zhou, “Atomic Structure of T6SS Reveals Interlaced Array Essential to Function”, Cell, vol. 160, no. 5. Elsevier BV, pp. 940–951, Feb. 2015. doi: 10.1016/j.cell.2015.02.005.*  
  
*P. Ge, Z. A. O. Durer, D. Kudryashov, Z. H. Zhouand E. Reisler, “Cryo-EM reveals different coronin binding modes for ADP– and ADP–BeFx actin filaments”, Nature Structural & Molecular Biology, vol. 21, no. 12. Springer Science and Business Media LLC, pp. 1075–1081, Nov. 02, 2014. doi: 10.1038/nsmb.2907.*  
  
*R. Kazi, J. Dai, C. Sweeney, H.-X. Zhouand L. P. Wollmuth, “Mechanical coupling maintains the fidelity of NMDA receptor–mediated currents”, Nature Neuroscience, vol. 17, no. 7. Springer Science and Business Media LLC, pp. 914–922, May 25, 2014. doi: 10.1038/nn.3724.*  
  
*M. D. Rasmussen, M. J. Hubisz, I. Gronauand A. Siepel, “Genome-Wide Inference of Ancestral Recombination Graphs”, PLoS Genetics, vol. 10, no. 5. Public Library of Science (PLoS), p. e1004342, May 15, 2014. doi: 10.1371/journal.pgen.1004342.*  
  
*K. S. Rahman, G. Cui, S. C. Harveyand N. A. McCarty, “Modeling the Conformational Changes Underlying Channel Opening in CFTR”, PLoS ONE, vol. 8, no. 9. Public Library of Science (PLoS), p. e74574, Sep. 27, 2013. doi: 10.1371/journal.pone.0074574.*  
  
*J. C. Jagodinsky and U. Akgun, “Characterizing the binding interactions between P‐glycoprotein and eight known cardiovascular transport substrates”, Pharmacology Research & Perspectives, vol. 3, no. 2. Wiley, Feb. 02, 2015. doi: 10.1002/prp2.114.*  
  
*C. Y. Cheng, F.-C. Chou, W. Kladwang, S. Tian, P. Corderoand R. Das, “Consistent global structures of complex RNA states through multidimensional chemical mapping”, eLife, vol. 4. eLife Sciences Publications, Ltd, Jun. 02, 2015. doi: 10.7554/elife.07600.*  
  
*F.-C. Chou, W. Kladwang, K. Kappeland R. Das, “Blind tests of RNA nearest-neighbor energy prediction”, Proceedings of the National Academy of Sciences, vol. 113, no. 30. Proceedings of the National Academy of Sciences, pp. 8430–8435, Jul. 08, 2016. doi: 10.1073/pnas.1523335113.*  
  
*Z. Miao, “RNA-Puzzles Round III: 3D RNA structure prediction of five riboswitches and one ribozyme”, RNA, vol. 23, no. 5. Cold Spring Harbor Laboratory, pp. 655–672, Jan. 30, 2017. doi: 10.1261/rna.060368.116.*  
  
*Z. Miao, “RNA-Puzzles Round II: assessment of RNA structure prediction programs applied to three large RNA structures”, RNA, vol. 21, no. 6. Cold Spring Harbor Laboratory, pp. 1066–1084, Apr. 16, 2015. doi: 10.1261/rna.049502.114.*  
  
*S. Lyskov, “Serverification of Molecular Modeling Applications: The Rosetta Online Server That Includes Everyone (ROSIE)”, PLoS ONE, vol. 8, no. 5. Public Library of Science (PLoS), p. e63906, May 22, 2013. doi: 10.1371/journal.pone.0063906.*  
  
*J. D. Yesselman and R. Das, “Modeling Small Noncanonical RNA Motifs with the Rosetta FARFAR Server”, RNA Structure Determination. Springer New York, pp. 187–198, 2016. doi: 10.1007/978-1-4939-6433-8\_12.*  
  
*I. Botos, “Structural and Functional Characterization of the LPS Transporter LptDE from Gram-Negative Pathogens”, Structure, vol. 24, no. 6. Elsevier BV, pp. 965–976, Jun. 2016. doi: 10.1016/j.str.2016.03.026.*  
  
*Y. Chen, B. W. Bauer, T. A. Rapoportand J. C. Gumbart, “Conformational Changes of the Clamp of the Protein Translocation ATPase SecA”, Journal of Molecular Biology, vol. 427, no. 14. Elsevier BV, pp. 2348–2359, Jul. 2015. doi: 10.1016/j.jmb.2015.05.003.*  
  
*J. Comer, J. C. Gumbart, J. Hénin, T. Lelièvre, A. Pohorilleand C. Chipot, “The Adaptive Biasing Force Method: Everything You Always Wanted To Know but Were Afraid To Ask”, The Journal of Physical Chemistry B, vol. 119, no. 3. American Chemical Society (ACS), pp. 1129–1151, Oct. 07, 2014. doi: 10.1021/jp506633n.*  
  
*Z. M. Darzynkiewicz, “Identification of Binding Sites for Efflux Pump Inhibitors of the AcrAB-TolC Component AcrA”, Biophysical Journal, vol. 116, no. 4. Elsevier BV, pp. 648–658, Feb. 2019. doi: 10.1016/j.bpj.2019.01.010.*  
  
*J. Deeng, “Dynamic Behavior of Trigger Factor on the Ribosome”, Journal of Molecular Biology, vol. 428, no. 18. Elsevier BV, pp. 3588–3602, Sep. 2016. doi: 10.1016/j.jmb.2016.06.007.*  
  
*J. Deeng, “Dynamic Behavior of Trigger Factor on the Ribosome”, Journal of Molecular Biology, vol. 428, no. 18. Elsevier BV, pp. 3588–3602, Sep. 2016. doi: 10.1016/j.jmb.2016.06.007.*  
  
*I. Z. Fernandez, “A novel human IL2RB mutation results in T and NK cell–driven immune dysregulation”, Journal of Experimental Medicine, vol. 216, no. 6. Rockefeller University Press, pp. 1255–1267, Apr. 30, 2019. doi: 10.1084/jem.20182015.*  
  
*J. C. Gumbart and C. Chipot, “Decrypting protein insertion through the translocon with free-energy calculations”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1858, no. 7. Elsevier BV, pp. 1663–1671, Jul. 2016. doi: 10.1016/j.bbamem.2016.02.017.*  
  
*H. Hwang, “Redox-Driven Conformational Dynamics in a Photosystem-II-Inspired β-Hairpin Maquette Determined through Spectroscopy and Simulation”, The Journal of Physical Chemistry B, vol. 121, no. 15. American Chemical Society (ACS), pp. 3536–3545, Feb. 13, 2017. doi: 10.1021/acs.jpcb.6b09481.*  
  
*H. Hwang, N. Paracini, J. M. Parks, J. H. Lakeyand J. C. Gumbart, “Distribution of mechanical stress in the Escherichia coli cell envelope”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1860, no. 12. Elsevier BV, pp. 2566–2575, Dec. 2018. doi: 10.1016/j.bbamem.2018.09.020.*  
  
*J. L. Johnson, “Structural and biophysical characterization of an epitope-specific engineered Fab fragment and complexation with membrane proteins: implications for co-crystallization”, Acta Crystallographica Section D Biological Crystallography, vol. 71, no. 4. International Union of Crystallography (IUCr), pp. 896–906, Mar. 27, 2015. doi: 10.1107/s1399004715001856.*  
  
*C. T. Lee, “Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds”, Journal of Chemical Information and Modeling, vol. 56, no. 4. American Chemical Society (ACS), pp. 721–733, Apr. 14, 2016. doi: 10.1021/acs.jcim.6b00022.*  
  
*K. Lundquist, C. Herndon, T. H. Hartyand J. C. Gumbart, “Accelerating the use of molecular modeling in the high school classroom with VMD Lite”, Biochemistry and Molecular Biology Education, vol. 44, no. 2. Wiley, pp. 124–129, Jan. 11, 2016. doi: 10.1002/bmb.20940.*  
  
*L. T. Nguyen, J. C. Gumbartand G. J. Jensen, “Coarse-Grained Molecular Dynamics Simulations of the Bacterial Cell Wall”, Methods in Molecular Biology. Springer New York, pp. 247–270, 2016. doi: 10.1007/978-1-4939-3676-2\_18.*  
  
*N. Noinaj, J. C. Gumbartand S. K. Buchanan, “The β-barrel assembly machinery in motion”, Nature Reviews Microbiology, vol. 15, no. 4. Springer Science and Business Media LLC, pp. 197–204, Apr. 2017. doi: 10.1038/nrmicro.2016.191.*  
  
*A. Pavlova, H. Hwang, K. Lundquist, C. Balusekand J. C. Gumbart, “Living on the edge: Simulations of bacterial outer-membrane proteins”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1858, no. 7. Elsevier BV, pp. 1753–1759, Jul. 2016. doi: 10.1016/j.bbamem.2016.01.020.*  
  
*A. Pavlova, J. M. Parks, A. K. Oyelereand J. C. Gumbart, “Toward the rational design of macrolide antibiotics to combat resistance”, Chemical Biology & Drug Design, vol. 90, no. 5. Wiley, pp. 641–652, May 16, 2017. doi: 10.1111/cbdd.13004.*  
  
*M. Coincon, “Crystal structures reveal the molecular basis of ion translocation in sodium/proton antiporters”, Nature Structural & Molecular Biology, vol. 23, no. 3. Springer Science and Business Media LLC, pp. 248–255, Feb. 01, 2016. doi: 10.1038/nsmb.3164.*  
  
*S. Fan, M. Linke, I. Paraskevakos, R. Gowers, M. Gechtand O. Beckstein, “PMDA - Parallel Molecular Dynamics Analysis”, Proceedings of the 18th Python in Science Conference. SciPy, 2019. doi: 10.25080/majora-7ddc1dd1-013.*  
  
*Y. Huang, W. Chen, D. L. Dotson, O. Becksteinand J. Shen, “Mechanism of pH-dependent activation of the sodium-proton antiporter NhaA”, Nature Communications, vol. 7, no. 1. Springer Science and Business Media LLC, Oct. 06, 2016. doi: 10.1038/ncomms12940.*  
  
*M. Khoshlessan, I. Paraskevakos, G. C. Fox, S. Jhaand O. Beckstein, “Parallel performance of molecular dynamics trajectory analysis”, Concurrency and Computation: Practice and Experience, vol. 32, no. 19. Wiley, Apr. 27, 2020. doi: 10.1002/cpe.5789.*  
  
*I. Paraskevakos, “Task-parallel Analysis of Molecular Dynamics Trajectories”, Proceedings of the 47th International Conference on Parallel Processing. ACM, Aug. 13, 2018. doi: 10.1145/3225058.3225128.*  
  
*S. L. Seyler, A. Kumar, M. F. Thorpeand O. Beckstein, “Path Similarity Analysis: A Method for Quantifying Macromolecular Pathways”, PLOS Computational Biology, vol. 11, no. 10. Public Library of Science (PLoS), p. e1004568, Oct. 21, 2015. doi: 10.1371/journal.pcbi.1004568.*  
  
*I. Winkelmann, “Structure and elevator mechanism of the mammalian sodium/proton exchanger NHE9”, The EMBO Journal, vol. 39, no. 24. EMBO, pp. 4541–4559, Oct. 29, 2020. doi: 10.15252/embj.2020105908.*  
  
*K. Akabori, “HIV-1 Tat membrane interactions probed using X-ray and neutron scattering, CD spectroscopy and MD simulations”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1838, no. 12. Elsevier BV, pp. 3078–3087, Dec. 2014. doi: 10.1016/j.bbamem.2014.08.014.*  
  
*C. A. English and A. E. García, “Charged Termini on the Trp-Cage Roughen the Folding Energy Landscape”, The Journal of Physical Chemistry B, vol. 119, no. 25. American Chemical Society (ACS), pp. 7874–7881, Jun. 09, 2015. doi: 10.1021/acs.jpcb.5b02040.*  
  
*H. D. Herce, A. E. Garciaand M. C. Cardoso, “Fundamental Molecular Mechanism for the Cellular Uptake of Guanidinium-Rich Molecules”, Journal of the American Chemical Society, vol. 136, no. 50. American Chemical Society (ACS), pp. 17459–17467, Dec. 01, 2014. doi: 10.1021/ja507790z.*  
  
*K. Huang and A. E. García, “Acceleration of Lateral Equilibration in Mixed Lipid Bilayers Using Replica Exchange with Solute Tempering”, Journal of Chemical Theory and Computation, vol. 10, no. 10. American Chemical Society (ACS), pp. 4264–4272, Sep. 26, 2014. doi: 10.1021/ct500305u.*  
  
*K. Huang and A. E. García, “Effects of truncating van der Waals interactions in lipid bilayer simulations”, The Journal of Chemical Physics, vol. 141, no. 10. AIP Publishing, p. 105101, Sep. 14, 2014. doi: 10.1063/1.4893965.*  
  
*R. C. Krafnick and A. E. García, “Efficient Schmidt number scaling in dissipative particle dynamics”, The Journal of Chemical Physics, vol. 143, no. 24. AIP Publishing, p. 243106, Dec. 28, 2015. doi: 10.1063/1.4930921.*  
  
*J. C. Miner, A. A. Chenand A. E. García, “Free-energy landscape of a hyperstable RNA tetraloop”, Proceedings of the National Academy of Sciences, vol. 113, no. 24. Proceedings of the National Academy of Sciences, pp. 6665–6670, May 27, 2016. doi: 10.1073/pnas.1603154113.*  
  
*J. C. Miner and A. E. García, “Equilibrium Denaturation and Preferential Interactions of an RNA Tetraloop with Urea”, The Journal of Physical Chemistry B, vol. 121, no. 15. American Chemical Society (ACS), pp. 3734–3746, Feb. 16, 2017. doi: 10.1021/acs.jpcb.6b10767.*  
  
*C. Neale, H. D. Herce, R. Pomèsand A. E. García, “Can Specific Protein-Lipid Interactions Stabilize an Active State of the Beta 2 Adrenergic Receptor?”, Biophysical Journal, vol. 109, no. 8. Elsevier BV, pp. 1652–1662, Oct. 2015. doi: 10.1016/j.bpj.2015.08.028.*  
  
*C. Neale, K. Huang, A. Garcíaand S. Tristram-Nagle, “Penetration of HIV-1 Tat47–57 into PC/PE Bilayers Assessed by MD Simulation and X-ray Scattering”, Membranes, vol. 5, no. 3. MDPI AG, pp. 473–494, Sep. 22, 2015. doi: 10.3390/membranes5030473.*  
  
*C. Neale, R. Pomèsand A. E. García, “Peptide Bond Isomerization in High-Temperature Simulations”, Journal of Chemical Theory and Computation, vol. 12, no. 4. American Chemical Society (ACS), pp. 1989–1999, Mar. 15, 2016. doi: 10.1021/acs.jctc.5b01022.*  
  
*D. J. Rosenman, C. Wangand A. E. García, “Characterization of Aβ Monomers through the Convergence of Ensemble Properties among Simulations with Multiple Force Fields”, The Journal of Physical Chemistry B, vol. 120, no. 2. American Chemical Society (ACS), pp. 259–277, Dec. 09, 2015. doi: 10.1021/acs.jpcb.5b09379.*  
  
*A. Saxena and A. E. García, “Multisite Ion Model in Concentrated Solutions of Divalent Cations (MgCl2 and CaCl2): Osmotic Pressure Calculations”, The Journal of Physical Chemistry B, vol. 119, no. 1. American Chemical Society (ACS), pp. 219–227, Dec. 22, 2014. doi: 10.1021/jp507008x.*  
  
*M. A. Sahai, “Combined in vitro and in silico approaches to the assessment of stimulant properties of novel psychoactive substances – The case of the benzofuran 5-MAPB”, Progress in Neuro-Psychopharmacology and Biological Psychiatry, vol. 75. Elsevier BV, pp. 1–9, Apr. 2017. doi: 10.1016/j.pnpbp.2016.11.004.*  
  
*B. J. DeKosky, “Large-scale sequence and structural comparisons of human naive and antigen-experienced antibody repertoires”, Proceedings of the National Academy of Sciences, vol. 113, no. 19. Proceedings of the National Academy of Sciences, Apr. 25, 2016. doi: 10.1073/pnas.1525510113.*  
  
*Q. Jiang, “Functional Loss of Semaphorin 3C and/or Semaphorin 3D and Their Epistatic Interaction with Ret Are Critical to Hirschsprung Disease Liability”, The American Journal of Human Genetics, vol. 96, no. 4. Elsevier BV, pp. 581–596, Apr. 2015. doi: 10.1016/j.ajhg.2015.02.014.*  
  
*K. P. Kilambi, K. Reddyand J. J. Gray, “Protein-Protein Docking with Dynamic Residue Protonation States”, PLoS Computational Biology, vol. 10, no. 12. Public Library of Science (PLoS), p. e1004018, Dec. 11, 2014. doi: 10.1371/journal.pcbi.1004018.*  
  
*D. Kuroda and J. J. Gray, “Shape complementarity and hydrogen bond preferences in protein–protein interfaces: implications for antibody modeling and protein–protein docking”, Bioinformatics, vol. 32, no. 16. Oxford University Press (OUP), pp. 2451–2456, Apr. 19, 2016. doi: 10.1093/bioinformatics/btw197.*  
  
*D. Kuroda and J. J. Gray, “Pushing the Backbone in Protein-Protein Docking”, Structure, vol. 24, no. 10. Elsevier BV, pp. 1821–1829, Oct. 2016. doi: 10.1016/j.str.2016.06.025.*  
  
*M. F. Lensink, “Blind prediction of interfacial water positions in CAPRI”, Proteins: Structure, Function, and Bioinformatics, vol. 82, no. 4. Wiley, pp. 620–632, Nov. 23, 2013. doi: 10.1002/prot.24439.*  
  
*M. F. Lensink, “Prediction of homoprotein and heteroprotein complexes by protein docking and template‐based modeling: A CASP‐CAPRI experiment”, Proteins: Structure, Function, and Bioinformatics, vol. 84, no. S1. Wiley, pp. 323–348, Jun. 2016. doi: 10.1002/prot.25007.*  
  
*N. A. Marze, J. R. Jeliazkov, S. S. Roy Burman, S. E. Boyken, F. DiMaioand J. J. Gray, “Modeling oblong proteins and water-mediated interfaces with RosettaDock in CAPRI rounds 28-35”, Proteins: Structure, Function, and Bioinformatics, vol. 85, no. 3. Wiley, pp. 479–486, Oct. 24, 2016. doi: 10.1002/prot.25168.*  
  
*N. A. Marze, S. Lyskovand J. J. Gray, “Improved prediction of antibody VL–VHorientation”, Protein Engineering Design and Selection, vol. 29, no. 10. Oxford University Press (OUP), pp. 409–418, Jun. 08, 2016. doi: 10.1093/protein/gzw013.*  
  
*B. D. Weitzner, R. L. Dunbrack Jr.and J. J. Gray, “The Origin of CDR H3 Structural Diversity”, Structure, vol. 23, no. 2. Elsevier BV, pp. 302–311, Feb. 2015. doi: 10.1016/j.str.2014.11.010.*  
  
*B. D. Weitzner and J. J. Gray, “Accurate Structure Prediction of CDR H3 Loops Enabled by a Novel Structure-Based C-Terminal Constraint”, The Journal of Immunology, vol. 198, no. 1. The American Association of Immunologists, pp. 505–515, Jan. 01, 2017. doi: 10.4049/jimmunol.1601137.*  
  
*B. D. Weitzner, “Modeling and docking of antibody structures with Rosetta”, Nature Protocols, vol. 12, no. 2. Springer Science and Business Media LLC, pp. 401–416, Jan. 26, 2017. doi: 10.1038/nprot.2016.180.*  
  
*B. D. Weitzner, D. Kuroda, N. Marze, J. Xuand J. J. Gray, “Blind prediction performance of RosettaAntibody 3.0: Grafting, relaxation, kinematic loop modeling, and full CDR optimization”, Proteins: Structure, Function, and Bioinformatics, vol. 82, no. 8. Wiley, pp. 1611–1623, Mar. 31, 2014. doi: 10.1002/prot.24534.*  
  
*I. G. Gould and A. A. Linninger, “Hematocrit Distribution and Tissue Oxygenation in Large Microcirculatory Networks”, Microcirculation, vol. 22, no. 1. Wiley, pp. 1–18, Jan. 2015. doi: 10.1111/micc.12156.*  
  
*A. A. Linninger, I. G. Gould, T. Marinnan, C.-Y. Hsu, M. Chojeckiand A. Alaraj, “Cerebral Microcirculation and Oxygen Tension in the Human Secondary Cortex”, Annals of Biomedical Engineering, vol. 41, no. 11. Springer Science and Business Media LLC, pp. 2264–2284, Jul. 11, 2013. doi: 10.1007/s10439-013-0828-0.*  
  
*D. Leung, “Integrative analysis of haplotype-resolved epigenomes across human tissues”, Nature, vol. 518, no. 7539. Springer Science and Business Media LLC, pp. 350–354, Feb. 18, 2015. doi: 10.1038/nature14217.*  
  
*M. D. Schultz, “Human body epigenome maps reveal noncanonical DNA methylation variation”, Nature, vol. 523, no. 7559. Springer Science and Business Media LLC, pp. 212–216, Jun. 01, 2015. doi: 10.1038/nature14465.*  
  
*C.-Y. Yang, “Identification of Potential Small Molecule Allosteric Modulator Sites on IL-1R1 Ectodomain Using Accelerated Conformational Sampling Method”, PLOS ONE, vol. 10, no. 2. Public Library of Science (PLoS), p. e0118671, Feb. 23, 2015. doi: 10.1371/journal.pone.0118671.*  
  
*C.-Y. Yang, “Conformational Sampling and Binding Site Assessment of Suppression of Tumorigenicity 2 Ectodomain”, PLOS ONE, vol. 11, no. 1. Public Library of Science (PLoS), p. e0146522, Jan. 06, 2016. doi: 10.1371/journal.pone.0146522.*  
  
*A. M. Jongco, “X-linked agammaglobulinemia presenting as polymicrobial pneumonia, including Pneumocystis jirovecii”, Annals of Allergy, Asthma & Immunology, vol. 112, no. 1. Elsevier BV, pp. 74–75.e2, Jan. 2014. doi: 10.1016/j.anai.2013.10.008.*  
  
*N. G. Crawford, “A phylogenomic analysis of turtles”, Molecular Phylogenetics and Evolution, vol. 83. Elsevier BV, pp. 250–257, Feb. 2015. doi: 10.1016/j.ympev.2014.10.021.*  
  
*R. J. Dotson, C. R. Smith, K. Bueche, G. Anglesand S. C. Pias, “Influence of Cholesterol on the Oxygen Permeability of Membranes: Insight from Atomistic Simulations”, Biophysical Journal, vol. 112, no. 11. Elsevier BV, pp. 2336–2347, Jun. 2017. doi: 10.1016/j.bpj.2017.04.046.*  
  
*R. Shea, C. Smithand S. C. Pias, “Magnification of Cholesterol-Induced Membrane Resistance on the Tissue Level: Implications for Hypoxia”, Advances in Experimental Medicine and Biology. Springer International Publishing, pp. 43–50, 2016. doi: 10.1007/978-3-319-38810-6\_6.*  
  
*W. Feinstein and M. Brylinski, “Structure-Based Drug Discovery Accelerated by Many-Core Devices”, Current Drug Targets, vol. 17, no. 14. Bentham Science Publishers Ltd., pp. 1595–1609, Sep. 30, 2016. doi: 10.2174/1389450117666160112112854.*  
  
*W. P. Feinstein and M. Brylinski, “Calculating an optimal box size for ligand docking and virtual screening against experimental and predicted binding pockets”, Journal of Cheminformatics, vol. 7, no. 1. Springer Science and Business Media LLC, May 15, 2015. doi: 10.1186/s13321-015-0067-5.*  
  
*W. P. Feinstein, J. Moreno, M. Jarrelland M. Brylinski, “Accelerating the Pace of Protein Functional Annotation With Intel Xeon Phi Coprocessors”, IEEE Transactions on NanoBioscience, vol. 14, no. 4. Institute of Electrical and Electronics Engineers (IEEE), pp. 429–439, Jun. 2015. doi: 10.1109/tnb.2015.2403776.*  
  
*B. R. Miller, C. A. Parishand E. Y. Wu, “Molecular Dynamics Study of the Opening Mechanism for DNA Polymerase I”, PLoS Computational Biology, vol. 10, no. 12. Public Library of Science (PLoS), p. e1003961, Dec. 04, 2014. doi: 10.1371/journal.pcbi.1003961.*  
  
*M. S. Jahan Sajib, P. Sarker, Y. Wei, X. Taoand T. Wei, “Protein Corona on Gold Nanoparticles Studied with Coarse-Grained Simulations”, Langmuir, vol. 36, no. 44. American Chemical Society (ACS), pp. 13356–13363, Oct. 30, 2020. doi: 10.1021/acs.langmuir.0c02767.*  
  
*C. Masato Nakano, M. S. J. Sajib, M. Samieegoharand T. Wei, “Field-induced stacking transition of biofunctionalized trilayer graphene”, Applied Physics Letters, vol. 108, no. 5. AIP Publishing, p. 051601, Feb. 2016. doi: 10.1063/1.4940893.*  
  
*C. M. Nakano, “iBET: Immersive visualization of biological electron-transfer dynamics”, Journal of Molecular Graphics and Modelling, vol. 65. Elsevier BV, pp. 94–99, Apr. 2016. doi: 10.1016/j.jmgm.2016.02.009.*  
  
*M. Samieegohar, F. Sha, A. Z. Clayborneand T. Wei, “ReaxFF MD Simulations of Peptide-Grafted Gold Nanoparticles”, Langmuir, vol. 35, no. 14. American Chemical Society (ACS), pp. 5029–5036, Mar. 14, 2019. doi: 10.1021/acs.langmuir.8b03951.*  
  
*N. P. van der Munnik, M. S. J. Sajib, M. A. Moss, T. Weiand M. J. Uline, “Determining the Potential of Mean Force for Amyloid-β Dimerization: Combining Self-Consistent Field Theory with Molecular Dynamics Simulation”, Journal of Chemical Theory and Computation, vol. 14, no. 5. American Chemical Society (ACS), pp. 2696–2704, Mar. 21, 2018. doi: 10.1021/acs.jctc.7b01057.*  
  
*T. Wei, H. Maand A. Nakano, “Decaheme Cytochrome MtrF Adsorption and Electron Transfer on Gold Surface”, The Journal of Physical Chemistry Letters, vol. 7, no. 5. American Chemical Society (ACS), pp. 929–936, Feb. 24, 2016. doi: 10.1021/acs.jpclett.5b02746.*  
  
*T. Wei, M. S. J. Sajib, M. Samieegohar, H. Maand K. Shing, “Self-Assembled Monolayers of an Azobenzene Derivative on Silica and Their Interactions with Lysozyme”, Langmuir, vol. 31, no. 50. American Chemical Society (ACS), pp. 13543–13552, Dec. 10, 2015. doi: 10.1021/acs.langmuir.5b03603.*  
  
*T. Wei, “Aromatic Polyamide Reverse-Osmosis Membrane: An Atomistic Molecular Dynamics Simulation”, The Journal of Physical Chemistry B, vol. 120, no. 39. American Chemical Society (ACS), pp. 10311–10318, Sep. 28, 2016. doi: 10.1021/acs.jpcb.6b06560.*  
  
*C. M. Nakano, H. Maand T. Wei, “Study of lysozyme mobility and binding free energy during adsorption on a graphene surface”, Applied Physics Letters, vol. 106, no. 15. AIP Publishing, p. 153701, Apr. 13, 2015. doi: 10.1063/1.4918292.*  
  
*M. S. J. Sajib, M. Samieegohar, T. Weiand K. Shing, “Atomic-Level Simulation Study of n-Hexane Pyrolysis on Silicon Carbide Surfaces”, Langmuir, vol. 33, no. 42. American Chemical Society (ACS), pp. 11102–11108, Oct. 03, 2017. doi: 10.1021/acs.langmuir.7b03102.*  
  
*M. Samieegohar, H. Ma, F. Sha, M. S. Jahan Sajib, G. I. Guerrero-Garcíaand T. Wei, “Understanding the interfacial behavior of lysozyme on Au (111) surfaces with multiscale simulations”, Applied Physics Letters, vol. 110, no. 7. AIP Publishing, p. 073703, Feb. 13, 2017. doi: 10.1063/1.4976516.*  
  
*T. Zhang, “Protein–Ligand Interaction Detection with a Novel Method of Transient Induced Molecular Electronic Spectroscopy (TIMES): Experimental and Theoretical Studies”, ACS Central Science, vol. 2, no. 11. American Chemical Society (ACS), pp. 834–842, Oct. 24, 2016. doi: 10.1021/acscentsci.6b00217.*  
  
*K. J. Boyd, P. Bansal, J. Fengand E. R. May, “Stability of Norwalk Virus Capsid Protein Interfaces Evaluated by in Silico Nanoindentation”, Frontiers in Bioengineering and Biotechnology, vol. 3. Frontiers Media SA, Jul. 30, 2015. doi: 10.3389/fbioe.2015.00103.*  
  
*S. Nangia and E. R. May, “Influence of membrane composition on the binding and folding of a membrane lytic peptide from the non-enveloped flock house virus”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1859, no. 7. Elsevier BV, pp. 1190–1199, Jul. 2017. doi: 10.1016/j.bbamem.2017.04.002.*  
  
*S. Nangia, J. G. Pattisand E. R. May, “Folding a viral peptide in different membrane environments: pathway and sampling analyses”, Journal of Biological Physics, vol. 44, no. 2. Springer Science and Business Media LLC, pp. 195–209, Apr. 11, 2018. doi: 10.1007/s10867-018-9490-y.*  
  
*J. G. Pattis and E. R. May, “Influence of RNA Binding on the Structure and Dynamics of the Lassa Virus Nucleoprotein”, Biophysical Journal, vol. 110, no. 6. Elsevier BV, pp. 1246–1254, Mar. 2016. doi: 10.1016/j.bpj.2016.02.008.*  
  
*M. D. Ward, S. Nangiaand E. R. May, “Evaluation of the hybrid resolution PACE model for the study of folding, insertion, and pore formation of membrane associated peptides”, Journal of Computational Chemistry, vol. 38, no. 16. Wiley, pp. 1462–1471, Jan. 19, 2017. doi: 10.1002/jcc.24694.*  
  
*A. T. Fenley, N. M. Henriksen, H. S. Muddanaand M. K. Gilson, “Bridging Calorimetry and Simulation through Precise Calculations of Cucurbituril–Guest Binding Enthalpies”, Journal of Chemical Theory and Computation, vol. 10, no. 9. American Chemical Society (ACS), pp. 4069–4078, Aug. 01, 2014. doi: 10.1021/ct5004109.*  
  
*K. Gao, J. Yin, N. M. Henriksen, A. T. Fenleyand M. K. Gilson, “Binding Enthalpy Calculations for a Neutral Host–Guest Pair Yield Widely Divergent Salt Effects across Water Models”, Journal of Chemical Theory and Computation, vol. 11, no. 10. American Chemical Society (ACS), pp. 4555–4564, Sep. 18, 2015. doi: 10.1021/acs.jctc.5b00676.*  
  
*N. M. Henriksen, A. T. Fenleyand M. K. Gilson, “Computational Calorimetry: High-Precision Calculation of Host–Guest Binding Thermodynamics”, Journal of Chemical Theory and Computation, vol. 11, no. 9. American Chemical Society (ACS), pp. 4377–4394, Aug. 26, 2015. doi: 10.1021/acs.jctc.5b00405.*  
  
*J. Yin, A. T. Fenley, N. M. Henriksenand M. K. Gilson, “Toward Improved Force-Field Accuracy through Sensitivity Analysis of Host-Guest Binding Thermodynamics”, The Journal of Physical Chemistry B, vol. 119, no. 32. American Chemical Society (ACS), pp. 10145–10155, Aug. 05, 2015. doi: 10.1021/acs.jpcb.5b04262.*  
  
*D. R. Barden and H. Vashisth, “Parameterization and atomistic simulations of biomimetic membranes”, Faraday Discussions, vol. 209. Royal Society of Chemistry (RSC), pp. 161–178, 2018. doi: 10.1039/c8fd00047f.*  
  
*Y.-. xiao . Shen, “Achieving high permeability and enhanced selectivity for Angstrom-scale separations using artificial water channel membranes”, Nature Communications, vol. 9, no. 1. Springer Science and Business Media LLC, Jun. 12, 2018. doi: 10.1038/s41467-018-04604-y.*  
  
*J. Wei, L. Czapla, M. A. Grosner, D. Swigonand W. K. Olson, “DNA topology confers sequence specificity to nonspecific architectural proteins”, Proceedings of the National Academy of Sciences, vol. 111, no. 47. Proceedings of the National Academy of Sciences, pp. 16742–16747, Nov. 10, 2014. doi: 10.1073/pnas.1405016111.*  
  
*A. Kapoor and A. Travesset, “Differential dynamics of RAS isoforms in GDP- and GTP-bound states”, Proteins: Structure, Function, and Bioinformatics, vol. 83, no. 6. Wiley, pp. 1091–1106, Apr. 22, 2015. doi: 10.1002/prot.24805.*  
  
*A. Kapoor and A. Travesset, “Mechanism of the Exchange Reaction in HRAS from Multiscale Modeling”, PLoS ONE, vol. 9, no. 10. Public Library of Science (PLoS), p. e108846, Oct. 01, 2014. doi: 10.1371/journal.pone.0108846.*  
  
*O. Laptenko, “The p53 C Terminus Controls Site-Specific DNA Binding and Promotes Structural Changes within the Central DNA Binding Domain”, Molecular Cell, vol. 57, no. 6. Elsevier BV, pp. 1034–1046, Mar. 2015. doi: 10.1016/j.molcel.2015.02.015.*  
  
*N. T. Pfister, “Mutant p53 cooperates with the SWI/SNF chromatin remodeling complex to regulate VEGFR2 in breast cancer cells”, Genes & Development, vol. 29, no. 12. Cold Spring Harbor Laboratory, pp. 1298–1315, Jun. 15, 2015. doi: 10.1101/gad.263202.115.*  
  
*Y. Zhu, K. Regunath, X. Jacqand C. Prives, “Cisplatin causes cell death via TAB1 regulation of p53/MDM2/MDMX circuitry”, Genes & Development, vol. 27, no. 16. Cold Spring Harbor Laboratory, pp. 1739–1751, Aug. 09, 2013. doi: 10.1101/gad.212258.112.*  
  
*N. Alexandrov, “SNP-Seek database of SNPs derived from 3000 rice genomes”, Nucleic Acids Research, vol. 43, no. D1. Oxford University Press (OUP), pp. D1023–D1027, Nov. 27, 2014. doi: 10.1093/nar/gku1039.*  
  
*H. Leung, “Allele mining and enhanced genetic recombination for rice breeding”, Rice, vol. 8, no. 1. Springer Science and Business Media LLC, Nov. 25, 2015. doi: 10.1186/s12284-015-0069-y.*  
  
*Q. Luan, A. Zelter, M. J. MacCoss, T. N. Davisand B. J. Nolen, “Identification of Wiskott-Aldrich syndrome protein (WASP) binding sites on the branched actin filament nucleator Arp2/3 complex”, Proceedings of the National Academy of Sciences, vol. 115, no. 7. Proceedings of the National Academy of Sciences, Jan. 31, 2018. doi: 10.1073/pnas.1716622115.*  
  
*J. Li, K. F. Jaimesand S. G. Aller, “Refined structures of mouse P-glycoprotein”, Protein Science, vol. 23, no. 1. Wiley, pp. 34–46, Nov. 15, 2013. doi: 10.1002/pro.2387.*  
  
*L. Pan and S. G. Aller, “Equilibrated Atomic Models of Outward-Facing P-glycoprotein and Effect of ATP Binding on Structural Dynamics”, Scientific Reports, vol. 5, no. 1. Springer Science and Business Media LLC, Jan. 20, 2015. doi: 10.1038/srep07880.*  
  
*J. Glaser, X. Zha, J. A. Anderson, S. C. Glotzerand A. Travesset, “Pressure in rigid body molecular dynamics”, Computational Materials Science, vol. 173. Elsevier BV, p. 109430, Feb. 2020. doi: 10.1016/j.commatsci.2019.109430.*  
  
*A. Kapoor and A. Travesset, “Folding and stability of helical bundle proteins from coarse-grained models”, Proteins: Structure, Function, and Bioinformatics, vol. 81, no. 7. Wiley, pp. 1200–1211, Apr. 10, 2013. doi: 10.1002/prot.24269.*  
  
*E. Macias, T. Waltmannand A. Travesset, “Assembly of nanocrystal clusters by solvent evaporation: icosahedral order and the breakdown of the Maxwell regime”, Soft Matter, vol. 16, no. 31. Royal Society of Chemistry (RSC), pp. 7350–7358, 2020. doi: 10.1039/d0sm00838a.*  
  
*S. Nayak, “Ordered Networks of Gold Nanoparticles Crosslinked by Dithiol-Oligomers”, Particle & Particle Systems Characterization, vol. 35, no. 8. Wiley, p. 1800097, Jun. 19, 2018. doi: 10.1002/ppsc.201800097.*  
  
*S. Nayak, “Interpolymer Complexation as a Strategy for Nanoparticle Assembly and Crystallization”, The Journal of Physical Chemistry C, vol. 123, no. 1. American Chemical Society (ACS), pp. 836–840, Dec. 07, 2018. doi: 10.1021/acs.jpcc.8b09647.*  
  
*B. K. Patra, H. Agrawal, J.-Y. Zheng, X. Zha, A. Travessetand E. C. Garnett, “Close-Packed Ultrasmooth Self-assembled Monolayer of CsPbBr3 Perovskite Nanocubes”, ACS Applied Materials & Interfaces, vol. 12, no. 28. American Chemical Society (ACS), pp. 31764–31769, Jun. 17, 2020. doi: 10.1021/acsami.0c05945.*  
  
*M. Pham and A. Travesset, “Ligand structure and adsorption free energy of nanocrystals on solid substrates”, The Journal of Chemical Physics, vol. 153, no. 20. AIP Publishing, p. 204701, Nov. 28, 2020. doi: 10.1063/5.0030529.*  
  
*A. Travesset, “Soft Skyrmions, Spontaneous Valence and Selection Rules in Nanoparticle Superlattices”, ACS Nano, vol. 11, no. 6. American Chemical Society (ACS), pp. 5375–5382, May 19, 2017. doi: 10.1021/acsnano.7b02219.*  
  
*A. Travesset, “Nanoparticle Superlattices as Quasi-Frank-Kasper Phases”, Physical Review Letters, vol. 119, no. 11. American Physical Society (APS), Sep. 14, 2017. doi: 10.1103/physrevlett.119.115701.*  
  
*C. Waltmann, N. Horstand A. Travesset, “Capping Ligand Vortices as “Atomic Orbitals” in Nanocrystal Self-Assembly”, ACS Nano, vol. 11, no. 11. American Chemical Society (ACS), pp. 11273–11282, Oct. 31, 2017. doi: 10.1021/acsnano.7b05694.*  
  
*C. Waltmann, N. Horstand A. Travesset, “Potential of mean force for two nanocrystals: Core geometry and size, hydrocarbon unsaturation, and universality with respect to the force field”, The Journal of Chemical Physics, vol. 149, no. 3. AIP Publishing, p. 034109, Jul. 21, 2018. doi: 10.1063/1.5039495.*  
  
*T. Waltmann, C. Waltmann, N. Horstand A. Travesset, “Many Body Effects and Icosahedral Order in Superlattice Self-Assembly”, Journal of the American Chemical Society, vol. 140, no. 26. American Chemical Society (ACS), pp. 8236–8245, Jun. 15, 2018. doi: 10.1021/jacs.8b03895.*  
  
*X. Zha and A. Travesset, “Stability and Free Energy of Nanocrystal Chains and Superlattices”, The Journal of Physical Chemistry C, vol. 122, no. 40. American Chemical Society (ACS), pp. 23153–23164, Sep. 13, 2018. doi: 10.1021/acs.jpcc.8b06996.*  
  
*X. Zha and A. Travesset, “The hard sphere diameter of nanocrystals (nanoparticles)”, The Journal of Chemical Physics, vol. 152, no. 9. AIP Publishing, p. 094502, Mar. 07, 2020. doi: 10.1063/1.5132747.*  
  
*B. R. Miller III, L. S. Beese, C. A. Parishand E. Y. Wu, “The Closing Mechanism of DNA Polymerase I at Atomic Resolution”, Structure, vol. 23, no. 9. Elsevier BV, pp. 1609–1620, Sep. 2015. doi: 10.1016/j.str.2015.06.016.*  
  
*E. Y. Wu, “A Conservative Isoleucine to Leucine Mutation Causes Major Rearrangements and Cold Sensitivity in KlenTaq1 DNA Polymerase”, Biochemistry, vol. 54, no. 3. American Chemical Society (ACS), pp. 881–889, Jan. 09, 2015. doi: 10.1021/bi501198f.*  
  
*A. Yeager, K. Humphries, E. Farmer, G. Clineand B. R. Miller III, “Investigation of Nascent Base Pair and Polymerase Behavior in the Presence of Mismatches in DNA Polymerase I Using Molecular Dynamics”, Journal of Chemical Information and Modeling, vol. 58, no. 2. American Chemical Society (ACS), pp. 338–349, Jan. 12, 2018. doi: 10.1021/acs.jcim.7b00516.*  
  
*A. V. Yeager, J. M. Swailsand B. R. Miller III, “Improved Accuracy for Constant pH-REMD Simulations through Modification of Carboxylate Effective Radii”, Journal of Chemical Theory and Computation, vol. 13, no. 10. American Chemical Society (ACS), pp. 4624–4635, Sep. 29, 2017. doi: 10.1021/acs.jctc.7b00638.*  
  
*H. Amir, “Spontaneous Single-Copy Loss of TP53 in Human Embryonic Stem Cells Markedly Increases Cell Proliferation and Survival”, Stem Cells, vol. 35, no. 4. Oxford University Press (OUP), pp. 872–885, Jan. 19, 2017. doi: 10.1002/stem.2550.*  
  
*R. Gonzalez, “Proof of Concept Studies Exploring the Safety and Functional Activity of Human Parthenogenetic-Derived Neural Stem Cells for the Treatment of Parkinson’s Disease”, Cell Transplantation, vol. 24, no. 4. SAGE Publications, pp. 681–690, Apr. 2015. doi: 10.3727/096368915x687769.*  
  
*H. Ma, “Metabolic rescue in pluripotent cells from patients with mtDNA disease”, Nature, vol. 524, no. 7564. Springer Science and Business Media LLC, pp. 234–238, Jul. 15, 2015. doi: 10.1038/nature14546.*  
  
*H. Ma, “Abnormalities in human pluripotent cells due to reprogramming mechanisms”, Nature, vol. 511, no. 7508. Springer Science and Business Media LLC, pp. 177–183, Jul. 02, 2014. doi: 10.1038/nature13551.*  
  
*S. Mora-Castilla, “Miniaturization Technologies for Efficient Single-Cell Library Preparation for Next-Generation Sequencing”, SLAS Technology, vol. 21, no. 4. Elsevier BV, pp. 557–567, Aug. 2016. doi: 10.1177/2211068216630741.*  
  
*L. Szabo, “Statistically based splicing detection reveals neural enrichment and tissue-specific induction of circular RNA during human fetal development”, Genome Biology, vol. 16, no. 1. Springer Science and Business Media LLC, Jun. 16, 2015. doi: 10.1186/s13059-015-0690-5.*  
  
*T. Touboul, “Stage-specific regulation of the WNT/β-catenin pathway enhances differentiation of hESCs into hepatocytes”, Journal of Hepatology, vol. 64, no. 6. Elsevier BV, pp. 1315–1326, Jun. 2016. doi: 10.1016/j.jhep.2016.02.028.*  
  
*A. Yokoi, “Mechanisms of nuclear content loading to exosomes”, Science Advances, vol. 5, no. 11. American Association for the Advancement of Science (AAAS), Nov. 2019. doi: 10.1126/sciadv.aax8849.*  
  
*T. Zdravkovic, “Human stem cells from single blastomeres reveal pathways of Embryonic or trophoblast fate specification”, Development. The Company of Biologists, Jan. 01, 2015. doi: 10.1242/dev.122846.*  
  
*M. Alwarawrah and J. Wereszczynski, “Investigation of the Effect of Bilayer Composition on PKCα-C2 Domain Docking Using Molecular Dynamics Simulations”, The Journal of Physical Chemistry B, vol. 121, no. 1. American Chemical Society (ACS), pp. 78–88, Dec. 20, 2016. doi: 10.1021/acs.jpcb.6b10188.*  
  
*S. Bowerman, R. J. Hickokand J. Wereszczynski, “Unique Dynamics in Asymmetric macroH2A–H2A Hybrid Nucleosomes Result in Increased Complex Stability”, The Journal of Physical Chemistry B, vol. 123, no. 2. American Chemical Society (ACS), pp. 419–427, Dec. 17, 2018. doi: 10.1021/acs.jpcb.8b10668.*  
  
*S. Bowerman, A. S. J. B. Rana, A. Rice, G. H. Pham, E. R. Strieterand J. Wereszczynski, “Determining Atomistic SAXS Models of Tri-Ubiquitin Chains from Bayesian Analysis of Accelerated Molecular Dynamics Simulations”, Journal of Chemical Theory and Computation, vol. 13, no. 6. American Chemical Society (ACS), pp. 2418–2429, May 17, 2017. doi: 10.1021/acs.jctc.7b00059.*  
  
*S. Bowerman and J. Wereszczynski, “Detecting Allosteric Networks Using Molecular Dynamics Simulation”, Methods in Enzymology. Elsevier, pp. 429–447, 2016. doi: 10.1016/bs.mie.2016.05.027.*  
  
*S. Bowerman and J. Wereszczynski, “Effects of MacroH2A and H2A.Z on Nucleosome Dynamics as Elucidated by Molecular Dynamics Simulations”, Biophysical Journal, vol. 110, no. 2. Elsevier BV, pp. 327–337, Jan. 2016. doi: 10.1016/j.bpj.2015.12.015.*  
  
*A. W. Jacobitz, “The “Lid” in the Streptococcus pneumoniae SrtC1 Sortase Adopts a Rigid Structure that Regulates Substrate Access to the Active Site”, The Journal of Physical Chemistry B, vol. 120, no. 33. American Chemical Society (ACS), pp. 8302–8312, May 05, 2016. doi: 10.1021/acs.jpcb.6b01930.*  
  
*K. M. Ma, E. S. Thomas, J. Wereszczynskiand N. Menhart, “Empirical and Computational Comparison of Alternative Therapeutic Exon Skip Repairs for Duchenne Muscular Dystrophy”, Biochemistry, vol. 58, no. 15. American Chemical Society (ACS), pp. 2061–2076, Mar. 21, 2019. doi: 10.1021/acs.biochem.9b00062.*  
  
*E. A. Morrison, S. Bowerman, K. L. Sylvers, J. Wereszczynskiand C. A. Musselman, “The conformation of the histone H3 tail inhibits association of the BPTF PHD finger with the nucleosome”, eLife, vol. 7. eLife Sciences Publications, Ltd, Apr. 12, 2018. doi: 10.7554/elife.31481.*  
  
*E. B. Naziga and J. Wereszczynski, “Molecular Mechanisms of the Binding and Specificity of Streptococcus Pneumoniae Sortase C Enzymes for Pilin Subunits”, Scientific Reports, vol. 7, no. 1. Springer Science and Business Media LLC, Oct. 13, 2017. doi: 10.1038/s41598-017-13135-3.*  
  
*A. Rice and J. Wereszczynski, “Probing the disparate effects of arginine and lysine residues on antimicrobial peptide/bilayer association”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1859, no. 10. Elsevier BV, pp. 1941–1950, Oct. 2017. doi: 10.1016/j.bbamem.2017.06.002.*  
  
*M. R. Ali and M. Mezei, “Quantum Signature of Anisotropic Singularities in Hydrogen Bond Breaking of Water Dimer”, []. Research Square Platform LLC, Jul. 09, 2020. doi: 10.21203/rs.3.rs-40070/v1.*  
  
*M. R. Ali and M. Mezei, “Observation of quantum signature in rivastigmine chemical bond break-up and quantum energetics, spectral studies of anti-Alzheimer inhibitors”, Journal of Biomolecular Structure and Dynamics, vol. 39, no. 1. Informa UK Limited, pp. 118–128, Jan. 10, 2020. doi: 10.1080/07391102.2019.1708462.*  
  
*M. R. Ali, M. Sadoqi, S. G. Møller, A. Boutajangoutand M. Mezei, “Assessing the binding of cholinesterase inhibitors by docking and molecular dynamics studies”, Journal of Molecular Graphics and Modelling, vol. 76. Elsevier BV, pp. 36–42, Sep. 2017. doi: 10.1016/j.jmgm.2017.06.027.*  
  
*R. Latif, “New Small Molecule Agonists to the Thyrotropin Receptor”, Thyroid, vol. 25, no. 1. Mary Ann Liebert Inc, pp. 51–62, Jan. 2015. doi: 10.1089/thy.2014.0119.*  
  
*M. Rejwan Ali, M. Sadoqi, A. Boutajangoutand M. Mezei, “Virtual screening of a natural compound library at orthosteric and allosteric binding sites of the neurotensin receptor”, Journal of Biomolecular Structure and Dynamics, vol. 37, no. 17. Informa UK Limited, pp. 4494–4506, Jan. 09, 2019. doi: 10.1080/07391102.2018.1552200.*  
  
*J. Chen, C. Lewis, D. Balamurugan, Z. Yang, L. Aiand D. Cai, “Theoretical analysis of a high performance protein imprint on a nanosensor”, Sensing and Bio-Sensing Research, vol. 7. Elsevier BV, pp. 12–19, Mar. 2016. doi: 10.1016/j.sbsr.2015.11.009.*  
  
*A. M. Smith, C. Papaleo, C. W. Reidand J. M. Bliss, “RNA-Seq reveals a central role for lectin, C1q and von Willebrand factor A domains in the defensive glue of a terrestrial slug”, Biofouling, vol. 33, no. 9. Informa UK Limited, pp. 741–754, Sep. 13, 2017. doi: 10.1080/08927014.2017.1361413.*  
  
*T. T. Joseph and J. S. Mincer, “Common Internal Allosteric Network Links Anesthetic Binding Sites in a Pentameric Ligand-Gated Ion Channel”, PLOS ONE, vol. 11, no. 7. Public Library of Science (PLoS), p. e0158795, Jul. 12, 2016. doi: 10.1371/journal.pone.0158795.*  
  
*K. A. Ball, “Non-degradative Ubiquitination of Protein Kinases”, PLOS Computational Biology, vol. 12, no. 6. Public Library of Science (PLoS), p. e1004898, Jun. 02, 2016. doi: 10.1371/journal.pcbi.1004898.*  
  
*C. R. Chen and G. I. Makhatadze, “ProteinVolume: calculating molecular van der Waals and void volumes in proteins”, BMC Bioinformatics, vol. 16, no. 1. Springer Science and Business Media LLC, Mar. 26, 2015. doi: 10.1186/s12859-015-0531-2.*  
  
*C. R. Chen and G. I. Makhatadze, “Molecular determinant of the effects of hydrostatic pressure on protein folding stability”, Nature Communications, vol. 8, no. 1. Springer Science and Business Media LLC, Feb. 07, 2017. doi: 10.1038/ncomms14561.*  
  
*S. Tripathi, A. E. Garcìaand G. I. Makhatadze, “Alterations of Nonconserved Residues Affect Protein Stability and Folding Dynamics through Charge–Charge Interactions”, The Journal of Physical Chemistry B, vol. 119, no. 41. American Chemical Society (ACS), pp. 13103–13112, Oct. 02, 2015. doi: 10.1021/acs.jpcb.5b08527.*  
  
*F. O. Tzul, K. L. Schweikerand G. I. Makhatadze, “Modulation of folding energy landscape by charge–charge interactions: Linking experiments with computational modeling”, Proceedings of the National Academy of Sciences, vol. 112, no. 3. Proceedings of the National Academy of Sciences, Jan. 06, 2015. doi: 10.1073/pnas.1410424112.*  
  
*L. Ingber, “Quantum Calcium-Ion Affective Influences Measured by EEG”, []. MDPI AG, Sep. 25, 2020. doi: 10.20944/preprints202009.0591.v1.*  
  
*L. Ingber, “Revisiting Our Quantum World”, []. MDPI AG, Sep. 25, 2020. doi: 10.20944/preprints202009.0590.v1.*  
  
*L. Ingber, “Forecasting COVID-19 with Importance-Sampling and Path-Integrals”, []. MDPI AG, Dec. 29, 2020. doi: 10.20944/preprints202012.0712.v1.*  
  
*H. Aguiar e Oliveira Junior, L. Ingber, A. Petraglia, M. Rembold Petragliaand M. Augusta Soares Machado, Stochastic Global Optimization and Its Applications with Fuzzy Adaptive Simulated Annealing. Springer Berlin Heidelberg, 2012. doi: 10.1007/978-3-642-27479-4.*  
  
*H. Aguiar e Oliveira Junior, L. Ingber, A. Petraglia, M. Rembold Petragliaand M. Augusta Soares Machado, Stochastic Global Optimization and Its Applications with Fuzzy Adaptive Simulated Annealing. Springer Berlin Heidelberg, 2012. doi: 10.1007/978-3-642-27479-4.*  
  
*L. Ingber, “Developing Bid-Ask Probabilities for High-Frequency Trading”, Virtual Economics, vol. 3, no. 2. The London Academy of Science and Business Limited, pp. 7–24, Apr. 30, 2020. doi: 10.34021/ve.2020.03.02(1).*  
  
*L. Ingber, “Computational Algorithms Derived from Multiple Scales of Neocortical Processing”, Cognitive Computation, vol. 4, no. 1. Springer Science and Business Media LLC, pp. 38–50, Aug. 05, 2011. doi: 10.1007/s12559-011-9105-4.*  
  
*L. Ingber, M. Pappaleporeand R. R. Stesiak, “Electroencephalographic field influence on calcium momentum waves”, Journal of Theoretical Biology, vol. 343. Elsevier BV, pp. 138–153, Feb. 2014. doi: 10.1016/j.jtbi.2013.11.002.*  
  
*L. Ingber, “Statistical mechanics of neocortical interactions: Large-scale EEG influences on molecular processes”, Journal of Theoretical Biology, vol. 395. Elsevier BV, pp. 144–152, Apr. 2016. doi: 10.1016/j.jtbi.2016.02.003.*  
  
*P. L. Nunez, R. Srinivasanand L. Ingber, “Theoretical and Experimental Electrophysiology in Human Neocortex: Multiscale Dynamic Correlates of Conscious Experience”, Multiscale Analysis and Nonlinear Dynamics. Wiley, pp. 147–177, Jul. 31, 2013. doi: 10.1002/9783527671632.ch06.*  
  
*R. Richards and R. E. Dempski, “Cysteine Substitution and Labeling Provide Insight into Channelrhodopsin-2 Ion Conductance”, Biochemistry, vol. 54, no. 37. American Chemical Society (ACS), pp. 5665–5668, Sep. 08, 2015. doi: 10.1021/acs.biochem.5b00738.*  
  
*R. Richards and R. E. Dempski, “Adjacent channelrhodopsin-2 residues within transmembranes 2 and 7 regulate cation selectivity and distribution of the two open states”, Journal of Biological Chemistry, vol. 292, no. 18. Elsevier BV, pp. 7314–7326, Mar. 2017. doi: 10.1074/jbc.m116.770321.*  
  
*A. M. Tarrant, M. F. Baumgartner, B. H. Hansen, D. Altin, T. Nordtugand A. J. Olsen, “Transcriptional profiling of reproductive development, lipid storage and molting throughout the last juvenile stage of the marine copepod Calanus finmarchicus”, Frontiers in Zoology, vol. 11, no. 1. Springer Science and Business Media LLC, Dec. 2014. doi: 10.1186/s12983-014-0091-8.*  
  
*Z. Tan, E. Gallicchio, M. Lapelosaand R. M. Levy, “Theory of binless multi-state free energy estimation with applications to protein-ligand binding”, The Journal of Chemical Physics, vol. 136, no. 14. AIP Publishing, p. 144102, Apr. 14, 2012. doi: 10.1063/1.3701175.*  
  
*E. E. Grintsevich, “Catastrophic disassembly of actin filaments via Mical-mediated oxidation”, Nature Communications, vol. 8, no. 1. Springer Science and Business Media LLC, Dec. 19, 2017. doi: 10.1038/s41467-017-02357-8.*  
  
*N. Poweleit, P. Ge, H. H. Nguyen, R. R. O. Loo, R. P. Gunsalusand Z. H. Zhou, “CryoEM structure of the Methanospirillum hungatei archaellum reveals structural features distinct from the bacterial flagellum and type IV pilus”, Nature Microbiology, vol. 2, no. 3. Springer Science and Business Media LLC, Dec. 05, 2016. doi: 10.1038/nmicrobiol.2016.222.*  
  
*P. Aprikian, “The Bacterial Fimbrial Tip Acts as a Mechanical Force Sensor”, PLoS Biology, vol. 9, no. 5. Public Library of Science (PLoS), p. e1000617, May 10, 2011. doi: 10.1371/journal.pbio.1000617.*  
  
*J. E. Baio, “Probing albumin adsorption onto calcium phosphates by x-ray photoelectron spectroscopy and time-of-flight secondary ion mass spectrometry”, Journal of Vacuum Science & Technology B, Nanotechnology and Microelectronics: Materials, Processing, Measurement, and Phenomena, vol. 29, no. 4. American Vacuum Society, pp. 04D113, Jul. 2011. doi: 10.1116/1.3613919.*  
  
*J. Chen, “Variable content of von Willebrand factor mutant monomer drives the phenotypic variability in a family with von Willebrand disease”, Blood, vol. 126, no. 2. American Society of Hematology, pp. 262–269, Jul. 09, 2015. doi: 10.1182/blood-2014-11-613935.*  
  
*M. A. Grant, “Identification of extant vertebrate Myxine glutinosa VWF: evolutionary conservation of primary hemostasis”, Blood, vol. 130, no. 23. American Society of Hematology, pp. 2548–2558, Dec. 07, 2017. doi: 10.1182/blood-2017-02-770792.*  
  
*G. Interlandi, “Destabilization of the von Willebrand factor A2 domain under oxidizing conditions investigated by molecular dynamics simulations”, PLOS ONE, vol. 13, no. 9. Public Library of Science (PLoS), p. e0203675, Sep. 17, 2018. doi: 10.1371/journal.pone.0203675.*  
  
*G. Interlandi, M. Ling, A. Y. Tu, D. W. Chungand W. E. Thomas, “Structural Basis of Type 2A von Willebrand Disease Investigated by Molecular Dynamics Simulations and Experiments”, PLoS ONE, vol. 7, no. 10. Public Library of Science (PLoS), p. e45207, Oct. 23, 2012. doi: 10.1371/journal.pone.0045207.*  
  
*G. Interlandi and W. Thomas, “The catch bond mechanism between von Willebrand factor and platelet surface receptors investigated by molecular dynamics simulations”, Proteins: Structure, Function, and Bioinformatics. Wiley, p. n/a–n/a, Apr. 28, 2010. doi: 10.1002/prot.22759.*  
  
*G. Interlandi, “Specific electrostatic interactions between charged amino acid residues regulate binding of von Willebrand factor to blood platelets”, Journal of Biological Chemistry, vol. 292, no. 45. Elsevier BV, pp. 18608–18617, Nov. 2017. doi: 10.1074/jbc.m117.797456.*  
  
*D. I. Kisiela, “Inhibition and Reversal of Microbial Attachment by an Antibody with Parasteric Activity against the FimH Adhesin of Uropathogenic E. coli”, PLOS Pathogens, vol. 11, no. 5. Public Library of Science (PLoS), p. e1004857, May 14, 2015. doi: 10.1371/journal.ppat.1004857.*  
  
*I. Le Trong, “Structural Basis for Mechanical Force Regulation of the Adhesin FimH via Finger Trap-like β Sheet Twisting”, Cell, vol. 141, no. 4. Elsevier BV, pp. 645–655, May 2010. doi: 10.1016/j.cell.2010.03.038.*  
  
*Y. Liu, “Tight Conformational Coupling between the Domains of the Enterotoxigenic Escherichia coli Fimbrial Adhesin CfaE Regulates Binding State Transition”, Journal of Biological Chemistry, vol. 288, no. 14. Elsevier BV, pp. 9993–10001, Apr. 2013. doi: 10.1074/jbc.m112.413534.*  
  
*E. N. Pederson and G. Interlandi, “Oxidation‐induced destabilization of the fibrinogen α C‐domain dimer investigated by molecular dynamics simulations”, Proteins: Structure, Function, and Bioinformatics, vol. 87, no. 10. Wiley, pp. 826–836, Jun. 14, 2019. doi: 10.1002/prot.25746.*  
  
*V. B. Rodriguez, B. A. Kidd, G. Interlandi, V. Tchesnokova, E. V. Sokurenkoand W. E. Thomas, “Allosteric Coupling in the Bacterial Adhesive Protein FimH”, Journal of Biological Chemistry, vol. 288, no. 33. Elsevier BV, pp. 24128–24139, Aug. 2013. doi: 10.1074/jbc.m113.461376.*  
  
*M. Yagi, “Heparin modulates the conformation and signaling of platelet integrin αIIbβ3”, Thrombosis Research, vol. 129, no. 6. Elsevier BV, pp. 743–749, Jun. 2012. doi: 10.1016/j.thromres.2011.11.054.*  
  
*N. Akyuz, “Transport domain unlocking sets the uptake rate of an aspartate transporter”, Nature, vol. 518, no. 7537. Springer Science and Business Media LLC, pp. 68–73, Feb. 2015. doi: 10.1038/nature14158.*  
  
*M. A. Cuendet, S. Stolzenberg, G. Khelashviliand H. Weinstein, “Molecular Dynamics Simulation Study of a Mutant Construct of the Archaeal Glutamate Transporter GltPh with Transport Rates as Fast as its Human Counterpart”, Biophysical Journal, vol. 108, no. 2. Elsevier BV, p. 198a, Jan. 2015. doi: 10.1016/j.bpj.2014.11.1092.*  
  
*Z.-R. Xie, J. Chenand Y. Wu, “A coarse-grained model for the simulations of biomolecular interactions in cellular environments”, The Journal of Chemical Physics, vol. 140, no. 5. AIP Publishing, p. 054112, Feb. 07, 2014. doi: 10.1063/1.4863992.*  
  
*K. Shieh, P. Ó. Broin, D. Rhee, M. Levyand A. Golden, “Using SAGA and the Open Science Grid to Search for Aptamers”, Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616517.*  
  
*T. D. Martin, E. H. Hill, D. G. Whitten, E. Y. Chiand D. G. Evans, “Oligomeric Conjugated Polyelectrolytes Display Site-Preferential Binding to an MS2 Viral Capsid”, Langmuir, vol. 32, no. 47. American Chemical Society (ACS), pp. 12542–12551, Aug. 29, 2016. doi: 10.1021/acs.langmuir.6b01667.*  
  
*H. K. Wayment-Steele, “Effects of Al3+ on Phosphocholine and Phosphoglycerol Containing Solid Supported Lipid Bilayers”, Langmuir, vol. 32, no. 7. American Chemical Society (ACS), pp. 1771–1781, Feb. 05, 2016. doi: 10.1021/acs.langmuir.5b03999.*  
  
*X. Mu, “Modeling Organochlorine Compounds and the σ-Hole Effect Using a Polarizable Multipole Force Field”, The Journal of Physical Chemistry B, vol. 118, no. 24. American Chemical Society (ACS), pp. 6456–6465, Feb. 20, 2014. doi: 10.1021/jp411671a.*  
  
*L.-P. Wang, “Systematic Improvement of a Classical Molecular Model of Water”, The Journal of Physical Chemistry B, vol. 117, no. 34. American Chemical Society (ACS), pp. 9956–9972, Aug. 14, 2013. doi: 10.1021/jp403802c.*  
  
*S. E. Gasanov, “Naja naja oxiana Cobra Venom Cytotoxins CTI and CTII Disrupt Mitochondrial Membrane Integrity: Implications for Basic Three-Fingered Cytotoxins”, PLOS ONE, vol. 10, no. 6. Public Library of Science (PLoS), p. e0129248, Jun. 19, 2015. doi: 10.1371/journal.pone.0129248.*  
  
*X. Lin, “Order and disorder control the functional rearrangement of influenza hemagglutinin”, Proceedings of the National Academy of Sciences, vol. 111, no. 33. Proceedings of the National Academy of Sciences, pp. 12049–12054, Jul. 31, 2014. doi: 10.1073/pnas.1412849111.*  
  
*X. Lin, J. K. Noel, N. R. Eddy, J. Maand J. N. Onuchic, “Investigation of the pH Induced Conformational Rearrangement of Influenza Hemagglutinin”, Biophysical Journal, vol. 110, no. 3. Elsevier BV, p. 13a, Feb. 2016. doi: 10.1016/j.bpj.2015.11.126.*  
  
*X. Lin, J. K. Noel, Q. Wang, J. Maand J. N. Onuchic, “Lowered pH Leads to Fusion Peptide Release and a Highly Dynamic Intermediate of Influenza Hemagglutinin”, The Journal of Physical Chemistry B, vol. 120, no. 36. American Chemical Society (ACS), pp. 9654–9660, Sep. 01, 2016. doi: 10.1021/acs.jpcb.6b06775.*  
  
*X. Lin, J. K. Noel, Q. Wang, J. Maand J. N. Onuchic, “Atomistic Simulations Reveal a Hindered Transition of the B-Loop Domain of Influenza Hemagglutinin”, Biophysical Journal, vol. 114, no. 3. Elsevier BV, p. 232a, Feb. 2018. doi: 10.1016/j.bpj.2017.11.1292.*  
  
*X. Lin, J. K. Noel, Q. Wang, J. Maand J. N. Onuchic, “Atomistic simulations indicate the functional loop-to-coiled-coil transition in influenza hemagglutinin is not downhill”, Proceedings of the National Academy of Sciences, vol. 115, no. 34. Proceedings of the National Academy of Sciences, Jul. 16, 2018. doi: 10.1073/pnas.1805442115.*  
  
*J. F. Cannon, “Novel phosphorylation‐dependent regulation in an unstructured protein”, Proteins: Structure, Function, and Bioinformatics, vol. 88, no. 2. Wiley, pp. 366–384, Oct. 2019. doi: 10.1002/prot.25812.*  
  
*J. M. Karp, S. Sparksand D. Cowburn, “Effects of FGFR2 kinase activation loop dynamics on catalytic activity”, PLOS Computational Biology, vol. 13, no. 2. Public Library of Science (PLoS), p. e1005360, Feb. 02, 2017. doi: 10.1371/journal.pcbi.1005360.*  
  
*B. Raveh, “Slide-and-exchange mechanism for rapid and selective transport through the nuclear pore complex”, Proceedings of the National Academy of Sciences, vol. 113, no. 18. Proceedings of the National Academy of Sciences, Apr. 18, 2016. doi: 10.1073/pnas.1522663113.*  
  
*S. C. DeSalvo, Y. Liu, G. S. Choudhary, D. Ren, S. Nangiaand R. Sureshkumar, “Signaling Factor Interactions with Polysaccharide Aggregates of Bacterial Biofilms”, Langmuir, vol. 31, no. 6. American Chemical Society (ACS), pp. 1958–1966, Feb. 03, 2015. doi: 10.1021/la504721b.*  
  
*K. N. Ibsen, H. Ma, A. Banerjee, E. E. L. Tanner, S. Nangiaand S. Mitragotri, “Mechanism of Antibacterial Activity of Choline-Based Ionic Liquids (CAGE)”, ACS Biomaterials Science & Engineering, vol. 4, no. 7. American Chemical Society (ACS), pp. 2370–2379, May 31, 2018. doi: 10.1021/acsbiomaterials.8b00486.*  
  
*F. J. Irudayanathan, N. Wang, X. Wangand S. Nangia, “Architecture of the paracellular channels formed by claudins of the blood–brain barrier tight junctions”, Annals of the New York Academy of Sciences, vol. 1405, no. 1. Wiley, pp. 131–146, Jun. 14, 2017. doi: 10.1111/nyas.13378.*  
  
*F. J. Irudayanathan, X. Wang, N. Wang, S. R. Willsey, I. A. Seddonand S. Nangia, “Self-Assembly Simulations of Classic Claudins—Insights into the Pore Structure, Selectivity, and Higher Order Complexes”, The Journal of Physical Chemistry B, vol. 122, no. 30. American Chemical Society (ACS), pp. 7463–7474, Jun. 05, 2018. doi: 10.1021/acs.jpcb.8b03842.*  
  
*W. Jiang, J. Luoand S. Nangia, “Multiscale Approach to Investigate Self-Assembly of Telodendrimer Based Nanocarriers for Anticancer Drug Delivery”, Langmuir, vol. 31, no. 14. American Chemical Society (ACS), pp. 4270–4280, Jan. 12, 2015. doi: 10.1021/la503949b.*  
  
*W. Jiang, X. Wang, D. Guo, J. Luoand S. Nangia, “Drug-Specific Design of Telodendrimer Architecture for Effective Doxorubicin Encapsulation”, The Journal of Physical Chemistry B, vol. 120, no. 36. American Chemical Society (ACS), pp. 9766–9777, Aug. 31, 2016. doi: 10.1021/acs.jpcb.6b06070.*  
  
*H. Ma, “Modeling Diversity in Structures of Bacterial Outer Membrane Lipids”, Journal of Chemical Theory and Computation, vol. 13, no. 2. American Chemical Society (ACS), pp. 811–824, Jan. 31, 2017. doi: 10.1021/acs.jctc.6b00856.*  
  
*H. Ma, A. Khanand S. Nangia, “Dynamics of OmpF Trimer Formation in the Bacterial Outer Membrane of Escherichia coli”, Langmuir, vol. 34, no. 19. American Chemical Society (ACS), pp. 5623–5634, Nov. 22, 2017. doi: 10.1021/acs.langmuir.7b02653.*  
  
*J. A. Scher, M. G. Bayne, A. Srihari, S. Nangiaand A. Chakraborty, “Development of effective stochastic potential method using random matrix theory for efficient conformational sampling of semiconductor nanoparticles at non-zero temperatures”, The Journal of Chemical Physics, vol. 149, no. 1. AIP Publishing, p. 014103, Jul. 07, 2018. doi: 10.1063/1.5026027.*  
  
*F. J. Irudayanathan, J. P. Trasatti, P. Karandeand S. Nangia, “Molecular Architecture of the Blood Brain Barrier Tight Junction Proteins–A Synergistic Computational and In Vitro Approach”, The Journal of Physical Chemistry B, vol. 120, no. 1. American Chemical Society (ACS), pp. 77–88, Dec. 29, 2015. doi: 10.1021/acs.jpcb.5b09977.*  
  
*H. Ma, F. J. Irudayanathan, W. Jiangand S. Nangia, “Simulating Gram-Negative Bacterial Outer Membrane: A Coarse Grain Model”, The Journal of Physical Chemistry B, vol. 119, no. 46. American Chemical Society (ACS), pp. 14668–14682, Sep. 25, 2015. doi: 10.1021/acs.jpcb.5b07122.*  
  
*C. M. Purcell, A. S. Seetharam, O. Snodgrass, S. Ortega-García, J. R. Hydeand A. J. Severin, “Insights into teleost sex determination from the Seriola dorsalis genome assembly”, BMC Genomics, vol. 19, no. 1. Springer Science and Business Media LLC, Jan. 08, 2018. doi: 10.1186/s12864-017-4403-1.*  
  
*A. Seetharam, A. Gomez, C. M. Purcell, J. R. Hyde, P. D. Bloodand A. J. Severin, “NCBI-BLAST programs optimization on XSEDE resources for sustainable aquaculture”, Proceedings of the 2015 XSEDE Conference on Scientific Advancements Enabled by Enhanced Cyberinfrastructure - XSEDE ’15. ACM Press, 2015. doi: 10.1145/2792745.2792749.*  
  
*E. Sjulstok, I. A. Solov’yovand P. L. Freddolino, “Applications of molecular modeling to flavoproteins: Insights and challenges”, Methods in Enzymology. Elsevier, pp. 277–314, 2019. doi: 10.1016/bs.mie.2019.03.014.*  
  
*P. S. Shen, “Rqc2p and 60 S ribosomal subunits mediate mRNA-independent elongation of nascent chains”, Science, vol. 347, no. 6217. American Association for the Advancement of Science (AAAS), pp. 75–78, Jan. 02, 2015. doi: 10.1126/science.1259724.*  
  
*R. Araya-Secchi, B. L. Neeland M. Sotomayor, “An elastic element in the protocadherin-15 tip link of the inner ear”, Nature Communications, vol. 7, no. 1. Springer Science and Business Media LLC, Nov. 18, 2016. doi: 10.1038/ncomms13458.*  
  
*R. Araya-Secchi and M. Sotomayor, “Structure of an Inner-Ear Protocadherin-15 Fragment with an Atypical Calcium-Free Linker”, Biophysical Journal, vol. 108, no. 2. Elsevier BV, p. 561a, Jan. 2015. doi: 10.1016/j.bpj.2014.11.3075.*  
  
*P. De-la-Torre, D. Choudhary, R. Araya-Secchi, Y. Naruiand M. Sotomayor, “A Mechanically Weak Extracellular Membrane-Adjacent Domain Induces Dimerization of Protocadherin-15”, Biophysical Journal, vol. 115, no. 12. Elsevier BV, pp. 2368–2385, Dec. 2018. doi: 10.1016/j.bpj.2018.11.010.*  
  
*Y. Narui and M. Sotomayor, “Structural and Biophysical Characterization of Inner Ear Tip Link Variants”, Biophysical Journal, vol. 108, no. 2. Elsevier BV, p. 562a, Jan. 2015. doi: 10.1016/j.bpj.2014.11.3078.*  
  
*Y. Narui and M. Sotomayor, “Tuning Inner-Ear Tip-Link Affinity Through Alternatively Spliced Variants of Protocadherin-15”, Biochemistry, vol. 57, no. 11. American Chemical Society (ACS), pp. 1702–1710, Feb. 14, 2018. doi: 10.1021/acs.biochem.7b01075.*  
  
*J. M. Nicoludis, “Interaction specificity of clustered protocadherins inferred from sequence covariation and structural analysis”, Proceedings of the National Academy of Sciences, vol. 116, no. 36. Proceedings of the National Academy of Sciences, pp. 17825–17830, Aug. 20, 2019. doi: 10.1073/pnas.1821063116.*  
  
*B. Pan, “TMC1 Forms the Pore of Mechanosensory Transduction Channels in Vertebrate Inner Ear Hair Cells”, Neuron, vol. 99, no. 4. Elsevier BV, pp. 736–753.e6, Aug. 2018. doi: 10.1016/j.neuron.2018.07.033.*  
  
*R. E. Powers, R. Gaudetand M. Sotomayor, “Structural Study of a Novel Partial Calcium-Free Linker and a Positively Selected Variation in Protocadherin-15: Implications for Hearing and Cell Adhesion”, Biophysical Journal, vol. 108, no. 2. Elsevier BV, p. 505a, Jan. 2015. doi: 10.1016/j.bpj.2014.11.2765.*  
  
*M. Sotomayor, “Mechanisms and Mechanosensitivity: Exceptional Cadherins for Hearing and Balance”, Biophysical Journal, vol. 108, no. 2. Elsevier BV, pp. 11a–12a, Jan. 2015. doi: 10.1016/j.bpj.2014.11.089.*  
  
*J. M. Cicchese, V. Dartois, D. E. Kirschnerand J. J. Linderman, “Both Pharmacokinetic Variability and Granuloma Heterogeneity Impact the Ability of the First-Line Antibiotics to Sterilize Tuberculosis Granulomas”, Frontiers in Pharmacology, vol. 11. Frontiers Media SA, Mar. 24, 2020. doi: 10.3389/fphar.2020.00333.*  
  
*J. Cicchese, A. Sambarey, D. Kirschner, J. Lindermanand S. Chandrasekaran, “A multi-scale pipeline linking drug transcriptomics with pharmacokinetics predicts in vivo interactions of tuberculosis drugs”, []. Cold Spring Harbor Laboratory, Sep. 04, 2020. doi: 10.1101/2020.09.03.281550.*  
  
*L. R. Joslyn, D. E. Kirschnerand J. J. Linderman, “CaliPro: A Calibration Protocol That Utilizes Parameter Density Estimation to Explore Parameter Space and Calibrate Complex Biological Models”, Cellular and Molecular Bioengineering, vol. 14, no. 1. Springer Science and Business Media LLC, pp. 31–47, Sep. 15, 2020. doi: 10.1007/s12195-020-00650-z.*  
  
*L. R. Joslyn, “Integrating Non-human Primate, Human, and Mathematical Studies to Determine the Influence of BCG Timing on H56 Vaccine Outcomes”, Frontiers in Microbiology, vol. 9. Frontiers Media SA, Aug. 17, 2018. doi: 10.3389/fmicb.2018.01734.*  
  
*D. Kirschner, E. Pienaar, S. Marinoand J. J. Linderman, “A review of computational and mathematical modeling contributions to our understanding of Mycobacterium tuberculosis within-host infection and treatment”, Current Opinion in Systems Biology, vol. 3. Elsevier BV, pp. 170–185, Jun. 2017. doi: 10.1016/j.coisb.2017.05.014.*  
  
*J. J. Linderman, N. A. Cilfone, E. Pienaar, C. Gongand D. E. Kirschner, “A multi-scale approach to designing therapeutics for tuberculosis”, Integrative Biology, vol. 7, no. 5. Oxford University Press (OUP), pp. 591–609, Apr. 30, 2015. doi: 10.1039/c4ib00295d.*  
  
*J. J. Linderman and D. E. Kirschner, “In silico models of M. tuberculosis infection provide a route to new therapies”, Drug Discovery Today: Disease Models, vol. 15. Elsevier BV, pp. 37–41, 2015. doi: 10.1016/j.ddmod.2014.02.006.*  
  
*S. Marino, “Computational and Empirical Studies Predict Mycobacterium tuberculosis-Specific T Cells as a Biomarker for Infection Outcome”, PLOS Computational Biology, vol. 12, no. 4. Public Library of Science (PLoS), p. e1004804, Apr. 11, 2016. doi: 10.1371/journal.pcbi.1004804.*  
  
*S. Marino, C. Hult, P. Wolberg, J. Lindermanand D. Kirschner, “The Role of Dimensionality in Understanding Granuloma Formation”, Computation, vol. 6, no. 4. MDPI AG, p. 58, Nov. 14, 2018. doi: 10.3390/computation6040058.*  
  
*S. Marino and D. Kirschner, “A Multi-Compartment Hybrid Computational Model Predicts Key Roles for Dendritic Cells in Tuberculosis Infection”, Computation, vol. 4, no. 4. MDPI AG, p. 39, Oct. 21, 2016. doi: 10.3390/computation4040039.*  
  
*E. Pienaar, V. Dartois, J. J. Lindermanand D. E. Kirschner, “In silico evaluation and exploration of antibiotic tuberculosis treatment regimens”, BMC Systems Biology, vol. 9, no. 1. Springer Science and Business Media LLC, Nov. 14, 2015. doi: 10.1186/s12918-015-0221-8.*  
  
*E. Pienaar, J. J. Lindermanand D. E. Kirschner, “Emergence and selection of isoniazid and rifampin resistance in tuberculosis granulomas”, PLOS ONE, vol. 13, no. 5. Public Library of Science (PLoS), p. e0196322, May 10, 2018. doi: 10.1371/journal.pone.0196322.*  
  
*M. Renardy, M. Eisenbergand D. Kirschner, “Predicting the second wave of COVID-19 in Washtenaw County, MI”, Journal of Theoretical Biology, vol. 507. Elsevier BV, p. 110461, Dec. 2020. doi: 10.1016/j.jtbi.2020.110461.*  
  
*M. Renardy and D. E. Kirschner, “Evaluating vaccination strategies for tuberculosis in endemic and non-endemic settings”, Journal of Theoretical Biology, vol. 469. Elsevier BV, pp. 1–11, May 2019. doi: 10.1016/j.jtbi.2019.02.020.*  
  
*M. Renardy and D. E. Kirschner, “A Framework for Network-Based Epidemiological Modeling of Tuberculosis Dynamics Using Synthetic Datasets”, Bulletin of Mathematical Biology, vol. 82, no. 6. Springer Science and Business Media LLC, Jun. 2020. doi: 10.1007/s11538-020-00752-9.*  
  
*M. Renardy, T. Wessler, S. Blemker, J. Linderman, S. Peirceand D. Kirschner, “Data-Driven Model Validation Across Dimensions”, Bulletin of Mathematical Biology, vol. 81, no. 6. Springer Science and Business Media LLC, pp. 1853–1866, Mar. 04, 2019. doi: 10.1007/s11538-019-00590-4.*  
  
*S. J. Rhodes, G. M. Knight, D. E. Kirschner, R. G. Whiteand T. G. Evans, “Dose finding for new vaccines: The role for immunostimulation/immunodynamic modelling”, Journal of Theoretical Biology, vol. 465. Elsevier BV, pp. 51–55, Mar. 2019. doi: 10.1016/j.jtbi.2019.01.017.*  
  
*J. Sarathy, “Fluoroquinolone Efficacy against Tuberculosis Is Driven by Penetration into Lesions and Activity against Resident Bacterial Populations”, Antimicrobial Agents and Chemotherapy, vol. 63, no. 5. American Society for Microbiology, May 2019. doi: 10.1128/aac.02516-18.*  
  
*E. A. Wong, “Low Levels of T Cell Exhaustion in Tuberculous Lung Granulomas”, Infection and Immunity, vol. 86, no. 9. American Society for Microbiology, Sep. 2018. doi: 10.1128/iai.00426-18.*  
  
*C. Ziraldo, C. Gong, D. E. Kirschnerand J. J. Linderman, “Strategic Priming with Multiple Antigens can Yield Memory Cell Phenotypes Optimized for Infection with Mycobacterium tuberculosis: A Computational Study”, Frontiers in Microbiology, vol. 6. Frontiers Media SA, Jan. 06, 2016. doi: 10.3389/fmicb.2015.01477.*  
  
*J. Yao and J. Wang, “Neither Two-State nor Three-State: Dimerization of Lambda Cro Repressor”, The Journal of Physical Chemistry Letters, vol. 6, no. 11. American Chemical Society (ACS), pp. 2022–2026, May 18, 2015. doi: 10.1021/acs.jpclett.5b00524.*  
  
*D. O. Holland, B. H. Shapiro, P. Xueand M. E. Johnson, “Protein-protein binding selectivity and network topology constrain global and local properties of interface binding networks”, Scientific Reports, vol. 7, no. 1. Springer Science and Business Media LLC, Jul. 17, 2017. doi: 10.1038/s41598-017-05686-2.*  
  
*A. M. Reilly, “Report on the sixth blind test of organic crystal structure prediction methods”, Acta Crystallographica Section B Structural Science, Crystal Engineering and Materials, vol. 72, no. 4. International Union of Crystallography (IUCr), pp. 439–459, Aug. 01, 2016. doi: 10.1107/s2052520616007447.*  
  
*P. Pandey, K. K. Royand R. J. Doerksen, “Negative allosteric modulators of cannabinoid receptor 2: protein modeling, binding site identification and molecular dynamics simulations in the presence of an orthosteric agonist”, Journal of Biomolecular Structure and Dynamics, vol. 38, no. 1. Informa UK Limited, pp. 32–47, Feb. 05, 2019. doi: 10.1080/07391102.2019.1567384.*  
  
*E. H. Brookes, “An Open Extensible Multi-Target Application Generation Tool for Simple Rapid Deployment of Multi-Scale Scientific Codes”, Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616560.*  
  
*E. H. Brookes, N. Anjum, J. E. Curtis, S. Marru, R. Singhand M. Pierce, “The GenApp framework integrated with Airavata for managed compute resource submissions”, Concurrency and Computation: Practice and Experience, vol. 27, no. 16. Wiley, pp. 4292–4303, May 20, 2015. doi: 10.1002/cpe.3519.*  
  
*E. H. Brookes, A. Kapoor, P. Patra, S. Marru, R. Singhand M. Pierce, “GSoC 2015 student contributions to GenApp and Airavata”, Concurrency and Computation: Practice and Experience, vol. 28, no. 7. Wiley, pp. 1960–1970, Oct. 31, 2015. doi: 10.1002/cpe.3689.*  
  
*S. J. Perkins, “Atomistic modelling of scattering data in the Collaborative Computational Project for Small Angle Scattering (CCP-SAS)”, Journal of Applied Crystallography, vol. 49, no. 6. International Union of Crystallography (IUCr), pp. 1861–1875, Oct. 14, 2016. doi: 10.1107/s160057671601517x.*  
  
*M. E. DeSantis, M. A. Cianfrocco, Z. M. Htet, P. T. Tran, S. L. Reck-Petersonand A. E. Leschziner, “Lis1 Has Two Opposing Modes of Regulating Cytoplasmic Dynein”, Cell, vol. 170, no. 6. Elsevier BV, pp. 1197–1208.e12, Sep. 2017. doi: 10.1016/j.cell.2017.08.037.*  
  
*S. Qin and H.-X. Zhou, “Fast Method for Computing Chemical Potentials and Liquid–Liquid Phase Equilibria of Macromolecular Solutions”, The Journal of Physical Chemistry B, vol. 120, no. 33. American Chemical Society (ACS), pp. 8164–8174, Jul. 05, 2016. doi: 10.1021/acs.jpcb.6b01607.*  
  
*M. A. Cuendet and H. Weinstein, “Dissecting Functional Correlates of a Double Mutation Enhancing GltPh Transport Efficiency using Alchemical Free Energy Calculations”, Biophysical Journal, vol. 110, no. 3. Elsevier BV, p. 627a, Feb. 2016. doi: 10.1016/j.bpj.2015.11.3360.*  
  
*S. Mukherjee, G. A. Pantelopulosand V. A. Voelz, “Markov models of the apo-MDM2 lid region reveal diffuse yet two-state binding dynamics and receptor poses for computational docking”, Scientific Reports, vol. 6, no. 1. Springer Science and Business Media LLC, Aug. 19, 2016. doi: 10.1038/srep31631.*  
  
*S. Mukherjee, G. Zhou, C. Micheland V. A. Voelz, “Insights into Peptoid Helix Folding Cooperativity from an Improved Backbone Potential”, The Journal of Physical Chemistry B, vol. 119, no. 50. American Chemical Society (ACS), pp. 15407–15417, Dec. 04, 2015. doi: 10.1021/acs.jpcb.5b09625.*  
  
*G. A. Pantelopulos, S. Mukherjeeand V. A. Voelz, “Microsecond simulations of mdm2 and its complex with p53 yield insight into force field accuracy and conformational dynamics”, Proteins: Structure, Function, and Bioinformatics, vol. 83, no. 9. Wiley, pp. 1665–1676, Jul. 21, 2015. doi: 10.1002/prot.24852.*  
  
*A. E. Wakefield, W. M. Wuestand V. A. Voelz, “Molecular Simulation of Conformational Pre-Organization in Cyclic RGD Peptides”, Journal of Chemical Information and Modeling, vol. 55, no. 4. American Chemical Society (ACS), pp. 806–813, Mar. 20, 2015. doi: 10.1021/ci500768u.*  
  
*H. Wan, Y. Ge, A. Razaviand V. A. Voelz, “Reconciling Simulated Ensembles of Apomyoglobin with Experimental Hydrogen/Deuterium Exchange Data Using Bayesian Inference and Multiensemble Markov State Models”, Journal of Chemical Theory and Computation, vol. 16, no. 2. American Chemical Society (ACS), pp. 1333–1348, Jan. 09, 2020. doi: 10.1021/acs.jctc.9b01240.*  
  
*H. Wan, G. Zhouand V. A. Voelz, “A Maximum-Caliber Approach to Predicting Perturbed Folding Kinetics Due to Mutations”, Journal of Chemical Theory and Computation, vol. 12, no. 12. American Chemical Society (ACS), pp. 5768–5776, Nov. 23, 2016. doi: 10.1021/acs.jctc.6b00938.*  
  
*G. Zhou, G. A. Pantelopulos, S. Mukherjeeand V. A. Voelz, “Bridging Microscopic and Macroscopic Mechanisms of p53-MDM2 Binding with Kinetic Network Models”, Biophysical Journal, vol. 113, no. 4. Elsevier BV, pp. 785–793, Aug. 2017. doi: 10.1016/j.bpj.2017.07.009.*  
  
*G. Zhou and V. A. Voelz, “Using Kinetic Network Models To Probe Non-Native Salt-Bridge Effects on α-Helix Folding”, The Journal of Physical Chemistry B, vol. 120, no. 5. American Chemical Society (ACS), pp. 926–935, Feb. 01, 2016. doi: 10.1021/acs.jpcb.5b11767.*  
  
*P. Ebrahimi, S. Kaur, L. Baronti, K. Petzoldand A. A. Chen, “A two-dimensional replica-exchange molecular dynamics method for simulating RNA folding using sparse experimental restraints”, Methods, vol. 162–163. Elsevier BV, pp. 96–107, Jun. 2019. doi: 10.1016/j.ymeth.2019.05.001.*  
  
*S. K. K. Galagedera, “Voltammetric Detection of Thrombin by Labeling with Osmium Tetroxide Bipyridine and Binding with Aptamers on a Gold Electrode”, Electroanalysis, vol. 30, no. 3. Wiley, pp. 398–401, Jan. 12, 2018. doi: 10.1002/elan.201700734.*  
  
*P. Haruehanroengra, S. Vangaveti, S. V. Ranganathan, R. Wang, A. Chenand J. Sheng, “Nature’s Selection of Geranyl Group as a tRNA Modification: The Effects of Chain Length on Base-Pairing Specificity”, ACS Chemical Biology, vol. 12, no. 6. American Chemical Society (ACS), pp. 1504–1513, Apr. 18, 2017. doi: 10.1021/acschembio.7b00108.*  
  
*J. L. Lippens, S. V. Ranganathan, R. J. D’Espositoand D. Fabris, “Modular calibrant sets for the structural analysis of nucleic acids by ion mobility spectrometry mass spectrometry”, The Analyst, vol. 141, no. 13. Royal Society of Chemistry (RSC), pp. 4084–4099, 2016. doi: 10.1039/c6an00453a.*  
  
*S. Mao, “Cyano Modification on Uridine Decreases Base‐Pairing Stability and Specificity through Neighboring Disruption in RNA Duplex”, ChemBioChem, vol. 19, no. 24. Wiley, pp. 2558–2565, Nov. 19, 2018. doi: 10.1002/cbic.201800399.*  
  
*C. A. Myers, R. J. D’Esposito, D. Fabris, S. V. Ranganathanand A. A. Chen, “CoSIMS: An Optimized Trajectory-Based Collision Simulator for Ion Mobility Spectrometry”, The Journal of Physical Chemistry B, vol. 123, no. 20. American Chemical Society (ACS), pp. 4347–4357, May 01, 2019. doi: 10.1021/acs.jpcb.9b01018.*  
  
*S. V. Ranganathan, K. Halvorsen, C. A. Myers, N. M. Robertson, M. V. Yigitand A. A. Chen, “Complex Thermodynamic Behavior of Single-Stranded Nucleic Acid Adsorption to Graphene Surfaces”, Langmuir, vol. 32, no. 24. American Chemical Society (ACS), pp. 6028–6034, Jun. 06, 2016. doi: 10.1021/acs.langmuir.6b00456.*  
  
*L. M. Seebald, “Cu(II)-Based Paramagnetic Probe to Study RNA–Protein Interactions by NMR”, Inorganic Chemistry, vol. 56, no. 7. American Chemical Society (ACS), pp. 3773–3780, Mar. 22, 2017. doi: 10.1021/acs.inorgchem.6b02286.*  
  
*M. K. Takahashi, “Using in-cell SHAPE-Seq and simulations to probe structure–function design principles of RNA transcriptional regulators”, RNA, vol. 22, no. 6. Cold Spring Harbor Laboratory, pp. 920–933, Apr. 21, 2016. doi: 10.1261/rna.054916.115.*  
  
*S. Vangaveti, R. J. D’Esposito, J. L. Lippens, D. Fabrisand S. V. Ranganathan, “A coarse-grained model for assisting the investigation of structure and dynamics of large nucleic acids by ion mobility spectrometry–mass spectrometry”, Physical Chemistry Chemical Physics, vol. 19, no. 23. Royal Society of Chemistry (RSC), pp. 14937–14946, 2017. doi: 10.1039/c7cp00717e.*  
  
*S. Vangaveti, S. V. Ranganathanand A. A. Chen, “Advances in RNA molecular dynamics: a simulator’s guide to RNA force fields”, Wiley Interdisciplinary Reviews: RNA, vol. 8, no. 2. Wiley, p. e1396, Oct. 04, 2016. doi: 10.1002/wrna.1396.*  
  
*R. Wang, “Construction and structure studies of DNA-bipyridine complexes as versatile scaffolds for site-specific incorporation of metal ions into DNA”, Journal of Biomolecular Structure and Dynamics, vol. 37, no. 3. Informa UK Limited, pp. 551–561, Feb. 22, 2018. doi: 10.1080/07391102.2018.1441071.*  
  
*R. Wang, “Synthesis, base pairing and structure studies of geranylated RNA”, Nucleic Acids Research, vol. 44, no. 13. Oxford University Press (OUP), pp. 6036–6045, Jun. 15, 2016. doi: 10.1093/nar/gkw544.*  
  
*A. M. Yu, P. M. Gasper, E. J. Strobel, K. E. Watters, A. A. Chenand J. B. Lucks, “Computationally Reconstructing Cotranscriptional RNA Folding Pathways from Experimental Data Reveals Rearrangement of Non-Native Folding Intermediates”, []. Cold Spring Harbor Laboratory, Jul. 28, 2018. doi: 10.1101/379222.*  
  
*R. Wang, S. V. Ranganathan, M. Basanta-Sanchez, F. Shen, A. Chenand J. Sheng, “Synthesis and base pairing studies of geranylated 2-thiothymidine, a natural variant of thymidine”, Chemical Communications, vol. 51, no. 91. Royal Society of Chemistry (RSC), pp. 16369–16372, 2015. doi: 10.1039/c5cc07479g.*  
  
*R. Wang, “Water-bridged hydrogen bond formation between 5-hydroxylmethylcytosine (5-hmC) and its 3′-neighbouring bases in A- and B-form DNA duplexes”, Chemical Communications, vol. 51, no. 91. Royal Society of Chemistry (RSC), pp. 16389–16392, 2015. doi: 10.1039/c5cc06563a.*  
  
*J. K. Noel, “SMOG 2: A Versatile Software Package for Generating Structure-Based Models”, PLOS Computational Biology, vol. 12, no. 3. Public Library of Science (PLoS), p. e1004794, Mar. 10, 2016. doi: 10.1371/journal.pcbi.1004794.*  
  
*D. Kilburg and E. Gallicchio, “Assessment of a Single Decoupling Alchemical Approach for the Calculation of the Absolute Binding Free Energies of Protein-Peptide Complexes”, Frontiers in Molecular Biosciences, vol. 5. Frontiers Media SA, Mar. 08, 2018. doi: 10.3389/fmolb.2018.00022.*  
  
*R. P. Murelli, “Synthetic α-hydroxytropolones as inhibitors of HIV reverse transcriptase ribonuclease H activity”, MedChemComm, vol. 7, no. 9. Royal Society of Chemistry (RSC), pp. 1783–1788, 2016. doi: 10.1039/c6md00238b.*  
  
*R. K. Pal and E. Gallicchio, “Perturbation potentials to overcome order/disorder transitions in alchemical binding free energy calculations”, The Journal of Chemical Physics, vol. 151, no. 12. AIP Publishing, p. 124116, Sep. 28, 2019. doi: 10.1063/1.5123154.*  
  
*R. K. Pal, “A combined treatment of hydration and dynamical effects for the modeling of host–guest binding thermodynamics: the SAMPL5 blinded challenge”, Journal of Computer-Aided Molecular Design, vol. 31, no. 1. Springer Science and Business Media LLC, pp. 29–44, Sep. 30, 2016. doi: 10.1007/s10822-016-9956-6.*  
  
*R. K. Pal, “Inclusion of enclosed hydration effects in the binding free energy estimation of dopamine D3 receptor complexes”, PLOS ONE, vol. 14, no. 9. Public Library of Science (PLoS), p. e0222902, Sep. 30, 2019. doi: 10.1371/journal.pone.0222902.*  
  
*B. Zhang, M. P. D’Erasmo, R. P. Murelliand E. Gallicchio, “Free Energy-Based Virtual Screening and Optimization of RNase H Inhibitors of HIV-1 Reverse Transcriptase”, ACS Omega, vol. 1, no. 3. American Chemical Society (ACS), pp. 435–447, Sep. 21, 2016. doi: 10.1021/acsomega.6b00123.*  
  
*J. Fu, “Computational and experimental analysis of short peptide motifs for enzyme inhibition”, PLOS ONE, vol. 12, no. 8. Public Library of Science (PLoS), p. e0182847, Aug. 15, 2017. doi: 10.1371/journal.pone.0182847.*  
  
*D. V. Prokopovich, J. W. Whittaker, M. M. Muthee, A. Ahmedand L. Larini, “Impact of Phosphorylation and Pseudophosphorylation on the Early Stages of Aggregation of the Microtubule-Associated Protein Tau”, The Journal of Physical Chemistry B, vol. 121, no. 9. American Chemical Society (ACS), pp. 2095–2103, Feb. 24, 2017. doi: 10.1021/acs.jpcb.7b00194.*  
  
*S.-H. Roh, M. M. Kasembeli, J. G. Galaz-Montoya, W. Chiuand D. J. Tweardy, “Chaperonin TRiC/CCT Recognizes Fusion Oncoprotein AML1-ETO through Subunit-Specific Interactions”, Biophysical Journal, vol. 110, no. 11. Elsevier BV, pp. 2377–2385, Jun. 2016. doi: 10.1016/j.bpj.2016.04.045.*  
  
*T. Zang, L. Yu, C. Zhangand J. Ma, “Parallel continuous simulated tempering and its applications in large-scale molecular simulations”, The Journal of Chemical Physics, vol. 141, no. 4. AIP Publishing, p. 044113, Jul. 28, 2014. doi: 10.1063/1.4890038.*  
  
*J. Comer, R. Chen, H. Poblete, A. Vergara-Jaqueand J. E. Riviere, “Predicting Adsorption Affinities of Small Molecules on Carbon Nanotubes Using Molecular Dynamics Simulation”, ACS Nano, vol. 9, no. 12. American Chemical Society (ACS), pp. 11761–11774, Nov. 09, 2015. doi: 10.1021/acsnano.5b03592.*  
  
*H. Poblete, “New Insights into Peptide–Silver Nanoparticle Interaction: Deciphering the Role of Cysteine and Lysine in the Peptide Sequence”, Langmuir, vol. 32, no. 1. American Chemical Society (ACS), pp. 265–273, Dec. 31, 2015. doi: 10.1021/acs.langmuir.5b03601.*  
  
*M. Doktorova, R. Dick, F. A. Heberle, G. W. Feigensonand V. M. Vogt, “Cholesterol Promotes the Peripheral Binding of Retroviral Proteins to Lipid Bilayers”, Biophysical Journal, vol. 110, no. 3. Elsevier BV, p. 356a, Feb. 2016. doi: 10.1016/j.bpj.2015.11.1921.*  
  
*M. Doktorova, “Cholesterol Promotes Protein Binding by Affecting Membrane Electrostatics and Solvation Properties”, Biophysical Journal, vol. 113, no. 9. Elsevier BV, pp. 2004–2015, Nov. 2017. doi: 10.1016/j.bpj.2017.08.055.*  
  
*J. Lin, R. Dargazanyand A. Alexander-Katz, “Lipid Flip-Flop and Pore Nucleation on Zwitterionic Bilayers are Asymmetric under Ionic Imbalance”, Small, vol. 13, no. 22. Wiley, p. 1603708, Apr. 20, 2017. doi: 10.1002/smll.201603708.*  
  
*J. T. Waters, H. D. Kim, J. C. Gumbart, X.-J. Luand S. C. Harvey, “DNA Scrunching in the Packaging of Viral Genomes”, The Journal of Physical Chemistry B, vol. 120, no. 26. American Chemical Society (ACS), pp. 6200–6207, May 26, 2016. doi: 10.1021/acs.jpcb.6b02149.*  
  
*J. T. Waters, “Transitions of Double-Stranded DNA Between the A- and B-Forms”, The Journal of Physical Chemistry B, vol. 120, no. 33. American Chemical Society (ACS), pp. 8449–8456, May 11, 2016. doi: 10.1021/acs.jpcb.6b02155.*  
  
*A. K. Gupta, “Multi‐target, ensemble‐based virtual screening yields novel allosteric KRAS inhibitors at high success rate”, Chemical Biology & Drug Design. Wiley, Apr. 29, 2019. doi: 10.1111/cbdd.13519.*  
  
*K. R. Levental, J. H. Lorent, X. Lin, A. A. Gorfeand I. Levental, “Dietary Fats Remodel Plasma Membrane Lipidome and Physical Properties to Regulate Phase Separation in Biological Membranes”, Biophysical Journal, vol. 110, no. 3. Elsevier BV, p. 584a, Feb. 2016. doi: 10.1016/j.bpj.2015.11.3119.*  
  
*K. R. Levental, “Polyunsaturated Lipids Regulate Membrane Domain Stability by Tuning Membrane Order”, Biophysical Journal, vol. 110, no. 8. Elsevier BV, pp. 1800–1810, Apr. 2016. doi: 10.1016/j.bpj.2016.03.012.*  
  
*X. Lin, Z. Liand A. A. Gorfe, “Reversible Effects of Peptide Concentration and Lipid Composition on H-Ras Lipid Anchor Clustering”, Biophysical Journal, vol. 109, no. 12. Elsevier BV, pp. 2467–2470, Dec. 2015. doi: 10.1016/j.bpj.2015.11.009.*  
  
*X. Lin, J. H. Lorent, K. R. Levental, A. A. Gorfeand I. Levental, “Order Differences between Coexisting Liquid Phases Driven by Lipid Unsaturation Determine Phase Separation in Biomimetic Membranes”, Biophysical Journal, vol. 110, no. 3. Elsevier BV, p. 71a, Feb. 2016. doi: 10.1016/j.bpj.2015.11.447.*  
  
*X. Lin, “Domain Stability in Biomimetic Membranes Driven by Lipid Polyunsaturation”, The Journal of Physical Chemistry B, vol. 120, no. 46. American Chemical Society (ACS), pp. 11930–11941, Nov. 10, 2016. doi: 10.1021/acs.jpcb.6b06815.*  
  
*J. H. Lorent, “Structural determinants and functional consequences of protein affinity for membrane rafts”, Nature Communications, vol. 8, no. 1. Springer Science and Business Media LLC, Oct. 31, 2017. doi: 10.1038/s41467-017-01328-3.*  
  
*M. McCarthy, P. Prakashand A. A. Gorfe, “Computational allosteric ligand binding site identification on Ras proteins”, Acta Biochimica et Biophysica Sinica, vol. 48, no. 1. China Science Publishing & Media Ltd., pp. 3–10, Jan. 01, 2016. doi: 10.1093/abbs/gmv100.*  
  
*P. Prakash, “Computational and biochemical characterization of two partially overlapping interfaces and multiple weak-affinity K-Ras dimers”, Scientific Reports, vol. 7, no. 1. Springer Science and Business Media LLC, Jan. 09, 2017. doi: 10.1038/srep40109.*  
  
*P. Prakash, A. Sayyed-Ahmadand A. A. Gorfe, “pMD-Membrane: A Method for Ligand Binding Site Identification in Membrane-Bound Proteins”, PLOS Computational Biology, vol. 11, no. 10. Public Library of Science (PLoS), p. e1004469, Oct. 27, 2015. doi: 10.1371/journal.pcbi.1004469.*  
  
*P. Prakash, Y. Zhou, H. Liang, J. F. Hancockand A. A. Gorfe, “Oncogenic K-Ras Binds to an Anionic Membrane in Two Distinct Orientations: A Molecular Dynamics Analysis”, Biophysical Journal, vol. 110, no. 5. Elsevier BV, pp. 1125–1138, Mar. 2016. doi: 10.1016/j.bpj.2016.01.019.*  
  
*S. Sarkar-Banerjee, “Spatiotemporal Analysis of K-Ras Plasma Membrane Interactions Reveals Multiple High Order Homo-oligomeric Complexes”, Journal of the American Chemical Society, vol. 139, no. 38. American Chemical Society (ACS), pp. 13466–13475, Sep. 18, 2017. doi: 10.1021/jacs.7b06292.*  
  
*A. Sayyed-Ahmad, K.-J. Cho, J. F. Hancockand A. A. Gorfe, “Computational Equilibrium Thermodynamic and Kinetic Analysis of K-Ras Dimerization through an Effector Binding Surface Suggests Limited Functional Role”, The Journal of Physical Chemistry B, vol. 120, no. 33. American Chemical Society (ACS), pp. 8547–8556, May 11, 2016. doi: 10.1021/acs.jpcb.6b02403.*  
  
*A. Sayyed-Ahmad and A. A. Gorfe, “Mixed-Probe Simulation and Probe-Derived Surface Topography Map Analysis for Ligand Binding Site Identification”, Journal of Chemical Theory and Computation, vol. 13, no. 4. American Chemical Society (ACS), pp. 1851–1861, Mar. 13, 2017. doi: 10.1021/acs.jctc.7b00130.*  
  
*Y. Zhou, P. Prakash, H. Liang, K.-J. Cho, A. A. Gorfeand J. F. Hancock, “Lipid-Sorting Specificity Encoded in K-Ras Membrane Anchor Regulates Signal Output”, Cell, vol. 168, no. 1–2. Elsevier BV, pp. 239–251.e16, Jan. 2017. doi: 10.1016/j.cell.2016.11.059.*  
  
*Y. Fu, O. N. Yogurtcu, R. Kothari, G. Thorkelsdottir, A. J. Sodtand M. E. Johnson, “An implicit lipid model for efficient reaction-diffusion simulations of protein binding to surfaces of arbitrary topology”, The Journal of Chemical Physics, vol. 151, no. 12. AIP Publishing, p. 124115, Sep. 28, 2019. doi: 10.1063/1.5120516.*  
  
*M. E. Johnson, “Modeling the Self-Assembly of Protein Complexes through a Rigid-Body Rotational Reaction–Diffusion Algorithm”, The Journal of Physical Chemistry B, vol. 122, no. 49. American Chemical Society (ACS), pp. 11771–11783, Sep. 26, 2018. doi: 10.1021/acs.jpcb.8b08339.*  
  
*M. J. Varga, Y. Fu, S. Loggia, O. N. Yogurtcuand M. E. Johnson, “NERDSS: A Nonequilibrium Simulator for Multibody Self-Assembly at the Cellular Scale”, Biophysical Journal, vol. 118, no. 12. Elsevier BV, pp. 3026–3040, Jun. 2020. doi: 10.1016/j.bpj.2020.05.002.*  
  
*O. N. Yogurtcu and M. E. Johnson, “Theory of bi-molecular association dynamics in 2D for accurate model and experimental parameterization of binding rates”, The Journal of Chemical Physics, vol. 143, no. 8. AIP Publishing, p. 084117, Aug. 28, 2015. doi: 10.1063/1.4929390.*  
  
*O. N. Yogurtcu and M. E. Johnson, “Cytosolic proteins can exploit membrane localization to trigger functional assembly”, PLOS Computational Biology, vol. 14, no. 3. Public Library of Science (PLoS), p. e1006031, Mar. 05, 2018. doi: 10.1371/journal.pcbi.1006031.*  
  
*S. Sukenik, T. V. Pogorelovand M. Gruebele, “Can Local Probes Go Global? A Joint Experiment–Simulation Analysis of λ6–85 Folding”, The Journal of Physical Chemistry Letters, vol. 7, no. 11. American Chemical Society (ACS), pp. 1960–1965, May 13, 2016. doi: 10.1021/acs.jpclett.6b00582.*  
  
*F. Pan, V. H. Man, C. Rolandand C. Sagui, “Structure and Dynamics of DNA and RNA Double Helices of CAG and GAC Trinucleotide Repeats”, Biophysical Journal, vol. 113, no. 1. Elsevier BV, pp. 19–36, Jul. 2017. doi: 10.1016/j.bpj.2017.05.041.*  
  
*Y. Zhang, V. H. Man, C. Rolandand C. Sagui, “Amyloid Properties of Asparagine and Glutamine in Prion-like Proteins”, ACS Chemical Neuroscience, vol. 7, no. 5. American Chemical Society (ACS), pp. 576–587, Mar. 03, 2016. doi: 10.1021/acschemneuro.5b00337.*  
  
*G. A. Cortina, J. M. Haysand P. M. Kasson, “Conformational Intermediate That Controls KPC-2 Catalysis and Beta-Lactam Drug Resistance”, ACS Catalysis, vol. 8, no. 4. American Chemical Society (ACS), pp. 2741–2747, Feb. 21, 2018. doi: 10.1021/acscatal.7b03832.*  
  
*J. M. Hays, M. K. Kieber, J. Z. Li, J. I. Han, L. Columbusand P. M. Kasson, “Refinement of Highly Flexible Protein Structures using Simulation‐Guided Spectroscopy”, Angewandte Chemie International Edition, vol. 57, no. 52. Wiley, pp. 17110–17114, Nov. 27, 2018. doi: 10.1002/anie.201810462.*  
  
*G. A. Pantelopulos and J. E. Straub, “Regimes of Complex Lipid Bilayer Phases Induced by Cholesterol Concentration in MD Simulation”, Biophysical Journal, vol. 115, no. 11. Elsevier BV, pp. 2167–2178, Dec. 2018. doi: 10.1016/j.bpj.2018.10.011.*  
  
*B. Xie, J. D. Clarkand D. D. L. Minh, “Efficiency of Stratification for Ensemble Docking Using Reduced Ensembles”, Journal of Chemical Information and Modeling, vol. 58, no. 9. American Chemical Society (ACS), pp. 1915–1925, Aug. 16, 2018. doi: 10.1021/acs.jcim.8b00314.*  
  
*B. Xie and D. D. L. Minh, “Alchemical Grid Dock (AlGDock) calculations in the D3R Grand Challenge 3”, Journal of Computer-Aided Molecular Design, vol. 33, no. 1. Springer Science and Business Media LLC, pp. 61–69, Aug. 06, 2018. doi: 10.1007/s10822-018-0143-9.*  
  
*D. D. L. Minh, “Alchemical Grid Dock (AlGDock): Binding Free Energy Calculations between Flexible Ligands and Rigid Receptors”, Journal of Computational Chemistry, vol. 41, no. 7. Wiley, pp. 715–730, Aug. 09, 2019. doi: 10.1002/jcc.26036.*  
  
*W. Menzer, B. Xieand D. D. L. Minh, “On Restraints in End-Point Protein-Ligand Binding Free Energy Calculations”, Biophysical Journal, vol. 116, no. 3. Elsevier BV, p. 47a, Feb. 2019. doi: 10.1016/j.bpj.2018.11.296.*  
  
*D. D. L. Minh, “Power transformations improve interpolation of grids for molecular mechanics interaction energies”, Journal of Computational Chemistry, vol. 39, no. 19. Wiley, pp. 1200–1207, Feb. 18, 2018. doi: 10.1002/jcc.25180.*  
  
*T. H. Nguyen and D. D. L. Minh, “Implicit ligand theory for relative binding free energies”, The Journal of Chemical Physics, vol. 148, no. 10. AIP Publishing, p. 104114, Mar. 14, 2018. doi: 10.1063/1.5017136.*  
  
*T. H. Nguyen, H.-X. Zhouand D. D. L. Minh, “Using the fast fourier transform in binding free energy calculations”, Journal of Computational Chemistry, vol. 39, no. 11. Wiley, pp. 621–636, Dec. 22, 2017. doi: 10.1002/jcc.25139.*  
  
*K. Mulholland and C. Wu, “Binding of Telomestatin to a Telomeric G-Quadruplex DNA Probed by All-Atom Molecular Dynamics Simulations with Explicit Solvent”, Journal of Chemical Information and Modeling, vol. 56, no. 10. American Chemical Society (ACS), pp. 2093–2102, Sep. 27, 2016. doi: 10.1021/acs.jcim.6b00473.*  
  
*C. Readmond and C. Wu, “Investigating detailed interactions between novel PAR1 antagonist F16357 and the receptor using docking and molecular dynamic simulations”, Journal of Molecular Graphics and Modelling, vol. 77. Elsevier BV, pp. 205–217, Oct. 2017. doi: 10.1016/j.jmgm.2017.08.019.*  
  
*K. L. Borrell, “An Experimental and Molecular Dynamics Study of Red Fluorescent Protein mCherry in Novel Aqueous Amino Acid Ionic Liquids”, The Journal of Physical Chemistry B, vol. 121, no. 18. American Chemical Society (ACS), pp. 4823–4832, Apr. 27, 2017. doi: 10.1021/acs.jpcb.7b03582.*  
  
*K. Mulholland, F. Siddiqueiand C. Wu, “Binding modes and pathway of RHPS4 to human telomeric G-quadruplex and duplex DNA probed by all-atom molecular dynamics simulations with explicit solvent”, Physical Chemistry Chemical Physics, vol. 19, no. 28. Royal Society of Chemistry (RSC), pp. 18685–18694, 2017. doi: 10.1039/c7cp03313c.*  
  
*S. Sader, J. Cai, A. C. G. Mullerand C. Wu, “Can human allergy drug fexofenadine, an antagonist of histamine (H1) receptor, be used to treat dog and cat? Homology modeling, docking and molecular dynamic Simulation of three H1 receptors in complex with fexofenadine”, Journal of Molecular Graphics and Modelling, vol. 75. Elsevier BV, pp. 106–116, Aug. 2017. doi: 10.1016/j.jmgm.2017.05.010.*  
  
*S. Sader and C. Wu, “Computational analysis of Amsacrine resistance in human topoisomerase II alpha mutants (R487K and E571K) using homology modeling, docking and all-atom molecular dynamics simulation in explicit solvent”, Journal of Molecular Graphics and Modelling, vol. 72. Elsevier BV, pp. 209–219, Mar. 2017. doi: 10.1016/j.jmgm.2016.11.019.*  
  
*Z. Shen, K. A. Mulholland, Y. Zhengand C. Wu, “Binding of anticancer drug daunomycin to a TGGGGT G-quadruplex DNA probed by all-atom molecular dynamics simulations: additional pure groove binding mode and implications on designing more selective G-quadruplex ligands”, Journal of Molecular Modeling, vol. 23, no. 9. Springer Science and Business Media LLC, Aug. 08, 2017. doi: 10.1007/s00894-017-3417-6.*  
  
*B. Machireddy, G. Kalra, S. Jonnalagadda, K. Ramanujacharyand C. Wu, “Probing the Binding Pathway of BRACO19 to a Parallel-Stranded Human Telomeric G-Quadruplex Using Molecular Dynamics Binding Simulation with AMBER DNA OL15 and Ligand GAFF2 Force Fields”, Journal of Chemical Information and Modeling, vol. 57, no. 11. American Chemical Society (ACS), pp. 2846–2864, Nov. 01, 2017. doi: 10.1021/acs.jcim.7b00287.*  
  
*S. Sader, K. Anantand C. Wu, “To probe interaction of morphine and IBNtxA with 7TM and 6TM variants of the human μ-opioid receptor using all-atom molecular dynamics simulations with an explicit membrane”, Physical Chemistry Chemical Physics, vol. 20, no. 3. Royal Society of Chemistry (RSC), pp. 1724–1741, 2018. doi: 10.1039/c7cp06745c.*  
  
*E. J. Alred, I. Lodangco, J. Gallaherand U. H. E. Hansmann, “Mutations Alter RNA-Mediated Conversion of Human Prions”, ACS Omega, vol. 3, no. 4. American Chemical Society (ACS), pp. 3936–3944, Apr. 09, 2018. doi: 10.1021/acsomega.7b02007.*  
  
*N. A. Bernhardt and U. H. E. Hansmann, “Multifunnel Landscape of the Fold-Switching Protein RfaH-CTD”, The Journal of Physical Chemistry B, vol. 122, no. 5. American Chemical Society (ACS), pp. 1600–1607, Jan. 24, 2018. doi: 10.1021/acs.jpcb.7b11352.*  
  
*N. A. Bernhardt, W. Xi, W. Wangand U. H. E. Hansmann, “Simulating Protein Fold Switching by Replica Exchange with Tunneling”, Journal of Chemical Theory and Computation, vol. 12, no. 11. American Chemical Society (ACS), pp. 5656–5666, Oct. 31, 2016. doi: 10.1021/acs.jctc.6b00826.*  
  
*M. Bhavaraju and U. H. E. Hansmann, “Effect of single point mutations in a form of systemic amyloidosis”, Protein Science, vol. 24, no. 9. Wiley, pp. 1451–1462, Jul. 14, 2015. doi: 10.1002/pro.2730.*  
  
*M. Bhavaraju, M. Phillips, D. Bowman, J. M. Aceves-Hernandezand U. H. E. Hansmann, “Binding of ACE-inhibitors to in vitro and patient-derived amyloid-β fibril models”, The Journal of Chemical Physics, vol. 144, no. 1. AIP Publishing, p. 015101, Jan. 07, 2016. doi: 10.1063/1.4938261.*  
  
*W. Wang, W. Xiand U. H. E. Hansmann, “Stability of the N-Terminal Helix and Its Role in Amyloid Formation of Serum Amyloid A”, ACS Omega, vol. 3, no. 11. American Chemical Society (ACS), pp. 16184–16190, Nov. 29, 2018. doi: 10.1021/acsomega.8b02377.*  
  
*W. Xi and U. H. E. Hansmann, “Conversion between parallel and antiparallel β-sheets in wild-type and Iowa mutant Aβ40 fibrils”, The Journal of Chemical Physics, vol. 148, no. 4. AIP Publishing, p. 045103, Jan. 28, 2018. doi: 10.1063/1.5016166.*  
  
*W. Xi, E. K. Vanderfordand U. H. E. Hansmann, “Out-of-Register Aβ42 Assemblies as Models for Neurotoxic Oligomers and Fibrils”, Journal of Chemical Theory and Computation, vol. 14, no. 2. American Chemical Society (ACS), pp. 1099–1110, Jan. 31, 2018. doi: 10.1021/acs.jctc.7b01106.*  
  
*H. Zhang, W. Xi, U. H. E. Hansmannand Y. Wei, “Fibril–Barrel Transitions in Cylindrin Amyloids”, Journal of Chemical Theory and Computation, vol. 13, no. 8. American Chemical Society (ACS), pp. 3936–3944, Jul. 17, 2017. doi: 10.1021/acs.jctc.7b00383.*  
  
*G. S. Jas, E. W. Childsand K. Kuczera, “Kinetic pathway analysis of an α-helix in two protonation states: Direct observation and optimal dimensionality reduction”, The Journal of Chemical Physics, vol. 150, no. 7. AIP Publishing, p. 074902, Feb. 21, 2019. doi: 10.1063/1.5082192.*  
  
*G. S. Jas and K. Kuczera, “Deprotonation of a Single Amino Acid Residue Induces Significant Stability in an α-Helical Heteropeptide”, The Journal of Physical Chemistry B, vol. 122, no. 49. American Chemical Society (ACS), pp. 11508–11518, Oct. 12, 2018. doi: 10.1021/acs.jpcb.8b07418.*  
  
*G. S. Jas and K. Kuczera, “Helix–Coil Transition Courses Through Multiple Pathways and Intermediates: Fast Kinetic Measurements and Dimensionality Reduction”, The Journal of Physical Chemistry B, vol. 122, no. 48. American Chemical Society (ACS), pp. 10806–10816, Nov. 05, 2018. doi: 10.1021/acs.jpcb.8b07924.*  
  
*D. P. Hoogerheide, P. A. Gurnev, T. K. Rostovtsevaand S. M. Bezrukov, “Mechanism of α-synuclein translocation through a VDAC nanopore revealed by energy landscape modeling of escape time distributions”, Nanoscale, vol. 9, no. 1. Royal Society of Chemistry (RSC), pp. 183–192, 2017. doi: 10.1039/c6nr08145b.*  
  
*M. C. Childers, C.-L. Towseand V. Daggett, “Molecular dynamics-derived rotamer libraries for d-amino acids within homochiral and heterochiral polypeptides”, Protein Engineering, Design and Selection, vol. 31, no. 6. Oxford University Press (OUP), pp. 191–204, Jun. 01, 2018. doi: 10.1093/protein/gzy016.*  
  
*H. R. Harrington, “Cotranslational Folding Stimulates Programmed Ribosomal Frameshifting in the Alphavirus Structural Polyprotein”, []. Cold Spring Harbor Laboratory, Oct. 02, 2019. doi: 10.1101/790444.*  
  
*M. J. M. Niesen, S. S. Marshall, T. F. Miller IIIand W. M. Clemons Jr., “Improving membrane protein expression by optimizing integration efficiency”, Journal of Biological Chemistry, vol. 292, no. 47. Elsevier BV, pp. 19537–19545, Nov. 2017. doi: 10.1074/jbc.m117.813469.*  
  
*M. J. M. Niesen, A. Müller-Lucks, R. Hedman, G. von Heijneand T. F. Miller III, “Forces on Nascent Polypeptides during Membrane Insertion and Translocation via the Sec Translocon”, Biophysical Journal, vol. 115, no. 10. Elsevier BV, pp. 1885–1894, Nov. 2018. doi: 10.1016/j.bpj.2018.10.002.*  
  
*M. J. M. Niesen, C. Y. Wang, R. C. Van Lehnand T. F. Miller, “Structurally detailed coarse-grained model for Sec-facilitated co-translational protein translocation and membrane integration”, PLOS Computational Biology, vol. 13, no. 3. Public Library of Science (PLoS), p. e1005427, Mar. 22, 2017. doi: 10.1371/journal.pcbi.1005427.*  
  
*F. A. Heberle, “The Molecular Structure of Sphingomyelin in Fluid Phase Bilayers Determined by the Joint Analysis of Neutron and X-Ray Scattering Data”, Biophysical Journal, vol. 112, no. 3. Elsevier BV, p. 223a, Feb. 2017. doi: 10.1016/j.bpj.2016.11.1231.*  
  
*R. Ali, R. Latif, T. Daviesand M. Mezei, “Predicting Transmembrane Dimerization and the Interfaces in Thyroid-Stimulating Hormone Receptor (TSHR) Using Brownian Dynamics Stimulation”, Biophysical Journal, vol. 100, no. 3. Elsevier BV, p. 158a, Feb. 2011. doi: 10.1016/j.bpj.2010.12.1076.*  
  
*H. L. Mays Jr., “Genomic Analysis of Demographic History and Ecological Niche Modeling in the Endangered Sumatran Rhinoceros Dicerorhinus sumatrensis”, Current Biology, vol. 28, no. 1. Elsevier BV, pp. 70–76.e4, Jan. 2018. doi: 10.1016/j.cub.2017.11.021.*  
  
*G. Janson, C. Zhang, M. G. Pradoand A. Paiardini, “PyMod 2.0: improvements in protein sequence-structure analysis and homology modeling within PyMOL”, Bioinformatics. Oxford University Press (OUP), p. btw638, Oct. 13, 2016. doi: 10.1093/bioinformatics/btw638.*  
  
*R. Yeasmin, M. Buck, A. Weinbergand L. Zhang, “Translocation of Human β Defensin Type 3 through a Neutrally Charged Lipid Membrane: A Free Energy Study”, The Journal of Physical Chemistry B, vol. 122, no. 50. American Chemical Society (ACS), pp. 11883–11894, Nov. 15, 2018. doi: 10.1021/acs.jpcb.8b08285.*  
  
*M. Freeberg and M. Heydarian, “Training Material For Chip-Seq Analysis”. Zenodo, Dec. 08, 2016. doi: 10.5281/ZENODO.197100.*  
  
*M. Freeberg and M. Heydarian, “Training Material For De Novo Transcriptome Reconstruction From Rna-Seq Data”. Zenodo, Jan. 20, 2017. doi: 10.5281/ZENODO.254485.*  
  
*N. E. Weiser, “MORC-1 Integrates Nuclear RNAi and Transgenerational Chromatin Architecture to Promote Germline Immortality”, Developmental Cell, vol. 41, no. 4. Elsevier BV, pp. 408–423.e7, May 2017. doi: 10.1016/j.devcel.2017.04.023.*  
  
*Q. L. He, “Exchange-biasing topological charges by antiferromagnetism”, Nature Communications, vol. 9, no. 1. Springer Science and Business Media LLC, Jul. 17, 2018. doi: 10.1038/s41467-018-05166-9.*  
  
*Q. L. He, “Topological Transitions Induced by Antiferromagnetism in a Thin-Film Topological Insulator”, Physical Review Letters, vol. 121, no. 9. American Physical Society (APS), Aug. 29, 2018. doi: 10.1103/physrevlett.121.096802.*  
  
*D. P. Hoogerheide, S. Y. Noskov, A. J. Kuszak, S. K. Buchanan, T. K. Rostovtsevaand H. Nanda, “Structure of voltage-dependent anion channel-tethered bilayer lipid membranes determined using neutron reflectivity”, Acta Crystallographica Section D Structural Biology, vol. 74, no. 12. International Union of Crystallography (IUCr), pp. 1219–1232, Nov. 30, 2018. doi: 10.1107/s2059798318011749.*  
  
*V. Jadhav, D. P. Hoogerheide, J. Korlachand M. Wanunu, “Porous Zero-Mode Waveguides for Picogram-Level DNA Capture”, Nano Letters, vol. 19, no. 2. American Chemical Society (ACS), pp. 921–929, Nov. 28, 2018. doi: 10.1021/acs.nanolett.8b04170.*  
  
*Q. Shao, “Exploring interfacial exchange coupling and sublattice effect in heavy metal/ferrimagnetic insulator heterostructures using Hall measurements, x-ray magnetic circular dichroism, and neutron reflectometry”, Physical Review B, vol. 99, no. 10. American Physical Society (APS), Mar. 04, 2019. doi: 10.1103/physrevb.99.104401.*  
  
*X. Zhai, A. J. Grutter, Y. Yun, Z. Cuiand Y. Lu, “Weak magnetism of Aurivillius-type multiferroic thin films probed by polarized neutron reflectivity”, Physical Review Materials, vol. 2, no. 4. American Physical Society (APS), Apr. 27, 2018. doi: 10.1103/physrevmaterials.2.044405.*  
  
*D. P. Hoogerheide, “Structural features and lipid binding domain of tubulin on biomimetic mitochondrial membranes”, Proceedings of the National Academy of Sciences, vol. 114, no. 18. Proceedings of the National Academy of Sciences, Apr. 18, 2017. doi: 10.1073/pnas.1619806114.*  
  
*T. C. Bidone, W. Jung, D. Maruri, C. Borau, R. D. Kammand T. Kim, “Morphological Transformation and Force Generation of Active Cytoskeletal Networks”, PLOS Computational Biology, vol. 13, no. 1. Public Library of Science (PLoS), p. e1005277, Jan. 23, 2017. doi: 10.1371/journal.pcbi.1005277.*  
  
*A.-R. Hassan, T. Bieland T. Kim, “Mechanical Model for Durotactic Cell Migration”, ACS Biomaterials Science & Engineering, vol. 5, no. 8. American Chemical Society (ACS), pp. 3954–3963, Mar. 12, 2019. doi: 10.1021/acsbiomaterials.8b01365.*  
  
*A.-R. Hassan, T. Biel, D. M. Umulisand T. Kim, “Interplay Between the Persistent Random Walk and the Contact Inhibition of Locomotion Leads to Collective Cell Behaviors”, Bulletin of Mathematical Biology, vol. 81, no. 8. Springer Science and Business Media LLC, pp. 3301–3321, Feb. 20, 2019. doi: 10.1007/s11538-019-00585-1.*  
  
*W. Jung, L. A. Fillenwarth, A. Matsuda, J. Li, Y. Inoueand T. Kim, “Collective and contractile filament motions in the myosin motility assay”, Soft Matter, vol. 16, no. 6. Royal Society of Chemistry (RSC), pp. 1548–1559, 2020. doi: 10.1039/c9sm02082a.*  
  
*W. Jung, A. P. Tabatabai, J. J. Thomas, S. M. A. Tabei, M. P. Murrelland T. Kim, “Dynamic motions of molecular motors in the actin cytoskeleton”, Cytoskeleton, vol. 76, no. 11–12. Wiley, pp. 517–531, Nov. 2019. doi: 10.1002/cm.21582.*  
  
*J. Li, T. Biel, P. Lomada, Q. Yuand T. Kim, “Buckling-induced F-actin fragmentation modulates the contraction of active cytoskeletal networks”, Soft Matter, vol. 13, no. 17. Royal Society of Chemistry (RSC), pp. 3213–3220, 2017. doi: 10.1039/c6sm02703b.*  
  
*A. Matsuda, J. Li, P. Brumm, T. Adachi, Y. Inoueand T. Kim, “Mobility of Molecular Motors Regulates Contractile Behaviors of Actin Networks”, Biophysical Journal, vol. 116, no. 11. Elsevier BV, pp. 2161–2171, Jun. 2019. doi: 10.1016/j.bpj.2019.04.018.*  
  
*K. M. Wisdom, D. Indana, P.-E. Chou, R. Desai, T. Kimand O. Chaudhuri, “Covalent cross-linking of basement membrane-like matrices physically restricts invasive protrusions in breast cancer cells”, Matrix Biology, vol. 85–86. Elsevier BV, pp. 94–111, Jan. 2020. doi: 10.1016/j.matbio.2019.05.006.*  
  
*Q. Yu, J. Li, M. P. Murrelland T. Kim, “Balance between Force Generation and Relaxation Leads to Pulsed Contraction of Actomyosin Networks”, Biophysical Journal, vol. 115, no. 10. Elsevier BV, pp. 2003–2013, Nov. 2018. doi: 10.1016/j.bpj.2018.10.008.*  
  
*K. W. East, “Allosteric Motions of the CRISPR–Cas9 HNH Nuclease Probed by NMR and Molecular Dynamics”, Journal of the American Chemical Society, vol. 142, no. 3. American Chemical Society (ACS), pp. 1348–1358, Dec. 30, 2019. doi: 10.1021/jacs.9b10521.*  
  
*C. G. Ricci, “Molecular mechanism of off-target effects in CRISPR-Cas9”, []. Cold Spring Harbor Laboratory, Sep. 19, 2018. doi: 10.1101/421537.*  
  
*R. E. S. Harrison, “Factor H-Inspired Design of Peptide Biomarkers of the Complement C3d Protein”, ACS Medicinal Chemistry Letters, vol. 11, no. 5. American Chemical Society (ACS), pp. 1054–1059, Feb. 28, 2020. doi: 10.1021/acsmedchemlett.9b00663.*  
  
*R. E. S. Harrison, “Factor H-Inspired Design of Peptide Biomarkers of the Complement C3d Protein”, ACS Medicinal Chemistry Letters, vol. 11, no. 5. American Chemical Society (ACS), pp. 1054–1059, Feb. 28, 2020. doi: 10.1021/acsmedchemlett.9b00663.*  
  
*B. P. Mitchell, R. V. Hsu, M. A. Medrano, N. T. Zewde, Y. B. Narkhedeand G. Palermo, “Spontaneous Embedding of DNA Mismatches Within the RNA:DNA Hybrid of CRISPR-Cas9”, Frontiers in Molecular Biosciences, vol. 7. Frontiers Media SA, Mar. 17, 2020. doi: 10.3389/fmolb.2020.00039.*  
  
*G. Palermo, “Structure and Dynamics of the CRISPR–Cas9 Catalytic Complex”, Journal of Chemical Information and Modeling, vol. 59, no. 5. American Chemical Society (ACS), pp. 2394–2406, Feb. 14, 2019. doi: 10.1021/acs.jcim.8b00988.*  
  
*G. Palermo, “Key role of the REC lobe during CRISPR–Cas9 activation by ‘sensing’, ‘regulating’, and ‘locking’ the catalytic HNH domain”, Quarterly Reviews of Biophysics, vol. 51. Cambridge University Press (CUP), 2018. doi: 10.1017/s0033583518000070.*  
  
*G. Palermo, Y. Miao, R. C. Walker, M. Jinekand J. A. McCammon, “Striking Plasticity of CRISPR-Cas9 and Key Role of Non-target DNA, as Revealed by Molecular Simulations”, ACS Central Science, vol. 2, no. 10. American Chemical Society (ACS), pp. 756–763, Sep. 09, 2016. doi: 10.1021/acscentsci.6b00218.*  
  
*G. Palermo, Y. Miao, R. C. Walker, M. Jinekand J. A. McCammon, “CRISPR-Cas9 conformational activation as elucidated from enhanced molecular simulations”, Proceedings of the National Academy of Sciences, vol. 114, no. 28. Proceedings of the National Academy of Sciences, pp. 7260–7265, Jun. 26, 2017. doi: 10.1073/pnas.1707645114.*  
  
*B. T. Castle, S. McCubbin, L. S. Prahl, J. N. Bernens, D. Septand D. J. Odde, “Mechanisms of kinetic stabilization by the drugs paclitaxel and vinblastine”, Molecular Biology of the Cell, vol. 28, no. 9. American Society for Cell Biology (ASCB), pp. 1238–1257, May 2017. doi: 10.1091/mbc.e16-08-0567.*  
  
*M. Hemmat, B. T. Castleand D. J. Odde, “Microtubule dynamics: moving toward a multi-scale approach”, Current Opinion in Cell Biology, vol. 50. Elsevier BV, pp. 8–13, Feb. 2018. doi: 10.1016/j.ceb.2017.12.013.*  
  
*S.-P. Chou and C. G. Danko, “AlleleHMM: a data-driven method to identify allele-specific differences in distributed functional genomic marks”, []. Cold Spring Harbor Laboratory, Aug. 10, 2018. doi: 10.1101/389262.*  
  
*C. G. Danko, “Dynamic evolution of regulatory element ensembles in primate CD4+ T cells”, Nature Ecology & Evolution, vol. 2, no. 3. Springer Science and Business Media LLC, pp. 537–548, Jan. 29, 2018. doi: 10.1038/s41559-017-0447-5.*  
  
*S. Horibata, “ER-positive breast cancer cells are poised for RET-mediated endocrine resistance”, PLOS ONE, vol. 13, no. 4. Public Library of Science (PLoS), p. e0194023, Apr. 02, 2018. doi: 10.1371/journal.pone.0194023.*  
  
*S. Horibata, “A bi-stable feedback loop between GDNF, EGR1, and ERα contribute to endocrine resistant breast cancer”, PLOS ONE, vol. 13, no. 4. Public Library of Science (PLoS), p. e0194522, Apr. 03, 2018. doi: 10.1371/journal.pone.0194522.*  
  
*Z. Wang, A. L. Martinsand C. G. Danko, “RTFBSDB: an integrated framework for transcription factor binding site analysis”, Bioinformatics, vol. 32, no. 19. Oxford University Press (OUP), pp. 3024–3026, Jun. 10, 2016. doi: 10.1093/bioinformatics/btw338.*  
  
*F. Pan, V. H. Man, C. Rolandand C. Sagui, “Structure and Dynamics of DNA and RNA Double Helices Obtained from the CCG and GGC Trinucleotide Repeats”, The Journal of Physical Chemistry B, vol. 122, no. 16. American Chemical Society (ACS), pp. 4491–4512, Apr. 04, 2018. doi: 10.1021/acs.jpcb.8b01658.*  
  
*F. Pan, Y. Zhang, V. H. Man, C. Rolandand C. Sagui, “E-motif formed by extrahelical cytosine bases in DNA homoduplexes of trinucleotide and hexanucleotide repeats”, Nucleic Acids Research, vol. 46, no. 2. Oxford University Press (OUP), pp. 942–955, Nov. 28, 2017. doi: 10.1093/nar/gkx1186.*  
  
*Y. Zhang, C. Rolandand C. Sagui, “Structural and Dynamical Characterization of DNA and RNA Quadruplexes Obtained from the GGGGCC and GGGCCT Hexanucleotide Repeats Associated with C9FTD/ALS and SCA36 Diseases”, ACS Chemical Neuroscience, vol. 9, no. 5. American Chemical Society (ACS), pp. 1104–1117, Dec. 27, 2017. doi: 10.1021/acschemneuro.7b00476.*  
  
*A. Mentes, “High-resolution cryo-EM structures of actin-bound myosin states reveal the mechanism of myosin force sensing”, Proceedings of the National Academy of Sciences, vol. 115, no. 6. Proceedings of the National Academy of Sciences, pp. 1292–1297, Jan. 22, 2018. doi: 10.1073/pnas.1718316115.*  
  
*A. Mentes, H. Shumanand E. M. Ostap, “Molecular Dynamics and Normal Mode Analysis of Myo1b and Myo1b Deletion Constructs Reveal Coupling between the Lever Arm Helix, N-Terminus, and Active Site”, Biophysical Journal, vol. 112, no. 3. Elsevier BV, pp. 265a–266a, Feb. 2017. doi: 10.1016/j.bpj.2016.11.1441.*  
  
*B. Fritch, “Origins of the Mechanochemical Coupling of Peptide Bond Formation to Protein Synthesis”, Journal of the American Chemical Society, vol. 140, no. 15. American Chemical Society (ACS), pp. 5077–5087, Mar. 26, 2018. doi: 10.1021/jacs.7b11044.*  
  
*S. M. Saladi, N. Javed, A. Müllerand W. M. Clemons Jr., “A statistical model for improved membrane protein expression using sequence-derived features”, Journal of Biological Chemistry, vol. 293, no. 13. Elsevier BV, pp. 4913–4927, Mar. 2018. doi: 10.1074/jbc.ra117.001052.*  
  
*B. He, S. M. Mortuza, Y. Wang, H.-B. Shenand Y. Zhang, “NeBcon: protein contact map prediction using neural network training coupled with naïve Bayes classifiers”, Bioinformatics, vol. 33, no. 15. Oxford University Press (OUP), pp. 2296–2306, Mar. 28, 2017. doi: 10.1093/bioinformatics/btx164.*  
  
*C. Zhang, P. L. Freddolinoand Y. Zhang, “COFACTOR: improved protein function prediction by combining structure, sequence and protein–protein interaction information”, Nucleic Acids Research, vol. 45, no. W1. Oxford University Press (OUP), pp. W291–W299, May 02, 2017. doi: 10.1093/nar/gkx366.*  
  
*Y. Li, C. Zhang, E. W. Bell, D. Yuand Y. Zhang, “Ensembling multiple raw coevolutionary features with deep residual neural networks for contact‐map prediction in CASP13”, Proteins: Structure, Function, and Bioinformatics, vol. 87, no. 12. Wiley, pp. 1082–1091, Aug. 22, 2019. doi: 10.1002/prot.25798.*  
  
*Y. Wang, “Fueling ab initio folding with marine metagenomics enables structure and function predictions of new protein families”, Genome Biology, vol. 20, no. 1. Springer Science and Business Media LLC, Nov. 01, 2019. doi: 10.1186/s13059-019-1823-z.*  
  
*Y. Wang, J. Virtanen, Z. Xueand Y. Zhang, “I-TASSER-MR: automated molecular replacement for distant-homology proteins using iterative fragment assembly and progressive sequence truncation”, Nucleic Acids Research, vol. 45, no. W1. Oxford University Press (OUP), pp. W429–W434, May 02, 2017. doi: 10.1093/nar/gkx349.*  
  
*X. Wei, C. Zhang, P. L. Freddolinoand Y. Zhang, “Detecting Gene Ontology misannotations using taxon-specific rate ratio comparisons”, Bioinformatics, vol. 36, no. 16. Oxford University Press (OUP), pp. 4383–4388, May 29, 2020. doi: 10.1093/bioinformatics/btaa548.*  
  
*C. Zhang, L. Lane, G. S. Omennand Y. Zhang, “Blinded Testing of Function Annotation for uPE1 Proteins by I-TASSER/COFACTOR Pipeline Using the 2018–2019 Additions to neXtProt and the CAFA3 Challenge”, Journal of Proteome Research, vol. 18, no. 12. American Chemical Society (ACS), pp. 4154–4166, Oct. 04, 2019. doi: 10.1021/acs.jproteome.9b00537.*  
  
*C. Zhang, S. M. Mortuza, B. He, Y. Wangand Y. Zhang, “Template‐based and free modeling of I‐TASSER and QUARK pipelines using predicted contact maps in CASP12”, Proteins: Structure, Function, and Bioinformatics, vol. 86, no. S1. Wiley, pp. 136–151, Nov. 14, 2017. doi: 10.1002/prot.25414.*  
  
*C. Zhang, X. Wei, G. S. Omennand Y. Zhang, “Structure and Protein Interaction-Based Gene Ontology Annotations Reveal Likely Functions of Uncharacterized Proteins on Human Chromosome 17”, Journal of Proteome Research, vol. 17, no. 12. American Chemical Society (ACS), pp. 4186–4196, Sep. 28, 2018. doi: 10.1021/acs.jproteome.8b00453.*  
  
*C. Zhang, W. Zheng, P. L. Freddolinoand Y. Zhang, “MetaGO: Predicting Gene Ontology of Non-homologous Proteins Through Low-Resolution Protein Structure Prediction and Protein–Protein Network Mapping”, Journal of Molecular Biology, vol. 430, no. 15. Elsevier BV, pp. 2256–2265, Jul. 2018. doi: 10.1016/j.jmb.2018.03.004.*  
  
*C. Zhang, W. Zheng, S. M. Mortuza, Y. Liand Y. Zhang, “DeepMSA: constructing deep multiple sequence alignment to improve contact prediction and fold-recognition for distant-homology proteins”, Bioinformatics, vol. 36, no. 7. Oxford University Press (OUP), pp. 2105–2112, Nov. 18, 2019. doi: 10.1093/bioinformatics/btz863.*  
  
*W. Zheng, Y. Li, C. Zhang, R. Pearce, S. M. Mortuzaand Y. Zhang, “Deep‐learning contact‐map guided protein structure prediction in CASP13”, Proteins: Structure, Function, and Bioinformatics, vol. 87, no. 12. Wiley, pp. 1149–1164, Aug. 14, 2019. doi: 10.1002/prot.25792.*  
  
*W. Zheng, “Detecting distant-homology protein structures by aligning deep neural-network based contact maps”, PLOS Computational Biology, vol. 15, no. 10. Public Library of Science (PLoS), p. e1007411, Oct. 17, 2019. doi: 10.1371/journal.pcbi.1007411.*  
  
*C. K. Abrams, “Alterations at Arg76of human connexin 46, a residue associated with cataract formation, cause loss of gap junction formation but preserve hemichannel function”, American Journal of Physiology-Cell Physiology, vol. 315, no. 5. American Physiological Society, pp. C623–C635, Nov. 01, 2018. doi: 10.1152/ajpcell.00157.2018.*  
  
*J. M. Valdez Capuccino, “The connexin26 human mutation N14K disrupts cytosolic intersubunit interactions and promotes channel opening”, The Journal of General Physiology, vol. 151, no. 3. Rockefeller University Press, pp. 328–341, Dec. 07, 2018. doi: 10.1085/jgp.201812219.*  
  
*A. Alsamarah, A. E. LaCuran, P. Oelschlaeger, J. Haoand Y. Luo, “Uncovering Molecular Bases Underlying Bone Morphogenetic Protein Receptor Inhibitor Selectivity”, PLOS ONE, vol. 10, no. 7. Public Library of Science (PLoS), p. e0132221, Jul. 02, 2015. doi: 10.1371/journal.pone.0132221.*  
  
*P. Chatterjee, “Can Relative Binding Free Energy Predict Selectivity of Reversible Covalent Inhibitors?”, Journal of the American Chemical Society, vol. 139, no. 49. American Chemical Society (ACS), pp. 17945–17952, Nov. 29, 2017. doi: 10.1021/jacs.7b08938.*  
  
*K. Chattrakun, D. P. Hoogerheide, C. Mao, L. L. Randalland G. M. King, “Protein Translocation Activity in Surface-Supported Lipid Bilayers”, Langmuir, vol. 35, no. 37. American Chemical Society (ACS), pp. 12246–12256, Aug. 25, 2019. doi: 10.1021/acs.langmuir.9b01928.*  
  
*D. P. Hoogerheide, P. A. Gurnev, T. K. Rostovtsevaand S. M. Bezrukov, “Real-Time Nanopore-Based Recognition of Protein Translocation Success”, Biophysical Journal, vol. 114, no. 4. Elsevier BV, pp. 772–776, Feb. 2018. doi: 10.1016/j.bpj.2017.12.019.*  
  
*E. D. Rus and J. A. Dura, “In Situ Neutron Reflectometry Study of Solid Electrolyte Interface (SEI) Formation on Tungsten Thin-Film Electrodes”, ACS Applied Materials & Interfaces, vol. 11, no. 50. American Chemical Society (ACS), pp. 47553–47563, Dec. 09, 2019. doi: 10.1021/acsami.9b16592.*  
  
*J. M. Vanegas, “Insertion of Dengue E into lipid bilayers studied by neutron reflectivity and molecular dynamics simulations”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1860, no. 5. Elsevier BV, pp. 1216–1230, May 2018. doi: 10.1016/j.bbamem.2018.02.012.*  
  
*B. W. Treece, P. A. Kienzle, D. P. Hoogerheide, C. F. Majkrzak, M. Löscheand F. Heinrich, “Optimization of reflectometry experiments using information theory”, Journal of Applied Crystallography, vol. 52, no. 1. International Union of Crystallography (IUCr), pp. 47–59, Feb. 01, 2019. doi: 10.1107/s1600576718017016.*  
  
*A. R. Crofts, S. W. Rose, R. L. Burton, A. V. Desai, P. J. A. Kenisand S. A. Dikanov, “The Q-Cycle Mechanism of the bc1 Complex: A Biologist’s Perspective on Atomistic Studies”, The Journal of Physical Chemistry B, vol. 121, no. 15. American Chemical Society (ACS), pp. 3701–3717, Mar. 14, 2017. doi: 10.1021/acs.jpcb.6b10524.*  
  
*A. Eskandari Nasrabad and R. Laghaei, “Thermodynamic and transport properties of nitrogen fluid: Molecular theory and computer simulations”, Chemical Physics, vol. 506. Elsevier BV, pp. 36–44, Apr. 2018. doi: 10.1016/j.chemphys.2018.03.026.*  
  
*A. E. Homan, R. Laghaei, M. Dittrichand S. D. Meriney, “Impact of spatiotemporal calcium dynamics within presynaptic active zones on synaptic delay at the frog neuromuscular junction”, Journal of Neurophysiology, vol. 119, no. 2. American Physiological Society, pp. 688–699, Feb. 01, 2018. doi: 10.1152/jn.00510.2017.*  
  
*R. Laghaei, “Transmitter release site organization can predict synaptic function at the neuromuscular junction”, Journal of Neurophysiology, vol. 119, no. 4. American Physiological Society, pp. 1340–1355, Apr. 01, 2018. doi: 10.1152/jn.00168.2017.*  
  
*B. G. Horan, G. H. Zerze, Y. C. Kim, D. Vavylonisand J. Mittal, “Computational modeling highlights the role of the disordered Formin Homology 1 domain in profilin‐actin transfer”, FEBS Letters, vol. 592, no. 11. Wiley, pp. 1804–1816, May 24, 2018. doi: 10.1002/1873-3468.13088.*  
  
*Z. A. Qadeer, “ATRX In-Frame Fusion Neuroblastoma Is Sensitive to EZH2 Inhibition via Modulation of Neuronal Gene Signatures”, Cancer Cell, vol. 36, no. 5. Elsevier BV, pp. 512–527.e9, Nov. 2019. doi: 10.1016/j.ccell.2019.09.002.*  
  
*E. Sendinc, “PCIF1 Catalyzes m6Am mRNA Methylation to Regulate Gene Expression”, Molecular Cell, vol. 75, no. 3. Elsevier BV, pp. 620–630.e9, Aug. 2019. doi: 10.1016/j.molcel.2019.05.030.*  
  
*C. F. Wong, “Steered molecular dynamics simulations for uncovering the molecular mechanisms of drug dissociation and for drug screening: A test on the focal adhesion kinase”, Journal of Computational Chemistry, vol. 39, no. 19. Wiley, pp. 1307–1318, Mar. 02, 2018. doi: 10.1002/jcc.25201.*  
  
*S. Liao, C. Floyd, N. Verratti, L. Leungand C. Wu, “Analysis of vismodegib resistance in D473G and W535L mutants of SMO receptor and design of novel drug derivatives using molecular dynamics simulations”, Life Sciences, vol. 244. Elsevier BV, p. 117302, Mar. 2020. doi: 10.1016/j.lfs.2020.117302.*  
  
*F. Liu, “Experimental and Simulation Identification of Xanthohumol as an Inhibitor and Substrate of ABCB1”, Applied Sciences, vol. 8, no. 5. MDPI AG, p. 681, Apr. 27, 2018. doi: 10.3390/app8050681.*  
  
*D. Montgomery, A. Campbell, H.-J. Sullivanand C. Wu, “Molecular dynamics simulation of biased agonists at the dopamine D2 receptor suggests the mechanism of receptor functional selectivity”, Journal of Biomolecular Structure and Dynamics, vol. 37, no. 12. Informa UK Limited, pp. 3206–3225, Nov. 13, 2018. doi: 10.1080/07391102.2018.1513378.*  
  
*H.-J. Sullivan, C. Readmond, C. Radicella, V. Persad, T. J. Fasanoand C. Wu, “Binding of Telomestatin, TMPyP4, BSU6037, and BRACO19 to a Telomeric G-Quadruplex–Duplex Hybrid Probed by All-Atom Molecular Dynamics Simulations with Explicit Solvent”, ACS Omega, vol. 3, no. 11. American Chemical Society (ACS), pp. 14788–14806, Nov. 05, 2018. doi: 10.1021/acsomega.8b01574.*  
  
*A. I. Ilitchev, “Hetero-oligomeric Amyloid Assembly and Mechanism: Prion Fragment PrP(106–126) Catalyzes the Islet Amyloid Polypeptide β-Hairpin”, Journal of the American Chemical Society, vol. 140, no. 30. American Chemical Society (ACS), pp. 9685–9695, Jul. 10, 2018. doi: 10.1021/jacs.8b05925.*  
  
*S. Bowerman, J. E. Curtis, J. Clayton, E. H. Brookesand J. Wereszczynski, “BEES: Bayesian Ensemble Estimation from SAS”, []. Cold Spring Harbor Laboratory, Aug. 25, 2018. doi: 10.1101/400168.*  
  
*S. Banerjee, M. Hashemi, Z. Lv, S. Maity, J.-C. Rochetand Y. L. Lyubchenko, “A novel pathway for amyloids self-assembly in aggregates at nanomolar concentration mediated by the interaction with surfaces”, Scientific Reports, vol. 7, no. 1. Springer Science and Business Media LLC, Mar. 30, 2017. doi: 10.1038/srep45592.*  
  
*S. Maity, M. Hashemiand Y. L. Lyubchenko, “Nano-assembly of amyloid β peptide: role of the hairpin fold”, Scientific Reports, vol. 7, no. 1. Springer Science and Business Media LLC, May 24, 2017. doi: 10.1038/s41598-017-02454-0.*  
  
*A. Dickson, P. Tiwaryand H. Vashisth, “Kinetics of Ligand Binding Through Advanced Computational Approaches: A Review”, Current Topics in Medicinal Chemistry, vol. 17, no. 23. Bentham Science Publishers Ltd., Aug. 08, 2017. doi: 10.2174/1568026617666170414142908.*  
  
*L. Levintov and H. Vashisth, “Ligand Recognition in Viral RNA Necessitates Rare Conformational Transitions”, The Journal of Physical Chemistry Letters, vol. 11, no. 14. American Chemical Society (ACS), pp. 5426–5432, Jun. 18, 2020. doi: 10.1021/acs.jpclett.0c01390.*  
  
*Y. Liu and H. Vashisth, “Conformational dynamics and interfacial interactions of peptide-appended pillar[5]arene water channels in biomimetic membranes”, Physical Chemistry Chemical Physics, vol. 21, no. 41. Royal Society of Chemistry (RSC), pp. 22711–22721, 2019. doi: 10.1039/c9cp04408f.*  
  
*H. Mohammadiarani, V. S. Shaw, R. R. Neubigand H. Vashisth, “Interpreting Hydrogen–Deuterium Exchange Events in Proteins Using Atomistic Simulations: Case Studies on Regulators of G-Protein Signaling Proteins”, The Journal of Physical Chemistry B, vol. 122, no. 40. American Chemical Society (ACS), pp. 9314–9323, Sep. 17, 2018. doi: 10.1021/acs.jpcb.8b07494.*  
  
*M. Mohammadi, H. Mohammadiarani, V. S. Shaw, R. R. Neubigand H. Vashisth, “Interplay of cysteine exposure and global protein dynamics in small‐molecule recognition by a regulator of G‐protein signaling protein”, Proteins: Structure, Function, and Bioinformatics, vol. 87, no. 2. Wiley, pp. 146–156, Dec. 26, 2018. doi: 10.1002/prot.25642.*  
  
*M. Mohammadi and H. Vashisth, “Pathways and Thermodynamics of Oxygen Diffusion in [FeFe]-Hydrogenase”, The Journal of Physical Chemistry B, vol. 121, no. 43. American Chemical Society (ACS), pp. 10007–10017, Oct. 18, 2017. doi: 10.1021/acs.jpcb.7b06489.*  
  
*S. Paul and H. Vashisth, “Self-assembly of lobed particles into amorphous and crystalline porous structures”, Soft Matter, vol. 16, no. 5. Royal Society of Chemistry (RSC), pp. 1142–1147, 2020. doi: 10.1039/c9sm01878f.*  
  
*K. D. Schuster, “Pharmacological and molecular dynamics analyses of differences in inhibitor binding to human and nematode PDE4: Implications for management of parasitic nematodes”, PLOS ONE, vol. 14, no. 3. Public Library of Science (PLoS), p. e0214554, Mar. 27, 2019. doi: 10.1371/journal.pone.0214554.*  
  
*V. S. Shaw, H. Mohammadiarani, H. Vashisthand R. R. Neubig, “Differential Protein Dynamics of Regulators of G-Protein Signaling: Role in Specificity of Small-Molecule Inhibitors”, Journal of the American Chemical Society, vol. 140, no. 9. American Chemical Society (ACS), pp. 3454–3460, Feb. 20, 2018. doi: 10.1021/jacs.7b13778.*  
  
*V. S. Shaw, M. Mohammadi, J. A. Quinn, H. Vashisthand R. R. Neubig, “An Interhelical Salt Bridge Controls Flexibility and Inhibitor Potency for Regulators of G-protein Signaling Proteins 4, 8, and 19”, Molecular Pharmacology, vol. 96, no. 6. American Society for Pharmacology & Experimental Therapeutics (ASPET), pp. 683–691, Sep. 22, 2019. doi: 10.1124/mol.119.117176.*  
  
*S. Tannir, “Functional Nanoassemblies with Mirror-Image Chiroptical Properties Templated by a Single Homochiral DNA Strand”, Chemistry of Materials, vol. 32, no. 6. American Chemical Society (ACS), pp. 2272–2281, Mar. 02, 2020. doi: 10.1021/acs.chemmater.9b04092.*  
  
*K. Huang, S. Xhani, A. V. Albrecht, V. L. T. Ha, S. Esakiand G. M. K. Poon, “Mechanism of cognate sequence discrimination by the ETS-family transcription factor ETS-1”, Journal of Biological Chemistry, vol. 294, no. 25. Elsevier BV, pp. 9666–9678, Jun. 2019. doi: 10.1074/jbc.ra119.007866.*  
  
*E. K. Asciutto and T. C. Pochapsky, “Some Surprising Implications of NMR-directed Simulations of Substrate Recognition and Binding by Cytochrome P450 cam (CYP101A1)”, Journal of Molecular Biology, vol. 430, no. 9. Elsevier BV, pp. 1295–1310, Apr. 2018. doi: 10.1016/j.jmb.2018.03.014.*  
  
*D. B. Berry, B. Regner, V. Galinsky, S. R. Wardand L. R. Frank, “Relationships between tissue microstructure and the diffusion tensor in simulated skeletal muscle”, Magnetic Resonance in Medicine, vol. 80, no. 1. Wiley, pp. 317–329, Oct. 31, 2017. doi: 10.1002/mrm.26993.*  
  
*A. Ray, I. Macwan, S. Singh, S. Silwaland P. Patra, “A Computational Approach for Understanding the Interactions between Graphene Oxide and Nucleoside Diphosphate Kinase with Implications for Heart Failure”, Nanomaterials, vol. 8, no. 2. MDPI AG, p. 57, Jan. 23, 2018. doi: 10.3390/nano8020057.*  
  
*D. G. Walgenbach, A. J. Gregoryand J. C. Klein, “Unique methionine-aromatic interactions govern the calmodulin redox sensor”, Biochemical and Biophysical Research Communications, vol. 505, no. 1. Elsevier BV, pp. 236–241, Oct. 2018. doi: 10.1016/j.bbrc.2018.09.052.*  
  
*A. J. Lee, “DAFi: A directed recursive data filtering and clustering approach for improving and interpreting data clustering identification of cell populations from polychromatic flow cytometry data”, Cytometry Part A, vol. 93, no. 6. Wiley, pp. 597–610, Apr. 17, 2018. doi: 10.1002/cyto.a.23371.*  
  
*R. H. Scheuermann, J. Bui, H.-Y. Wangand Y. Qian, “Automated Analysis of Clinical Flow Cytometry Data”, Clinics in Laboratory Medicine, vol. 37, no. 4. Elsevier BV, pp. 931–944, Dec. 2017. doi: 10.1016/j.cll.2017.07.011.*  
  
*M. Chen, “Let It Catch: A Short‐Branched Protein for Efficiently Capturing Polysulfides in Lithium–Sulfur Batteries”, Advanced Energy Materials, vol. 10, no. 9. Wiley, p. 1903642, Jan. 31, 2020. doi: 10.1002/aenm.201903642.*  
  
*H. Deng, P. Duttaand J. Liu, “Stochastic simulations of nanoparticle internalization through transferrin receptor dependent clathrin-mediated endocytosis”, Biochimica et Biophysica Acta (BBA) - General Subjects, vol. 1862, no. 9. Elsevier BV, pp. 2104–2111, Sep. 2018. doi: 10.1016/j.bbagen.2018.06.018.*  
  
*H. Deng, P. Duttaand J. Liu, “Entry modes of ellipsoidal nanoparticles on a membrane during clathrin-mediated endocytosis”, Soft Matter, vol. 15, no. 25. Royal Society of Chemistry (RSC), pp. 5128–5137, 2019. doi: 10.1039/c9sm00751b.*  
  
*H. Deng, P. Duttaand J. Liu, “Stochastic modeling of nanoparticle internalization and expulsion through receptor-mediated transcytosis”, Nanoscale, vol. 11, no. 23. Royal Society of Chemistry (RSC), pp. 11227–11235, 2019. doi: 10.1039/c9nr02710f.*  
  
*X. Fu, “Building Ion-Conduction Highways in Polymeric Electrolytes by Manipulating Protein Configuration”, ACS Applied Materials & Interfaces, vol. 10, no. 5. American Chemical Society (ACS), pp. 4726–4736, Jan. 27, 2018. doi: 10.1021/acsami.7b17156.*  
  
*X. Fu, C. Li, Y. Wang, L. Scudiero, J. Liuand W.-H. Zhong, “Self-Assembled Protein Nanofilter for Trapping Polysulfides and Promoting Li+ Transport in Lithium–Sulfur Batteries”, The Journal of Physical Chemistry Letters, vol. 9, no. 10. American Chemical Society (ACS), pp. 2450–2459, Apr. 24, 2018. doi: 10.1021/acs.jpclett.8b00836.*  
  
*Y. Jewel, P. Duttaand J. Liu, “Exploration of conformational changes in lactose permease upon sugar binding and proton transfer through coarse‐grained simulations”, Proteins: Structure, Function, and Bioinformatics, vol. 85, no. 10. Wiley, pp. 1856–1865, Jul. 06, 2017. doi: 10.1002/prot.25340.*  
  
*Y. Jewel, J. Liuand P. Dutta, “Coarse-grained simulations of conformational changes in the multidrug efflux transporter AcrB”, Molecular BioSystems, vol. 13, no. 10. Royal Society of Chemistry (RSC), pp. 2006–2014, 2017. doi: 10.1039/c7mb00276a.*  
  
*Y. Jewel, Q. Van Dinh, J. Liuand P. Dutta, “Substrate‐dependent transport mechanism in AcrB of multidrug resistant bacteria”, Proteins: Structure, Function, and Bioinformatics, vol. 88, no. 7. Wiley, pp. 853–864, Feb. 08, 2020. doi: 10.1002/prot.25877.*  
  
*C. Li, X. Fu, W. Zhongand J. Liu, “Dissipative Particle Dynamics Simulations of a Protein-Directed Self-Assembly of Nanoparticles”, ACS Omega, vol. 4, no. 6. American Chemical Society (ACS), pp. 10216–10224, Jun. 12, 2019. doi: 10.1021/acsomega.9b01078.*  
  
*A. Ahuja, “Validated Computational Model to Compute Re-apposition Pressures for Treating Type-B Aortic Dissections”, Frontiers in Physiology, vol. 9. Frontiers Media SA, May 09, 2018. doi: 10.3389/fphys.2018.00513.*  
  
*M. S. Avestan, A. Javidi, L. P. Ganote, J. M. Brownand G. Stan, “Kinetic effects in directional proteasomal degradation of the green fluorescent protein”, The Journal of Chemical Physics, vol. 153, no. 10. AIP Publishing, p. 105101, Sep. 14, 2020. doi: 10.1063/5.0015191.*  
  
*A. Javidialesaadi, S. M. Flournoyand G. Stan, “Role of Diffusion in Unfolding and Translocation of Multidomain Titin I27 Substrates by a Clp ATPase Nanomachine”, The Journal of Physical Chemistry B, vol. 123, no. 12. American Chemical Society (ACS), pp. 2623–2635, Jan. 25, 2019. doi: 10.1021/acs.jpcb.8b10282.*  
  
*J. S. Shore, H. J. Hamam, P. D. J. Chafe, J. D. J. Labonne, P. M. Henningand A. G. McCubbin, “The long and short of the S ‐locus in Turnera (Passifloraceae)”, New Phytologist, vol. 224, no. 3. Wiley, pp. 1316–1329, Jul. 15, 2019. doi: 10.1111/nph.15970.*  
  
*N. B. M. Athreya, A. Sarathyand J.-P. Leburton, “Large Scale Parallel DNA Detection by Two-Dimensional Solid-State Multipore Systems”, ACS Sensors, vol. 3, no. 5. American Chemical Society (ACS), pp. 1032–1039, Apr. 17, 2018. doi: 10.1021/acssensors.8b00192.*  
  
*A. Sarathy, N. B. Athreya, L. R. Varshneyand J.-P. Leburton, “Classification of Epigenetic Biomarkers with Atomically Thin Nanopores”, The Journal of Physical Chemistry Letters, vol. 9, no. 19. American Chemical Society (ACS), pp. 5718–5725, Sep. 18, 2018. doi: 10.1021/acs.jpclett.8b02200.*  
  
*S. K. Tabatabaei, “DNA Punch Cards: Storing Data on Native DNA Sequences via Nicking”, []. Cold Spring Harbor Laboratory, Jun. 15, 2019. doi: 10.1101/672394.*  
  
*A. Bacolla, “Heritable pattern of oxidized DNA base repair coincides with pre-targeting of repair complexes to open chromatin”, Nucleic Acids Research, vol. 49, no. 1. Oxford University Press (OUP), pp. 221–243, Dec. 09, 2020. doi: 10.1093/nar/gkaa1120.*  
  
*A. Bacolla, Z. Ye, Z. Ahmedand J. A. Tainer, “Cancer mutational burden is shaped by G4 DNA, replication stress and mitochondrial dysfunction”, Progress in Biophysics and Molecular Biology, vol. 147. Elsevier BV, pp. 47–61, Oct. 2019. doi: 10.1016/j.pbiomolbio.2019.03.004.*  
  
*J. P. Lees-Miller, “Uncovering DNA-PKcs ancient phylogeny, unique sequence motifs and insights for human disease”, Progress in Biophysics and Molecular Biology, vol. 163. Elsevier BV, pp. 87–108, Aug. 2021. doi: 10.1016/j.pbiomolbio.2020.09.010.*  
  
*S. H. Seo, “Replication‐Based Rearrangements Are a Common Mechanism for SNCA Duplication in Parkinson’s Disease”, Movement Disorders, vol. 35, no. 5. Wiley, pp. 868–876, Feb. 10, 2020. doi: 10.1002/mds.27998.*  
  
*B. Apsel Winger, “ATP-Competitive Inhibitors Midostaurin and Avapritinib Have Distinct Resistance Profiles in Exon 17–Mutant KIT”, Cancer Research, vol. 79, no. 16. American Association for Cancer Research (AACR), pp. 4283–4292, Aug. 15, 2019. doi: 10.1158/0008-5472.can-18-3139.*  
  
*R. A. Charafeddine, “Tau repeat regions contain conserved histidine residues that modulate microtubule-binding in response to changes in pH”, Journal of Biological Chemistry, vol. 294, no. 22. Elsevier BV, pp. 8779–8790, May 2019. doi: 10.1074/jbc.ra118.007004.*  
  
*E. Brookes and M. Rocco, “Recent advances in the UltraScan SOlution MOdeller (US-SOMO) hydrodynamic and small-angle scattering data analysis and simulation suite”, European Biophysics Journal, vol. 47, no. 7. Springer Science and Business Media LLC, pp. 855–864, Mar. 28, 2018. doi: 10.1007/s00249-018-1296-0.*  
  
*E. Brookes and A. Savelyev, “GenApp Integrated with OpenStack Supports Elastic Computing on Jetstream”, Proceedings of the Practice and Experience in Advanced Research Computing 2017 on Sustainability, Success and Impact. ACM, Jul. 09, 2017. doi: 10.1145/3093338.3093356.*  
  
*E. Brookes and J. Stubbs, “GenApp, Containers and Abaco”, Proceedings of the Practice and Experience in Advanced Research Computing on Rise of the Machines (learning). ACM, Jul. 28, 2019. doi: 10.1145/3332186.3332191.*  
  
*A. Savelyev and E. Brookes, “GenApp: Extensible tool for rapid generation of web and native GUI applications”, Future Generation Computer Systems, vol. 94. Elsevier BV, pp. 929–936, May 2019. doi: 10.1016/j.future.2017.09.069.*  
  
*T. D. Martin, G. Brinkley, D. G. Whitten, E. Y. Chiand D. G. Evans, “Computational Investigation of the Binding Dynamics of Oligo p-Phenylene Ethynylene Fluorescence Sensors and Aβ Oligomers”, ACS Chemical Neuroscience, vol. 11, no. 22. American Chemical Society (ACS), pp. 3761–3771, Nov. 03, 2020. doi: 10.1021/acschemneuro.0c00360.*  
  
*T. E. Speltz, J. M. Danes, J. D. Stender, J. Frasorand T. W. Moore, “A Cell-Permeable Stapled Peptide Inhibitor of the Estrogen Receptor/Coactivator Interaction”, ACS Chemical Biology, vol. 13, no. 3. American Chemical Society (ACS), pp. 676–684, Jan. 08, 2018. doi: 10.1021/acschembio.7b01016.*  
  
*T. E. Speltz, “A “cross-stitched” peptide with improved helicity and proteolytic stability”, Organic & Biomolecular Chemistry, vol. 16, no. 20. Royal Society of Chemistry (RSC), pp. 3702–3706, 2018. doi: 10.1039/c8ob00790j.*  
  
*D. Karandur, “Breakage of the Oligomeric CaMKII Hub by the Regulatory Segment of the Kinase”, []. Cold Spring Harbor Laboratory, Apr. 16, 2020. doi: 10.1101/2020.04.15.043067.*  
  
*A. H. Beaven, A. J. Sodt, R. W. Pastor, R. E. Koeppe II, O. S. Andersenand W. Im, “Characterizing Residue-Bilayer Interactions Using Gramicidin A as a Scaffold and Tryptophan Substitutions as Probes”, Journal of Chemical Theory and Computation, vol. 13, no. 10. American Chemical Society (ACS), pp. 5054–5064, Sep. 22, 2017. doi: 10.1021/acs.jctc.7b00400.*  
  
*P. Blasco, D. S. Patel, O. Engström, W. Imand G. Widmalm, “Conformational Dynamics of the Lipopolysaccharide from Escherichia coli O91 Revealed by Nuclear Magnetic Resonance Spectroscopy and Molecular Simulations”, Biochemistry, vol. 56, no. 29. American Chemical Society (ACS), pp. 3826–3839, Jun. 27, 2017. doi: 10.1021/acs.biochem.7b00106.*  
  
*A. Blázquez-Moreno, S. Park, W. Im, M. J. Call, M. E. Calland H. T. Reyburn, “Transmembrane features governing Fc receptor CD16A assembly with CD16A signaling adaptor molecules”, Proceedings of the National Academy of Sciences, vol. 114, no. 28. Proceedings of the National Academy of Sciences, Jun. 26, 2017. doi: 10.1073/pnas.1706483114.*  
  
*M. S. Feigman, “Synthetic Immunotherapeutics against Gram-negative Pathogens”, Cell Chemical Biology, vol. 25, no. 10. Elsevier BV, pp. 1185–1194.e5, Oct. 2018. doi: 10.1016/j.chembiol.2018.05.019.*  
  
*P. Hsu, “CHARMM‐GUI Martini Maker for modeling and simulation of complex bacterial membranes with lipopolysaccharides”, Journal of Computational Chemistry, vol. 38, no. 27. Wiley, pp. 2354–2363, Aug. 03, 2017. doi: 10.1002/jcc.24895.*  
  
*S. Jo, “Multiple Conformational States Contribute to the 3D Structure of a Glucan Decasaccharide: A Combined SAXS and MD Simulation Study”, The Journal of Physical Chemistry B, vol. 122, no. 3. American Chemical Society (ACS), pp. 1169–1175, Jan. 09, 2018. doi: 10.1021/acs.jpcb.7b11085.*  
  
*S. Kim, J. Lee, S. Jo, C. L. Brooks III, H. S. Leeand W. Im, “CHARMM-GUI ligand reader and modeler for CHARMM force field generation of small molecules”, Journal of Computational Chemistry, vol. 38, no. 21. Wiley, pp. 1879–1886, May 11, 2017. doi: 10.1002/jcc.24829.*  
  
*H. S. Lee and W. Im, “Transmembrane motions of PglB induced by LLO are coupled with EL5 loop conformational changes necessary for OST activity”, Glycobiology, vol. 27, no. 8. Oxford University Press (OUP), pp. 734–742, Jun. 16, 2017. doi: 10.1093/glycob/cwx052.*  
  
*H. S. Lee and W. Im, “Effects of N-Glycan Composition on Structure and Dynamics of IgG1 Fc and Their Implications for Antibody Engineering”, Scientific Reports, vol. 7, no. 1. Springer Science and Business Media LLC, Oct. 04, 2017. doi: 10.1038/s41598-017-12830-5.*  
  
*J. Lee, Z. Ren, M. Zhouand W. Im, “Molecular Simulation and Biochemical Studies Support an Elevator-type Transport Mechanism in EIIC”, Biophysical Journal, vol. 112, no. 11. Elsevier BV, pp. 2249–2252, Jun. 2017. doi: 10.1016/j.bpj.2017.04.040.*  
  
*A. Machen, “Asymmetric Cryo-EM Structure of Anthrax Toxin Protective Antigen Pore with Lethal Factor N-Terminal Domain”, Toxins, vol. 9, no. 10. MDPI AG, p. 298, Sep. 22, 2017. doi: 10.3390/toxins9100298.*  
  
*K. A. Matthias, “Heterogeneity in non‐epitope loop sequence and outer membrane protein complexes alters antibody binding to the major porin protein PorB in serogroup B Neisseria meningitidis”, Molecular Microbiology, vol. 105, no. 6. Wiley, pp. 934–953, Aug. 2017. doi: 10.1111/mmi.13747.*  
  
*D. Min, “Unfolding of a ClC chloride transporter retains memory of its evolutionary history”, Nature Chemical Biology, vol. 14, no. 5. Springer Science and Business Media LLC, pp. 489–496, Mar. 26, 2018. doi: 10.1038/s41589-018-0025-4.*  
  
*N. I. Nissen, “Augmenting the antinociceptive effects of nicotinic acetylcholine receptor activity through lynx1 modulation”, PLOS ONE, vol. 13, no. 7. Public Library of Science (PLoS), p. e0199643, Jul. 03, 2018. doi: 10.1371/journal.pone.0199643.*  
  
*S. Park and W. Im, “Quantitative Characterization of Cholesterol Partitioning between Binary Bilayers”, Journal of Chemical Theory and Computation, vol. 14, no. 6. American Chemical Society (ACS), pp. 2829–2833, May 07, 2018. doi: 10.1021/acs.jctc.8b00140.*  
  
*S. Park, L. Krshnan, M. J. Call, M. E. Calland W. Im, “Structural Conservation and Effects of Alterations in T Cell Receptor Transmembrane Interfaces”, Biophysical Journal, vol. 114, no. 5. Elsevier BV, pp. 1030–1035, Mar. 2018. doi: 10.1016/j.bpj.2018.01.004.*  
  
*S.-J. Park, “Glycan Reader is improved to recognize most sugar types and chemical modifications in the Protein Data Bank”, Bioinformatics, vol. 33, no. 19. Oxford University Press (OUP), pp. 3051–3057, Jun. 05, 2017. doi: 10.1093/bioinformatics/btx358.*  
  
*Z. Ren, “Structure of an EIIC sugar transporter trapped in an inward-facing conformation”, Proceedings of the National Academy of Sciences, vol. 115, no. 23. Proceedings of the National Academy of Sciences, pp. 5962–5967, May 21, 2018. doi: 10.1073/pnas.1800647115.*  
  
*L. Shi, X. Meng, E. Tseng, M. Mascagniand Z. Wang, “SpaRC: scalable sequence clustering using Apache Spark”, Bioinformatics, vol. 35, no. 5. Oxford University Press (OUP), pp. 760–768, Aug. 23, 2018. doi: 10.1093/bioinformatics/bty733.*  
  
*E. G. Shcherbakova, “Supramolecular Sensors for Opiates and Their Metabolites”, Journal of the American Chemical Society, vol. 139, no. 42. American Chemical Society (ACS), pp. 14954–14960, Sep. 08, 2017. doi: 10.1021/jacs.7b06371.*  
  
*D. K. Das, R. Govindan, I. Nikić-Spiegel, F. Krammer, E. A. Lemkeand J. B. Munro, “Direct Visualization of the Conformational Dynamics of Single Influenza Hemagglutinin Trimers”, Cell, vol. 174, no. 4. Elsevier BV, pp. 926–937.e12, Aug. 2018. doi: 10.1016/j.cell.2018.05.050.*  
  
*B. Machireddy, H.-J. Sullivanand C. Wu, “Binding of BRACO19 to a Telomeric G-Quadruplex DNA Probed by All-Atom Molecular Dynamics Simulations with Explicit Solvent”, Molecules, vol. 24, no. 6. MDPI AG, p. 1010, Mar. 13, 2019. doi: 10.3390/molecules24061010.*  
  
*K. Mulholland, H.-J. Sullivan, J. Garner, J. Cai, B. Chenand C. Wu, “Three-Dimensional Structure of RNA Monomeric G-Quadruplex Containing ALS and FTD Related G4C2 Repeat and Its Binding with TMPyP4 Probed by Homology Modeling based on Experimental Constraints and Molecular Dynamics Simulations”, ACS Chemical Neuroscience, vol. 11, no. 1. American Chemical Society (ACS), pp. 57–75, Dec. 04, 2019. doi: 10.1021/acschemneuro.9b00572.*  
  
*H.-J. Sullivan, A. Tursi, K. Moore, A. Campbell, C. Floydand C. Wu, “Binding Interactions of Ergotamine and Dihydroergotamine to 5-Hydroxytryptamine Receptor 1B (5-HT1b) Using Molecular Dynamics Simulations and Dynamic Network Analysis”, Journal of Chemical Information and Modeling, vol. 60, no. 3. American Chemical Society (ACS), pp. 1749–1765, Feb. 20, 2020. doi: 10.1021/acs.jcim.9b01082.*  
  
*H.-J. Sullivan, X. Wang, S. Nogle, S. Liaoand C. Wu, “To Probe Full and Partial Activation of Human Peroxisome Proliferator-Activated Receptors by Pan-Agonist Chiglitazar Using Molecular Dynamics Simulations”, PPAR Research, vol. 2020. Hindawi Limited, pp. 1–24, Apr. 01, 2020. doi: 10.1155/2020/5314187.*  
  
*A. I. Uba, “Binding of agonist WAY-267,464 and antagonist WAY-methylated to oxytocin receptor probed by all-atom molecular dynamics simulations”, Life Sciences, vol. 252. Elsevier BV, p. 117643, Jul. 2020. doi: 10.1016/j.lfs.2020.117643.*  
  
*G. Cingolani, “Structural basis for the homotypic fusion of chlamydial inclusions by the SNARE-like protein IncA”, Nature Communications, vol. 10, no. 1. Springer Science and Business Media LLC, Jun. 21, 2019. doi: 10.1038/s41467-019-10806-9.*  
  
*R. A. Dick, “Author Correction: Inositol phosphates are assembly co-factors for HIV-1”, Nature, vol. 563, no. 7731. Springer Science and Business Media LLC, pp. E22–E22, Aug. 29, 2018. doi: 10.1038/s41586-018-0505-4.*  
  
*R. A. Dick, “Inositol phosphates are assembly co-factors for HIV-1”, Nature, vol. 560, no. 7719. Springer Science and Business Media LLC, pp. 509–512, Aug. 2018. doi: 10.1038/s41586-018-0396-4.*  
  
*J. A. Hadden, J. R. Perilla, C. J. Schlicksup, B. Venkatakrishnan, A. Zlotnickand K. Schulten, “All-atom molecular dynamics of the HBV capsid reveals insights into biological function and cryo-EM resolution limits”, eLife, vol. 7. eLife Sciences Publications, Ltd, Apr. 27, 2018. doi: 10.7554/elife.32478.*  
  
*J. L. Martin, “Critical Role of the Human T-Cell Leukemia Virus Type 1 Capsid N-Terminal Domain for Gag-Gag Interactions and Virus Particle Assembly”, Journal of Virology, vol. 92, no. 14. American Society for Microbiology, Jul. 15, 2018. doi: 10.1128/jvi.00333-18.*  
  
*C. M. Quinn, “Dynamic regulation of HIV-1 capsid interaction with the restriction factor TRIM5α identified by magic-angle spinning NMR and molecular dynamics simulations”, Proceedings of the National Academy of Sciences, vol. 115, no. 45. Proceedings of the National Academy of Sciences, pp. 11519–11524, Oct. 17, 2018. doi: 10.1073/pnas.1800796115.*  
  
*S. S. Smaga, C. Xu, B. J. Summers, K. M. Digianantonio, J. R. Perillaand Y. Xiong, “MxB Restricts HIV-1 by Targeting the Tri-hexamer Interface of the Viral Capsid”, Structure, vol. 27, no. 8. Elsevier BV, pp. 1234–1245.e5, Aug. 2019. doi: 10.1016/j.str.2019.04.015.*  
  
*R. A. Dick, “Structures of immature EIAV Gag lattices reveal a conserved role for IP6 in lentivirus assembly”, PLOS Pathogens, vol. 16, no. 1. Public Library of Science (PLoS), p. e1008277, Jan. 27, 2020. doi: 10.1371/journal.ppat.1008277.*  
  
*T. Burgin and H. B. Mayes, “Mechanism of oligosaccharide synthesis via a mutant GH29 fucosidase”, Reaction Chemistry & Engineering, vol. 4, no. 2. Royal Society of Chemistry (RSC), pp. 402–409, 2019. doi: 10.1039/c8re00240a.*  
  
*T. Burgin, J. Ståhlbergand H. B. Mayes, “Advantages of a distant cellulase catalytic base”, Journal of Biological Chemistry, vol. 293, no. 13. Elsevier BV, pp. 4680–4687, Mar. 2018. doi: 10.1074/jbc.ra117.001186.*  
  
*J. V. Vermaas, “The dissociation mechanism of processive cellulases”, Proceedings of the National Academy of Sciences, vol. 116, no. 46. Proceedings of the National Academy of Sciences, pp. 23061–23067, Oct. 30, 2019. doi: 10.1073/pnas.1913398116.*  
  
*J. Yang, “Biochemical and Genetic Analysis Identify CSLD3 as a beta-1,4-Glucan Synthase That Functions during Plant Cell Wall Synthesis”, The Plant Cell, vol. 32, no. 5. Oxford University Press (OUP), pp. 1749–1767, Mar. 13, 2020. doi: 10.1105/tpc.19.00637.*  
  
*I. V. Pivkin, Z. Peng, G. E. Karniadakis, P. A. Buffet, M. Daoand S. Suresh, “Biomechanics of red blood cells in human spleen and consequences for physiology and disease”, Proceedings of the National Academy of Sciences, vol. 113, no. 28. Proceedings of the National Academy of Sciences, pp. 7804–7809, Jun. 27, 2016. doi: 10.1073/pnas.1606751113.*  
  
*Y. Miao, A. Bhattarai, A. T. N. Nguyen, A. Christopoulosand L. T. May, “Structural Basis for Binding of Allosteric Drug Leads in the Adenosine A1 Receptor”, Scientific Reports, vol. 8, no. 1. Springer Science and Business Media LLC, Nov. 15, 2018. doi: 10.1038/s41598-018-35266-x.*  
  
*K. Niu and R. A. Marcus, “Sum frequency generation, calculation of absolute intensities, comparison with experiments, and two-field relaxation-based derivation”, Proceedings of the National Academy of Sciences, vol. 117, no. 6. Proceedings of the National Academy of Sciences, pp. 2805–2814, Jan. 29, 2020. doi: 10.1073/pnas.1906243117.*  
  
*S. Baral, I. Leventaland E. Lyman, “Composition dependence of cholesterol flip-flop rates in physiological mixtures”, Chemistry and Physics of Lipids, vol. 232. Elsevier BV, p. 104967, Oct. 2020. doi: 10.1016/j.chemphyslip.2020.104967.*  
  
*S. Baral, “Ultrafast Formation of the Charge Transfer State of Prodan Reveals Unique Aspects of the Chromophore Environment”, The Journal of Physical Chemistry B, vol. 124, no. 13. American Chemical Society (ACS), pp. 2643–2651, Mar. 11, 2020. doi: 10.1021/acs.jpcb.0c00121.*  
  
*J. H. Lorent, “Plasma membranes are asymmetric in lipid unsaturation, packing and protein shape”, Nature Chemical Biology, vol. 16, no. 6. Springer Science and Business Media LLC, pp. 644–652, May 04, 2020. doi: 10.1038/s41589-020-0529-6.*  
  
*C. McGraw, L. Yang, I. Levental, E. Lymanand A. S. Robinson, “Membrane cholesterol depletion reduces downstream signaling activity of the adenosine A2A receptor”, Biochimica et Biophysica Acta (BBA) - Biomembranes, vol. 1861, no. 4. Elsevier BV, pp. 760–767, Apr. 2019. doi: 10.1016/j.bbamem.2019.01.001.*  
  
*K. Pinkwart, “Nanoscale dynamics of cholesterol in the cell membrane”, Journal of Biological Chemistry, vol. 294, no. 34. Elsevier BV, pp. 12599–12609, Aug. 2019. doi: 10.1074/jbc.ra119.009683.*  
  
*E. Rouviere, C. Arnarezand E. Lyman, “Automated Identification of Cholesterol Interaction Sites on G-Protein Coupled Receptors by Coarse-Grained Simulation”, Biophysical Journal, vol. 112, no. 3. Elsevier BV, p. 392a, Feb. 2017. doi: 10.1016/j.bpj.2016.11.2128.*  
  
*E. Rouviere, C. Arnarez, L. Yangand E. Lyman, “Identification of Two New Cholesterol Interaction Sites on the A2A Adenosine Receptor”, Biophysical Journal, vol. 113, no. 11. Elsevier BV, pp. 2415–2424, Dec. 2017. doi: 10.1016/j.bpj.2017.09.027.*  
  
*L. Yang and E. Lyman, “Local Enrichment of Unsaturated Chains around the A2A Adenosine Receptor”, Biochemistry, vol. 58, no. 39. American Chemical Society (ACS), pp. 4096–4105, Sep. 09, 2019. doi: 10.1021/acs.biochem.9b00607.*  
  
*A. Zgorski, R. W. Pastorand E. Lyman, “Surface Shear Viscosity and Interleaflet Friction from Nonequilibrium Simulations of Lipid Bilayers”, Journal of Chemical Theory and Computation, vol. 15, no. 11. American Chemical Society (ACS), pp. 6471–6481, Sep. 02, 2019. doi: 10.1021/acs.jctc.9b00683.*  
  
*L. Hong, B. P. Vani, E. H. Thiede, M. J. Rustand A. R. Dinner, “Molecular dynamics simulations of nucleotide release from the circadian clock protein KaiC reveal atomic-resolution functional insights”, Proceedings of the National Academy of Sciences, vol. 115, no. 49. Proceedings of the National Academy of Sciences, Nov. 15, 2018. doi: 10.1073/pnas.1812555115.*  
  
*S. Sensale, Z. Pengand H.-C. Chang, “Acceleration of DNA melting kinetics using alternating electric fields”, The Journal of Chemical Physics, vol. 149, no. 8. AIP Publishing, p. 085102, Aug. 28, 2018. doi: 10.1063/1.5039887.*  
  
*S. Sensale, Z. Pengand H.-C. Chang, “Biphasic signals during nanopore translocation of DNA and nanoparticles due to strong ion cloud deformation”, Nanoscale, vol. 11, no. 47. Royal Society of Chemistry (RSC), pp. 22772–22779, 2019. doi: 10.1039/c9nr05223b.*  
  
*S. Sensale, C. Wangand H.-C. Chang, “Resistive amplitude fingerprints during translocation of linear molecules through charged solid-state nanopores”, The Journal of Chemical Physics, vol. 153, no. 3. AIP Publishing, p. 035102, Jul. 21, 2020. doi: 10.1063/5.0013195.*  
  
*M. Adeli Koudehi, D. M. Rutkowskiand D. Vavylonis, “Organization of associating or crosslinked actin filaments in confinement”, Cytoskeleton, vol. 76, no. 11–12. Wiley, pp. 532–548, Oct. 31, 2019. doi: 10.1002/cm.21565.*  
  
*B. G. Horan, A. R. Halland D. Vavylonis, “Insights into Actin Polymerization and Nucleation Using a Coarse-Grained Model”, Biophysical Journal, vol. 119, no. 3. Elsevier BV, pp. 553–566, Aug. 2020. doi: 10.1016/j.bpj.2020.06.019.*  
  
*T. Litschel, “Reconstitution of contractile actomyosin rings in vesicles”, []. Cold Spring Harbor Laboratory, Jul. 01, 2020. doi: 10.1101/2020.06.30.180901.*  
  
*Z. Ghaemi, J. R. Peterson, M. Gruebeleand Z. Luthey-Schulten, “An in-silico human cell model reveals the influence of spatial organization on RNA splicing”, PLOS Computational Biology, vol. 16, no. 3. Public Library of Science (PLoS), p. e1007717, Mar. 25, 2020. doi: 10.1371/journal.pcbi.1007717.*  
  
*J. Lai, Z. Ghaemiand Z. Luthey-Schulten, “The Conformational Change in Elongation Factor Tu Involves Separation of Its Domains”, Biochemistry, vol. 56, no. 45. American Chemical Society (ACS), pp. 5972–5979, Oct. 27, 2017. doi: 10.1021/acs.biochem.7b00591.*  
  
*K. A. Alexander and M. J. García-García, “Imprinted gene expression at theDlk1-Dio3cluster is controlled by both maternal and paternalIG-DMRs in a tissue-specific fashion”, []. Cold Spring Harbor Laboratory, Jan. 31, 2019. doi: 10.1101/536102.*  
  
*J. G. Azofeifa, M. A. Allen, J. R. Hendrix, T. Read, J. D. Rubinand R. D. Dowell, “Enhancer RNA profiling predicts transcription factor activity”, Genome Research, vol. 28, no. 3. Cold Spring Harbor Laboratory, pp. 334–344, Feb. 15, 2018. doi: 10.1101/gr.225755.117.*  
  
*L. Barros de Andrade e Sousa, “Kinetics of Xist-induced gene silencing can be predicted from combinations of epigenetic and genomic features”, Genome Research, vol. 29, no. 7. Cold Spring Harbor Laboratory, pp. 1087–1099, Jun. 07, 2019. doi: 10.1101/gr.245027.118.*  
  
*T. A. Hait, D. Amar, R. Shamirand R. Elkon, “FOCS: a novel method for analyzing enhancer and gene activity patterns infers an extensive enhancer–promoter map”, Genome Biology, vol. 19, no. 1. Springer Science and Business Media LLC, May 01, 2018. doi: 10.1186/s13059-018-1432-2.*  
  
*Y. Li, W. Shiand W. W. Wasserman, “Genome-wide prediction of cis-regulatory regions using supervised deep learning methods”, BMC Bioinformatics, vol. 19, no. 1. Springer Science and Business Media LLC, May 31, 2018. doi: 10.1186/s12859-018-2187-1.*  
  
*R. Lozano, “RNA polymerase mapping in plants identifies enhancers enriched in causal variants”, []. Cold Spring Harbor Laboratory, Jul. 24, 2018. doi: 10.1101/376640.*  
  
*J. Ray, “Chromatin conformation remains stable upon extensive transcriptional changes driven by heat shock”, Proceedings of the National Academy of Sciences, vol. 116, no. 39. Proceedings of the National Academy of Sciences, pp. 19431–19439, Sep. 10, 2019. doi: 10.1073/pnas.1901244116.*  
  
*S. Rennie, “Transcription start site analysis reveals widespread divergent transcription in D. melanogaster and core promoter-encoded enhancer activities”, Nucleic Acids Research, vol. 46, no. 11. Oxford University Press (OUP), pp. 5455–5469, Apr. 06, 2018. doi: 10.1093/nar/gky244.*  
  
*K. M. Sathyan, B. D. McKenna, W. D. Anderson, F. M. Duarte, L. Coreand M. J. Guertin, “An improved auxin-inducible degron system preserves native protein levels and enables rapid and specific protein depletion”, Genes & Development, vol. 33, no. 19–20. Cold Spring Harbor Laboratory, pp. 1441–1455, Aug. 29, 2019. doi: 10.1101/gad.328237.119.*  
  
*I. J. Tripodi, M. Chowdhuryand R. Dowell, “ATAC-seq signal processing and recurrent neural networks can identify RNA polymerase activity”, []. Cold Spring Harbor Laboratory, Jan. 26, 2019. doi: 10.1101/531517.*  
  
*A. Vihervaara, D. B. Mahat, S. Himanen, M. Blom, J. T. Lisand L. Sistonen, “Stress-Induced Transcriptional Memory Accelerates Promoter-Proximal Pause-Release and Decelerates Termination Over Mitotic Divisions”, SSRN Electronic Journal. Elsevier BV, 2019. doi: 10.2139/ssrn.3399580.*  
  
*J. Wang, Y. Zhao, X. Zhou, S. W. Hiebert, Q. Liuand Y. Shyr, “Nascent RNA sequencing analysis provides insights into enhancer-mediated gene regulation”, BMC Genomics, vol. 19, no. 1. Springer Science and Business Media LLC, Aug. 23, 2018. doi: 10.1186/s12864-018-5016-z.*  
  
*Z. Wang, “Building a Science Gateway For Processing and Modeling Sequencing Data Via Apache Airavata”, Proceedings of the Practice and Experience on Advanced Research Computing. ACM, Jul. 22, 2018. doi: 10.1145/3219104.3219141.*  
  
*D. Devaurs, “Using parallelized incremental meta-docking can solve the conformational sampling issue when docking large ligands to proteins”, BMC Molecular and Cell Biology, vol. 20, no. 1. Springer Science and Business Media LLC, Sep. 05, 2019. doi: 10.1186/s12860-019-0218-z.*  
  
*M. Razizadeh, M. Nikfar, R. Pauland Y. Liu, “Coarse-Grained Modeling of Pore Dynamics on the Red Blood Cell Membrane under Large Deformations”, Biophysical Journal, vol. 119, no. 3. Elsevier BV, pp. 471–482, Aug. 2020. doi: 10.1016/j.bpj.2020.06.016.*  
  
*E. A. Solares, Y. Tao, A. D. Longand B. S. Gaut, “HapSolo: an optimization approach for removing secondary haplotigs during diploid genome assembly and scaffolding”, BMC Bioinformatics, vol. 22, no. 1. Springer Science and Business Media LLC, Jan. 06, 2021. doi: 10.1186/s12859-020-03939-y.*  
  
*X. Chi, “Universal concept signature analysis: genome-wide quantification of new biological and pathological functions of genes and pathways”, Briefings in Bioinformatics, vol. 21, no. 5. Oxford University Press (OUP), pp. 1717–1732, Oct. 18, 2019. doi: 10.1093/bib/bbz093.*  
  
*S. Lee, “Landscape analysis of adjacent gene rearrangements reveals BCL2L14–ETV6 gene fusions in more aggressive triple-negative breast cancer”, Proceedings of the National Academy of Sciences, vol. 117, no. 18. Proceedings of the National Academy of Sciences, pp. 9912–9921, Apr. 22, 2020. doi: 10.1073/pnas.1921333117.*  
  
*A. Bhattarai, S. Devkota, S. Bhattarai, M. S. Wolfeand Y. Miao, “Mechanisms of γ-Secretase Activation and Substrate Processing”, ACS Central Science, vol. 6, no. 6. American Chemical Society (ACS), pp. 969–983, Jun. 04, 2020. doi: 10.1021/acscentsci.0c00296.*  
  
*A. Bhattarai and Y. Miao, “Gaussian accelerated molecular dynamics for elucidation of drug pathways”, Expert Opinion on Drug Discovery, vol. 13, no. 11. Informa UK Limited, pp. 1055–1065, Oct. 29, 2018. doi: 10.1080/17460441.2018.1538207.*  
  
*A. Bhattarai, J. Wangand Y. Miao, “G‐Protein‐Coupled Receptor–Membrane Interactions Depend on the Receptor Activation State”, Journal of Computational Chemistry, vol. 41, no. 5. Wiley, pp. 460–471, Oct. 10, 2019. doi: 10.1002/jcc.26082.*  
  
*J. Wang and Y. Miao, “Mechanistic Insights into Specific G Protein Interactions with Adenosine Receptors Revealed by Accelerated Molecular Simulations”, []. Cold Spring Harbor Laboratory, Feb. 05, 2019. doi: 10.1101/541250.*  
  
*J. Wang and Y. Miao, “Recent advances in computational studies of GPCR-G protein interactions”, Advances in Protein Chemistry and Structural Biology. Elsevier, pp. 397–419, 2019. doi: 10.1016/bs.apcsb.2018.11.011.*  
  
*R. Laghmach, M. Di Pierroand D. A. Potoyan, “Mesoscale Liquid Model of Chromatin Recapitulates Nuclear Order of Eukaryotes”, Biophysical Journal, vol. 118, no. 9. Elsevier BV, pp. 2130–2140, May 2020. doi: 10.1016/j.bpj.2019.09.013.*  
  
*L. Clark, D. Leatherby, E. Krilich, A. J. Ropelewskiand J. Perozich, “In silico analysis of class I adenylate-forming enzymes reveals family and group-specific conservations”, PLOS ONE, vol. 13, no. 9. Public Library of Science (PLoS), p. e0203218, Sep. 04, 2018. doi: 10.1371/journal.pone.0203218.*  
  
*L. Clark, D. Leatherby, E. Krilich, A. J. Ropelewskiand J. Perozich, “In silico analysis of class I adenylate-forming enzymes reveals family and group-specific conservations”, PLOS ONE, vol. 13, no. 9. Public Library of Science (PLoS), p. e0203218, Sep. 04, 2018. doi: 10.1371/journal.pone.0203218.*  
  
*M. Alonge, “RaGOO: fast and accurate reference-guided scaffolding of draft genomes”, Genome Biology, vol. 20, no. 1. Springer Science and Business Media LLC, Oct. 28, 2019. doi: 10.1186/s13059-019-1829-6.*  
  
*C. J. Anaya, H. J. Zander, R. D. Graham, V. Sankarasubramanianand S. F. Lempka, “Evoked Potentials Recorded From the Spinal Cord During Neurostimulation for Pain: A Computational Modeling Study”, Neuromodulation: Technology at the Neural Interface, vol. 23, no. 1. Elsevier BV, pp. 64–73, Jan. 2020. doi: 10.1111/ner.12965.*  
  
*B. W. Treece, F. Heinrich, A. Ramanathanand M. Lösche, “Steering Molecular Dynamics Simulations of Membrane-Associated Proteins with Neutron Reflection Results”, Journal of Chemical Theory and Computation, vol. 16, no. 5. American Chemical Society (ACS), pp. 3408–3419, Apr. 08, 2020. doi: 10.1021/acs.jctc.0c00136.*  
  
*C. Lin, “Specific inter-domain interactions stabilize a compact HIV-1 Gag conformation”, PLOS ONE, vol. 14, no. 8. Public Library of Science (PLoS), p. e0221256, Aug. 22, 2019. doi: 10.1371/journal.pone.0221256.*  
  
*Y. Gao, “Plug-and-Play Protein Modification Using Homology-Independent Universal Genome Engineering”, Neuron, vol. 103, no. 4. Elsevier BV, pp. 583–597.e8, Aug. 2019. doi: 10.1016/j.neuron.2019.05.047.*  
  
*A. J. Wisdom, “Neutrophils promote tumor resistance to radiation therapy”, Proceedings of the National Academy of Sciences, vol. 116, no. 37. Proceedings of the National Academy of Sciences, pp. 18584–18589, Aug. 28, 2019. doi: 10.1073/pnas.1901562116.*  
  
*Y. Xiang, Y. Ye, Z. Zhangand L. Han, “Maximizing the Utility of Cancer Transcriptomic Data”, Trends in Cancer, vol. 4, no. 12. Elsevier BV, pp. 823–837, Dec. 2018. doi: 10.1016/j.trecan.2018.09.009.*  
  
*K. M. Bultman, A. G. Cecere, T. Miyashiro, A. N. Septerand M. J. Mandel, “Draft Genome Sequences of Type VI Secretion System-Encoding Vibrio fischeri Strains FQ-A001 and ES401”, Microbiology Resource Announcements, vol. 8, no. 20. American Society for Microbiology, May 16, 2019. doi: 10.1128/mra.00385-19.*  
  
*S. Ballweg, “Regulation of lipid saturation without sensing membrane fluidity”, Nature Communications, vol. 11, no. 1. Springer Science and Business Media LLC, Feb. 06, 2020. doi: 10.1038/s41467-020-14528-1.*  
  
*F. A. Heberle, M. Doktorova, H. L. Scott, A. Skinkle, M. N. Waxhamand I. Levental, “Direct label-free imaging of nanodomains in biomimetic and biological membranes by cryogenic electron microscopy”, []. Cold Spring Harbor Laboratory, Feb. 05, 2020. doi: 10.1101/2020.02.05.935551.*  
  
*H. Bagheri, U. Muppirala, R. E. Masonbrink, A. J. Severinand H. Rajan, “Shared data science infrastructure for genomics data”, BMC Bioinformatics, vol. 20, no. 1. Springer Science and Business Media LLC, Aug. 22, 2019. doi: 10.1186/s12859-019-2967-2.*  
  
*K. Bafna, C. Narayanan, S. C. Chennubhotla, N. Doucetand P. K. Agarwal, “Nucleotide substrate binding characterization in human pancreatic-type ribonucleases”, PLOS ONE, vol. 14, no. 8. Public Library of Science (PLoS), p. e0220037, Aug. 08, 2019. doi: 10.1371/journal.pone.0220037.*  
  
*K. P. Hester, K. Bhattarai, H. Jiang, P. K. Agarwaland C. Pope, “Engineering Dynamic Surface Peptide Networks on ButyrylcholinesteraseG117H for Enhanced Organophosphosphorus Anticholinesterase Catalysis”, Chemical Research in Toxicology, vol. 32, no. 9. American Chemical Society (ACS), pp. 1801–1810, Aug. 14, 2019. doi: 10.1021/acs.chemrestox.9b00146.*  
  
*N. M. Hoitsma, “AP-endonuclease 1 sculpts DNA through an anchoring tyrosine residue on the DNA intercalating loop”, Nucleic Acids Research. Oxford University Press (OUP), Jun. 15, 2020. doi: 10.1093/nar/gkaa496.*  
  
*P. Kumar, P. K. Agarwal, M. B. Waddell, T. Mittag, E. H. Serpersuand M. J. Cuneo, “Low‐Barrier and Canonical Hydrogen Bonds Modulate Activity and Specificity of a Catalytic Triad”, Angewandte Chemie, vol. 131, no. 45. Wiley, pp. 16406–16412, Sep. 24, 2019. doi: 10.1002/ange.201908535.*  
  
*C. Narayanan, “Insights into Structural and Dynamical Changes Experienced by Human RNase 6 upon Ligand Binding”, Biochemistry, vol. 59, no. 6. American Chemical Society (ACS), pp. 755–765, Jan. 07, 2020. doi: 10.1021/acs.biochem.9b00888.*  
  
*B. J. Levandowski, R. T. Rainesand K. N. Houk, “Hyperconjugative π → σ*CF Interactions Stabilize the Enol Form of Perfluorinated Cyclic Keto–Enol Systems”, *The Journal of Organic Chemistry*, vol. 84, no. 10. American Chemical Society (ACS), pp. 6432–6436, Apr. 16, 2019. doi: 10.1021/acs.joc.9b00825.  
  
A. Saadat, C. J. Guidoand E. S. G. Shaqfeh, “Effect of Cytoplasmic Viscosity on Red Blood Cell Migration in Small Arteriole-level Confinements”, *[]*. Cold Spring Harbor Laboratory, Mar. 21, 2019. doi: 10.1101/572933.  
  
A. Saadat, “A system for the high-throughput measurement of the shear modulus distribution of human red blood cells”, *Lab on a Chip*, vol. 20, no. 16. Royal Society of Chemistry (RSC), pp. 2927–2936, 2020. doi: 10.1039/d0lc00283f.  
  
A. O. Valdivia, P. K. Agarwaland S. K. Bhattacharya, “Myelin Basic Protein Phospholipid Complexation Likely Competes with Deimination in Experimental Autoimmune Encephalomyelitis Mouse Model”, *ACS Omega*, vol. 5, no. 25. American Chemical Society (ACS), pp. 15454–15467, Jun. 16, 2020. doi: 10.1021/acsomega.0c01590.  
  
F. Heinrich, P. A. Kienzle, D. P. Hoogerheideand M. Lösche, “Information gain from isotopic contrast variation in neutron reflectometry on protein–membrane complex structures”, *Journal of Applied Crystallography*, vol. 53, no. 3. International Union of Crystallography (IUCr), pp. 800–810, May 29, 2020. doi: 10.1107/s1600576720005634.  
  
B. W. Treece, F. Heinrich, A. Ramanathanand M. Lösche, “Steering Molecular Dynamics Simulations of Membrane-Associated Proteins with Neutron Reflection Results”, *Journal of Chemical Theory and Computation*, vol. 16, no. 5. American Chemical Society (ACS), pp. 3408–3419, Apr. 08, 2020. doi: 10.1021/acs.jctc.0c00136.  
  
E.-M. Zangerl-Plessl, “Atomistic basis of opening and conduction in mammalian inward rectifier potassium (Kir2.2) channels”, *The Journal of General Physiology*. Rockefeller University Press, p. jgp.201912422, Nov. 19, 2019. doi: 10.1085/jgp.201912422.  
  
M. D. Chen, I. J. Fucci, K. Sinhaand G. S. Rule, “dGMP Binding to Thymidylate Kinase from *Plasmodium falciparum* Shows Half-Site Binding and Induces Protein Dynamics at the Dimer Interface”, *Biochemistry*, vol. 59, no. 5. American Chemical Society (ACS), pp. 694–703, Jan. 14, 2020. doi: 10.1021/acs.biochem.9b00898.  
  
Y. Wu, “Metagenomic analysis reveals gestational diabetes mellitus-related microbial regulators of glucose tolerance”, *Acta Diabetologica*, vol. 57, no. 5. Springer Science and Business Media LLC, pp. 569–581, Dec. 09, 2019. doi: 10.1007/s00592-019-01434-2.  
  
N. Tobin and K. B. Manning, “Large-Eddy Simulations of Flow in the FDA Benchmark Nozzle Geometry to Predict Hemolysis”, *Cardiovascular Engineering and Technology*, vol. 11, no. 3. Springer Science and Business Media LLC, pp. 254–267, Apr. 15, 2020. doi: 10.1007/s13239-020-00461-3.  
  
Y. Zhang, “ProDCoNN: Protein design using a convolutional neural network”, *Proteins: Structure, Function, and Bioinformatics*, vol. 88, no. 7. Wiley, pp. 819–829, Jan. 06, 2020. doi: 10.1002/prot.25868.  
  
M. M. Papasergi-Scott, M. J. Robertson, A. B. Seven, O. Panova, J. M. Mathiesenand G. Skiniotis, “Structures of metabotropic GABAB receptor”, *Nature*, vol. 584, no. 7820. Springer Science and Business Media LLC, pp. 310–314, Jun. 24, 2020. doi: 10.1038/s41586-020-2469-4.  
  
V. Padilla-Sanchez, “In silico analysis of SARS-CoV-2 spike glycoprotein and insights into antibody binding”, *Research Ideas and Outcomes*, vol. 6. Pensoft Publishers, Jun. 16, 2020. doi: 10.3897/rio.6.e55281.  
  
E. Becket, “Draft Genome Sequences of Bacillus glennii V44-8, Bacillus saganii V47-23a, *Bacillus* sp. Strain V59.32b, *Bacillus* sp. Strain MER\_TA\_151, and *Paenibacillus* sp. Strain MER\_111, Isolated from Cleanrooms Where the Viking and Mars Exploration Rover Spacecraft Were Assembled”, *Microbiology Resource Announcements*, vol. 9, no. 26. American Society for Microbiology, Jun. 25, 2020. doi: 10.1128/mra.00354-20.  
  
S. Kim and J. M. J. Swanson, “The Surface and Hydration Properties of Lipid Droplets”, *Biophysical Journal*, vol. 119, no. 10. Elsevier BV, pp. 1958–1969, Nov. 2020. doi: 10.1016/j.bpj.2020.10.001.  
  
N. Li, N. Shan, L. Luand Z. Wang, “tRFtarget: a database for transfer RNA-derived fragment targets”, *Nucleic Acids Research*, vol. 49, no. D1. Oxford University Press (OUP), pp. D254–D260, Oct. 09, 2020. doi: 10.1093/nar/gkaa831.  
  
D. M. Eckmann, R. P. Bradley, S. K. Kandy, K. Patil, P. A. Janmeyand R. Radhakrishnan, “Multiscale modeling of protein membrane interactions for nanoparticle targeting in drug delivery”, *Current Opinion in Structural Biology*, vol. 64. Elsevier BV, pp. 104–110, Oct. 2020. doi: 10.1016/j.sbi.2020.06.023.  
  
M. H. Peters, O. Bastidas, D. S. Kokronand C. Henze, “Static All-Atom Energetic Mappings of the SARS-Cov-2 Spike Protein with Potential Latch Identification of the Down State Protomer”, *[]*. Cold Spring Harbor Laboratory, May 12, 2020. doi: 10.1101/2020.05.12.091090.  
  
M. Gur, E. Taka, S. Z. Yilmaz, C. Kilinc, U. Aktasand M. Golcuk, “Conformational transition of SARS-CoV-2 spike glycoprotein between its closed and open states”, *The Journal of Chemical Physics*, vol. 153, no. 7. AIP Publishing, p. 075101, Aug. 21, 2020. doi: 10.1063/5.0011141.  
  
U. Singh and E. S. Wurtele, “Differential expression of COVID-19-related genes in European Americans and African Americans”, *[]*. Cold Spring Harbor Laboratory, Jun. 10, 2020. doi: 10.1101/2020.06.09.143271.  
  
M. Vohra and S. Mahadevan, “Discovering the active subspace for efficient UQ of molecular dynamics simulations of phonon transport in silicon”, *International Journal of Heat and Mass Transfer*, vol. 132. Elsevier BV, pp. 577–586, Apr. 2019. doi: 10.1016/j.ijheatmasstransfer.2018.11.171.  
  
M. Vohra, A. Y. Nobakht, S. Shinand S. Mahadevan, “Uncertainty quantification in non-equilibrium molecular dynamics simulations of thermal transport”, *International Journal of Heat and Mass Transfer*, vol. 127. Elsevier BV, pp. 297–307, Dec. 2018. doi: 10.1016/j.ijheatmasstransfer.2018.07.073.  
  
Y. Chen and M. Ostoja-Starzewski, “MRI-based finite element modeling of head trauma: spherically focusing shear waves”, *Acta Mechanica*, vol. 213, no. 1–2. Springer Science and Business Media LLC, pp. 155–167, Feb. 03, 2010. doi: 10.1007/s00707-009-0274-0.  
  
P. N. Demmie and M. Ostoja-Starzewski, “Local and nonlocal material models, spatial randomness, and impact loading”, *Archive of Applied Mechanics*, vol. 86, no. 1–2. Springer Science and Business Media LLC, pp. 39–58, Dec. 31, 2015. doi: 10.1007/s00419-015-1095-3.  
  
H. Joumaa and M. Ostoja-Starzewski, “Acoustic-elastodynamic interaction in isotropic fractal media”, *The European Physical Journal Special Topics*, vol. 222, no. 8. Springer Science and Business Media LLC, pp. 1951–1960, Sep. 2013. doi: 10.1140/epjst/e2013-01976-x.  
  
S. Kale and M. Ostoja–Starzewski, “Representing stochastic damage evolution in disordered media as a jump Markov process using the fiber bundle model”, *International Journal of Damage Mechanics*, vol. 26, no. 1. SAGE Publications, pp. 147–161, Jul. 28, 2016. doi: 10.1177/1056789516650249.  
  
S. Kale, F. A. Sabet, I. Jasiukand M. Ostoja-Starzewski, “Tunneling-percolation behavior of polydisperse prolate and oblate ellipsoids”, *Journal of Applied Physics*, vol. 118, no. 15. AIP Publishing, p. 154306, Oct. 21, 2015. doi: 10.1063/1.4933100.  
  
S. Kale, A. Saharan, S. Koricand M. Ostoja-Starzewski, “Scaling and bounds in thermal conductivity of planar Gaussian correlated microstructures”, *Journal of Applied Physics*, vol. 117, no. 10. AIP Publishing, p. 104301, Mar. 14, 2015. doi: 10.1063/1.4914128.  
  
A. Malyarenko and M. Ostoja-Starzewski, “Spectral expansions of homogeneous and isotropic tensor-valued random fields”, *Zeitschrift für angewandte Mathematik und Physik*, vol. 67, no. 3. Springer Science and Business Media LLC, May 03, 2016. doi: 10.1007/s00033-016-0657-8.  
  
V. V. Nishawala and M. Ostoja-Starzewski, “Peristatic solutions for finite one- and two-dimensional systems”, *Mathematics and Mechanics of Solids*, vol. 22, no. 8. SAGE Publications, pp. 1639–1653, Apr. 21, 2016. doi: 10.1177/1081286516641180.  
  
V. V. Nishawala, M. Ostoja-Starzewski, M. J. Leamyand P. N. Demmie, “Simulation of elastic wave propagation using cellular automata and peridynamics, and comparison with experiments”, *Wave Motion*, vol. 60. Elsevier BV, pp. 73–83, Jan. 2016. doi: 10.1016/j.wavemoti.2015.08.005.  
  
M. Ostoja-Starzewski, “Second law violations, continuum mechanics, and permeability”, *Continuum Mechanics and Thermodynamics*, vol. 28, no. 1–2. Springer Science and Business Media LLC, pp. 489–501, Jun. 27, 2015. doi: 10.1007/s00161-015-0451-4.  
  
M. Ostoja-Starzewski and L. Costa, “Shock waves in random viscoelastic media”, *Acta Mechanica*, vol. 223, no. 8. Springer Science and Business Media LLC, pp. 1777–1788, May 01, 2012. doi: 10.1007/s00707-012-0658-4.  
  
M. Ostoja-Starzewski, L. Costaand S. I. Ranganathan, “Scale-Dependent Homogenization of Random Hyperbolic Thermoelastic Solids”, *Journal of Elasticity*, vol. 118, no. 2. Springer Science and Business Media LLC, pp. 243–250, Jun. 10, 2014. doi: 10.1007/s10659-014-9483-4.  
  
M. Ostoja-Starzewski and B. Venkatesh Raghavan, “Continuum mechanics versus violations of the second law of thermodynamics”, *Journal of Thermal Stresses*, vol. 39, no. 6. Informa UK Limited, pp. 734–749, May 11, 2016. doi: 10.1080/01495739.2016.1169140.  
  
L. Shen, M. Ostoja-Starzewskiand E. Porcu, “Harmonic oscillator driven by random processes having fractal and Hurst effects”, *Acta Mechanica*, vol. 226, no. 11. Springer Science and Business Media LLC, pp. 3653–3672, Jul. 17, 2015. doi: 10.1007/s00707-015-1385-4.  
  
L. Shen, M. Ostoja-Starzewskiand E. Porcu, “Elastic Rods and Shear Beams with Random Field Properties under Random Field Loads: Fractal and Hurst Effects”, *Journal of Engineering Mechanics*, vol. 141, no. 7. American Society of Civil Engineers (ASCE), Jul. 2015. doi: 10.1061/(asce)em.1943-7889.0000906.  
  
L. Shen, M. Ostoja-Starzewskiand E. Porcu, “Responses of first-order dynamical systems to Matérn, Cauchy, and Dagum excitations”, *Mathematics and Mechanics of Complex Systems*, vol. 3, no. 1. Mathematical Sciences Publishers, pp. 27–41, Feb. 13, 2015. doi: 10.2140/memocs.2015.3.27.  
  
D. Zhang and M. Ostoja-Starzewski, “Finite Element Solutions to the Bending Stiffness of a Single-Layered Helically Wound Cable With Internal Friction”, *Journal of Applied Mechanics*, vol. 83, no. 3. ASME International, Dec. 10, 2015. doi: 10.1115/1.4032023.  
  
J. Zhang and M. Ostoja-Starzewski, “Mesoscale bounds in viscoelasticity of random composites”, *Mechanics Research Communications*, vol. 68. Elsevier BV, pp. 98–104, Sep. 2015. doi: 10.1016/j.mechrescom.2015.05.005.  
  
J. Zhang and M. Ostoja-Starzewski, “Frequency-dependent scaling from mesoscale to macroscale in viscoelastic random composites”, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 472, no. 2188. The Royal Society, p. 20150801, Apr. 2016. doi: 10.1098/rspa.2015.0801.  
  
T. Al-Mulla and M. J. Buehler, “Folding creases through bending”, *Nature Materials*, vol. 14, no. 4. Springer Science and Business Media LLC, pp. 366–368, Mar. 24, 2015. doi: 10.1038/nmat4258.  
  
B. An, S.-W. Chang, C. Hoop, J. Baum, M. J. Buehlerand D. L. Kaplan, “Structural Insights into the Glycine Pair Motifs in Type III Collagen”, *ACS Biomaterials Science & Engineering*, vol. 3, no. 3. American Chemical Society (ACS), pp. 269–278, Jan. 09, 2017. doi: 10.1021/acsbiomaterials.6b00512.  
  
P. D. Boyer, “Delivering Single-Walled Carbon Nanotubes to the Nucleus Using Engineered Nuclear Protein Domains”, *ACS Applied Materials & Interfaces*, vol. 8, no. 5. American Chemical Society (ACS), pp. 3524–3534, Feb. 01, 2016. doi: 10.1021/acsami.5b12602.  
  
M. J. Buehler and G. M. Genin, “Integrated multiscale biomaterials experiment and modelling: a perspective”, *Interface Focus*, vol. 6, no. 1. The Royal Society, p. 20150098, Feb. 06, 2016. doi: 10.1098/rsfs.2015.0098.  
  
C.-T. Chen, C. Chuang, J. Cao, V. Ball, D. Ruchand M. J. Buehler, “Excitonic effects from geometric order and disorder explain broadband optical absorption in eumelanin”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, May 22, 2014. doi: 10.1038/ncomms4859.  
  
C.-T. Chen, F. J. Martin-Martinez, G. S. Jungand M. J. Buehler, “Polydopamine and eumelanin molecular structures investigated with ab initio calculations”, *Chemical Science*, vol. 8, no. 2. Royal Society of Chemistry (RSC), pp. 1631–1641, 2017. doi: 10.1039/c6sc04692d.  
  
C.-C. Chou, E. Lepore, P. Antonaci, N. Pugnoand M. J. Buehler, “Mechanics of trichocyte alpha-keratin fibers: Experiment, theory, and simulation”, *Journal of Materials Research*, vol. 30, no. 1. Springer Science and Business Media LLC, pp. 26–35, Jan. 14, 2015. doi: 10.1557/jmr.2014.267.  
  
C.-C. Chou, “Ion Effect and Metal-Coordinated Cross-Linking for Multiscale Design of *Nereis* Jaw Inspired Mechanomutable Materials”, *ACS Nano*, vol. 11, no. 2. American Chemical Society (ACS), pp. 1858–1868, Feb. 15, 2017. doi: 10.1021/acsnano.6b07878.  
  
B. Depalle, Z. Qin, S. J. Shefelbineand M. J. Buehler, “Influence of cross-link structure, density and mechanical properties in the mesoscale deformation mechanisms of collagen fibrils”, *Journal of the Mechanical Behavior of Biomedical Materials*, vol. 52. Elsevier BV, pp. 1–13, Dec. 2015. doi: 10.1016/j.jmbbm.2014.07.008.  
  
B. Depalle, Z. Qin, S. J. Shefelbineand M. J. Buehler, “Large Deformation Mechanisms, Plasticity, and Failure of an Individual Collagen Fibril With Different Mineral Content”, *Journal of Bone and Mineral Research*, vol. 31, no. 2. Wiley, pp. 380–390, Feb. 2016. doi: 10.1002/jbmr.2705.  
  
L. S. Dimas, D. Venezianoand M. J. Buehler, “The Effective Modulus of Random Checkerboard Plates”, *Journal of Applied Mechanics*, vol. 83, no. 1. ASME International, Nov. 05, 2015. doi: 10.1115/1.4031744.  
  
L. S. Dimas, D. Venezianoand M. J. Buehler, “Strength and fracture toughness of heterogeneous blocks with joint lognormal modulus and failure strain”, *Journal of the Mechanics and Physics of Solids*, vol. 92. Elsevier BV, pp. 72–86, Jul. 2016. doi: 10.1016/j.jmps.2016.03.026.  
  
L. S. Dimas, D. Veneziano, T. Giesaand M. J. Buehler, “Random Bulk Properties of Heterogeneous Rectangular Blocks With Lognormal Young’s Modulus: Effective Moduli”, *Journal of Applied Mechanics*, vol. 82, no. 1. ASME International, Jan. 01, 2015. doi: 10.1115/1.4028783.  
  
L. S. Dimas, D. Veneziano, T. Giesaand M. J. Buehler, “Probability distribution of fracture elongation, strength and toughness of notched rectangular blocks with lognormal Young’s modulus”, *Journal of the Mechanics and Physics of Solids*, vol. 84. Elsevier BV, pp. 116–129, Nov. 2015. doi: 10.1016/j.jmps.2015.06.016.  
  
N. Dinjaski, D. Ebrahimi, S. Ling, S. Shah, M. J. Buehlerand D. L. Kaplan, “Integrated Modeling and Experimental Approaches to Control Silica Modification of Design Silk-Based Biomaterials”, *ACS Biomaterials Science & Engineering*, vol. 3, no. 11. American Chemical Society (ACS), pp. 2877–2888, Aug. 23, 2016. doi: 10.1021/acsbiomaterials.6b00236.  
  
S. Ganesh, “The tail domain of lamin B1 is more strongly modulated by divalent cations than lamin A”, *Nucleus*, vol. 6, no. 3. Informa UK Limited, pp. 203–211, Mar. 25, 2015. doi: 10.1080/19491034.2015.1031436.  
  
T. Giesa, C. C. Perryand M. J. Buehler, “Secondary Structure Transition and Critical Stress for a Model of Spider Silk Assembly”, *Biomacromolecules*, vol. 17, no. 2. American Chemical Society (ACS), pp. 427–436, Jan. 13, 2016. doi: 10.1021/acs.biomac.5b01246.  
  
G. X. Gu, L. Dimas, Z. Qinand M. J. Buehler, “Optimization of Composite Fracture Properties: Method, Validation, and Applications”, *Journal of Applied Mechanics*, vol. 83, no. 7. ASME International, May 05, 2016. doi: 10.1115/1.4033381.  
  
G. X. Gu, M. Takaffoli, A. J. Hsiehand M. J. Buehler, “Biomimetic additive manufactured polymer composites for improved impact resistance”, *Extreme Mechanics Letters*, vol. 9. Elsevier BV, pp. 317–323, Dec. 2016. doi: 10.1016/j.eml.2016.09.006.  
  
W. Huang, “Synergistic Integration of Experimental and Simulation Approaches for the *de Novo* Design of Silk-Based Materials”, *Accounts of Chemical Research*, vol. 50, no. 4. American Chemical Society (ACS), pp. 866–876, Feb. 13, 2017. doi: 10.1021/acs.accounts.6b00616.  
  
W. Huang, “Design of Multistimuli Responsive Hydrogels Using Integrated Modeling and Genetically Engineered Silk–Elastin‐Like Proteins”, *Advanced Functional Materials*, vol. 26, no. 23. Wiley, pp. 4113–4123, Apr. 15, 2016. doi: 10.1002/adfm.201600236.  
  
K. Jin, Z. Qinand M. J. Buehler, “Molecular deformation mechanisms of the wood cell wall material”, *Journal of the Mechanical Behavior of Biomedical Materials*, vol. 42. Elsevier BV, pp. 198–206, Feb. 2015. doi: 10.1016/j.jmbbm.2014.11.010.  
  
G. Jung, Z. Qinand M. J. Buehler, “Molecular mechanics of polycrystalline graphene with enhanced fracture toughness”, *Extreme Mechanics Letters*, vol. 2. Elsevier BV, pp. 52–59, Mar. 2015. doi: 10.1016/j.eml.2015.01.007.  
  
G. Jung, Z. Qinand M. J. Buehler, “Mechanical Properties and Failure of Biopolymers: Atomistic Reactions to Macroscale Response”, *Topics in Current Chemistry*. Springer International Publishing, pp. 317–343, 2015. doi: 10.1007/128\_2015\_643.  
  
F. Libonati, G. X. Gu, Z. Qin, L. Verganiand M. J. Buehler, “Bone-Inspired Materials by Design: Toughness Amplification Observed Using 3D Printing and Testing”, *Advanced Engineering Materials*, vol. 18, no. 8. Wiley, pp. 1354–1363, May 23, 2016. doi: 10.1002/adem.201600143.  
  
S. Ling, N. Dinjaski, D. Ebrahimi, J. Y. Wong, D. L. Kaplanand M. J. Buehler, “Conformation Transitions of Recombinant Spidroins via Integration of Time-Resolved FTIR Spectroscopy and Molecular Dynamic Simulation”, *ACS Biomaterials Science & Engineering*, vol. 2, no. 8. American Chemical Society (ACS), pp. 1298–1308, Jul. 01, 2016. doi: 10.1021/acsbiomaterials.6b00234.  
  
S. Ling, K. Jin, D. L. Kaplanand M. J. Buehler, “Ultrathin Free-Standing *Bombyx mori* Silk Nanofibril Membranes”, *Nano Letters*, vol. 16, no. 6. American Chemical Society (ACS), pp. 3795–3800, May 17, 2016. doi: 10.1021/acs.nanolett.6b01195.  
  
S. Ling, C. Li, K. Jin, D. L. Kaplanand M. J. Buehler, “Liquid Exfoliated Natural Silk Nanofibrils: Applications in Optical and Electrical Devices”, *Advanced Materials*, vol. 28, no. 35. Wiley, pp. 7783–7790, Jun. 28, 2016. doi: 10.1002/adma.201601783.  
  
S. Ling, Z. Qin, W. Huang, S. Cao, D. L. Kaplanand M. J. Buehler, “Design and function of biomimetic multilayer water purification membranes”, *Science Advances*, vol. 3, no. 4. American Association for the Advancement of Science (AAAS), Apr. 07, 2017. doi: 10.1126/sciadv.1601939.  
  
S. Ling, Q. Zhang, D. L. Kaplan, F. Omenetto, M. J. Buehlerand Z. Qin, “Printing of stretchable silk membranes for strain measurements”, *Lab on a Chip*, vol. 16, no. 13. Royal Society of Chemistry (RSC), pp. 2459–2466, 2016. doi: 10.1039/c6lc00519e.  
  
T. Li, “Studies of chain substitution caused sub-fibril level differences in stiffness and ultrastructure of wildtype and oim/oim collagen fibers using multifrequency-AFM and molecular modeling”, *Biomaterials*, vol. 107. Elsevier BV, pp. 15–22, Nov. 2016. doi: 10.1016/j.biomaterials.2016.08.038.  
  
F. J. Martín-Martínez, E. H. Finiand M. J. Buehler, “Molecular asphaltene models based on Clar sextet theory”, *RSC Advances*, vol. 5, no. 1. Royal Society of Chemistry (RSC), pp. 753–759, 2015. doi: 10.1039/c4ra05694a.  
  
A. Masic, “Osmotic pressure induced tensile forces in tendon collagen”, *Nature Communications*, vol. 6, no. 1. Springer Science and Business Media LLC, Jan. 22, 2015. doi: 10.1038/ncomms6942.  
  
R. Mirzaeifar, L. S. Dimas, Z. Qinand M. J. Buehler, “Defect-Tolerant Bioinspired Hierarchical Composites: Simulation and Experiment”, *ACS Biomaterials Science & Engineering*, vol. 1, no. 5. American Chemical Society (ACS), pp. 295–304, Apr. 14, 2015. doi: 10.1021/ab500120f.  
  
R. Mirzaeifar, Z. Qinand M. J. Buehler, “Mesoscale mechanics of twisting carbon nanotube yarns”, *Nanoscale*, vol. 7, no. 12. Royal Society of Chemistry (RSC), pp. 5435–5445, 2015. doi: 10.1039/c4nr06669c.  
  
A. K. Nair, A. Gautieriand M. J. Buehler, “Role of Intrafibrillar Collagen Mineralization in Defining the Compressive Properties of Nascent Bone”, *Biomacromolecules*, vol. 15, no. 7. American Chemical Society (ACS), pp. 2494–2500, Jun. 23, 2014. doi: 10.1021/bm5003416.  
  
S. D. Palkovic, D. B. Brommer, K. Kupwade-Patil, A. Masic, M. J. Buehlerand O. Büyüköztürk, “Roadmap across the mesoscale for durable and sustainable cement paste – A bioinspired approach”, *Construction and Building Materials*, vol. 115. Elsevier BV, pp. 13–31, Jul. 2016. doi: 10.1016/j.conbuildmat.2016.04.020.  
  
M. Parambath, Q. S. Hanley, F. J. Martin-Martinez, T. Giesa, M. J. Buehlerand C. C. Perry, “The nature of the silicaphilic fluorescence of PDMPO”, *Physical Chemistry Chemical Physics*, vol. 18, no. 8. Royal Society of Chemistry (RSC), pp. 5938–5948, 2016. doi: 10.1039/c5cp05105c.  
  
Z. Qin and M. J. Buehler, “Nonlinear Viscous Water at Nanoporous Two-Dimensional Interfaces Resists High-Speed Flow through Cooperativity”, *Nano Letters*, vol. 15, no. 6. American Chemical Society (ACS), pp. 3939–3944, May 22, 2015. doi: 10.1021/acs.nanolett.5b00809.  
  
Z. Qin, B. G. Compton, J. A. Lewisand M. J. Buehler, “Structural optimization of 3D-printed synthetic spider webs for high strength”, *Nature Communications*, vol. 6, no. 1. Springer Science and Business Media LLC, May 15, 2015. doi: 10.1038/ncomms8038.  
  
Z. Qin, K. Jinand M. J. Buehler, “Molecular Modeling and Mechanics of Acrylic Adhesives on a Graphene Substrate with Roughness”, *BioNanoScience*, vol. 6, no. 3. Springer Science and Business Media LLC, pp. 177–184, Jun. 09, 2016. doi: 10.1007/s12668-016-0205-1.  
  
Z. Qin, G. S. Jung, M. J. Kangand M. J. Buehler, “The mechanics and design of a lightweight three-dimensional graphene assembly”, *Science Advances*, vol. 3, no. 1. American Association for the Advancement of Science (AAAS), Jan. 06, 2017. doi: 10.1126/sciadv.1601536.  
  
I. Su and M. J. Buehler, “Nanomechanics of silk: the fundamentals of a strong, tough and versatile material”, *Nanotechnology*, vol. 27, no. 30. IOP Publishing, p. 302001, Jun. 16, 2016. doi: 10.1088/0957-4484/27/30/302001.  
  
I. Su and M. J. Buehler, “Dynamic mechanics”, *Nature Materials*, vol. 15, no. 10. Springer Science and Business Media LLC, pp. 1054–1055, Jul. 25, 2016. doi: 10.1038/nmat4721.  
  
A. M. Sultan, “Aqueous Peptide–TiO2 Interfaces: Isoenergetic Binding via Either Entropically or Enthalpically Driven Mechanisms”, *ACS Applied Materials & Interfaces*, vol. 8, no. 28. American Chemical Society (ACS), pp. 18620–18630, Jul. 11, 2016. doi: 10.1021/acsami.6b05200.  
  
A. Tarakanova, W. Huang, A. S. Weiss, D. L. Kaplanand M. J. Buehler, “Computational smart polymer design based on elastin protein mutability”, *Biomaterials*, vol. 127. Elsevier BV, pp. 49–60, May 2017. doi: 10.1016/j.biomaterials.2017.01.041.  
  
S. Wang, “Atomically Sharp Crack Tips in Monolayer MoS2 and Their Enhanced Toughness by Vacancy Defects”, *ACS Nano*, vol. 10, no. 11. American Chemical Society (ACS), pp. 9831–9839, Sep. 30, 2016. doi: 10.1021/acsnano.6b05435.  
  
Y. Wang, Z. Qin, M. J. Buehlerand Z. Xu, “Intercalated water layers promote thermal dissipation at bio–nano interfaces”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Sep. 23, 2016. doi: 10.1038/ncomms12854.  
  
G. X. Gu, I. Su, S. Sharma, J. L. Voros, Z. Qinand M. J. Buehler, “Three-Dimensional-Printing of Bio-Inspired Composites”, *Journal of Biomechanical Engineering*, vol. 138, no. 2. ASME International, Jan. 27, 2016. doi: 10.1115/1.4032423.  
  
G. C. Yeo, A. Tarakanova, C. Baldock, S. G. Wise, M. J. Buehlerand A. S. Weiss, “Subtle balance of tropoelastin molecular shape and flexibility regulates dynamics and hierarchical assembly”, *Science Advances*, vol. 2, no. 2. American Association for the Advancement of Science (AAAS), Feb. 05, 2016. doi: 10.1126/sciadv.1501145.  
  
J. L. Zitnay, “Molecular level detection and localization of mechanical damage in collagen enabled by collagen hybridizing peptides”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Mar. 22, 2017. doi: 10.1038/ncomms14913.  
  
C. Ariyaratana and L. A. Fahnestock, “Evaluation of buckling-restrained braced frame seismic performance considering reserve strength”, *Engineering Structures*, vol. 33, no. 1. Elsevier BV, pp. 77–89, Jan. 2011. doi: 10.1016/j.engstruct.2010.09.020.  
  
S. T. Hoffman and L. A. Fahnestock, “Behavior of multi-story steel buildings under dynamic column loss scenarios”, *Steel and Composite Structures*, vol. 11, no. 2, pp. 149–168, Mar. 2011, doi: 10.12989/SCS.2011.11.2.149.  
  
D. Jang, X. Li, H. Gaoand J. R. Greer, “Deformation mechanisms in nanotwinned metal nanopillars”, *Nature Nanotechnology*, vol. 7, no. 9. Springer Science and Business Media LLC, pp. 594–601, Jul. 15, 2012. doi: 10.1038/nnano.2012.116.  
  
S. Kumar, X. Li, A. Haqueand H. Gao, “Is Stress Concentration Relevant for Nanocrystalline Metals?”, *Nano Letters*, vol. 11, no. 6. American Chemical Society (ACS), pp. 2510–2516, May 18, 2011. doi: 10.1021/nl201083t.  
  
X. Li, Y. Wei, L. Lu, K. Luand H. Gao, “Dislocation nucleation governed softening and maximum strength in nano-twinned metals”, *Nature*, vol. 464, no. 7290. Springer Science and Business Media LLC, pp. 877–880, Apr. 08, 2010. doi: 10.1038/nature08929.  
  
L. Zhu, H. Ruan, X. Li, M. Dao, H. Gaoand J. Lu, “Modeling grain size dependent optimal twin spacing for achieving ultimate high strength and related high ductility in nanotwinned metals”, *Acta Materialia*, vol. 59, no. 14. Elsevier BV, pp. 5544–5557, Aug. 2011. doi: 10.1016/j.actamat.2011.05.027.  
  
L. Xiong, Q. Deng, G. Tucker, D. L. McDowelland Y. Chen, “A concurrent scheme for passing dislocations from atomistic to continuum domains”, *Acta Materialia*, vol. 60, no. 3. Elsevier BV, pp. 899–913, Feb. 2012. doi: 10.1016/j.actamat.2011.11.002.  
  
Q. Qin, “Recoverable plasticity in penta-twinned metallic nanowires governed by dislocation nucleation and retraction”, *Nature Communications*, vol. 6, no. 1. Springer Science and Business Media LLC, Jan. 13, 2015. doi: 10.1038/ncomms6983.  
  
Y. A. Shin, “Nanotwin-governed toughening mechanism in hierarchically structured biological materials”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Feb. 17, 2016. doi: 10.1038/ncomms10772.  
  
T. Zhang, X. Liand H. Gao, “Defects controlled wrinkling and topological design in graphene”, *Journal of the Mechanics and Physics of Solids*, vol. 67. Elsevier BV, pp. 2–13, Jul. 2014. doi: 10.1016/j.jmps.2014.02.005.  
  
T. Zhang, X. Liand H. Gao, “Designing graphene structures with controlled distributions of topological defects: A case study of toughness enhancement in graphene ruga”, *Extreme Mechanics Letters*, vol. 1. Elsevier BV, pp. 3–8, Dec. 2014. doi: 10.1016/j.eml.2014.12.007.  
  
H. Zhou and H. Gao, “A Plastic Deformation Mechanism by Necklace Dislocations Near Crack-like Defects in Nanotwinned Metals”, *Journal of Applied Mechanics*, vol. 82, no. 7. ASME International, Jul. 01, 2015. doi: 10.1115/1.4030417.  
  
H. Zhou, X. Li, S. Qu, W. Yangand H. Gao, “A Jogged Dislocation Governed Strengthening Mechanism in Nanotwinned Metals”, *Nano Letters*, vol. 14, no. 9. American Chemical Society (ACS), pp. 5075–5080, Aug. 22, 2014. doi: 10.1021/nl501755q.  
  
H. Zhou, X. Li, Y. Wang, Z. Liu, W. Yangand H. Gao, “Torsional Detwinning Domino in Nanotwinned One-Dimensional Nanostructures”, *Nano Letters*, vol. 15, no. 9. American Chemical Society (ACS), pp. 6082–6087, Aug. 04, 2015. doi: 10.1021/acs.nanolett.5b02330.  
  
W. Zhu, “Nanomechanical mechanism for lipid bilayer damage induced by carbon nanotubes confined in intracellular vesicles”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 44. Proceedings of the National Academy of Sciences, pp. 12374–12379, Oct. 17, 2016. doi: 10.1073/pnas.1605030113.  
  
D. J. Borello and L. A. Fahnestock, “Seismic Design and Analysis of Steel Plate Shear Walls with Coupling”, *Journal of Structural Engineering*, vol. 139, no. 8. American Society of Civil Engineers (ASCE), pp. 1263–1273, Aug. 2013. doi: 10.1061/(asce)st.1943-541x.0000576.  
  
K. Mathur, L. A. Fahnestock, T. Okazakiand M. J. Parkolap, “Impact of Residual Stresses and Initial Imperfections on the Seismic Response of Steel Moment Frames”, *Journal of Structural Engineering*, vol. 138, no. 7. American Society of Civil Engineers (ASCE), pp. 942–951, Jul. 2012. doi: 10.1061/(asce)st.1943-541x.0000512.  
  
C. D. Stoakes and L. A. Fahnestock, “Cyclic flexural analysis and behavior of beam-column connections with gusset plates”, *Journal of Constructional Steel Research*, vol. 72. Elsevier BV, pp. 227–239, May 2012. doi: 10.1016/j.jcsr.2011.12.008.  
  
S. Szyniszewski, B. H. Smith, J. F. Hajjar, S. R. Arwadeand B. W. Schafer, “Local buckling strength of steel foam sandwich panels”, *Thin-Walled Structures*, vol. 59. Elsevier BV, pp. 11–19, Oct. 2012. doi: 10.1016/j.tws.2012.04.014.  
  
B. H. Smith, S. Szyniszewski, J. F. Hajjar, B. W. Schaferand S. R. Arwade, “Steel foam for structures: A review of applications, manufacturing and material properties”, *Journal of Constructional Steel Research*, vol. 71. Elsevier BV, pp. 1–10, Apr. 2012. doi: 10.1016/j.jcsr.2011.10.028.  
  
A. Ural, P. Bruno, B. Zhou, X. T. Shiand X. E. Guo, “A new fracture assessment approach coupling HR-pQCT imaging and fracture mechanics-based finite element modeling”, *Journal of Biomechanics*, vol. 46, no. 7. Elsevier BV, pp. 1305–1311, Apr. 2013. doi: 10.1016/j.jbiomech.2013.02.009.  
  
A. J. Golman, K. A. Danelson, J. P. Gaewskyand J. D. Stitzel, “Implementation and validation of thoracic side impact injury prediction metrics in a human body model”, *Computer Methods in Biomechanics and Biomedical Engineering*, vol. 18, no. 10. Informa UK Limited, pp. 1044–1055, Feb. 12, 2014. doi: 10.1080/10255842.2013.869319.  
  
A. J. Golman, K. A. Danelson, L. E. Millerand J. D. Stitzel, “Injury prediction in a side impact crash using human body model simulation”, *Accident Analysis & Prevention*, vol. 64. Elsevier BV, pp. 1–8, Mar. 2014. doi: 10.1016/j.aap.2013.10.026.  
  
A. J. Golman, K. A. Danelson, L. E. Millerand J. D. Stitzel, “Injury prediction in a side impact crash using human body model simulation”, *Accident Analysis & Prevention*, vol. 64. Elsevier BV, pp. 1–8, Mar. 2014. doi: 10.1016/j.aap.2013.10.026.  
  
J. Patalak, M. Davis, J. Gaewsky, J. Stitzeland M. Harper, “Influence of Driver Position and Seat Design on Thoracolumbar Loading During Frontal Impacts”, *SAE Technical Paper Series*. SAE International, Apr. 03, 2018. doi: 10.4271/2018-01-0544.  
  
X. Ye, “Numerical investigation of driver lower extremity injuries in finite element frontal crash reconstruction”, *Traffic Injury Prevention*, vol. 19, no. sup1. Informa UK Limited, pp. S21–S28, Feb. 28, 2018. doi: 10.1080/15389588.2017.1376051.  
  
J. A. Hernandez and I. L. Al-Qadi, “Hyperelastic Modeling of Wide-Base Tire and Prediction of Its Contact Stresses”, *Journal of Engineering Mechanics*, vol. 142, no. 2. American Society of Civil Engineers (ASCE), Feb. 2016. doi: 10.1061/(asce)em.1943-7889.0001007.  
  
J. A. Hernandez and I. L. Al-Qadi, “Tire–pavement interaction modelling: hyperelastic tire and elastic pavement”, *Road Materials and Pavement Design*, vol. 18, no. 5. Informa UK Limited, pp. 1067–1083, Jul. 19, 2016. doi: 10.1080/14680629.2016.1206485.  
  
J. A. Hernandez, I. L. Al-Qadiand H. Ozer, “Baseline rolling resistance for tires’ on-road fuel efficiency using finite element modeling”, *International Journal of Pavement Engineering*, vol. 18, no. 5. Informa UK Limited, pp. 424–432, Oct. 29, 2015. doi: 10.1080/10298436.2015.1095298.  
  
A. Harpale and H. B. Chew, “Hydrogen-plasma patterning of multilayer graphene: Mechanisms and modeling”, *Carbon*, vol. 117. Elsevier BV, pp. 82–91, Jun. 2017. doi: 10.1016/j.carbon.2017.02.062.  
  
A. Harpale, M. Panesiand H. B. Chew, “Communication: Surface-to-bulk diffusion of isolated versus interacting C atoms in Ni(111) and Cu(111) substrates: A first principle investigation”, *The Journal of Chemical Physics*, vol. 142, no. 6. AIP Publishing, p. 061101, Feb. 14, 2015. doi: 10.1063/1.4907716.  
  
A. Harpale, M. Panesiand H. B. Chew, “Plasma-graphene interaction and its effects on nanoscale patterning”, *Physical Review B*, vol. 93, no. 3. American Physical Society (APS), Jan. 11, 2016. doi: 10.1103/physrevb.93.035416.  
  
A. Harpale, S. Sawant, R. Kumar, D. Levinand H. B. Chew, “Ablative thermal protection systems: Pyrolysis modeling by scale-bridging molecular dynamics”, *Carbon*, vol. 130. Elsevier BV, pp. 315–324, Apr. 2018. doi: 10.1016/j.carbon.2017.12.099.  
  
R. Li and H. B. Chew, “Deformation twinning and plastic recovery in Cu/Ag nanolayers under uniaxial tensile straining”, *Philosophical Magazine Letters*, vol. 94, no. 5. Informa UK Limited, pp. 260–268, Mar. 31, 2014. doi: 10.1080/09500839.2014.893063.  
  
R. Li and H. B. Chew, “Closed and open-ended stacking fault tetrahedra formation along the interfaces of Cu–Al nanolayered metals”, *Philosophical Magazine*, vol. 95, no. 25. Informa UK Limited, pp. 2747–2763, Aug. 26, 2015. doi: 10.1080/14786435.2015.1077283.  
  
R. Li and H. B. Chew, “Planar-to-wavy transition of Cu–Ag nanolayered metals: a precursor mechanism to twinning”, *Philosophical Magazine*, vol. 95, no. 10. Informa UK Limited, pp. 1029–1048, Mar. 16, 2015. doi: 10.1080/14786435.2015.1006290.  
  
R. Li and H. B. Chew, “Grain Boundary Traction Signatures: Quantitative Predictors of Dislocation Emission”, *Physical Review Letters*, vol. 117, no. 8. American Physical Society (APS), Aug. 15, 2016. doi: 10.1103/physrevlett.117.085502.  
  
R. Li and H. B. Chew, “Grain boundary traction signatures: Quantifying the asymmetrical dislocation emission processes under tension and compression”, *Journal of the Mechanics and Physics of Solids*, vol. 103. Elsevier BV, pp. 142–154, Jun. 2017. doi: 10.1016/j.jmps.2017.03.009.  
  
H. Wang and H. B. Chew, “Molecular dynamics simulations of plasticity and cracking in lithiated silicon electrodes”, *Extreme Mechanics Letters*, vol. 9. Elsevier BV, pp. 503–513, Dec. 2016. doi: 10.1016/j.eml.2016.02.020.  
  
H. Wang and H. B. Chew, “Nanoscale Mechanics of the Solid Electrolyte Interphase on Lithiated-Silicon Electrodes”, *ACS Applied Materials & Interfaces*, vol. 9, no. 31. American Chemical Society (ACS), pp. 25662–25667, Jul. 25, 2017. doi: 10.1021/acsami.7b07626.  
  
H. Wang, B. Hou, X. Wang, S. Xiaand H. B. Chew, “Atomic-Scale Mechanisms of Sliding along an Interdiffused Li–Si–Cu Interface”, *Nano Letters*, vol. 15, no. 3. American Chemical Society (ACS), pp. 1716–1721, Feb. 06, 2015. doi: 10.1021/nl5043837.  
  
H. Wang, X. Wang, S. Xiaand H. B. Chew, “Brittle-to-ductile transition of lithiated silicon electrodes: Crazing to stable nanopore growth”, *The Journal of Chemical Physics*, vol. 143, no. 10. AIP Publishing, p. 104703, Sep. 14, 2015. doi: 10.1063/1.4930856.  
  
C. Yi, “Direct nanomechanical characterization of carbon nanotubes - titanium interfaces”, *Carbon*, vol. 132. Elsevier BV, pp. 548–555, Jun. 2018. doi: 10.1016/j.carbon.2018.02.069.  
  
J. Wang, “Near-ideal theoretical strength in gold nanowires containing angstrom scale twins”, *Nature Communications*, vol. 4, no. 1. Springer Science and Business Media LLC, Apr. 23, 2013. doi: 10.1038/ncomms2768.  
  
P. Bhattacharya, “Trends in Thermoresponsive Behavior of Lipophilic Polymers”, *Industrial & Engineering Chemistry Research*, vol. 55, no. 51. American Chemical Society (ACS), pp. 12983–12990, Dec. 14, 2016. doi: 10.1021/acs.iecr.6b03812.  
  
K. Hasz, Z. Ye, A. Martiniand R. W. Carpick, “Experiments and simulations of the humidity dependence of friction between nanoasperities and graphite: The role of interfacial contact quality”, *Physical Review Materials*, vol. 2, no. 12. American Physical Society (APS), Dec. 07, 2018. doi: 10.1103/physrevmaterials.2.126001.  
  
X. Hu, N. Chan, A. Martiniand P. Egberts, “Tip convolution on HOPG surfaces measured in AM-AFM and interpreted using a combined experimental and simulation approach”, *Nanotechnology*, vol. 28, no. 2. IOP Publishing, p. 025702, Dec. 01, 2016. doi: 10.1088/0957-4484/28/2/025702.  
  
X. Hu, P. Egberts, Y. Dongand A. Martini, “Molecular dynamics simulation of amplitude modulation atomic force microscopy”, *Nanotechnology*, vol. 26, no. 23. IOP Publishing, p. 235705, May 20, 2015. doi: 10.1088/0957-4484/26/23/235705.  
  
M. Luisier, “Investigation of ripple-limited low-field mobility in large-scale graphene nanoribbons”, *Applied Physics Letters*, vol. 102, no. 25. AIP Publishing, p. 253506, Jun. 24, 2013. doi: 10.1063/1.4811761.  
  
U. S. Ramasamy, M. Lenand A. Martini, “Correlating Molecular Structure to the Behavior of Linear Styrene–Butadiene Viscosity Modifiers”, *Tribology Letters*, vol. 65, no. 4. Springer Science and Business Media LLC, Oct. 10, 2017. doi: 10.1007/s11249-017-0926-5.  
  
U. S. Ramasamy, S. Lichterand A. Martini, “Effect of Molecular-Scale Features on the Polymer Coil Size of Model Viscosity Index Improvers”, *Tribology Letters*, vol. 62, no. 2. Springer Science and Business Media LLC, Mar. 31, 2016. doi: 10.1007/s11249-016-0672-0.  
  
M. R. Vazirisereshk, “Origin of Nanoscale Friction Contrast between Supported Graphene, MoS2, and a Graphene/MoS2 Heterostructure”, *Nano Letters*, vol. 19, no. 8. American Chemical Society (ACS), pp. 5496–5505, Jul. 03, 2019. doi: 10.1021/acs.nanolett.9b02035.  
  
Z. Ye, A. Balkanci, A. Martiniand M. Z. Baykara, “Effect of roughness on the layer-dependent friction of few-layer graphene”, *Physical Review B*, vol. 96, no. 11. American Physical Society (APS), Sep. 01, 2017. doi: 10.1103/physrevb.96.115401.  
  
Z. Ye, P. Egberts, G. H. Han, A. T. C. Johnson, R. W. Carpickand A. Martini, “Load-Dependent Friction Hysteresis on Graphene”, *ACS Nano*, vol. 10, no. 5. American Chemical Society (ACS), pp. 5161–5168, Apr. 28, 2016. doi: 10.1021/acsnano.6b00639.  
  
Z. Ye and A. Martini, “Atomistic Simulation of the Load Dependence of Nanoscale Friction on Suspended and Supported Graphene”, *Langmuir*, vol. 30, no. 49. American Chemical Society (ACS), pp. 14707–14711, Dec. 01, 2014. doi: 10.1021/la503329u.  
  
Z. Ye and A. Martini, “Atomic friction at exposed and buried graphite step edges: Experiments and simulations”, *Applied Physics Letters*, vol. 106, no. 23. AIP Publishing, p. 231603, Jun. 08, 2015. doi: 10.1063/1.4922485.  
  
J. A. El-Awady, “Unravelling the physics of size-dependent dislocation-mediated plasticity”, *Nature Communications*, vol. 6, no. 1. Springer Science and Business Media LLC, Jan. 06, 2015. doi: 10.1038/ncomms6926.  
  
M. S. Manivannan and M. N. Silberstein, “Theoretical framework and design of mechanochemically augmented polymer composites”, *Extreme Mechanics Letters*, vol. 19. Elsevier BV, pp. 27–38, Mar. 2018. doi: 10.1016/j.eml.2017.12.005.  
  
S. Bae, O. Galant, C. E. Diesendruckand M. N. Silberstein, “Tailoring single chain polymer nanoparticle thermo-mechanical behavior by cross-link density”, *Soft Matter*, vol. 13, no. 15. Royal Society of Chemistry (RSC), pp. 2808–2816, 2017. doi: 10.1039/c7sm00360a.  
  
S. Bae, O. Galant, C. E. Diesendruckand M. N. Silberstein, “The Effect of Intrachain Cross-Linking on the Thermomechanical Behavior of Bulk Polymers Assembled Solely from Single Chain Polymer Nanoparticles”, *Macromolecules*, vol. 51, no. 18. American Chemical Society (ACS), pp. 7160–7168, Sep. 10, 2018. doi: 10.1021/acs.macromol.8b01027.  
  
M. R. Buche and M. N. Silberstein, “Statistical mechanical constitutive theory of polymer networks: The inextricable links between distribution, behavior, and ensemble”, *Physical Review E*, vol. 102, no. 1. American Physical Society (APS), Jul. 02, 2020. doi: 10.1103/physreve.102.012501.  
  
O. Galant, S. Bae, M. N. Silbersteinand C. E. Diesendruck, “Highly Stretchable Polymers: Mechanical Properties Improvement by Balancing Intra‐ and Intermolecular Interactions”, *Advanced Functional Materials*, vol. 30, no. 18. Wiley, p. 1901806, Apr. 18, 2019. doi: 10.1002/adfm.201901806.  
  
M. S. Manivannan and M. N. Silberstein, “Computational investigation of shear driven mechanophore activation at interfaces”, *Extreme Mechanics Letters*, vol. 8. Elsevier BV, pp. 6–12, Sep. 2016. doi: 10.1016/j.eml.2015.10.003.  
  
Y. Vidavsky, “Tuning the Mechanical Properties of Metallopolymers via Ligand Interactions: A Combined Experimental and Theoretical Study”, *Macromolecules*, vol. 53, no. 6. American Chemical Society (ACS), pp. 2021–2030, Mar. 05, 2020. doi: 10.1021/acs.macromol.9b02756.  
  
C. S. Thompson, “Bring the NLACE model online using XSEDE and HUBzero”, *Proceedings of the 2015 XSEDE Conference on Scientific Advancements Enabled by Enhanced Cyberinfrastructure - XSEDE ’15*. ACM Press, 2015. doi: 10.1145/2792745.2792781.  
  
A. M. Hussein, S. I. Rao, M. D. Uchic, D. M. Dimidukand J. A. El-Awady, “Microstructurally based cross-slip mechanisms and their effects on dislocation microstructure evolution in fcc crystals”, *Acta Materialia*, vol. 85. Elsevier BV, pp. 180–190, Feb. 2015. doi: 10.1016/j.actamat.2014.10.067.  
  
S. S. Duan and A. M. Mohammed, “Computer Simulation of Multibody Dynamical Systems in a TeraGrid Environment”, *Volume 11: New Developments in Simulation Methods and Software for Engineering Applications; Safety Engineering, Risk Analysis and Reliability Methods; Transportation Systems*. ASMEDC, Jan. 01, 2010. doi: 10.1115/imece2010-40000.  
  
B. Noble, A. Ovcharenkoand B. Raeymaekers, “Quantifying lubricant droplet spreading on a flat substrate using molecular dynamics”, *Applied Physics Letters*, vol. 105, no. 15. AIP Publishing, p. 151601, Oct. 13, 2014. doi: 10.1063/1.4898140.  
  
H. Babaei, A. Basakand V. I. Levitas, “Algorithmic aspects and finite element solutions for advanced phase field approach to martensitic phase transformation under large strains”, *Computational Mechanics*, vol. 64, no. 4. Springer Science and Business Media LLC, pp. 1177–1197, Apr. 03, 2019. doi: 10.1007/s00466-019-01699-y.  
  
S. E. Esfahani, I. Ghamarian, V. I. Levitasand P. C. Collins, “Microscale phase field modeling of the martensitic transformation during cyclic loading of NiTi single crystal”, *International Journal of Solids and Structures*, vol. 146. Elsevier BV, pp. 80–96, Aug. 2018. doi: 10.1016/j.ijsolstr.2018.03.022.  
  
C.-T. Lu, A. Weerasinghe, D. Maroudasand A. Ramasubramaniam, “A Comparison of the Elastic Properties of Graphene- and Fullerene-Reinforced Polymer Composites: The Role of Filler Morphology and Size”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Aug. 22, 2016. doi: 10.1038/srep31735.  
  
S. Xu, R. Che, L. Xiong, Y. Chenand D. L. McDowell, “A quasistatic implementation of the concurrent atomistic-continuum method for FCC crystals”, *International Journal of Plasticity*, vol. 72. Elsevier BV, pp. 91–126, Sep. 2015. doi: 10.1016/j.ijplas.2015.05.007.  
  
C. Kunka, A. Awasthiand G. Subhash, “Crystallographic and spectral equivalence of boron-carbide polymorphs”, *Scripta Materialia*, vol. 122. Elsevier BV, pp. 82–85, Sep. 2016. doi: 10.1016/j.scriptamat.2016.05.010.  
  
G. Subhash, A. P. Awasthi, C. Kunka, P. Jannottiand M. DeVries, “In search of amorphization-resistant boron carbide”, *Scripta Materialia*, vol. 123. Elsevier BV, pp. 158–162, Oct. 2016. doi: 10.1016/j.scriptamat.2016.06.012.  
  
A. Awasthi and G. Subhash, “Deformation behavior and amorphization in icosahedral boron-rich ceramics”, *Progress in Materials Science*, vol. 112. Elsevier BV, p. 100664, Jul. 2020. doi: 10.1016/j.pmatsci.2020.100664.  
  
B. A. Noble, C. M. Mateand B. Raeymaekers, “Spreading Kinetics of Ultrathin Liquid Films Using Molecular Dynamics”, *Langmuir*, vol. 33, no. 14. American Chemical Society (ACS), pp. 3476–3483, Mar. 27, 2017. doi: 10.1021/acs.langmuir.7b00334.  
  
B. A. Noble, A. Ovcharenkoand B. Raeymaekers, “Terraced spreading of nanometer-thin lubricant using molecular dynamics”, *Polymer*, vol. 84. Elsevier BV, pp. 286–292, Feb. 2016. doi: 10.1016/j.polymer.2016.01.016.  
  
X. Fu, Y. Jewel, Y. Wang, J. Liuand W.-H. Zhong, “Decoupled Ion Transport in a Protein-Based Solid Ion Conductor”, *The Journal of Physical Chemistry Letters*, vol. 7, no. 21. American Chemical Society (ACS), pp. 4304–4310, Oct. 19, 2016. doi: 10.1021/acs.jpclett.6b02071.  
  
Y. Jewel, P. Duttaand J. Liu, “Coarse-grained simulations of proton-dependent conformational changes in lactose permease”, *Proteins: Structure, Function, and Bioinformatics*, vol. 84, no. 8. Wiley, pp. 1067–1074, May 03, 2016. doi: 10.1002/prot.25053.  
  
T. Bucher, C. Bolger, M. Zhang, C. J. Chenand Y. Lawrence Yao, “Effect of Geometrical Modeling on the Prediction of Laser-Induced Heat Transfer in Metal Foam”, *Journal of Manufacturing Science and Engineering*, vol. 138, no. 12. ASME International, Jul. 27, 2016. doi: 10.1115/1.4033927.  
  
Z. Shen, M. Röding, M. Krögerand Y. Li, “Carbon Nanotube Length Governs the Viscoelasticity and Permeability of Buckypaper”, *Polymers*, vol. 9, no. 12. MDPI AG, p. 115, Mar. 23, 2017. doi: 10.3390/polym9040115.  
  
Z. Shen, H. Ye, M. Krögerand Y. Li, “Self-assembled core–polyethylene glycol–lipid shell nanoparticles demonstrate high stability in shear flow”, *Physical Chemistry Chemical Physics*, vol. 19, no. 20. Royal Society of Chemistry (RSC), pp. 13294–13306, 2017. doi: 10.1039/c7cp01530e.  
  
Y. Liu, W. Sun, Z. Yuanand J. Fish, “A nonlocal multiscale discrete-continuum model for predicting mechanical behavior of granular materials”, *International Journal for Numerical Methods in Engineering*, vol. 106, no. 2. Wiley, pp. 129–160, Nov. 03, 2015. doi: 10.1002/nme.5139.  
  
Y. Wang and A. Ural, “Mineralized collagen fibril network spatial arrangement influences cortical bone fracture behavior”, *Journal of Biomechanics*, vol. 66. Elsevier BV, pp. 70–77, Jan. 2018. doi: 10.1016/j.jbiomech.2017.10.038.  
  
Y. Wang and A. Ural, “Effect of modifications in mineralized collagen fibril and extra-fibrillar matrix material properties on submicroscale mechanical behavior of cortical bone”, *Journal of the Mechanical Behavior of Biomedical Materials*, vol. 82. Elsevier BV, pp. 18–26, Jun. 2018. doi: 10.1016/j.jmbbm.2018.03.013.  
  
X. Zhang, A. Acharya, N. J. Walkingtonand J. Bielak, “A single theory for some quasi-static, supersonic, atomic, and tectonic scale applications of dislocations”, *Journal of the Mechanics and Physics of Solids*, vol. 84. Elsevier BV, pp. 145–195, Nov. 2015. doi: 10.1016/j.jmps.2015.07.004.  
  
L. K. Aagesen, “PRISMS: An Integrated, Open-Source Framework for Accelerating Predictive Structural Materials Science”, *JOM*, vol. 70, no. 10. Springer Science and Business Media LLC, pp. 2298–2314, Aug. 30, 2018. doi: 10.1007/s11837-018-3079-6.  
  
P. Motamarri and V. Gavini, “Configurational forces in electronic structure calculations using Kohn-Sham density functional theory”, *Physical Review B*, vol. 97, no. 16. American Physical Society (APS), Apr. 20, 2018. doi: 10.1103/physrevb.97.165132.  
  
H. M. Paranjape, “Influences of granular constraints and surface effects on the heterogeneity of elastic, superelastic, and plastic responses of polycrystalline shape memory alloys”, *Journal of the Mechanics and Physics of Solids*, vol. 102. Elsevier BV, pp. 46–66, May 2017. doi: 10.1016/j.jmps.2017.02.007.  
  
A. Mesgarnejad and A. Karma, “Phase field modeling of chemomechanical fracture of intercalation electrodes: Role of charging rate and dimensionality”, *Journal of the Mechanics and Physics of Solids*, vol. 132. Elsevier BV, p. 103696, Nov. 2019. doi: 10.1016/j.jmps.2019.103696.  
  
A. P. Awasthi and G. Subhash, “High-pressure deformation and amorphization in boron carbide”, *Journal of Applied Physics*, vol. 125, no. 21. AIP Publishing, p. 215901, Jun. 07, 2019. doi: 10.1063/1.5091795.  
  
A. A. Cheenady, A. Awasthiand G. Subhash, “Intrinsic hardness of boron carbide: Influence of polymorphism and stoichiometry”, *Journal of the American Ceramic Society*, vol. 103, no. 12. Wiley, pp. 7127–7134, Sep. 2020. doi: 10.1111/jace.17420.  
  
M. DeVries, G. Subhashand A. Awasthi, “Shocked ceramics melt: An atomistic analysis of thermodynamic behavior of boron carbide”, *Physical Review B*, vol. 101, no. 14. American Physical Society (APS), Apr. 27, 2020. doi: 10.1103/physrevb.101.144107.  
  
C. Kunka, “Nanotwinning and amorphization of boron suboxide”, *Acta Materialia*, vol. 147. Elsevier BV, pp. 195–202, Apr. 2018. doi: 10.1016/j.actamat.2018.01.048.  
  
C. Kunka, A. Awasthiand G. Subhash, “Evaluating boron-carbide constituents with simulated Raman spectra”, *Scripta Materialia*, vol. 138. Elsevier BV, pp. 32–34, Sep. 2017. doi: 10.1016/j.scriptamat.2017.05.030.  
  
C. Kunka, X. Yang, Q. Anand G. Subhash, “Icosahedral superstrength at the nanoscale”, *Physical Review Materials*, vol. 2, no. 6. American Physical Society (APS), Jun. 27, 2018. doi: 10.1103/physrevmaterials.2.063606.  
  
J. Yu, M. Wangand S. Lin, “Probing the Soft and Nanoductile Mechanical Nature of Single and Polycrystalline Organic–Inorganic Hybrid Perovskites for Flexible Functional Devices”, *ACS Nano*, vol. 10, no. 12. American Chemical Society (ACS), pp. 11044–11057, Dec. 09, 2016. doi: 10.1021/acsnano.6b05913.  
  
J. H. Lee, “Flexible Conductive Composite Integrated with Personal Earphone for Wireless, Real-Time Monitoring of Electrophysiological Signs”, *ACS Applied Materials & Interfaces*, vol. 10, no. 25. American Chemical Society (ACS), pp. 21184–21190, Jun. 05, 2018. doi: 10.1021/acsami.8b06484.  
  
A. T. Zehnder, R. H. Randand S. Krylov, “Locking of electrostatically coupled thermo-optically driven MEMS limit cycle oscillators”, *International Journal of Non-Linear Mechanics*, vol. 102. Elsevier BV, pp. 92–100, Jun. 2018. doi: 10.1016/j.ijnonlinmec.2018.03.009.  
  
H. M. Paranjape, “In situ, 3D characterization of the deformation mechanics of a superelastic NiTi shape memory alloy single crystal under multiscale constraint”, *Acta Materialia*, vol. 144. Elsevier BV, pp. 748–757, Feb. 2018. doi: 10.1016/j.actamat.2017.11.026.  
  
P. P. Paul, M. Fortman, H. M. Paranjape, P. M. Anderson, A. P. Stebnerand L. C. Brinson, “Influence of Structure and Microstructure on Deformation Localization and Crack Growth in NiTi Shape Memory Alloys”, *Shape Memory and Superelasticity*, vol. 4, no. 2. Springer Science and Business Media LLC, pp. 285–293, Apr. 12, 2018. doi: 10.1007/s40830-018-0172-1.  
  
H. Chen, S. Xu, W. Li, R. Ji, T. Phanand L. Xiong, “A spatial decomposition parallel algorithm for a concurrent atomistic-continuum simulator and its preliminary applications”, *Computational Materials Science*, vol. 144. Elsevier BV, pp. 1–10, Mar. 2018. doi: 10.1016/j.commatsci.2017.11.051.  
  
V. I. Levitas, H. Chenand L. Xiong, “Triaxial-Stress-Induced Homogeneous Hysteresis-Free First-Order Phase Transformations with Stable Intermediate Phases”, *Physical Review Letters*, vol. 118, no. 2. American Physical Society (APS), Jan. 11, 2017. doi: 10.1103/physrevlett.118.025701.  
  
V. I. Levitas, H. Chenand L. Xiong, “Lattice instability during phase transformations under multiaxial stress: Modified transformation work criterion”, *Physical Review B*, vol. 96, no. 5. American Physical Society (APS), Aug. 29, 2017. doi: 10.1103/physrevb.96.054118.  
  
S. Xu, “PyCAC: The concurrent atomistic-continuum simulation environment”, *Journal of Materials Research*, vol. 33, no. 7. Springer Science and Business Media LLC, pp. 857–871, Jan. 30, 2018. doi: 10.1557/jmr.2018.8.  
  
S. Xu, L. Xiong, Y. Chenand D. L. McDowell, “Comparing EAM Potentials to Model Slip Transfer of Sequential Mixed Character Dislocations Across Two Symmetric Tilt Grain Boundaries in Ni”, *JOM*, vol. 69, no. 5. Springer Science and Business Media LLC, pp. 814–821, Mar. 10, 2017. doi: 10.1007/s11837-017-2302-1.  
  
S. Xu, L. Xiong, Y. Chenand D. L. McDowell, “Shear stress- and line length-dependent screw dislocation cross-slip in FCC Ni”, *Acta Materialia*, vol. 122. Elsevier BV, pp. 412–419, Jan. 2017. doi: 10.1016/j.actamat.2016.10.005.  
  
T. A. Engstrom, T. Zhang, A. K. Lawton, A. L. Joynerand J. M. Schwarz, “Buckling without Bending: A New Paradigm in Morphogenesis”, *Physical Review X*, vol. 8, no. 4. American Physical Society (APS), Dec. 21, 2018. doi: 10.1103/physrevx.8.041053.  
  
J. Sui, J. Chen, X. Zhang, G. Nieand T. Zhang, “Symplectic Analysis of Wrinkles in Elastic Layers With Graded Stiffnesses”, *Journal of Applied Mechanics*, vol. 86, no. 1. ASME International, Oct. 18, 2018. doi: 10.1115/1.4041620.  
  
T. Zhang, “Deriving a lattice model for neo-Hookean solids from finite element methods”, *Extreme Mechanics Letters*, vol. 26. Elsevier BV, pp. 40–45, Jan. 2019. doi: 10.1016/j.eml.2018.11.007.  
  
S. Hajilar and B. Shafei, “Structure, orientation, and dynamics of water-soluble ions adsorbed to basal surfaces of calcium monosulfoaluminate hydrates”, *Physical Chemistry Chemical Physics*, vol. 20, no. 38. Royal Society of Chemistry (RSC), pp. 24681–24694, 2018. doi: 10.1039/c8cp03872d.  
  
S. Hajilar and B. Shafei, “Atomic-scale investigation of physical adsorption of water molecules and aggressive ions to ettringite’s surfaces”, *Journal of Colloid and Interface Science*, vol. 513. Elsevier BV, pp. 104–116, Mar. 2018. doi: 10.1016/j.jcis.2017.09.019.  
  
L. He and N. Abdolrahim, “Stress-Assisted Structural Phase Transformation Enhances Ductility in Mo/Cu Bicontinuous Intertwined Composites”, *ACS Applied Nano Materials*, vol. 2, no. 4. American Chemical Society (ACS), pp. 1890–1897, Feb. 05, 2019. doi: 10.1021/acsanm.8b02219.  
  
A. Neogi, L. Heand N. Abdolrahim, “Atomistic simulations of shock compression of single crystal and core-shell Cu@Ni nanoporous metals”, *Journal of Applied Physics*, vol. 126, no. 1. AIP Publishing, p. 015901, Jul. 07, 2019. doi: 10.1063/1.5100261.  
  
H. Babaei and V. I. Levitas, “Phase-field approach for stress- and temperature-induced phase transformations that satisfies lattice instability conditions. Part 2. simulations of phase transformations Si I Si II”, *International Journal of Plasticity*, vol. 107. Elsevier BV, pp. 223–245, Aug. 2018. doi: 10.1016/j.ijplas.2018.04.006.  
  
H. Babaei and V. I. Levitas, “Stress-Measure Dependence of Phase Transformation Criterion under Finite Strains: Hierarchy of Crystal Lattice Instabilities for Homogeneous and Heterogeneous Transformations”, *Physical Review Letters*, vol. 124, no. 7. American Physical Society (APS), Feb. 21, 2020. doi: 10.1103/physrevlett.124.075701.  
  
H. Babaei and V. I. Levitas, “Finite-strain scale-free phase-field approach to multivariant martensitic phase transformations with stress-dependent effective thresholds”, *Journal of the Mechanics and Physics of Solids*, vol. 144. Elsevier BV, p. 104114, Nov. 2020. doi: 10.1016/j.jmps.2020.104114.  
  
A. Basak and V. I. Levitas, “Finite element procedure and simulations for a multiphase phase field approach to martensitic phase transformations at large strains and with interfacial stresses”, *Computer Methods in Applied Mechanics and Engineering*, vol. 343. Elsevier BV, pp. 368–406, Jan. 2019. doi: 10.1016/j.cma.2018.08.006.  
  
A. Basak and V. I. Levitas, “An exact formulation for exponential-logarithmic transformation stretches in a multiphase phase field approach to martensitic transformations”, *Mathematics and Mechanics of Solids*, vol. 25, no. 6. SAGE Publications, pp. 1219–1246, Feb. 14, 2020. doi: 10.1177/1081286520905352.  
  
A. Basak and V. I. Levitas, “Matrix-precipitate interface-induced martensitic transformation within nanoscale phase field approach: Effect of energy and dimensionless interface width”, *Acta Materialia*, vol. 189. Elsevier BV, pp. 255–265, May 2020. doi: 10.1016/j.actamat.2020.02.047.  
  
S. Ehsan Esfahani, I. Ghamarianand V. I. Levitas, “Strain-induced multivariant martensitic transformations: A scale-independent simulation of interaction between localized shear bands and microstructure”, *Acta Materialia*, vol. 196. Elsevier BV, pp. 430–443, Sep. 2020. doi: 10.1016/j.actamat.2020.06.059.  
  
H. Zhu, A. J. Whittle, R. J.-M. Pellenqand K. Ioannidou, “Mesoscale simulation of aggregation of imogolite nanotubes from potential of mean force interactions”, *Molecular Physics*, vol. 117, no. 22. Informa UK Limited, pp. 3445–3455, Sep. 06, 2019. doi: 10.1080/00268976.2019.1660817.  
  
S. Huang, I. J. Beyerleinand C. Zhou, “Nanograin size effects on the strength of biphase nanolayered composites”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Sep. 12, 2017. doi: 10.1038/s41598-017-10064-z.  
  
S. Huang and C. Zhou, “Modeling and Simulation of Nanoindentation”, *JOM*, vol. 69, no. 11. Springer Science and Business Media LLC, pp. 2256–2263, Aug. 22, 2017. doi: 10.1007/s11837-017-2541-1.  
  
W. Xu and L. P. Dávila, “Tensile nanomechanics and the Hall-Petch effect in nanocrystalline aluminium”, *Materials Science and Engineering: A*, vol. 710. Elsevier BV, pp. 413–418, Jan. 2018. doi: 10.1016/j.msea.2017.10.021.  
  
Z. Gao, “Graphene reinforced carbon fibers”, *Science Advances*, vol. 6, no. 17. American Association for the Advancement of Science (AAAS), Apr. 24, 2020. doi: 10.1126/sciadv.aaz4191.  
  
B. K. Wittmaack, A. N. Volkovand L. V. Zhigilei, “Phase transformation as the mechanism of mechanical deformation of vertically aligned carbon nanotube arrays: Insights from mesoscopic modeling”, *Carbon*, vol. 143. Elsevier BV, pp. 587–597, Mar. 2019. doi: 10.1016/j.carbon.2018.11.066.  
  
A. Kazemi and S. Yang, “Atomistic Study of the Effect of Magnesium Dopants on the Strength of Nanocrystalline Aluminum”, *JOM*, vol. 71, no. 4. Springer Science and Business Media LLC, pp. 1209–1214, Feb. 19, 2019. doi: 10.1007/s11837-019-03373-3.  
  
W. Li, X. Chenand S. Yang, “Phonon Transport Across Coherent and Incoherent Interfaces”, *JOM*, vol. 71, no. 11. Springer Science and Business Media LLC, pp. 3885–3891, Aug. 22, 2019. doi: 10.1007/s11837-019-03731-1.  
  
H. M. Johlas, L. A. Martínez-Tossas, M. A. Lackner, D. P. Schmidtand M. J. Churchfield, “Large eddy simulations of offshore wind turbine wakes for two floating platform types”, *Journal of Physics: Conference Series*, vol. 1452, no. 1. IOP Publishing, p. 012034, Jan. 01, 2020. doi: 10.1088/1742-6596/1452/1/012034.  
  
S. Kumar, S.-J. Parkand S. Sitharama Iyengar, “A loss-event driven scalable fluid simulation method for high-speed networks”, *Computer Networks*, vol. 54, no. 1. Elsevier BV, pp. 112–132, Jan. 2010. doi: 10.1016/j.comnet.2009.08.018.  
  
Y. Wu, S. Kumarand S.-J. Park, “Measurement and performance issues of transport protocols over 10Gbps high-speed optical networks”, *Computer Networks*, vol. 54, no. 3. Elsevier BV, pp. 475–488, Feb. 2010. doi: 10.1016/j.comnet.2009.09.017.  
  
A. A. Awan, J. Bedorf, C.-H. Chu, H. Subramoniand D. K. Panda, “Scalable Distributed DNN Training using TensorFlow and CUDA-Aware MPI: Characterization, Designs, and Performance Evaluation”, *2019 19th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGRID)*. IEEE, May 2019. doi: 10.1109/ccgrid.2019.00064.  
  
A. A. Awan, K. Hamidouche, J. M. Hashmiand D. K. Panda, “S-Caffe”, *Proceedings of the 22nd ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming*. ACM, Jan. 26, 2017. doi: 10.1145/3018743.3018769.  
  
A. A. Awan, K. Hamidouche, A. Venkateshand D. K. Panda, “Efficient Large Message Broadcast using NCCL and CUDA-Aware MPI for Deep Learning”, *Proceedings of the 23rd European MPI Users’ Group Meeting*. ACM, Sep. 25, 2016. doi: 10.1145/2966884.2966912.  
  
A. A. Awan, A. Jain, Q. Anthony, H. Subramoniand D. K. Panda, “HyPar-Flow: Exploiting MPI and Keras for Scalable Hybrid-Parallel DNN Training with TensorFlow”, *Lecture Notes in Computer Science*. Springer International Publishing, pp. 83–103, 2020. doi: 10.1007/978-3-030-50743-5\_5.  
  
A. A. Awan, A. Jain, C.-H. Chu, H. Subramoniand D. K. Panda, “Communication Profiling and Characterization of Deep-Learning Workloads on Clusters With High-Performance Interconnects”, *IEEE Micro*, vol. 40, no. 1. Institute of Electrical and Electronics Engineers (IEEE), pp. 35–43, Jan. 01, 2020. doi: 10.1109/mm.2019.2949986.  
  
A. A. Awan, K. V. Manian, C.-H. Chu, H. Subramoniand D. K. Panda, “Optimized large-message broadcast for deep learning workloads: MPI, MPI+NCCL, or NCCL2?”, *Parallel Computing*, vol. 85. Elsevier BV, pp. 141–152, Jul. 2019. doi: 10.1016/j.parco.2019.03.005.  
  
M. Bayatpour, S. Chakraborty, H. Subramoni, X. Luand D. K. (DK) . Panda, “Scalable reduction collectives with data partitioning-based multi-leader design”, *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*. ACM, Nov. 12, 2017. doi: 10.1145/3126908.3126954.  
  
S. Chakraborty, H. Subramoni, A. Moody, A. Venkatesh, J. Perkinsand D. K. Panda, “Non-Blocking PMI Extensions for Fast MPI Startup”, *2015 15th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing*. IEEE, May 2015. doi: 10.1109/ccgrid.2015.151.  
  
S. Chakraborty, H. Subramoniand D. K. Panda, “Contention-Aware Kernel-Assisted MPI Collectives for Multi-/Many-Core Systems”, *2017 IEEE International Conference on Cluster Computing (CLUSTER)*. IEEE, Sep. 2017. doi: 10.1109/cluster.2017.106.  
  
S. Chakraborty, H. Subramoni, J. Perkins, A. A. Awanand D. K. Panda, “On-demand Connection Management for OpenSHMEM and OpenSHMEM+MPI”, *2015 IEEE International Parallel and Distributed Processing Symposium Workshop*. IEEE, May 2015. doi: 10.1109/ipdpsw.2015.104.  
  
S. Chakraborty, H. Subramoni, J. Perkins, A. Moody, M. Arnoldand D. K. Panda, “PMI Extensions for Scalable MPI Startup”, *Proceedings of the 21st European MPI Users’ Group Meeting*. ACM, Sep. 09, 2014. doi: 10.1145/2642769.2642780.  
  
R. R. Chandrasekar, A. Venkatesh, K. Hamidoucheand D. K. Panda, “Power-Check: An Energy-Efficient Checkpointing Framework for HPC Clusters”, *2015 15th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing*. IEEE, May 2015. doi: 10.1109/ccgrid.2015.169.  
  
D. J. Choi, G. K. Lockwood, R. S. Sinkovitsand M. Tatineni, “Performance of Applications using Dual-Rail InfiniBand 3D Torus network on the Gordon Supercomputer”, *Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment*. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616541.  
  
C.-H. Chu, K. Hamidouche, A. Venkatesh, D. S. Banerjee, H. Subramoniand D. K. Panda, “Exploiting Maximal Overlap for Non-Contiguous Data Movement Processing on Modern GPU-Enabled Systems”, *2016 IEEE International Parallel and Distributed Processing Symposium (IPDPS)*. IEEE, May 2016. doi: 10.1109/ipdps.2016.99.  
  
C.-H. Chu, J. M. Hashmi, K. S. Khorassani, H. Subramoniand D. K. Panda, “High-Performance Adaptive MPI Derived Datatype Communication for Modern Multi-GPU Systems”, *2019 IEEE 26th International Conference on High Performance Computing, Data, and Analytics (HiPC)*. IEEE, Dec. 2019. doi: 10.1109/hipc.2019.00041.  
  
C.-H. Chu, P. Kousha, A. A. Awan, K. S. Khorassani, H. Subramoniand D. K. (D K. Panda, “NV-group”, *Proceedings of the 34th ACM International Conference on Supercomputing*. ACM, Jun. 29, 2020. doi: 10.1145/3392717.3392771.  
  
A. Gómez-Iglesias, D. Pekurovsky, K. Hamidouche, J. Zhangand J. Vienne, “Porting scientific libraries to PGAS in XSEDE resources”, *Proceedings of the 2015 XSEDE Conference on Scientific Advancements Enabled by Enhanced Cyberinfrastructure - XSEDE ‘15*. ACM Press, 2015. doi: 10.1145/2792745.2792785.  
  
K. Hamidouche, S. Potluri, H. Subramoni, K. Kandallaand D. K. Panda, “MIC-RO”, *Proceedings of the 27th international ACM conference on International conference on supercomputing*. ACM, Jun. 10, 2013. doi: 10.1145/2464996.2465445.  
  
J. M. Hashmi, S. Chakraborty, M. Bayatpour, H. Subramoniand D. K. Panda, “Design and Characterization of Shared Address Space MPI Collectives on Modern Architectures”, *2019 19th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGRID)*. IEEE, May 2019. doi: 10.1109/ccgrid.2019.00055.  
  
J. M. Hashmi, S. Chakraborty, M. Bayatpour, H. Subramoniand D. K. Panda, “FALCON: Efficient Designs for Zero-Copy MPI Datatype Processing on Emerging Architectures”, *2019 IEEE International Parallel and Distributed Processing Symposium (IPDPS)*. IEEE, May 2019. doi: 10.1109/ipdps.2019.00045.  
  
J. M. Hashmi, S. Xu, B. Ramesh, M. Bayatpour, H. Subramoniand D. K. D. Panda, “Machine-agnostic and Communication-aware Designs for MPI on Emerging Architectures”, *2020 IEEE International Parallel and Distributed Processing Symposium (IPDPS)*. IEEE, May 2020. doi: 10.1109/ipdps47924.2020.00014.  
  
N. S. Islam, M. Wasi-ur-Rahman, X. Luand D. K. Panda, “High Performance Design for HDFS with Byte-Addressability of NVM and RDMA”, *Proceedings of the 2016 International Conference on Supercomputing*. ACM, Jun. 2016. doi: 10.1145/2925426.2926290.  
  
A. Jain, A. A. Awan, Q. Anthony, H. Subramoniand D. K. D. Panda, “Performance Characterization of DNN Training using TensorFlow and PyTorch on Modern Clusters”, *2019 IEEE International Conference on Cluster Computing (CLUSTER)*. IEEE, Sep. 2019. doi: 10.1109/cluster.2019.8891042.  
  
M. Li, J. Lin, X. Lu, K. Hamidouche, K. Tomkoand D. K. Panda, “Scalable MiniMD Design with Hybrid MPI and OpenSHMEM”, *Proceedings of the 8th International Conference on Partitioned Global Address Space Programming Models*. ACM, Oct. 06, 2014. doi: 10.1145/2676870.2676893.  
  
M. Luo, X. Lu, K. Hamidouche, K. Kandallaand D. K. Panda, “Initial study of multi-endpoint runtime for MPI+OpenMP hybrid programming model on multi-core systems”, *Proceedings of the 19th ACM SIGPLAN symposium on Principles and practice of parallel programming*. ACM, Feb. 06, 2014. doi: 10.1145/2555243.2555287.  
  
X. Lu, D. Shankar, S. Gugnaniand D. K. Panda, “High-performance design of apache spark with RDMA and its benefits on various workloads”, *2016 IEEE International Conference on Big Data (Big Data)*. IEEE, Dec. 2016. doi: 10.1109/bigdata.2016.7840611.  
  
X. Lu, D. Shankar, S. Gugnani, H. Subramoniand D. K. Panda, “Impact of HPC Cloud Networking Technologies on Accelerating Hadoop RPC and HBase”, *2016 IEEE International Conference on Cloud Computing Technology and Science (CloudCom)*. IEEE, Dec. 2016. doi: 10.1109/cloudcom.2016.0057.  
  
K. V. Manian, A. A. Ammar, A. Ruhela, C.-H. Chu, H. Subramoniand D. K. Panda, “Characterizing CUDA Unified Memory (UM)-Aware MPI Designs on Modern GPU Architectures”, *Proceedings of the 12th Workshop on General Purpose Processing Using GPUs*. ACM, Apr. 13, 2019. doi: 10.1145/3300053.3319419.  
  
R. Rajachandrasekar, J. Perkins, K. Hamidouche, M. Arnoldand D. K. (DK) . Panda, “Understanding the Memory-Utilization of MPI Libraries”, *Proceedings of the 21st European MPI Users’ Group Meeting*. ACM, Sep. 09, 2014. doi: 10.1145/2642769.2642782.  
  
A. Ruhela, H. Subramoni, S. Chakraborty, M. Bayatpour, P. Koushaand D. K. Panda, “Efficient Asynchronous Communication Progress for MPI without Dedicated Resources”, *Proceedings of the 25th European MPI Users’ Group Meeting*. ACM, Sep. 23, 2018. doi: 10.1145/3236367.3236376.  
  
A. Ruhela, H. Subramoni, S. Chakraborty, M. Bayatpour, P. Koushaand D. K. (DK) Panda, “Efficient design for MPI asynchronous progress without dedicated resources”, *Parallel Computing*, vol. 85. Elsevier BV, pp. 13–26, Jul. 2019. doi: 10.1016/j.parco.2019.03.003.  
  
D. Shankar, X. Lu, N. Islam, M. Wasi-Ur-Rahmanand D. K. Panda, “High-Performance Hybrid Key-Value Store on Modern Clusters with RDMA Interconnects and SSDs: Non-blocking Extensions, Designs, and Benefits”, *2016 IEEE International Parallel and Distributed Processing Symposium (IPDPS)*. IEEE, May 2016. doi: 10.1109/ipdps.2016.112.  
  
D. Shankar, X. Luand D. K. Panda, “Boldio: A hybrid and resilient burst-buffer over lustre for accelerating big data I/O”, *2016 IEEE International Conference on Big Data (Big Data)*. IEEE, Dec. 2016. doi: 10.1109/bigdata.2016.7840630.  
  
D. Shankar, X. Luand D. K. Panda, “High-Performance and Resilient Key-Value Store with Online Erasure Coding for Big Data Workloads”, *2017 IEEE 37th International Conference on Distributed Computing Systems (ICDCS)*. IEEE, Jun. 2017. doi: 10.1109/icdcs.2017.224.  
  
H. Shi, X. Lu, D. Shankarand D. K. (DK) . Panda, “High-Performance Multi-Rail Erasure Coding Library over Modern Data Center Architectures”, *Proceedings of the ACM Symposium on Cloud Computing*. ACM, Oct. 11, 2018. doi: 10.1145/3267809.3275472.  
  
K. Vadambacheri Manian, C.-H. Chu, A. Ahmad Awan, K. Shafie Khorassani, H. Subramoniand D. K. Panda, “OMB-UM: Design, Implementation, and Evaluation of CUDA Unified Memory Aware MPI Benchmarks”, *2019 IEEE/ACM Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems (PMBS)*. IEEE, Nov. 2019. doi: 10.1109/pmbs49563.2019.00015.  
  
A. Venkatesh, “A case for application-oblivious energy-efficient MPI runtime”, *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*. ACM, Nov. 15, 2015. doi: 10.1145/2807591.2807658.  
  
M. Wasi-ur-Rahman, N. S. Islam, X. Luand D. K. Panda, “A Comprehensive Study of MapReduce Over Lustre for Intermediate Data Placement and Shuffle Strategies on HPC Clusters”, *IEEE Transactions on Parallel and Distributed Systems*, vol. 28, no. 3. Institute of Electrical and Electronics Engineers (IEEE), pp. 633–646, Mar. 01, 2017. doi: 10.1109/tpds.2016.2591947.  
  
J. Zhang, X. Lu, C.-H. Chuand D. K. Panda, “C-GDR: High-Performance Container-Aware GPUDirect MPI Communication Schemes on RDMA Networks”, *2019 IEEE International Parallel and Distributed Processing Symposium (IPDPS)*. IEEE, May 2019. doi: 10.1109/ipdps.2019.00034.  
  
J. Zhang, X. Luand D. K. Panda, “High Performance MPI Library for Container-Based HPC Cloud on InfiniBand Clusters”, *2016 45th International Conference on Parallel Processing (ICPP)*. IEEE, Aug. 2016. doi: 10.1109/icpp.2016.38.  
  
J. Zhang, X. Luand D. K. Panda, “Performance Characterization of Hypervisor-and Container-Based Virtualization for HPC on SR-IOV Enabled InfiniBand Clusters”, *2016 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*. IEEE, May 2016. doi: 10.1109/ipdpsw.2016.178.  
  
J. Zhang, X. Luand D. K. Panda, “High-Performance Virtual Machine Migration Framework for MPI Applications on SR-IOV Enabled InfiniBand Clusters”, *2017 IEEE International Parallel and Distributed Processing Symposium (IPDPS)*. IEEE, May 2017. doi: 10.1109/ipdps.2017.43.  
  
J. Zhang, X. Luand D. K. (DK) . Panda, “Designing Locality and NUMA Aware MPI Runtime for Nested Virtualization based HPC Cloud with SR-IOV Enabled InfiniBand”, *Proceedings of the 13th ACM SIGPLAN/SIGOPS International Conference on Virtual Execution Environments*. ACM, Apr. 08, 2017. doi: 10.1145/3050748.3050765.  
  
C.-H. Chu, X. Lu, A. A. Awan, H. Subramoni, B. Eltonand D. K. Panda, “Exploiting Hardware Multicast and GPUDirect RDMA for Efficient Broadcast”, *IEEE Transactions on Parallel and Distributed Systems*, vol. 30, no. 3. Institute of Electrical and Electronics Engineers (IEEE), pp. 575–588, Mar. 01, 2019. doi: 10.1109/tpds.2018.2867222.  
  
K. Benson, A. Dainotti, . kc . Claffyand E. Aben, “Gaining insight into AS-level outages through analysis of internet background radiation”, *Proceedings of the 2012 ACM conference on CoNEXT student workshop*. ACM, Dec. 10, 2012. doi: 10.1145/2413247.2413285.  
  
A. Dainotti, R. Amman, E. Abenand K. C. Claffy, “Extracting benefit from harm”, *ACM SIGCOMM Computer Communication Review*, vol. 42, no. 1. Association for Computing Machinery (ACM), pp. 31–39, Jan. 16, 2012. doi: 10.1145/2096149.2096154.  
  
A. Dainotti, “Estimating internet address space usage through passive measurements”, *ACM SIGCOMM Computer Communication Review*, vol. 44, no. 1. Association for Computing Machinery (ACM), pp. 42–49, Dec. 31, 2013. doi: 10.1145/2567561.2567568.  
  
A. Dainotti, A. Kingand K. Claffy, “Analysis of internet-wide probing using darknets”, *Proceedings of the 2012 ACM Workshop on Building analysis datasets and gathering experience returns for security*. ACM, Oct. 15, 2012. doi: 10.1145/2382416.2382423.  
  
A. Dainotti, A. King, K. Claffy, F. Papaleand A. Pescape, “Analysis of a “/0” Stealth Scan From a Botnet”, *IEEE/ACM Transactions on Networking*, vol. 23, no. 2. Institute of Electrical and Electronics Engineers (IEEE), pp. 341–354, Apr. 2015. doi: 10.1109/tnet.2013.2297678.  
  
A. Dainotti, A. King, . kc . Claffy, F. Papaleand A. Pescapè, “Analysis of a”/0” stealth scan from a botnet”, *Proceedings of the 2012 Internet Measurement Conference*. ACM, Nov. 14, 2012. doi: 10.1145/2398776.2398778.  
  
A. Dainotti, “Analysis of country-wide internet outages caused by censorship”, *Proceedings of the 2011 ACM SIGCOMM conference on Internet measurement conference*. ACM, Nov. 02, 2011. doi: 10.1145/2068816.2068818.  
  
A. Dainotti, “Analysis of Country-Wide Internet Outages Caused by Censorship”, *IEEE/ACM Transactions on Networking*, vol. 22, no. 6. Institute of Electrical and Electronics Engineers (IEEE), pp. 1964–1977, Dec. 2014. doi: 10.1109/tnet.2013.2291244.  
  
L. Romero, D. A. Siegel, J. C. McWilliams, Y. Uchiyamaand C. Jones, “Characterizing storm water dispersion and dilution from small coastal streams”, *Journal of Geophysical Research: Oceans*, vol. 121, no. 6. American Geophysical Union (AGU), pp. 3926–3943, Jun. 2016. doi: 10.1002/2015jc011323.  
  
L. Renault, C. Deutsch, J. C. McWilliams, H. Frenzel, J.-H. Liangand F. Colas, “Partial decoupling of primary productivity from upwelling in the California Current system”, *Nature Geoscience*, vol. 9, no. 7. Springer Science and Business Media LLC, pp. 505–508, May 30, 2016. doi: 10.1038/ngeo2722.  
  
J. C. McWilliams, E. Huckle, J. Liangand P. P. Sullivan, “Langmuir Turbulence in Swell”, *Journal of Physical Oceanography*, vol. 44, no. 3. American Meteorological Society, pp. 870–890, Mar. 01, 2014. doi: 10.1175/jpo-d-13-0122.1.  
  
A. C. Subramanian, A. J. Miller, B. D. Cornuelle, E. Di Lorenzo, R. A. Wellerand F. Straneo, “A data assimilative perspective of oceanic mesoscale eddy evolution during VOCALS-REx”, *Atmospheric Chemistry and Physics*, vol. 13, no. 6. Copernicus GmbH, pp. 3329–3344, Mar. 25, 2013. doi: 10.5194/acp-13-3329-2013.  
  
A. Roland, “A fully coupled 3D wave-current interaction model on unstructured grids”, *Journal of Geophysical Research: Oceans*, vol. 117, no. C11. American Geophysical Union (AGU), p. n/a–n/a, Sep. 29, 2012. doi: 10.1029/2012jc007952.  
  
Y. J. Zhang, R. C. Witterand G. R. Priest, “Tsunami–tide interaction in 1964 Prince William Sound tsunami”, *Ocean Modelling*, vol. 40, no. 3–4. Elsevier BV, pp. 246–259, Jan. 2011. doi: 10.1016/j.ocemod.2011.09.005.  
  
R. Briganti, “Advances in numerical modelling of swash zone dynamics”, *Coastal Engineering*, vol. 115. Elsevier BV, pp. 26–41, Sep. 2016. doi: 10.1016/j.coastaleng.2016.05.001.  
  
J. Chauchat, Z. Cheng, T. Nagel, C. Bonamyand T.-J. Hsu, “SedFoam-2.0: a 3-D two-phase flow numerical model for sediment transport”, *Geoscientific Model Development*, vol. 10, no. 12. Copernicus GmbH, pp. 4367–4392, Nov. 30, 2017. doi: 10.5194/gmd-10-4367-2017.  
  
Z. Cheng, J. Chauchat, T.-J. Hsuand J. Calantoni, “Eddy interaction model for turbulent suspension in Reynolds-averaged Euler–Lagrange simulations of steady sheet flow”, *Advances in Water Resources*, vol. 111. Elsevier BV, pp. 435–451, Jan. 2018. doi: 10.1016/j.advwatres.2017.11.019.  
  
Z. Cheng, T.-J. Hsuand J. Chauchat, “An Eulerian two-phase model for steady sheet flow using large-eddy simulation methodology”, *Advances in Water Resources*, vol. 111. Elsevier BV, pp. 205–223, Jan. 2018. doi: 10.1016/j.advwatres.2017.11.016.  
  
Z. Cheng, X. Yu, T.-J. Hsuand S. Balachandar, “A numerical investigation of fine sediment resuspension in the wave boundary layer—Uncertainties in particle inertia and hindered settling”, *Computers & Geosciences*, vol. 83. Elsevier BV, pp. 176–192, Oct. 2015. doi: 10.1016/j.cageo.2015.07.009.  
  
Z. Cheng, X. Yu, T.-J. Hsu, C. E. Ozdemirand S. Balachandar, “On the transport modes of fine sediment in the wave boundary layer due to resuspension/deposition: A turbulence-resolving numerical investigation”, *Journal of Geophysical Research: Oceans*, vol. 120, no. 3. American Geophysical Union (AGU), pp. 1918–1936, Mar. 2015. doi: 10.1002/2014jc010623.  
  
Y. Kim, Z. Cheng, T. Hsuand J. Chauchat, “A Numerical Study of Sheet Flow Under Monochromatic Nonbreaking Waves Using a Free Surface Resolving Eulerian Two‐Phase Flow Model”, *Journal of Geophysical Research: Oceans*, vol. 123, no. 7. American Geophysical Union (AGU), pp. 4693–4719, Jul. 2018. doi: 10.1029/2018jc013930.  
  
Y. Kim, Z. Zhou, T. Hsuand J. A. Puleo, “Large eddy simulation of dam‐break‐driven swash on a rough‐planar beach”, *Journal of Geophysical Research: Oceans*, vol. 122, no. 2. American Geophysical Union (AGU), pp. 1274–1296, Feb. 2017. doi: 10.1002/2016jc012366.  
  
C. E. Ozdemir, T.-J. Hsuand S. Balachandar, “Simulation of fine sediment transport in oscillatory boundary layer”, *Journal of Hydro-environment Research*, vol. 3, no. 4. Elsevier BV, pp. 247–259, Mar. 2010. doi: 10.1016/j.jher.2009.10.013.  
  
C. E. Ozdemir, T.-J. Hsuand S. Balachandar, “Direct numerical simulations of instability and boundary layer turbulence under a solitary wave”, *Journal of Fluid Mechanics*, vol. 731. Cambridge University Press (CUP), pp. 545–578, Aug. 28, 2013. doi: 10.1017/jfm.2013.361.  
  
C. E. Ozdemir, T.-J. Hsuand S. Balachandar, “Direct numerical simulations of transition and turbulence in smooth-walled Stokes boundary layer”, *Physics of Fluids*, vol. 26, no. 4. AIP Publishing, p. 045108, Apr. 2014. doi: 10.1063/1.4871020.  
  
L. Yue, Z. Chengand T. Hsu, “A Turbulence‐Resolving Numerical Investigation of Wave‐Supported Gravity Flows”, *Journal of Geophysical Research: Oceans*, vol. 125, no. 2. American Geophysical Union (AGU), Feb. 2020. doi: 10.1029/2019jc015220.  
  
X. Yu, T.-J. Hsuand S. Balachandar, “A spectral-like turbulence-resolving scheme for fine sediment transport in the bottom boundary layer”, *Computers & Geosciences*, vol. 61. Elsevier BV, pp. 11–22, Dec. 2013. doi: 10.1016/j.cageo.2013.07.021.  
  
X. Yu, T.-J. Hsuand S. Balachandar, “Convective instability in sedimentation: 3-D numerical study”, *Journal of Geophysical Research: Oceans*, vol. 119, no. 11. American Geophysical Union (AGU), pp. 8141–8161, Nov. 2014. doi: 10.1002/2014jc010123.  
  
Z. Zhou, T. Hsu, D. Coxand X. Liu, “Large‐eddy simulation of wave‐breaking induced turbulent coherent structures and suspended sediment transport on a barred beach”, *Journal of Geophysical Research: Oceans*, vol. 122, no. 1. American Geophysical Union (AGU), pp. 207–235, Jan. 2017. doi: 10.1002/2016jc011884.  
  
L. Zheng, “Implications from the comparisons between two- and three-dimensional model simulations of the Hurricane Ike storm surge”, *Journal of Geophysical Research: Oceans*, vol. 118, no. 7. American Geophysical Union (AGU), pp. 3350–3369, Jul. 2013. doi: 10.1002/jgrc.20248.  
  
C. C. Wall, D. A. Mann, C. Lembke, C. Taylor, R. Heand T. Kellison, “Mapping the Soundscape Off the Southeastern USA by Using Passive Acoustic Glider Technology”, *Marine and Coastal Fisheries*, vol. 9, no. 1. Wiley, pp. 23–37, Jan. 2017. doi: 10.1080/19425120.2016.1255685.  
  
J. Wilkin, “Advancing coastal ocean modelling, analysis, and prediction for the US Integrated Ocean Observing System”, *Journal of Operational Oceanography*, vol. 10, no. 2. Informa UK Limited, pp. 115–126, Apr. 03, 2017. doi: 10.1080/1755876x.2017.1322026.  
  
Y. Yuan, R. M. Castelaoand R. He, “Variability in along-shelf and cross-shelf circulation in the South Atlantic Bight”, *Continental Shelf Research*, vol. 134. Elsevier BV, pp. 52–62, Feb. 2017. doi: 10.1016/j.csr.2017.01.006.  
  
C. Akan, A. E. Tejada-Martínez, C. E. Groschand G. Martinat, “Scalar transport in large-eddy simulation of Langmuir turbulence in shallowwater”, *Continental Shelf Research*, vol. 55. Elsevier BV, pp. 1–16, Mar. 2013. doi: 10.1016/j.csr.2012.12.009.  
  
A. E. Tejada-Martínez, C. E. Grosch, N. Sinha, C. Akanand G. Martinat, “Disruption of the bottom log layer in large-eddy simulations of full-depth Langmuir circulation”, *Journal of Fluid Mechanics*, vol. 699. Cambridge University Press (CUP), pp. 79–93, Mar. 27, 2012. doi: 10.1017/jfm.2012.84.  
  
J. D. Flanagan, T. Radko, W. J. Shawand T. P. Stanton, “Dynamic and Double-Diffusive Instabilities in a Weak Pycnocline. Part II: Direct Numerical Simulations and Flux Laws”, *Journal of Physical Oceanography*, vol. 44, no. 8. American Meteorological Society, pp. 1992–2012, Aug. 01, 2014. doi: 10.1175/jpo-d-13-043.1.  
  
T. Radko, “Thermohaline layering in dynamically and diffusively stable shear flows”, *Journal of Fluid Mechanics*, vol. 805. Cambridge University Press (CUP), pp. 147–170, Sep. 16, 2016. doi: 10.1017/jfm.2016.547.  
  
T. Radko, “Suppression of internal waves by thermohaline staircases”, *Journal of Fluid Mechanics*, vol. 902. Cambridge University Press (CUP), Sep. 07, 2020. doi: 10.1017/jfm.2020.563.  
  
T. Radko, A. Bulters, J. D. Flanaganand J.-M. Campin, “Double-Diffusive Recipes. Part I: Large-Scale Dynamics of Thermohaline Staircases”, *Journal of Physical Oceanography*, vol. 44, no. 5. American Meteorological Society, pp. 1269–1284, Apr. 24, 2014. doi: 10.1175/jpo-d-13-0155.1.  
  
T. Radko and E. Edwards, “Diapycnal Velocity in the Double-Diffusive Thermocline”, *Fluids*, vol. 1, no. 3. MDPI AG, p. 25, Aug. 25, 2016. doi: 10.3390/fluids1030025.  
  
T. Radko, J. D. Flanagan, S. Stellmachand M.-L. Timmermans, “Double-Diffusive Recipes. Part II: Layer-Merging Events”, *Journal of Physical Oceanography*, vol. 44, no. 5. American Meteorological Society, pp. 1285–1305, Apr. 24, 2014. doi: 10.1175/jpo-d-13-0156.1.  
  
T. Radko and C. Sisti, “Life and Demise of Intrathermocline Mesoscale Vortices”, *Journal of Physical Oceanography*, vol. 47, no. 12. American Meteorological Society, pp. 3087–3103, Dec. 2017. doi: 10.1175/jpo-d-17-0044.1.  
  
A. S. Delman, J. L. McClean, J. Sprintall, L. D. Talley, E. Yulaevaand S. R. Jayne, “Effects of Eddy Vorticity Forcing on the Mean State of the Kuroshio Extension”, *Journal of Physical Oceanography*, vol. 45, no. 5. American Meteorological Society, pp. 1356–1375, May 2015. doi: 10.1175/jpo-d-13-0259.1.  
  
R. Barkan, K. B. Wintersand S. G. Llewellyn Smith, “Rotating horizontal convection”, *Journal of Fluid Mechanics*, vol. 723. Cambridge University Press (CUP), pp. 556–586, Apr. 16, 2013. doi: 10.1017/jfm.2013.136.  
  
R. Barkan, K. B. Wintersand S. G. Llewellyn Smith, “Energy Cascades and Loss of Balance in a Reentrant Channel Forced by Wind Stress and Buoyancy Fluxes”, *Journal of Physical Oceanography*, vol. 45, no. 1. American Meteorological Society, pp. 272–293, Jan. 2015. doi: 10.1175/jpo-d-14-0068.1.  
  
H. T. Pham, S. Sarkarand K. B. Winters, “Large-Eddy Simulation of Deep-Cycle Turbulence in an Equatorial Undercurrent Model”, *Journal of Physical Oceanography*, vol. 43, no. 11. American Meteorological Society, pp. 2490–2502, Nov. 01, 2013. doi: 10.1175/jpo-d-13-016.1.  
  
E. Arobone and S. Sarkar, “Evolution of a stratified rotating shear layer with horizontal shear. Part 2. Nonlinear evolution”, *Journal of Fluid Mechanics*, vol. 732. Cambridge University Press (CUP), pp. 373–400, Sep. 06, 2013. doi: 10.1017/jfm.2013.383.  
  
K. B. Winters, “Tidally-forced flow in a rotating, stratified, shoaling basin”, *Ocean Modelling*, vol. 90. Elsevier BV, pp. 72–81, Jun. 2015. doi: 10.1016/j.ocemod.2015.04.004.  
  
K. B. Winters, “Tidally driven mixing and dissipation in the stratified boundary layer above steep submarine topography”, *Geophysical Research Letters*, vol. 42, no. 17. American Geophysical Union (AGU), pp. 7123–7130, Sep. 03, 2015. doi: 10.1002/2015gl064676.  
  
K. B. Winters and L. Armi, “The response of a continuously stratified fluid to an oscillating flow past an obstacle”, *Journal of Fluid Mechanics*, vol. 727. Cambridge University Press (CUP), pp. 83–118, Jun. 14, 2013. doi: 10.1017/jfm.2013.247.  
  
K. B. Winters and L. Armi, “Topographic control of stratified flows: upstream jets, blocking and isolating layers”, *Journal of Fluid Mechanics*, vol. 753. Cambridge University Press (CUP), pp. 80–103, Jul. 16, 2014. doi: 10.1017/jfm.2014.363.  
  
K. B. Winters and A. de la Fuente, “Modelling rotating stratified flows at laboratory-scale using spectrally-based DNS”, *Ocean Modelling*, vol. 49–50. Elsevier BV, pp. 47–59, Jun. 2012. doi: 10.1016/j.ocemod.2012.04.001.  
  
R. C. Martyr-Koller, “Application of an unstructured 3D finite volume numerical model to flows and salinity dynamics in the San Francisco Bay-Delta”, *Estuarine, Coastal and Shelf Science*, vol. 192. Elsevier BV, pp. 86–107, Jun. 2017. doi: 10.1016/j.ecss.2017.04.024.  
  
D. Giglio, V. Lyubchichand M. R. Mazloff, “Estimating Oxygen in the Southern Ocean Using Argo Temperature and Salinity”, *Journal of Geophysical Research: Oceans*, vol. 123, no. 6. American Geophysical Union (AGU), pp. 4280–4297, Jun. 2018. doi: 10.1029/2017jc013404.  
  
T. Ito, M. Woloszynand M. Mazloff, “Anthropogenic carbon dioxide transport in the Southern Ocean driven by Ekman flow”, *Nature*, vol. 463, no. 7277. Springer Science and Business Media LLC, pp. 80–83, Jan. 2010. doi: 10.1038/nature08687.  
  
R. Johnson, P. G. Strutton, S. W. Wright, A. McMinnand K. M. Meiners, “Three improved satellite chlorophyll algorithms for the Southern Ocean”, *Journal of Geophysical Research: Oceans*, vol. 118, no. 7. American Geophysical Union (AGU), pp. 3694–3703, Jul. 2013. doi: 10.1002/jgrc.20270.  
  
P. Landschützer, “The reinvigoration of the Southern Ocean carbon sink”, *Science*, vol. 349, no. 6253. American Association for the Advancement of Science (AAAS), pp. 1221–1224, Sep. 11, 2015. doi: 10.1126/science.aab2620.  
  
Y.-C. Liang, M. R. Mazloff, I. Rosso, S.-W. Fangand J.-Y. Yu, “A Multivariate Empirical Orthogonal Function Method to Construct Nitrate Maps in the Southern Ocean”, *Journal of Atmospheric and Oceanic Technology*, vol. 35, no. 7. American Meteorological Society, pp. 1505–1519, Jul. 2018. doi: 10.1175/jtech-d-18-0018.1.  
  
J. Masich, M. R. Mazloffand T. K. Chereskin, “Interfacial Form Stress in the Southern Ocean State Estimate”, *Journal of Geophysical Research: Oceans*, vol. 123, no. 5. American Geophysical Union (AGU), pp. 3368–3385, May 2018. doi: 10.1029/2018jc013844.  
  
M. R. Mazloff, B. D. Cornuelle, S. T. Gilleand A. Verdy, “Correlation Lengths for Estimating the Large‐Scale Carbon and Heat Content of the Southern Ocean”, *Journal of Geophysical Research: Oceans*, vol. 123, no. 2. American Geophysical Union (AGU), pp. 883–901, Feb. 2018. doi: 10.1002/2017jc013408.  
  
R. C. Musgrave, R. Pinkel, J. A. MacKinnon, M. R. Mazloffand W. R. Young, “Stratified tidal flow over a tall ridge above and below the turning latitude”, *Journal of Fluid Mechanics*, vol. 793. Cambridge University Press (CUP), pp. 933–957, Mar. 29, 2016. doi: 10.1017/jfm.2016.150.  
  
I. Rosso, M. R. Mazloff, A. Verdyand L. D. Talley, “Space and time variability of the S outhern O cean carbon budget”, *Journal of Geophysical Research: Oceans*, vol. 122, no. 9. American Geophysical Union (AGU), pp. 7407–7432, Sep. 2017. doi: 10.1002/2016jc012646.  
  
J. L. Russell, “Metrics for the Evaluation of the Southern Ocean in Coupled Climate Models and Earth System Models”, *Journal of Geophysical Research: Oceans*, vol. 123, no. 5. American Geophysical Union (AGU), pp. 3120–3143, May 2018. doi: 10.1002/2017jc013461.  
  
V. Tamsitt, R. P. Abernathey, M. R. Mazloff, J. Wangand L. D. Talley, “Transformation of Deep Water Masses Along Lagrangian Upwelling Pathways in the Southern Ocean”, *Journal of Geophysical Research: Oceans*, vol. 123, no. 3. American Geophysical Union (AGU), pp. 1994–2017, Mar. 2018. doi: 10.1002/2017jc013409.  
  
V. Tamsitt, “Spiraling pathways of global deep waters to the surface of the Southern Ocean”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Aug. 02, 2017. doi: 10.1038/s41467-017-00197-0.  
  
E. van Sebille, P. Spence, M. R. Mazloff, M. H. England, S. R. Rintouland O. A. Saenko, “Abyssal connections of Antarctic Bottom Water in a Southern Ocean State Estimate”, *Geophysical Research Letters*, vol. 40, no. 10. American Geophysical Union (AGU), pp. 2177–2182, May 28, 2013. doi: 10.1002/grl.50483.  
  
A. Verdy, B. Cornuelle, M. R. Mazloffand D. L. Rudnick, “Estimation of the Tropical Pacific Ocean State 2010–13”, *Journal of Atmospheric and Oceanic Technology*, vol. 34, no. 7. American Meteorological Society, pp. 1501–1517, Jul. 2017. doi: 10.1175/jtech-d-16-0223.1.  
  
A. Verdy and M. R. Mazloff, “A data assimilating model for estimating S outhern O cean biogeochemistry”, *Journal of Geophysical Research: Oceans*, vol. 122, no. 9. American Geophysical Union (AGU), pp. 6968–6988, Sep. 2017. doi: 10.1002/2016jc012650.  
  
A. Verdy and M. R. Mazloff, “A data assimilating model for estimating S outhern O cean biogeochemistry”, *Journal of Geophysical Research: Oceans*, vol. 122, no. 9. American Geophysical Union (AGU), pp. 6968–6988, Sep. 2017. doi: 10.1002/2016jc012650.  
  
T. Wang, S. T. Gille, M. R. Mazloff, N. V. Zilbermanand Y. Du, “Numerical Simulations to Project Argo Float Positions in the Middepth and Deep Southwest Pacific”, *Journal of Atmospheric and Oceanic Technology*, vol. 35, no. 7. American Meteorological Society, pp. 1425–1440, Jul. 2018. doi: 10.1175/jtech-d-17-0214.1.  
  
M. Woloszyn, M. Mazloffand T. Ito, “Testing an eddy-permitting model of the Southern Ocean carbon cycle against observations”, *Ocean Modelling*, vol. 39, no. 1–2. Elsevier BV, pp. 170–182, Jan. 2011. doi: 10.1016/j.ocemod.2010.12.004.  
  
C. Hu, “Developing a Smart Semantic Web With Linked Data and Models for Near-Real-Time Monitoring of Red Tides in the Eastern Gulf of Mexico”, *IEEE Systems Journal*, vol. 10, no. 3. Institute of Electrical and Electronics Engineers (IEEE), pp. 1282–1290, Sep. 2016. doi: 10.1109/jsyst.2015.2440782.  
  
Y. Liu, R. H. Weisberg, J. M. Lenes, L. Zheng, K. Hubbardand J. J. Walsh, “Offshore forcing on the “pressure point” of the West Florida Shelf: Anomalous upwelling and its influence on harmful algal blooms”, *Journal of Geophysical Research: Oceans*, vol. 121, no. 8. American Geophysical Union (AGU), pp. 5501–5515, Aug. 2016. doi: 10.1002/2016jc011938.  
  
Y. Liu, R. H. Weisberg, S. Vignudelliand G. T. Mitchum, “Patterns of the loop current system and regions of sea surface height variability in the eastern Gulf of Mexico revealed by the self‐organizing maps”, *Journal of Geophysical Research: Oceans*, vol. 121, no. 4. American Geophysical Union (AGU), pp. 2347–2366, Apr. 2016. doi: 10.1002/2015jc011493.  
  
D. A. Mayer, R. H. Weisberg, L. Zhengand Y. Liu, “Winds on the West Florida Shelf: Regional comparisons between observations and model estimates”, *Journal of Geophysical Research: Oceans*, vol. 122, no. 2. American Geophysical Union (AGU), pp. 834–846, Feb. 2017. doi: 10.1002/2016jc012112.  
  
C. Pan, L. Zheng, R. H. Weisberg, Y. Liuand C. E. Lembke, “Comparisons of different ensemble schemes for glider data assimilation on West Florida Shelf”, *Ocean Modelling*, vol. 81. Elsevier BV, pp. 13–24, Sep. 2014. doi: 10.1016/j.ocemod.2014.06.005.  
  
J. J. Walsh, “A simulation analysis of the plankton fate of the Deepwater Horizon oil spills”, *Continental Shelf Research*, vol. 107. Elsevier BV, pp. 50–68, Sep. 2015. doi: 10.1016/j.csr.2015.07.002.  
  
R. H. Weisberg, L. Zhengand Y. Liu, “Basic Tenets for Coastal Ocean Ecosystems Monitoring”, *Coastal Ocean Observing Systems*. Elsevier, pp. 40–57, 2015. doi: 10.1016/b978-0-12-802022-7.00004-3.  
  
R. H. Weisberg, “Karenia brevis blooms on the West Florida Shelf: A comparative study of the robust 2012 bloom and the nearly null 2013 event”, *Continental Shelf Research*, vol. 120. Elsevier BV, pp. 106–121, Jun. 2016. doi: 10.1016/j.csr.2016.03.011.  
  
R. H. Weisberg, L. Zheng, Y. Liu, C. Lembke, J. M. Lenesand J. J. Walsh, “Why no red tide was observed on the West Florida Continental Shelf in 2010”, *Harmful Algae*, vol. 38. Elsevier BV, pp. 119–126, Sep. 2014. doi: 10.1016/j.hal.2014.04.010.  
  
R. H. Weisberg, L. Zheng, Y. Liu, S. Murawski, C. Huand J. Paul, “Did Deepwater Horizon hydrocarbons transit to the west Florida continental shelf?”, *Deep Sea Research Part II: Topical Studies in Oceanography*, vol. 129. Elsevier BV, pp. 259–272, Jul. 2016. doi: 10.1016/j.dsr2.2014.02.002.  
  
R. H. Weisberg, L. Zhengand E. Peebles, “Gag grouper larvae pathways on the West Florida Shelf”, *Continental Shelf Research*, vol. 88. Elsevier BV, pp. 11–23, Oct. 2014. doi: 10.1016/j.csr.2014.06.003.  
  
J. Zhu, R. H. Weisberg, L. Zhengand S. Han, “Influences of Channel Deepening and Widening on the Tidal and Nontidal Circulations of Tampa Bay”, *Estuaries and Coasts*, vol. 38, no. 1. Springer Science and Business Media LLC, pp. 132–150, Apr. 22, 2014. doi: 10.1007/s12237-014-9815-4.  
  
J. Zhu, R. H. Weisberg, L. Zhengand S. Han, “On the Flushing of Tampa Bay”, *Estuaries and Coasts*, vol. 38, no. 1. Springer Science and Business Media LLC, pp. 118–131, Apr. 01, 2014. doi: 10.1007/s12237-014-9793-6.  
  
J. Zhu, R. H. Weisberg, L. Zhengand H. Qi, “On the salt balance of Tampa Bay”, *Continental Shelf Research*, vol. 107. Elsevier BV, pp. 115–131, Sep. 2015. doi: 10.1016/j.csr.2015.07.001.  
  
R. H. Weisberg, Z. Lianyuanand Y. Liu, “On the movement of Deepwater Horizon Oil to northern Gulf beaches”, *Ocean Modelling*, vol. 111. Elsevier BV, pp. 81–97, Mar. 2017. doi: 10.1016/j.ocemod.2017.02.002.  
  
R. H. Weisberg, L. Zhengand Y. Liu, “West Florida shelf upwelling: Origins and pathways”, *Journal of Geophysical Research: Oceans*, vol. 121, no. 8. American Geophysical Union (AGU), pp. 5672–5681, Aug. 2016. doi: 10.1002/2015jc011384.  
  
M. Jalali and S. Sarkar, “Large Eddy Simulation of Flow and Turbulence at the Steep Topography of Luzon Strait”, *Geophysical Research Letters*, vol. 44, no. 18. American Geophysical Union (AGU), pp. 9440–9448, Sep. 25, 2017. doi: 10.1002/2017gl074119.  
  
M. Jalali, A. VanDine, V. K. Chalamallaand S. Sarkar, “Oscillatory stratified flow over supercritical topography: Wave energetics and turbulence”, *Computers & Fluids*, vol. 158. Elsevier BV, pp. 39–48, Nov. 2017. doi: 10.1016/j.compfluid.2016.12.019.  
  
S. Sarkar and A. Scotti, “From Topographic Internal Gravity Waves to Turbulence”, *Annual Review of Fluid Mechanics*, vol. 49, no. 1. Annual Reviews, pp. 195–220, Jan. 03, 2017. doi: 10.1146/annurev-fluid-010816-060013.  
  
P. Cessi, “The Effect of Northern Hemisphere Winds on the Meridional Overturning Circulation and Stratification”, *Journal of Physical Oceanography*, vol. 48, no. 10. American Meteorological Society, pp. 2495–2506, Oct. 2018. doi: 10.1175/jpo-d-18-0085.1.  
  
D. Ferreira, “Atlantic-Pacific Asymmetry in Deep Water Formation”, *Annual Review of Earth and Planetary Sciences*, vol. 46, no. 1. Annual Reviews, pp. 327–352, May 30, 2018. doi: 10.1146/annurev-earth-082517-010045.  
  
C. S. Jones and P. Cessi, “Components of Upper-Ocean Salt Transport by the Gyres and the Meridional Overturning Circulation”, *Journal of Physical Oceanography*, vol. 48, no. 10. American Meteorological Society, pp. 2445–2456, Oct. 2018. doi: 10.1175/jpo-d-18-0005.1.  
  
C. L. Wolfe and P. Cessi, “Multiple Regimes and Low-Frequency Variability in the Quasi-Adiabatic Overturning Circulation”, *Journal of Physical Oceanography*, vol. 45, no. 6. American Meteorological Society, pp. 1690–1708, Jun. 2015. doi: 10.1175/jpo-d-14-0095.1.  
  
T. Kärnä, A. M. Baptista, J. E. Lopez, P. J. Turner, C. McNeiland T. B. Sanford, “Numerical modeling of circulation in high-energy estuaries: A Columbia River estuary benchmark”, *Ocean Modelling*, vol. 88. Elsevier BV, pp. 54–71, Apr. 2015. doi: 10.1016/j.ocemod.2015.01.001.  
  
J. U. Pein, E. V. Stanevand Y. J. Zhang, “The tidal asymmetries and residual flows in Ems Estuary”, *Ocean Dynamics*, vol. 64, no. 12. Springer Science and Business Media LLC, pp. 1719–1741, Oct. 26, 2014. doi: 10.1007/s10236-014-0772-z.  
  
G. R. Priest, R. C. Witter, Y. J. Zhang, C. Goldfinger, K. Wangand J. C. Allan, “New constraints on coseismic slip during southern Cascadia subduction zone earthquakes over the past 4600 years implied by tsunami deposits and marine turbidites”, *Natural Hazards*, vol. 88, no. 1. Springer Science and Business Media LLC, pp. 285–313, Apr. 29, 2017. doi: 10.1007/s11069-017-2864-9.  
  
G. R. Priest, R. C. Witter, Y. J. Zhang, C. Goldfinger, K. Wangand J. C. Allan, “New constraints on coseismic slip during southern Cascadia subduction zone earthquakes over the past 4600 years implied by tsunami deposits and marine turbidites”, *Natural Hazards*, vol. 88, no. 1. Springer Science and Business Media LLC, pp. 285–313, Apr. 29, 2017. doi: 10.1007/s11069-017-2864-9.  
  
H.-C. Yu, “Simulating multi-scale oceanic processes around Taiwan on unstructured grids”, *Ocean Modelling*, vol. 119. Elsevier BV, pp. 72–93, Nov. 2017. doi: 10.1016/j.ocemod.2017.09.007.  
  
Y. J. Zhang, E. Ateljevich, H.-C. Yu, C. H. Wuand J. C. S. Yu, “A new vertical coordinate system for a 3D unstructured-grid model”, *Ocean Modelling*, vol. 85. Elsevier BV, pp. 16–31, Jan. 2015. doi: 10.1016/j.ocemod.2014.10.003.  
  
Y. J. Zhang, E. V. Stanevand S. Grashorn, “Unstructured-grid model for the North Sea and Baltic Sea: Validation against observations”, *Ocean Modelling*, vol. 97. Elsevier BV, pp. 91–108, Jan. 2016. doi: 10.1016/j.ocemod.2015.11.009.  
  
Y. J. Zhang, F. Ye, E. V. Stanevand S. Grashorn, “Seamless cross-scale modeling with SCHISM”, *Ocean Modelling*, vol. 102. Elsevier BV, pp. 64–81, Jun. 2016. doi: 10.1016/j.ocemod.2016.05.002.  
  
S. Bassim and B. Allam, “SNP hot-spots in the clam parasite QPX”, *BMC Genomics*, vol. 19, no. 1. Springer Science and Business Media LLC, Jun. 20, 2018. doi: 10.1186/s12864-018-4866-8.  
  
L. Deike, W. K. Melvilleand S. Popinet, “Air entrainment and bubble statistics in breaking waves”, *Journal of Fluid Mechanics*, vol. 801. Cambridge University Press (CUP), pp. 91–129, Jul. 19, 2016. doi: 10.1017/jfm.2016.372.  
  
K. Alizad, “Dynamic responses and implications to coastal wetlands and the surrounding regions under sea level rise”, *PLOS ONE*, vol. 13, no. 10. Public Library of Science (PLoS), p. e0205176, Oct. 12, 2018. doi: 10.1371/journal.pone.0205176.  
  
K. Alizad, S. C. Hagen, J. T. Morris, S. C. Medeiros, M. V. Bilskieand J. F. Weishampel, “Coastal wetland response to sea‐level rise in a fluvial estuarine system”, *Earth’s Future*, vol. 4, no. 11. American Geophysical Union (AGU), pp. 483–497, Nov. 2016. doi: 10.1002/2016ef000385.  
  
M. V. Bilskie, D. Coggin, S. C. Hagenand S. C. Medeiros, “Terrain-driven unstructured mesh development through semi-automatic vertical feature extraction”, *Advances in Water Resources*, vol. 86. Elsevier BV, pp. 102–118, Dec. 2015. doi: 10.1016/j.advwatres.2015.09.020.  
  
M. V. Bilskie, “Dynamic simulation and numerical analysis of hurricane storm surge under sea level rise with geomorphologic changes along the northern Gulf of Mexico”, *Earth’s Future*, vol. 4, no. 5. American Geophysical Union (AGU), pp. 177–193, May 2016. doi: 10.1002/2015ef000347.  
  
M. V. Bilskie, S. C. Hagenand J. L. Irish, “Development of Return Period Stillwater Floodplains for the Northern Gulf of Mexico under the Coastal Dynamics of Sea Level Rise”, *Journal of Waterway, Port, Coastal, and Ocean Engineering*, vol. 145, no. 2. American Society of Civil Engineers (ASCE), Mar. 2019. doi: 10.1061/(asce)ww.1943-5460.0000468.  
  
M. V. Bilskie, S. C. Hagen, S. C. Medeiros, A. T. Cox, M. Salisburyand D. Coggin, “Data and numerical analysis of astronomic tides, wind‐waves, and hurricane storm surge along the northern Gulf of Mexico”, *Journal of Geophysical Research: Oceans*, vol. 121, no. 5. American Geophysical Union (AGU), pp. 3625–3658, May 2016. doi: 10.1002/2015jc011400.  
  
D. L. Passeri, S. C. Hagen, N. G. Plant, M. V. Bilskie, S. C. Medeirosand K. Alizad, “Tidal hydrodynamics under future sea level rise and coastal morphology in the Northern Gulf of Mexico”, *Earth’s Future*, vol. 4, no. 5. American Geophysical Union (AGU), pp. 159–176, May 2016. doi: 10.1002/2015ef000332.  
  
C. G. Siverd, “Assessment of the temporal evolution of storm surge across coastal Louisiana”, *Coastal Engineering*, vol. 150. Elsevier BV, pp. 59–78, Aug. 2019. doi: 10.1016/j.coastaleng.2019.04.010.  
  
C. G. Siverd, S. C. Hagen, M. V. Bilskie, D. H. Braud, R. H. Peeleand R. R. Twilley, “Hydrodynamic storm surge model simplification via application of land to water isopleths in coastal Louisiana”, *Coastal Engineering*, vol. 137. Elsevier BV, pp. 28–42, Jul. 2018. doi: 10.1016/j.coastaleng.2018.03.006.  
  
Y. Wang and A. L. Stewart, “Eddy dynamics over continental slopes under retrograde winds: Insights from a model inter-comparison”, *Ocean Modelling*, vol. 121. Elsevier BV, pp. 1–18, Jan. 2018. doi: 10.1016/j.ocemod.2017.11.006.  
  
L. Deike, “Dynamics of jets produced by bursting bubbles”, *Physical Review Fluids*, vol. 3, no. 1. American Physical Society (APS), Jan. 25, 2018. doi: 10.1103/physrevfluids.3.013603.  
  
L. Deike, N. Pizzoand W. K. Melville, “Lagrangian transport by breaking surface waves”, *Journal of Fluid Mechanics*, vol. 829. Cambridge University Press (CUP), pp. 364–391, Sep. 19, 2017. doi: 10.1017/jfm.2017.548.  
  
C.-Y. Lai, J. Eggersand L. Deike, “Bubble Bursting: Universal Cavity and Jet Profiles”, *Physical Review Letters*, vol. 121, no. 14. American Physical Society (APS), Oct. 02, 2018. doi: 10.1103/physrevlett.121.144501.  
  
E. Turkoz, J. M. Lopez-Herrera, J. Eggers, C. B. Arnoldand L. Deike, “Axisymmetric simulation of viscoelastic filament thinning with the Oldroyd-B model”, *Journal of Fluid Mechanics*, vol. 851. Cambridge University Press (CUP), Jul. 18, 2018. doi: 10.1017/jfm.2018.514.  
  
A. M. Baptista, “Infrastructure for collaborative science and societal applications in the Columbia River estuary”, *Frontiers of Earth Science*, vol. 9, no. 4. Springer Science and Business Media LLC, pp. 659–682, Oct. 01, 2015. doi: 10.1007/s11707-015-0540-5.  
  
L. Renault, M. J. Molemaker, J. Gula, S. Massonand J. C. McWilliams, “Control and Stabilization of the Gulf Stream by Oceanic Current Interaction with the Atmosphere”, *Journal of Physical Oceanography*, vol. 46, no. 11. American Meteorological Society, pp. 3439–3453, Nov. 2016. doi: 10.1175/jpo-d-16-0115.1.  
  
F. Kessouri, “Configuration and validation of an oceanic physical and biogeochemical model to investigate coastal eutrophication: case study in the Southern California Bight”, *[]*. Wiley, Aug. 20, 2020. doi: 10.1002/essoar.10504012.1.  
  
J. Daily and M. J. Hoffman, “Modeling the three-dimensional transport and distribution of multiple microplastic polymer types in Lake Erie”, *Marine Pollution Bulletin*, vol. 154. Elsevier BV, p. 111024, May 2020. doi: 10.1016/j.marpolbul.2020.111024.  
  
S. A. Mason, “High levels of pelagic plastic pollution within the surface waters of Lakes Erie and Ontario”, *Journal of Great Lakes Research*, vol. 46, no. 2. Elsevier BV, pp. 277–288, Apr. 2020. doi: 10.1016/j.jglr.2019.12.012.  
  
I. Pasmans, A. L. Kurapov, J. A. Barth, A. Ignatov, P. M. Kosroand R. K. Shearman, “Why Gliders Appreciate Good Company: Glider Assimilation in the Oregon‐Washington Coastal Ocean 4DVAR System With and Without Surface Observations”, *Journal of Geophysical Research: Oceans*, vol. 124, no. 1. American Geophysical Union (AGU), pp. 750–772, Jan. 2019. doi: 10.1029/2018jc014230.  
  
F. Da, M. Friedrichsand P. St. Laurent, “Associated dataset: Impacts of Atmospheric Nitrogen Deposition and Coastal Nitrogen Fluxes on Oxygen Concentrations in Chesapeake Bay”. Virginia Institute of Marine Science, College of William & Mary, 2018. doi: 10.21220/GAWW-M696.  
  
M. A. M. and S.-L. Friedrichs, “Associated dataset: Ocean circulation causes strong variability in the Mid-Atlantic Bight nitrogen budget”. Virginia Institute of Marine Science, 2018. doi: 10.25773/2F36-PN56.  
  
I. D. Irby, M. A. M. Friedrichs, F. Daand K. E. Hinson, “The competing impacts of climate change and nutrient reductions on dissolved oxygen in Chesapeake Bay”, *[]*. Copernicus GmbH, Oct. 17, 2017. doi: 10.5194/bg-2017-416.  
  
I. D. Irby, “Challenges associated with modeling low-oxygen waters in Chesapeake Bay: a multiple model comparison”, *Biogeosciences*, vol. 13, no. 7. Copernicus GmbH, pp. 2011–2028, Apr. 06, 2016. doi: 10.5194/bg-13-2011-2016.  
  
P. St‐Laurent, “Impacts of Atmospheric Nitrogen Deposition on Surface Waters of the Western North Atlantic Mitigated by Multiple Feedbacks”, *Journal of Geophysical Research: Oceans*, vol. 122, no. 11. American Geophysical Union (AGU), pp. 8406–8426, Nov. 2017. doi: 10.1002/2017jc013072.  
  
F. Kessouri, D. Bianchi, L. Renault, J. C. McWilliams, H. Frenzeland C. A. Deutsch, “Submesoscale Currents Modulate the Seasonal Cycle of Nutrients and Productivity in the California Current System”, *Global Biogeochemical Cycles*, vol. 34, no. 10. American Geophysical Union (AGU), Oct. 2020. doi: 10.1029/2020gb006578.  
  
G. E. Manucharyan, A. F. Thompsonand M. A. Spall, “Eddy Memory Mode of Multidecadal Variability in Residual-Mean Ocean Circulations with Application to the Beaufort Gyre”, *Journal of Physical Oceanography*, vol. 47, no. 4. American Meteorological Society, pp. 855–866, Apr. 2017. doi: 10.1175/jpo-d-16-0194.1.  
  
J. M. Moriarty, C. K. Harris, K. Fennel, M. A. M. Friedrichs, K. Xuand C. Rabouille, “The roles of resuspension, diffusion and biogeochemical processes on oxygen dynamics offshore of the Rhône River, France: a numerical modeling study”, *Biogeosciences*, vol. 14, no. 7. Copernicus GmbH, pp. 1919–1946, Apr. 07, 2017. doi: 10.5194/bg-14-1919-2017.  
  
B. S. Santos, D. M. Kaplan, M. A. M. Friedrichs, S. G. Barco, K. L. Mansfieldand J. P. Manning, “Consequences of drift and carcass decomposition for estimating sea turtle mortality hotspots”, *Ecological Indicators*, vol. 84. Elsevier BV, pp. 319–336, Jan. 2018. doi: 10.1016/j.ecolind.2017.08.064.  
  
G. E. Manucharyan and P. E. Isachsen, “Critical Role of Continental Slopes in Halocline and Eddy Dynamics of the Ekman‐Driven Beaufort Gyre”, *Journal of Geophysical Research: Oceans*, vol. 124, no. 4. American Geophysical Union (AGU), pp. 2679–2696, Apr. 2019. doi: 10.1029/2018jc014624.  
  
K. Fennel and A. Laurent, “N and P as ultimate and proximate limiting nutrients in the northern Gulf of Mexico: Implications for hypoxia reduction strategies”, *[]*. Copernicus GmbH, Nov. 06, 2017. doi: 10.5194/bg-2017-470.  
  
A. Laurent, K. Fennel, W. Cai, W. Huang, L. Barberoand R. Wanninkhof, “Eutrophication‐induced acidification of coastal waters in the northern Gulf of Mexico: Insights into origin and processes from a coupled physical‐biogeochemical model”, *Geophysical Research Letters*, vol. 44, no. 2. American Geophysical Union (AGU), pp. 946–956, Jan. 28, 2017. doi: 10.1002/2016gl071881.  
  
R. Luettich Jr., “A Test Bed for Coastal and Ocean Modeling”, *Eos*. American Geophysical Union (AGU), Aug. 04, 2017. doi: 10.1029/2017eo078243.  
  
J. Chen, R. H. Weisberg, Y. Liu, L. Zhengand J. Zhu, “On the Momentum Balance of Tampa Bay”, *Journal of Geophysical Research: Oceans*, vol. 124, no. 7. American Geophysical Union (AGU), pp. 4492–4510, Jul. 2019. doi: 10.1029/2018jc014890.  
  
Y. Liu, R. H. Weisbergand L. Zheng, “Impacts of Hurricane Irma on the Circulation and Transport in Florida Bay and the Charlotte Harbor Estuary”, *Estuaries and Coasts*, vol. 43, no. 5. Springer Science and Business Media LLC, pp. 1194–1216, Oct. 25, 2019. doi: 10.1007/s12237-019-00647-6.  
  
R. H. Weisberg and Y. Liu, “On the Loop Current Penetration into the Gulf of Mexico”, *Journal of Geophysical Research: Oceans*, vol. 122, no. 12. American Geophysical Union (AGU), pp. 9679–9694, Dec. 2017. doi: 10.1002/2017jc013330.  
  
J. Chen, R. H. Weisberg, Y. Liuand L. Zheng, “The Tampa Bay Coastal Ocean Model Performance for Hurricane Irma”, *Marine Technology Society Journal*, vol. 52, no. 3. Marine Technology Society, pp. 33–42, May 01, 2018. doi: 10.4031/mtsj.52.3.6.  
  
C.-H. Lee and Z. Huang, “A two-phase flow model for submarine granular flows: With an application to collapse of deeply-submerged granular columns”, *Advances in Water Resources*, vol. 115. Elsevier BV, pp. 286–300, May 2018. doi: 10.1016/j.advwatres.2017.12.012.  
  
N. Bednaršek, “Systematic Review and Meta-Analysis Toward Synthesis of Thresholds of Ocean Acidification Impacts on Calcifying Pteropods and Interactions With Warming”, *Frontiers in Marine Science*, vol. 6. Frontiers Media SA, May 09, 2019. doi: 10.3389/fmars.2019.00227.  
  
C. Deutsch, “Biogeochemical variability in the California Current System”, *Progress in Oceanography*, vol. 196. Elsevier BV, p. 102565, Aug. 2021. doi: 10.1016/j.pocean.2021.102565.  
  
B. Quach, Y. Glaser, J. E. Stopa, A. A. Moucheand P. Sadowski, “Deep Learning for Predicting Significant Wave Height From Synthetic Aperture Radar”, *IEEE Transactions on Geoscience and Remote Sensing*, vol. 59, no. 3. Institute of Electrical and Electronics Engineers (IEEE), pp. 1859–1867, Mar. 2021. doi: 10.1109/tgrs.2020.3003839.  
  
O. Asselin, L. N. Thomas, W. R. Youngand L. Rainville, “Refraction and Straining of Near-Inertial Waves by Barotropic Eddies”, *Journal of Physical Oceanography*, vol. 50, no. 12. American Meteorological Society, pp. 3439–3454, Dec. 2020. doi: 10.1175/jpo-d-20-0109.1.  
  
O. Asselin and W. R. Young, “Penetration of Wind-Generated Near-Inertial Waves into a Turbulent Ocean”, *Journal of Physical Oceanography*, vol. 50, no. 6. American Meteorological Society, pp. 1699–1716, Jun. 2020. doi: 10.1175/jpo-d-19-0319.1.  
  
J. Egger, “A high-pressure hydrogen time projection chamber for the MuCap experiment”, *The European Physical Journal A*, vol. 50, no. 10. Springer Science and Business Media LLC, Oct. 2014. doi: 10.1140/epja/i2014-14163-1.  
  
R. J. Hill, P. Kammel, W. J. Marcianoand A. Sirlin, “Nucleon axial radius and muonic hydrogen—a new analysis and review”, *Reports on Progress in Physics*, vol. 81, no. 9. IOP Publishing, p. 096301, Jul. 30, 2018. doi: 10.1088/1361-6633/aac190.  
  
P. Kammel, “Muon capture in hydrogen”, *Nuclear Physics A*, vol. 844, no. 1–4. Elsevier BV, pp. 181c–184c, Nov. 2010. doi: 10.1016/j.nuclphysa.2010.05.032.  
  
P. Kammel and K. Kubodera, “Precision Muon Capture”, *Annual Review of Nuclear and Particle Science*, vol. 60, no. 1. Annual Reviews, pp. 327–353, Nov. 23, 2010. doi: 10.1146/annurev-nucl-100809-131946.  
  
M. C. Babiuc, J. Winicourand Y. Zlochower, “Binary black hole waveform extraction at null infinity”, *Classical and Quantum Gravity*, vol. 28, no. 13. IOP Publishing, p. 134006, Jun. 16, 2011. doi: 10.1088/0264-9381/28/13/134006.  
  
M. Campanelli, C. O. Lousto, B. C. Mundim, H. Nakano, Y. Zlochowerand H.-P. Bischof, “Advances in simulations of generic black-hole binaries”, *Classical and Quantum Gravity*, vol. 27, no. 8. IOP Publishing, p. 084034, Apr. 06, 2010. doi: 10.1088/0264-9381/27/8/084034.  
  
V. Cardoso, “NR/HEP: roadmap for the future”, *Classical and Quantum Gravity*, vol. 29, no. 24. IOP Publishing, p. 244001, Nov. 21, 2012. doi: 10.1088/0264-9381/29/24/244001.  
  
J. Healy, C. O. Loustoand Y. Zlochower, “Remnant mass, spin, and recoil from spin aligned black-hole binaries”, *Physical Review D*, vol. 90, no. 10. American Physical Society (APS), Nov. 06, 2014. doi: 10.1103/physrevd.90.104004.  
  
B. Ireland, B. C. Mundim, H. Nakanoand M. Campanelli, “Inspiralling, nonprecessing, spinning black hole binary spacetime via asymptotic matching”, *Physical Review D*, vol. 93, no. 10. American Physical Society (APS), May 27, 2016. doi: 10.1103/physrevd.93.104057.  
  
B. J. Kelly, W. Tichy, Y. Zlochower, M. Campanelliand B. Whiting, “Post-Newtonian initial data with waves: progress in evolution”, *Classical and Quantum Gravity*, vol. 27, no. 11. IOP Publishing, p. 114005, May 11, 2010. doi: 10.1088/0264-9381/27/11/114005.  
  
C. O. Lousto, M. Campanelli, Y. Zlochowerand H. Nakano, “Remnant masses, spins and recoils from the merger of generic black hole binaries”, *Classical and Quantum Gravity*, vol. 27, no. 11. IOP Publishing, p. 114006, May 10, 2010. doi: 10.1088/0264-9381/27/11/114006.  
  
C. O. Lousto and J. Healy, “Flip-Flopping Binary Black Holes”, *Physical Review Letters*, vol. 114, no. 14. American Physical Society (APS), Apr. 06, 2015. doi: 10.1103/physrevlett.114.141101.  
  
C. O. Lousto and J. Healy, “Unstable flip-flopping spinning binary black holes”, *Physical Review D*, vol. 93, no. 12. American Physical Society (APS), Jun. 30, 2016. doi: 10.1103/physrevd.93.124074.  
  
C. O. Lousto, J. Healyand H. Nakano, “Spin flips in generic black hole binaries”, *Physical Review D*, vol. 93, no. 4. American Physical Society (APS), Feb. 10, 2016. doi: 10.1103/physrevd.93.044031.  
  
C. O. Lousto and Y. Zlochower, “Where angular momentum goes in a precessing black-hole binary”, *Physical Review D*, vol. 89, no. 2. American Physical Society (APS), Jan. 06, 2014. doi: 10.1103/physrevd.89.021501.  
  
B. C. Mundim, B. J. Kelly, Y. Zlochower, H. Nakanoand M. Campanelli, “Hybrid black-hole binary initial data”, *Classical and Quantum Gravity*, vol. 28, no. 13. IOP Publishing, p. 134003, Jun. 16, 2011. doi: 10.1088/0264-9381/28/13/134003.  
  
H. Nakano, M. Campanelli, C. O. Loustoand Y. Zlochower, “Perturbative effects of spinning black holes in the extreme mass-ratio limit”, *Classical and Quantum Gravity*, vol. 28, no. 13. IOP Publishing, p. 134005, Jun. 16, 2011. doi: 10.1088/0264-9381/28/13/134005.  
  
H. Nakano, J. Healy, C. O. Loustoand Y. Zlochower, “Perturbative extraction of gravitational waveforms generated with numerical relativity”, *Physical Review D*, vol. 91, no. 10. American Physical Society (APS), May 18, 2015. doi: 10.1103/physrevd.91.104022.  
  
M. Ponce, C. Loustoand Y. Zlochower, “Seeking for toroidal event horizons from initially stationary BH configurations”, *Classical and Quantum Gravity*, vol. 28, no. 14. IOP Publishing, p. 145027, Jun. 20, 2011. doi: 10.1088/0264-9381/28/14/145027.  
  
M. Zilhão and S. C. Noble, “Dynamic fisheye grids for binary black hole simulations”, *Classical and Quantum Gravity*, vol. 31, no. 6. IOP Publishing, p. 065013, Feb. 27, 2014. doi: 10.1088/0264-9381/31/6/065013.  
  
Y. Zlochower, M. Campanelliand C. O. Lousto, “Modeling gravitational recoil from black-hole binaries using numerical relativity”, *Classical and Quantum Gravity*, vol. 28, no. 11. IOP Publishing, p. 114015, May 20, 2011. doi: 10.1088/0264-9381/28/11/114015.  
  
Y. Zlochower and C. O. Lousto, “Modeling the remnant mass, spin, and recoil from unequal-mass, precessing black-hole binaries: The intermediate mass ratio regime”, *Physical Review D*, vol. 92, no. 2. American Physical Society (APS), Jul. 13, 2015. doi: 10.1103/physrevd.92.024022.  
  
Y. Zlochower, H. Nakano, B. C. Mundim, M. Campanelli, S. Nobleand M. Zilhão, “Inspiraling black-hole binary spacetimes: Challenges in transitioning from analytical to numerical techniques”, *Physical Review D*, vol. 93, no. 12. American Physical Society (APS), Jun. 29, 2016. doi: 10.1103/physrevd.93.124072.  
  
P. Ajith, “The NINJA-2 catalog of hybrid post-Newtonian/numerical-relativity waveforms for non-precessing black-hole binaries”, *Classical and Quantum Gravity*, vol. 29, no. 12. IOP Publishing, p. 124001, Jun. 01, 2012. doi: 10.1088/0264-9381/29/12/124001.  
  
B. P. Abbott et al., “Observation of Gravitational Waves from a Binary Black Hole Merger”, *Centennial of General Relativity*. WORLD SCIENTIFIC, pp. 291–311, Feb. 05, 2017. doi: 10.1142/9789814699662\_0011.  
  
J. Healy and C. O. Lousto, “Remnant of binary black-hole mergers: New simulations and peak luminosity studies”, *Physical Review D*, vol. 95, no. 2. American Physical Society (APS), Jan. 30, 2017. doi: 10.1103/physrevd.95.024037.  
  
J. Healy and C. O. Lousto, “Hangup effect in unequal mass binary black hole mergers and further studies of their gravitational radiation and remnant properties”, *Physical Review D*, vol. 97, no. 8. American Physical Society (APS), Apr. 02, 2018. doi: 10.1103/physrevd.97.084002.  
  
J. Healy, C. O. Lousto, H. Nakanoand Y. Zlochower, “Post-Newtonian quasicircular initial orbits for numerical relativity”, *Classical and Quantum Gravity*, vol. 34, no. 14. IOP Publishing, p. 145011, Jun. 29, 2017. doi: 10.1088/1361-6382/aa7929.  
  
J. Healy, C. O. Lousto, I. Ruchlinand Y. Zlochower, “Evolutions of unequal mass, highly spinning black hole binaries”, *Physical Review D*, vol. 97, no. 10. American Physical Society (APS), May 18, 2018. doi: 10.1103/physrevd.97.104026.  
  
J. Healy, C. O. Loustoand Y. Zlochower, “Nonspinning binary black hole merger scenario revisited”, *Physical Review D*, vol. 96, no. 2. American Physical Society (APS), Jul. 21, 2017. doi: 10.1103/physrevd.96.024031.  
  
J. Healy, C. O. Loustoand Y. Zlochower, “Nonspinning binary black hole merger scenario revisited”, *Physical Review D*, vol. 96, no. 2. American Physical Society (APS), Jul. 21, 2017. doi: 10.1103/physrevd.96.024031.  
  
C. O. Lousto, Y. Zlochowerand M. Campanelli, “Modeling the Black Hole Merger of QSO 3C 186”, *The Astrophysical Journal*, vol. 841, no. 2. American Astronomical Society, p. L28, Jun. 01, 2017. doi: 10.3847/2041-8213/aa733c.  
  
Y. Zlochower, J. Healy, C. O. Loustoand I. Ruchlin, “Evolutions of nearly maximally spinning black hole binaries using the moving puncture approach”, *Physical Review D*, vol. 96, no. 4. American Physical Society (APS), Aug. 03, 2017. doi: 10.1103/physrevd.96.044002.  
  
T. Blake, S. Meineland D. van Dyk, “Bayesian analysis of Wilson coefficients using the full angular distribution of decays”, *Physical Review D*, vol. 101, no. 3. American Physical Society (APS), Feb. 19, 2020. doi: 10.1103/physrevd.101.035023.  
  
Z. S. Brown, W. Detmold, S. Meineland K. Orginos, “Charmed bottom baryon spectroscopy from lattice QCD”, *Physical Review D*, vol. 90, no. 9. American Physical Society (APS), Nov. 19, 2014. doi: 10.1103/physrevd.90.094507.  
  
A. Datta, S. Kamali, S. Meineland A. Rashed, “Phenomenology of

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$$ {\Lambda}\_b\to {\Lambda}\_c\tau {\overline{\nu}}\_{\tau } $$ using lattice QCD calculations”, *Journal of High Energy Physics*, vol. 2017, no. 8. Springer Science and Business Media LLC, Aug. 2017. doi: 10.1007/jhep08(2017)131.  
  
W. Detmold, C. Lehnerand S. Meinel, “andform factors from lattice QCD with relativistic heavy quarks”, *Physical Review D*, vol. 92, no. 3. American Physical Society (APS), Aug. 04, 2015. doi: 10.1103/physrevd.92.034503.  
  
W. Detmold, C.-J. D. Linand S. Meinel, “Calculation of the heavy-hadron axial couplings,, andusing lattice QCD”, *Physical Review D*, vol. 85, no. 11. American Physical Society (APS), Jun. 18, 2012. doi: 10.1103/physrevd.85.114508.  
  
W. Detmold, C.-J. D. Linand S. Meinel, “Axial Couplings and Strong Decay Widths of Heavy Hadrons”, *Physical Review Letters*, vol. 108, no. 17. American Physical Society (APS), Apr. 27, 2012. doi: 10.1103/physrevlett.108.172003.  
  
W. Detmold, C.-J. D. Lin, S. Meineland M. Wingate, “form factors from lattice QCD with staticquarks”, *Physical Review D*, vol. 88, no. 1. American Physical Society (APS), Jul. 23, 2013. doi: 10.1103/physrevd.88.014512.  
  
W. Detmold, C.-J. D. Lin, S. Meineland M. Wingate, “form factors and differential branching fraction from lattice QCD”, *Physical Review D*, vol. 87, no. 7. American Physical Society (APS), Apr. 05, 2013. doi: 10.1103/physrevd.87.074502.  
  
W. Detmold and S. Meinel, “form factors, differential branching fraction, and angular observables from lattice QCD with relativisticquarks”, *Physical Review D*, vol. 93, no. 7. American Physical Society (APS), Apr. 01, 2016. doi: 10.1103/physrevd.93.074501.  
  
W. Detmold, S. Meineland Z. Shi, “Quarkonium at nonzero isospin density”, *Physical Review D*, vol. 87, no. 9. American Physical Society (APS), May 10, 2013. doi: 10.1103/physrevd.87.094504.  
  
L. Leskovec, S. Meinel, M. Pflaumerand M. Wagner, “Lattice QCD investigation of a doubly-bottom tetraquark with quantum numbers ”, *Physical Review D*, vol. 100, no. 1. American Physical Society (APS), Jul. 12, 2019. doi: 10.1103/physrevd.100.014503.  
  
S. Meinel, “Bottomonium spectrum at orderfrom domain-wall lattice QCD: Precise results for hyperfine splittings”, *Physical Review D*, vol. 82, no. 11. American Physical Society (APS), Dec. 01, 2010. doi: 10.1103/physrevd.82.114502.  
  
S. Meinel, “Prediction of themass from lattice QCD”, *Physical Review D*, vol. 82, no. 11. American Physical Society (APS), Dec. 29, 2010. doi: 10.1103/physrevd.82.114514.  
  
S. Meinel, “Excited-state spectroscopy of triply bottom baryons from lattice QCD”, *Physical Review D*, vol. 85, no. 11. American Physical Society (APS), Jun. 25, 2012. doi: 10.1103/physrevd.85.114510.  
  
S. Meinel, “ form factors from lattice QCD and phenomenology of and decays”, *Physical Review D*, vol. 97, no. 3. American Physical Society (APS), Feb. 23, 2018. doi: 10.1103/physrevd.97.034511.  
  
S. Barraza-Lopez, “Coherent electron transport through freestanding graphene junctions with metal contacts: a materials approach”, *Journal of Computational Electronics*, vol. 12, no. 2. Springer Science and Business Media LLC, pp. 145–164, Mar. 14, 2013. doi: 10.1007/s10825-013-0447-x.  
  
S. Barraza-Lopez, M. Kindermannand M. Y. Chou, “Charge Transport through Graphene Junctions with Wetting Metal Leads”, *Nano Letters*, vol. 12, no. 7. American Chemical Society (ACS), pp. 3424–3430, Jun. 12, 2012. doi: 10.1021/nl3004122.  
  
S. Barraza-Lopez, A. A. Pacheco Sanjuan, Z. Wangand M. Vanević, “Strain-engineering of graphene’s electronic structure beyond continuum elasticity”, *Solid State Communications*, vol. 166. Elsevier BV, pp. 70–75, Jul. 2013. doi: 10.1016/j.ssc.2013.05.002.  
  
D. Choudhury, “Anomalous charge and negative-charge-transfer insulating state in cuprate chain compound”, *Physical Review B*, vol. 92, no. 20. American Physical Society (APS), Nov. 19, 2015. doi: 10.1103/physrevb.92.201108.  
  
K. T. He, J. C. Koepke, S. Barraza-Lopezand J. W. Lyding, “Separation-Dependent Electronic Transparency of Monolayer Graphene Membranes on III−V Semiconductor Substrates”, *Nano Letters*, vol. 10, no. 9. American Chemical Society (ACS), pp. 3446–3452, Aug. 18, 2010. doi: 10.1021/nl101527e.  
  
J. C. Koepke, J. D. Wood, C. M. Horvath, J. W. Lydingand S. Barraza-Lopez, “Preserving the 7 × 7 surface reconstruction of clean Si(111) by graphene adsorption”, *Applied Physics Letters*, vol. 107, no. 7. AIP Publishing, p. 071603, Aug. 17, 2015. doi: 10.1063/1.4928930.  
  
M. Mehboudi, “Two-Dimensional Disorder in Black Phosphorus and Monochalcogenide Monolayers”, *Nano Letters*, vol. 16, no. 3. American Chemical Society (ACS), pp. 1704–1712, Feb. 16, 2016. doi: 10.1021/acs.nanolett.5b04613.  
  
M. Mehboudi, K. Utt, H. Terrones, E. O. Harriss, A. A. Pacheco SanJuanand S. Barraza-Lopez, “Strain and the optoelectronic properties of nonplanar phosphorene monolayers”, *Proceedings of the National Academy of Sciences*, vol. 112, no. 19. Proceedings of the National Academy of Sciences, pp. 5888–5892, Apr. 27, 2015. doi: 10.1073/pnas.1500633112.  
  
S. Middey, “Polarity compensation in ultra-thin films of complex oxides: The case of a perovskite nickelate”, *Scientific Reports*, vol. 4, no. 1. Springer Science and Business Media LLC, Oct. 29, 2014. doi: 10.1038/srep06819.  
  
G. G. Naumis, S. Barraza-Lopez, M. Oliva-Leyvaand H. Terrones, “Electronic and optical properties of strained graphene and other strained 2D materials: a review”, *Reports on Progress in Physics*, vol. 80, no. 9. IOP Publishing, p. 096501, Aug. 21, 2017. doi: 10.1088/1361-6633/aa74ef.  
  
A. A. Pacheco Sanjuan, M. Mehboudi, E. O. Harriss, H. Terronesand S. Barraza-Lopez, “Quantitative Chemistry and the Discrete Geometry of Conformal Atom-Thin Crystals”, *ACS Nano*, vol. 8, no. 2. American Chemical Society (ACS), pp. 1136–1146, Jan. 13, 2014. doi: 10.1021/nn406532z.  
  
P. Rivero, “Systematic pseudopotentials from reference eigenvalue sets for DFT calculations”, *Computational Materials Science*, vol. 98. Elsevier BV, pp. 372–389, Feb. 2015. doi: 10.1016/j.commatsci.2014.11.026.  
  
P. Rivero, C. M. Horvath, Z. Zhu, J. Guan, D. Tománekand S. Barraza-Lopez, “Simulated scanning tunneling microscopy images of few-layer phosphorus capped by graphene and hexagonal boron nitride monolayers”, *Physical Review B*, vol. 91, no. 11. American Physical Society (APS), Mar. 10, 2015. doi: 10.1103/physrevb.91.115413.  
  
P. Rivero, “Systematic pseudopotentials from reference eigenvalue sets for DFT calculations: Pseudopotential files”, *Data in Brief*, vol. 3. Elsevier BV, pp. 21–23, Jun. 2015. doi: 10.1016/j.dib.2014.12.005.  
  
K. L. Utt, “Intrinsic Defects, Fluctuations of the Local Shape, and the Photo-Oxidation of Black Phosphorus”, *ACS Central Science*, vol. 1, no. 6. American Chemical Society (ACS), pp. 320–327, Aug. 06, 2015. doi: 10.1021/acscentsci.5b00244.  
  
J.-A. Yan, M. A. D. Cruz, S. Barraza-Lopezand L. Yang, “Strain-tunable topological quantum phase transition in buckled honeycomb lattices”, *Applied Physics Letters*, vol. 106, no. 18. AIP Publishing, p. 183107, May 04, 2015. doi: 10.1063/1.4919885.  
  
L. Barack, “Black holes, gravitational waves and fundamental physics: a roadmap”, *Classical and Quantum Gravity*, vol. 36, no. 14. IOP Publishing, p. 143001, Jun. 20, 2019. doi: 10.1088/1361-6382/ab0587.  
  
E. Barausse, “Prospects for fundamental physics with LISA”, *General Relativity and Gravitation*, vol. 52, no. 8. Springer Science and Business Media LLC, Aug. 2020. doi: 10.1007/s10714-020-02691-1.  
  
E. Berti, “Topical collection: Testing the Kerr spacetime with gravitational-wave and electromagnetic observations”, *General Relativity and Gravitation*, vol. 51, no. 11. Springer Science and Business Media LLC, Oct. 31, 2019. doi: 10.1007/s10714-019-2622-2.  
  
E. Berti, “Testing general relativity with present and future astrophysical observations”, *Classical and Quantum Gravity*, vol. 32, no. 24. IOP Publishing, p. 243001, Dec. 01, 2015. doi: 10.1088/0264-9381/32/24/243001.  
  
E. Berti, V. Cardoso, L. C. B. Crispino, L. Gualtieri, C. Herdeiroand U. Sperhake, “Numerical relativity and high energy physics: Recent developments”, *International Journal of Modern Physics D*, vol. 25, no. 9. World Scientific Pub Co Pte Lt, p. 1641022, Aug. 2016. doi: 10.1142/s0218271816410224.  
  
E. Berti, “Semianalytical estimates of scattering thresholds and gravitational radiation in ultrarelativistic black hole encounters”, *Physical Review D*, vol. 81, no. 10. American Physical Society (APS), May 27, 2010. doi: 10.1103/physrevd.81.104048.  
  
E. Berti, M. Kesdenand U. Sperhake, “Effects of post-Newtonian spin alignment on the distribution of black-hole recoils”, *Physical Review D*, vol. 85, no. 12. American Physical Society (APS), Jun. 21, 2012. doi: 10.1103/physrevd.85.124049.  
  
Y. Bouffanais, “Constraining the Fraction of Binary Black Holes Formed in Isolation and Young Star Clusters with Gravitational-wave Data”, *The Astrophysical Journal*, vol. 886, no. 1. American Astronomical Society, p. 25, Nov. 15, 2019. doi: 10.3847/1538-4357/ab4a79.  
  
R. Brito, V. Cardosoand H. Okawa, “Accretion of Dark Matter by Stars”, *Physical Review Letters*, vol. 115, no. 11. American Physical Society (APS), Sep. 09, 2015. doi: 10.1103/physrevlett.115.111301.  
  
D. Brizuela, J. M. Martín-García, U. Sperhakeand K. D. Kokkotas, “High-order perturbations of a spherical collapsing star”, *Physical Review D*, vol. 82, no. 10. American Physical Society (APS), Nov. 17, 2010. doi: 10.1103/physrevd.82.104039.  
  
V. Cardoso, V. F. Foitand M. Kleban, “Gravitational wave echoes from black hole area quantization”, *Journal of Cosmology and Astroparticle Physics*, vol. 2019, no. 8. IOP Publishing, pp. 006–006, Aug. 05, 2019. doi: 10.1088/1475-7516/2019/08/006.  
  
L. G. Collodel, B. Kleihaus, J. Kunzand E. Berti, “Spinning and excited black holes in Einstein-scalar-Gauss–Bonnet theory”, *Classical and Quantum Gravity*, vol. 37, no. 7. IOP Publishing, p. 075018, Mar. 05, 2020. doi: 10.1088/1361-6382/ab74f9.  
  
W. G. Cook, P. Figueras, M. Kunesch, U. Sperhakeand S. Tunyasuvunakool, “Dimensional reduction in numerical relativity: Modified Cartoon formalism and regularization”, *International Journal of Modern Physics D*, vol. 25, no. 9. World Scientific Pub Co Pte Lt, p. 1641013, Aug. 2016. doi: 10.1142/s0218271816410133.  
  
W. G. Cook and U. Sperhake, “Extraction of gravitational-wave energy in higher dimensional numerical relativity using the Weyl tensor”, *Classical and Quantum Gravity*, vol. 34, no. 3. IOP Publishing, p. 035010, Jan. 10, 2017. doi: 10.1088/1361-6382/aa5294.  
  
W. G. Cook, D. Wangand U. Sperhake, “Orbiting black-hole binaries and apparent horizons in higher dimensions”, *Classical and Quantum Gravity*, vol. 35, no. 23. IOP Publishing, p. 235008, Nov. 09, 2018. doi: 10.1088/1361-6382/aae995.  
  
P. Figueras, M. Kuneschand S. Tunyasuvunakool, “End Point of Black Ring Instabilities and the Weak Cosmic Censorship Conjecture”, *Physical Review Letters*, vol. 116, no. 7. American Physical Society (APS), Feb. 18, 2016. doi: 10.1103/physrevlett.116.071102.  
  
D. Gerosa, “Precessional Instability in Binary Black Holes with Aligned Spins”, *Physical Review Letters*, vol. 115, no. 14. American Physical Society (APS), Oct. 02, 2015. doi: 10.1103/physrevlett.115.141102.  
  
D. Gerosa, M. Kesden, U. Sperhake, E. Bertiand R. O’Shaughnessy, “Multi-timescale analysis of phase transitions in precessing black-hole binaries”, *Physical Review D*, vol. 92, no. 6. American Physical Society (APS), Sep. 14, 2015. doi: 10.1103/physrevd.92.064016.  
  
D. Gerosa, A. Lima, E. Berti, U. Sperhake, M. Kesdenand R. O’Shaughnessy, “Wide nutation: binary black-hole spins repeatedly oscillating from full alignment to full anti-alignment”, *Classical and Quantum Gravity*, vol. 36, no. 10. IOP Publishing, p. 105003, Apr. 15, 2019. doi: 10.1088/1361-6382/ab14ae.  
  
D. Gerosa and C. J. Moore, “Black Hole Kicks as New Gravitational Wave Observables”, *Physical Review Letters*, vol. 117, no. 1. American Physical Society (APS), Jun. 29, 2016. doi: 10.1103/physrevlett.117.011101.  
  
D. Gerosa, U. Sperhakeand J. Vošmera, “On the equal-mass limit of precessing black-hole binaries”, *Classical and Quantum Gravity*, vol. 34, no. 6. IOP Publishing, p. 064004, Mar. 02, 2017. doi: 10.1088/1361-6382/aa5e58.  
  
M. Horbatsch, “Tensor-multi-scalar theories: relativistic stars and 3 + 1 decomposition”, *Classical and Quantum Gravity*, vol. 32, no. 20. IOP Publishing, p. 204001, Sep. 23, 2015. doi: 10.1088/0264-9381/32/20/204001.  
  
M. Kesden, D. Gerosa, R. O’Shaughnessy, E. Bertiand U. Sperhake, “Effective Potentials and Morphological Transitions for Binary Black Hole Spin Precession”, *Physical Review Letters*, vol. 114, no. 8. American Physical Society (APS), Feb. 24, 2015. doi: 10.1103/physrevlett.114.081103.  
  
M. Kesden, U. Sperhakeand E. Berti, “Final spins from the merger of precessing binary black holes”, *Physical Review D*, vol. 81, no. 8. American Physical Society (APS), Apr. 29, 2010. doi: 10.1103/physrevd.81.084054.  
  
M. Kesden, U. Sperhakeand E. Berti, “RELATIVISTIC SUPPRESSION OF BLACK HOLE RECOILS”, *The Astrophysical Journal*, vol. 715, no. 2. American Astronomical Society, pp. 1006–1011, May 05, 2010. doi: 10.1088/0004-637x/715/2/1006.  
  
G. Lovelace, “Momentum flow in black-hole binaries. II. Numerical simulations of equal-mass, head-on mergers with antiparallel spins”, *Physical Review D*, vol. 82, no. 6. American Physical Society (APS), Sep. 24, 2010. doi: 10.1103/physrevd.82.064031.  
  
C. Reisswig, C. D. Ott, U. Sperhakeand E. Schnetter, “Gravitational wave extraction in simulations of rotating stellar core collapse”, *Physical Review D*, vol. 83, no. 6. American Physical Society (APS), Mar. 08, 2011. doi: 10.1103/physrevd.83.064008.  
  
R. Rosca-Mead, C. J. Moore, M. Agathosand U. Sperhake, “Inverse-chirp signals and spontaneous scalarisation with self-interacting potentials in stellar collapse”, *Classical and Quantum Gravity*, vol. 36, no. 13. IOP Publishing, p. 134003, Jun. 18, 2019. doi: 10.1088/1361-6382/ab256f.  
  
R. Rosca-Mead, C. J. Moore, U. Sperhake, M. Agathosand D. Gerosa, “Structure of Neutron Stars in Massive Scalar-Tensor Gravity”, *Symmetry*, vol. 12, no. 9. MDPI AG, p. 1384, Aug. 19, 2020. doi: 10.3390/sym12091384.  
  
R. Rosca-Mead, U. Sperhake, C. J. Moore, M. Agathos, D. Gerosaand C. D. Ott, “Core collapse in massive scalar-tensor gravity”, *Physical Review D*, vol. 102, no. 4. American Physical Society (APS), Aug. 06, 2020. doi: 10.1103/physrevd.102.044010.  
  
U. Sperhake, “Numerical relativity: the role of black holes in gravitational wave physics, astrophysics and high-energy physics”, *General Relativity and Gravitation*, vol. 46, no. 5. Springer Science and Business Media LLC, Apr. 17, 2014. doi: 10.1007/s10714-014-1689-z.  
  
U. Sperhake, “Gravitational Recoil and Astrophysical Impact”, *Gravitational Wave Astrophysics*. Springer International Publishing, pp. 185–202, Nov. 10, 2014. doi: 10.1007/978-3-319-10488-1\_16.  
  
U. Sperhake, “The numerical relativity breakthrough for binary black holes”, *Classical and Quantum Gravity*, vol. 32, no. 12. IOP Publishing, p. 124011, Jun. 01, 2015. doi: 10.1088/0264-9381/32/12/124011.  
  
U. SPERHAKE, “NUMERICAL RELATIVITY IN HIGHER DIMENSIONS”, *The Thirteenth Marcel Grossmann Meeting*. WORLD SCIENTIFIC, Jan. 29, 2015. doi: 10.1142/9789814623995\_0025.  
  
U. Sperhake, E. Bertiand V. Cardoso, “Numerical simulations of black-hole binaries and gravitational wave emission”, *Comptes Rendus Physique*, vol. 14, no. 4. Elsevier BV, pp. 306–317, Apr. 2013. doi: 10.1016/j.crhy.2013.01.004.  
  
U. Sperhake, E. Berti, V. Cardosoand F. Pretorius, “Gravity-dominated unequal-mass black hole collisions”, *Physical Review D*, vol. 93, no. 4. American Physical Society (APS), Feb. 04, 2016. doi: 10.1103/physrevd.93.044012.  
  
U. Sperhake, E. Berti, V. Cardoso, F. Pretoriusand N. Yunes, “Superkicks in ultrarelativistic encounters of spinning black holes”, *Physical Review D*, vol. 83, no. 2. American Physical Society (APS), Jan. 28, 2011. doi: 10.1103/physrevd.83.024037.  
  
U. Sperhake, B. Brügmann, D. Müllerand C. F. Sopuerta, “11-orbit inspiral of a mass ratio 4:1 black-hole binary”, *Classical and Quantum Gravity*, vol. 28, no. 13. IOP Publishing, p. 134004, Jun. 16, 2011. doi: 10.1088/0264-9381/28/13/134004.  
  
U. Sperhake, V. Cardoso, C. D. Ott, E. Schnetterand H. Witek, “Collisions of unequal mass black holes and the point particle limit”, *Physical Review D*, vol. 84, no. 8. American Physical Society (APS), Oct. 18, 2011. doi: 10.1103/physrevd.84.084038.  
  
D. Trifirò, “Distinguishing black-hole spin-orbit resonances by their gravitational wave signatures. II. Full parameter estimation”, *Physical Review D*, vol. 93, no. 4. American Physical Society (APS), Feb. 26, 2016. doi: 10.1103/physrevd.93.044071.  
  
H. Witek, “Black holes in a box”, *Journal of Physics: Conference Series*, vol. 229. IOP Publishing, p. 012072, May 01, 2010. doi: 10.1088/1742-6596/229/1/012072.  
  
H. Witek, V. Cardoso, L. Gualtieri, C. Herdeiro, U. Sperhakeand M. Zilhão, “Head-on collisions of unequal mass black holes indimensions”, *Physical Review D*, vol. 83, no. 4. American Physical Society (APS), Feb. 08, 2011. doi: 10.1103/physrevd.83.044017.  
  
H. Witek, V. Cardoso, L. Gualtieri, C. Herdeiro, U. Sperhakeand M. Zilhão, “Numerical Relativity in*D*dimensional space-times: Collisions of unequal mass black holes”, *Journal of Physics: Conference Series*, vol. 314. IOP Publishing, p. 012104, Sep. 22, 2011. doi: 10.1088/1742-6596/314/1/012104.  
  
H. Witek, V. Cardoso, C. Herdeiro, A. Nerozzi, U. Sperhakeand M. Zilhão, “Black holes in a box: Toward the numerical evolution of black holes in AdS space-times”, *Physical Review D*, vol. 82, no. 10. American Physical Society (APS), Nov. 18, 2010. doi: 10.1103/physrevd.82.104037.  
  
H. Witek, D. Hilditchand U. Sperhake, “Stability of the puncture method with a generalized Baumgarte-Shapiro-Shibata-Nakamura formulation”, *Physical Review D*, vol. 83, no. 10. American Physical Society (APS), May 20, 2011. doi: 10.1103/physrevd.83.104041.  
  
H. Witek, “Numerical relativity fordimensional space-times: Head-on collisions of black holes and gravitational wave extraction”, *Physical Review D*, vol. 82, no. 10. American Physical Society (APS), Nov. 05, 2010. doi: 10.1103/physrevd.82.104014.  
  
K. W. K. Wong, V. Baibhavand E. Berti, “Binary radial velocity measurements with space-based gravitational-wave detectors”, *Monthly Notices of the Royal Astronomical Society*, vol. 488, no. 4. Oxford University Press (OUP), pp. 5665–5670, Jul. 30, 2019. doi: 10.1093/mnras/stz2077.  
  
M. Zilhão, “Higher-dimensional puncture initial data”, *Physical Review D*, vol. 84, no. 8. American Physical Society (APS), Oct. 18, 2011. doi: 10.1103/physrevd.84.084039.  
  
M. Zilhão, “Simulations of black holes in compactified spacetimes”, *Journal of Physics: Conference Series*, vol. 314. IOP Publishing, p. 012103, Sep. 22, 2011. doi: 10.1088/1742-6596/314/1/012103.  
  
M. Zilhão, V. Cardoso, L. Gualtieri, C. Herdeiro, U. Sperhakeand H. Witek, “Black Hole Collisions in Asymptotically de Sitter Spacetimes”, *Springer Proceedings in Physics*. Springer International Publishing, pp. 247–254, 2014. doi: 10.1007/978-3-319-06761-2\_31.  
  
M. Zilhão, V. Cardoso, C. Herdeiro, L. Lehnerand U. Sperhake, “Testing the nonlinear stability of Kerr-Newman black holes”, *Physical Review D*, vol. 90, no. 12. American Physical Society (APS), Dec. 30, 2014. doi: 10.1103/physrevd.90.124088.  
  
M. ZILHÃO, V. CARDOSO, C. HERDEIRO, L. LEHNERand U. SPERHAKE, “DYNAMICS OF CHARGED BLACK HOLES”, *The Thirteenth Marcel Grossmann Meeting*. WORLD SCIENTIFIC, Jan. 29, 2015. doi: 10.1142/9789814623995\_0061.  
  
M. Zilhão, “Numerical relativity in higher dimensions”, *Journal of Physics: Conference Series*, vol. 229. IOP Publishing, p. 012074, May 01, 2010. doi: 10.1088/1742-6596/229/1/012074.  
  
M. Zilhão, “Numerical relativity fordimensional axially symmetric space-times: Formalism and code tests”, *Physical Review D*, vol. 81, no. 8. American Physical Society (APS), Apr. 29, 2010. doi: 10.1103/physrevd.81.084052.  
  
A. P. Hickman, D. O. Kashinski, R. F. Malenda, F. Gattiand D. Talbi, “Calculation of dissociating autoionizing states using the block diagonalization method: Application to N2H”, *Journal of Physics: Conference Series*, vol. 300. IOP Publishing, p. 012016, Jul. 20, 2011. doi: 10.1088/1742-6596/300/1/012016.  
  
D. O. Kashinski, D. Talbiand A. P. Hickman, “Ab initio calculations of autoionizing states using block diagonalization: Collinear diabatic states for dissociative recombination of electrons with”, *Chemical Physics Letters*, vol. 529. Elsevier BV, pp. 10–15, Mar. 2012. doi: 10.1016/j.cplett.2012.01.037.  
  
D. O. Kashinski, “A theoretical study of the dissociative recombination of SH+with electrons through the2Π states of SH”, *The Journal of Chemical Physics*, vol. 146, no. 20. AIP Publishing, p. 204109, May 28, 2017. doi: 10.1063/1.4983690.  
  
R. F. Malenda, F. Gatti, H.-D. Meyer, D. Talbiand A. P. Hickman, “Comparison of the multi-configuration, time-dependent Hartree (MCTDH) method with the Arthurs and Dalgarno coupled-channel method for rotationally inelastic scattering”, *Chemical Physics Letters*, vol. 585. Elsevier BV, pp. 184–188, Oct. 2013. doi: 10.1016/j.cplett.2013.08.083.  
  
A. Kumar and R. T. Fisher, “The astrochemical evolution of turbulent giant molecular clouds: physical processes and method of solution for hydrodynamic, embedded starless clouds”, *Monthly Notices of the Royal Astronomical Society*, vol. 431, no. 1. Oxford University Press (OUP), pp. 455–476, Feb. 28, 2013. doi: 10.1093/mnras/stt171.  
  
P. S. Barklem, “Inelastic e+Mg collision data and its impact on modelling stellar and supernova spectra”, *Astronomy & Astrophysics*, vol. 606. EDP Sciences, p. A11, Sep. 26, 2017. doi: 10.1051/0004-6361/201730864.  
  
K. Bartschat, “Electron collisions—experiment, theory, and applications”, *Journal of Physics B: Atomic, Molecular and Optical Physics*, vol. 51, no. 13. IOP Publishing, p. 132001, Jun. 12, 2018. doi: 10.1088/1361-6455/aac5aa.  
  
K. Bartschat, X. Guan, C. J. Noble, B. I. Schneiderand O. Zatsarinny, “Multi-Photon Single and Double Ionization of Complex Atoms by Ultrashort Intense Laser Pulses”, *Quantum Dynamic Imaging*. Springer New York, pp. 13–22, 2011. doi: 10.1007/978-1-4419-9491-2\_2.  
  
K. Bartschat and M. J. Kushner, “Electron collisions with atoms, ions, molecules, and surfaces: Fundamental science empowering advances in technology”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 26. Proceedings of the National Academy of Sciences, pp. 7026–7034, Jun. 17, 2016. doi: 10.1073/pnas.1606132113.  
  
K. Bartschat, J. Tennysonand O. Zatsarinny, “Quantum-Mechanical Calculations of Cross Sections for Electron Collisions With Atoms and Molecules”, *Plasma Processes and Polymers*, vol. 14, no. 1–2. Wiley, p. 1600093, Sep. 05, 2016. doi: 10.1002/ppap.201600093.  
  
C. J. Bostock, D. V. Fursa, I. Brayand K. Bartschat, “Calculation of the polarization fraction and electron-impact excitation cross section for thestate”, *Physical Review A*, vol. 90, no. 1. American Physical Society (APS), Jul. 21, 2014. doi: 10.1103/physreva.90.012707.  
  
C. J. Bostock, D. V. Fursa, I. Brayand K. Bartschat, “Calculation of the polarization fraction and electron-impact excitation cross section for thestate”, *Physical Review A*, vol. 90, no. 1. American Physical Society (APS), Jul. 21, 2014. doi: 10.1103/physreva.90.012707.  
  
J. E. Calvert, “The interaction of excited atoms and few-cycle laser pulses”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Sep. 26, 2016. doi: 10.1038/srep34101.  
  
Z. Chen, X. Li, O. Zatsarinny, K. Bartschatand C. D. Lin, “Ratios of double to single ionization of He and Ne by strong 400-nm laser pulses using the quantitative rescattering theory”, *Physical Review A*, vol. 97, no. 1. American Physical Society (APS), Jan. 29, 2018. doi: 10.1103/physreva.97.013425.  
  
Z. Chen, “Numerical simulation of the double-to-single ionization ratio for the helium atom in strong laser fields”, *Physical Review A*, vol. 92, no. 6. American Physical Society (APS), Dec. 29, 2015. doi: 10.1103/physreva.92.063427.  
  
H.-K. Chung, “Uncertainty estimates for theoretical atomic and molecular data”, *Journal of Physics D: Applied Physics*, vol. 49, no. 36. IOP Publishing, p. 363002, Aug. 17, 2016. doi: 10.1088/0022-3727/49/36/363002.  
  
Dipti, “Recommended electron-impact excitation and ionization cross sections for Be I”, *Atomic Data and Nuclear Data Tables*, vol. 127–128. Elsevier BV, pp. 1–21, May 2019. doi: 10.1016/j.adt.2018.11.001.  
  
N. Douguet and K. Bartschat, “Dynamics of tunneling ionization using Bohmian mechanics”, *Physical Review A*, vol. 97, no. 1. American Physical Society (APS), Jan. 08, 2018. doi: 10.1103/physreva.97.013402.  
  
N. Douguet, A. N. Grum-Grzhimailoand K. Bartschat, “Above-threshold ionization in neon produced by combining optical and bichromatic XUV femtosecond laser pulses”, *Physical Review A*, vol. 95, no. 1. American Physical Society (APS), Jan. 19, 2017. doi: 10.1103/physreva.95.013407.  
  
N. Douguet, A. N. Grum-Grzhimailo, E. V. Gryzlova, E. I. Staroselskaya, J. Venzkeand K. Bartschat, “Photoelectron angular distributions in bichromatic atomic ionization induced by circularly polarized VUV femtosecond pulses”, *Physical Review A*, vol. 93, no. 3. American Physical Society (APS), Mar. 02, 2016. doi: 10.1103/physreva.93.033402.  
  
M. L. Dubernet, “The virtual atomic and molecular data centre (VAMDC) consortium”, *Journal of Physics B: Atomic, Molecular and Optical Physics*, vol. 49, no. 7. IOP Publishing, p. 074003, Mar. 17, 2016. doi: 10.1088/0953-4075/49/7/074003.  
  
L. Fernández-Menchero, O. Zatsarinnyand K. Bartschat, “Electron impact excitation of N3+using the*B*-spline*R*-matrix method: importance of the target structure description and the size of the close-coupling expansion”, *Journal of Physics B: Atomic, Molecular and Optical Physics*, vol. 50, no. 6. IOP Publishing, p. 065203, Mar. 09, 2017. doi: 10.1088/1361-6455/aa5fc4.  
  
V. Gedeon, S. Gedeon, V. Lazur, E. Nagy, O. Zatsarinnyand K. Bartschat, “-spline-matrix-with-pseudostates calculations for electron collisions with aluminum”, *Physical Review A*, vol. 92, no. 5. American Physical Society (APS), Nov. 02, 2015. doi: 10.1103/physreva.92.052701.  
  
V. Gedeon, S. Gedeon, V. Lazur, E. Nagy, O. Zatsarinnyand K. Bartschat, “Low-energy outer-shell photo-detachment of the negative ion of aluminum”, *Journal of Physics B: Atomic, Molecular and Optical Physics*, vol. 51, no. 3. IOP Publishing, p. 035004, Jan. 10, 2018. doi: 10.1088/1361-6455/aa9c37.  
  
L. Giannessi, “Coherent control schemes for the photoionization of neon and helium in the Extreme Ultraviolet spectral region”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, May 17, 2018. doi: 10.1038/s41598-018-25833-7.  
  
A. N. Grum-Grzhimailo, “Photoelectron angular distribution in bichromatic atomic ionization”, *Journal of Physics: Conference Series*, vol. 635, no. 1. IOP Publishing, p. 012008, Sep. 07, 2015. doi: 10.1088/1742-6596/635/1/012008.  
  
A. N. Grum-Grzhimailo, E. V. Gryzlova, E. I. Staroselskaya, J. Venzkeand K. Bartschat, “Erratum: Interfering one-photon and two-photon ionization by femtosecond VUV pulses in the region of an intermediate resonance [Phys. Rev. A**91**, 063418 (2015)]”, *Physical Review A*, vol. 93, no. 1. American Physical Society (APS), Jan. 20, 2016. doi: 10.1103/physreva.93.019901.  
  
E. V. Gryzlova, A. N. Grum-Grzhimailo, E. I. Staroselskaya, N. Douguetand K. Bartschat, “Quantum coherent control of the photoelectron angular distribution in bichromatic-field ionization of atomic neon”, *Physical Review A*, vol. 97, no. 1. American Physical Society (APS), Jan. 26, 2018. doi: 10.1103/physreva.97.013420.  
  
X. Guan, K. Bartschatand B. I. Schneider, “Benchmark calculations for multi-photon ionization of the hydrogen molecule and the hydrogen molecular ion by short-pulse intense laser radiation”, *Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment: Bridging from the eXtreme to the campus and beyond*. ACM, Jul. 16, 2012. doi: 10.1145/2335755.2335813.  
  
X. Guan, K. Bartschat, B. I. Schneiderand L. Koesterke, “Alignment and pulse-duration effects in two-photon double ionization ofby femtosecond XUV laser pulses”, *Physical Review A*, vol. 90, no. 4. American Physical Society (APS), Oct. 24, 2014. doi: 10.1103/physreva.90.043416.  
  
X. Guan, K. Bartschat, B. I. Schneiderand L. Koesterke, “Alignment and pulse-duration effects in two-photon double ionization ofby femtosecond XUV laser pulses”, *Physical Review A*, vol. 90, no. 4. American Physical Society (APS), Oct. 24, 2014. doi: 10.1103/physreva.90.043416.  
  
X. Guan, K. Bartschat, B. I. Schneiderand L. Koesterke, “Alignment and pulse-duration effects in two-photon double ionization ofby femtosecond XUV laser pulses”, *Physical Review A*, vol. 90, no. 4. American Physical Society (APS), Oct. 24, 2014. doi: 10.1103/physreva.90.043416.  
  
X. Guan, K. Bartschat, B. I. Schneiderand L. Koesterke, “Alignment and pulse-duration effects in two-photon double ionization ofby femtosecond XUV laser pulses”, *Physical Review A*, vol. 90, no. 4. American Physical Society (APS), Oct. 24, 2014. doi: 10.1103/physreva.90.043416.  
  
X. Guan, K. Bartschat, B. I. Schneiderand L. Koesterke, “Effects of autoionizing states on two-photon double ionization of the H2molecule”, *Journal of Physics: Conference Series*, vol. 488, no. 1. IOP Publishing, p. 012024, Apr. 10, 2014. doi: 10.1088/1742-6596/488/1/012024.  
  
L. R. Hargreaves, “Polarization correlations for electron-impact excitation of neon at 50 eV”, *Journal of Physics B: Atomic, Molecular and Optical Physics*, vol. 48, no. 18. IOP Publishing, p. 185201, Jul. 29, 2015. doi: 10.1088/0953-4075/48/18/185201.  
  
M. Ilchen, “Circular Dichroism in Multiphoton Ionization of Resonantly ExcitedIons”, *Physical Review Letters*, vol. 118, no. 1. American Physical Society (APS), Jan. 05, 2017. doi: 10.1103/physrevlett.118.013002.  
  
I. A. Ivanov, “Displacement effect in strong-field atomic ionization by an XUV pulse”, *Physical Review A*, vol. 90, no. 4. American Physical Society (APS), Oct. 03, 2014. doi: 10.1103/physreva.90.043401.  
  
I. A. Ivanov, “Displacement effect in strong-field atomic ionization by an XUV pulse”, *Physical Review A*, vol. 90, no. 4. American Physical Society (APS), Oct. 03, 2014. doi: 10.1103/physreva.90.043401.  
  
M. Kurka, “Differential cross sections for non-sequential double ionization of He by 52 eV photons from the Free Electron Laser in Hamburg, FLASH”, *New Journal of Physics*, vol. 12, no. 7. IOP Publishing, p. 073035, Jul. 27, 2010. doi: 10.1088/1367-2630/12/7/073035.  
  
N. L. S. Martin, C. M. Weaver, B. N. Kim, B. A. deHarak, O. Zatsarinnyand K. Bartschat, “Out-of-plane ( ) measurements and calculations on He autoionizing levels as a function of incident-electron energy”, *Physical Review A*, vol. 97, no. 5. American Physical Society (APS), May 29, 2018. doi: 10.1103/physreva.97.052710.  
  
L. C. Pitchford, “LXCat: an Open-Access, Web-Based Platform for Data Needed for Modeling Low Temperature Plasmas”, *Plasma Processes and Polymers*, vol. 14, no. 1–2. Wiley, p. 1600098, Sep. 01, 2016. doi: 10.1002/ppap.201600098.  
  
K. C. Prince, “Coherent control with a short-wavelength free-electron laser”, *Nature Photonics*, vol. 10, no. 3. Springer Science and Business Media LLC, pp. 176–179, Feb. 22, 2016. doi: 10.1038/nphoton.2016.13.  
  
X. Ren, “Kinematically complete study of low-energy electron-impact ionization of neon: Internormalized cross sections in three-dimensional kinematics”, *Physical Review A*, vol. 91, no. 3. American Physical Society (APS), Mar. 18, 2015. doi: 10.1103/physreva.91.032707.  
  
X. Ren, “Kinematically complete study of low-energy electron-impact ionization of argon: Internormalized cross sections in three-dimensional kinematics”, *Physical Review A*, vol. 93, no. 6. American Physical Society (APS), Jun. 13, 2016. doi: 10.1103/physreva.93.062704.  
  
X. Ren, “Erratum: Low-energy electron-impact ionization of argon: Three-dimensional cross section [Phys. Rev. A 85, 032702 (2012)]”, *Physical Review A*, vol. 92, no. 1. American Physical Society (APS), Jul. 13, 2015. doi: 10.1103/physreva.92.019901.  
  
X. Ren, “Propensity for distinguishing two free electrons with equal energies in electron-impact ionization of helium”, *Physical Review A*, vol. 92, no. 5. American Physical Society (APS), Nov. 16, 2015. doi: 10.1103/physreva.92.052707.  
  
S. B. Santra and P. Ray, “XXVII IUPAP Conference on Computational Physics (CCP2015)”, *Journal of Physics: Conference Series*, vol. 759. IOP Publishing, p. 011001, Oct. 2016. doi: 10.1088/1742-6596/759/1/011001.  
  
B. I. Schneider, K. Bartschatand X. Guan, “Time Propagation of Partial Differential Equations Using the Short Iterative Lanczos Method and Finite-Element Discrete Variable Representation”, *Proceedings of the XSEDE16 Conference on Diversity, Big Data, and Science at Scale*. ACM, Jul. 17, 2016. doi: 10.1145/2949550.2949565.  
  
B. I. Schneider, K. R. Bartschat, X. Guan, D. Federand L. A. Collins, “Time-Dependent Computational Methods for Matter Under Extreme Conditions”, *Advances in Chemical Physics*. John Wiley & Sons, Inc., pp. 195–214, Dec. 12, 2014. doi: 10.1002/9781118959602.ch16.  
  
B. I. Schneider, L. A. Collins, K. Bartschat, X. Guanand S. X. Hu, “A few selected contributions to electron and photon collisions with H2and ${{\rm{H}}}\_{2}^{+}$”, *Journal of Physics B: Atomic, Molecular and Optical Physics*, vol. 50, no. 21. IOP Publishing, p. 214002, Oct. 23, 2017. doi: 10.1088/1361-6455/aa8e6d.  
  
B. I. Schneider, “Recent Advances in Computational Methods for the Solution of the Time-Dependent Schrödinger Equation for the Interaction of Short, Intense Radiation with One and Two Electron Systems”, *Quantum Dynamic Imaging*. Springer New York, pp. 149–208, 2011. doi: 10.1007/978-1-4419-9491-2\_10.  
  
B. I. Schneider, X. Guanand K. Bartschat, “Time Propagation of Partial Differential Equations Using the Short Iterative Lanczos Method and Finite-Element Discrete Variable Representation”, *Concepts of Mathematical Physics in Chemistry: A Tribute to Frank E. Harris - Part B*. Elsevier, pp. 95–127, 2016. doi: 10.1016/bs.aiq.2015.12.002.  
  
B. I. Schneider, J. Segura, A. Gil, X. Guanand K. Bartschat, “A new Fortran 90 program to compute regular and irregular associated Legendre functions”, *Computer Physics Communications*, vol. 181, no. 12. Elsevier BV, pp. 2091–2097, Dec. 2010. doi: 10.1016/j.cpc.2010.08.038.  
  
S. S. Tayal and O. Zatsarinny, “-spline-matrix-with-pseudostates approach for excitation and ionization of atomic oxygen by electron collisions”, *Physical Review A*, vol. 94, no. 4. American Physical Society (APS), Oct. 21, 2016. doi: 10.1103/physreva.94.042707.  
  
J. Tennyson, “QDB: a new database of plasma chemistries and reactions”, *Plasma Sources Science and Technology*, vol. 26, no. 5. IOP Publishing, p. 055014, Apr. 04, 2017. doi: 10.1088/1361-6595/aa6669.  
  
W. C. Wallace, “Precise and Accurate Measurements of Strong-Field Photoionization and a Transferable Laser Intensity Calibration Standard”, *Physical Review Letters*, vol. 117, no. 5. American Physical Society (APS), Jul. 29, 2016. doi: 10.1103/physrevlett.117.053001.  
  
K. Wang, L. Fernández-Menchero, O. Zatsarinnyand K. Bartschat, “Calculations for electron-impact excitation of ”, *Physical Review A*, vol. 95, no. 4. American Physical Society (APS), Apr. 21, 2017. doi: 10.1103/physreva.95.042709.  
  
K. Wang, O. Zatsarinnyand K. Bartschat, “Low-energy outer-shell photodetachment of the negative ion of boron”, *The European Physical Journal D*, vol. 70, no. 4. Springer Science and Business Media LLC, Apr. 2016. doi: 10.1140/epjd/e2016-70017-9.  
  
K. Wang, O. Zatsarinnyand K. Bartschat, “Low-energy photodetachment ofand elastic electron scattering from neutral Ga”, *Physical Review A*, vol. 94, no. 2. American Physical Society (APS), Aug. 01, 2016. doi: 10.1103/physreva.94.023402.  
  
K. Wang, O. Zatsarinnyand K. Bartschat, “Electron-impact excitation and ionization of atomic boron at low and intermediate energies”, *Physical Review A*, vol. 93, no. 5. American Physical Society (APS), May 24, 2016. doi: 10.1103/physreva.93.052715.  
  
Y. Wang, O. Zatsarinnyand K. Bartschat, “-spline-matrix-with-pseudostates calculations for electron-impact excitation and ionization of nitrogen”, *Physical Review A*, vol. 89, no. 6. American Physical Society (APS), Jun. 23, 2014. doi: 10.1103/physreva.89.062714.  
  
Y. Wang, O. Zatsarinnyand K. Bartschat, “-spline-matrix-with-pseudostates calculations for electron-impact excitation and ionization of nitrogen”, *Physical Review A*, vol. 89, no. 6. American Physical Society (APS), Jun. 23, 2014. doi: 10.1103/physreva.89.062714.  
  
Y. Wang, O. Zatsarinnyand K. Bartschat, “-spline-matrix-with-pseudostates calculations for electron-impact excitation and ionization of nitrogen”, *Physical Review A*, vol. 89, no. 6. American Physical Society (APS), Jun. 23, 2014. doi: 10.1103/physreva.89.062714.  
  
Y. Wang, O. Zatsarinnyand K. Bartschat, “-spline-matrix-with-pseudostates calculations for electron-impact excitation and ionization of nitrogen”, *Physical Review A*, vol. 89, no. 6. American Physical Society (APS), Jun. 23, 2014. doi: 10.1103/physreva.89.062714.  
  
Y. Wang, O. Zatsarinnyand K. Bartschat, “-spline-matrix-with-pseudostates calculations for electron-impact excitation and ionization of nitrogen”, *Physical Review A*, vol. 89, no. 6. American Physical Society (APS), Jun. 23, 2014. doi: 10.1103/physreva.89.062714.  
  
O. Zatsarinny and K. Bartschat, “Benchmark calculations for electron collisions with complex atoms”, *Journal of Physics: Conference Series*, vol. 488, no. 1. IOP Publishing, p. 012044, Apr. 10, 2014. doi: 10.1088/1742-6596/488/1/012044.  
  
O. Zatsarinny and K. Bartschat, “Nonperturbative-spline-matrix-with-pseudostates calculations for electron-impact ionization-excitation of helium to thestates of”, *Physical Review A*, vol. 93, no. 1. American Physical Society (APS), Jan. 25, 2016. doi: 10.1103/physreva.93.012712.  
  
O. Zatsarinny, K. Bartschat, D. V. Fursaand I. Bray, “Calculations for electron-impact excitation and ionization of beryllium”, *Journal of Physics B: Atomic, Molecular and Optical Physics*, vol. 49, no. 23. IOP Publishing, p. 235701, Nov. 18, 2016. doi: 10.1088/0953-4075/49/23/235701.  
  
L. B. Zhao, O. Zatsarinnyand K. Bartschat, “Continuous spectra of atomic hydrogen in a strong magnetic field”, *Physical Review A*, vol. 94, no. 3. American Physical Society (APS), Sep. 29, 2016. doi: 10.1103/physreva.94.033422.  
  
J. D. Brown, “Numerical simulations with a first-order BSSN formulation of Einstein’s field equations”, *Physical Review D*, vol. 85, no. 8. American Physical Society (APS), Apr. 02, 2012. doi: 10.1103/physrevd.85.084004.  
  
S. Bourouaine and G. G. Howes, “The development of magnetic field line wander in gyrokinetic plasma turbulence: dependence on amplitude of turbulence”, *Journal of Plasma Physics*, vol. 83, no. 3. Cambridge University Press (CUP), May 02, 2017. doi: 10.1017/s0022377817000319.  
  
G. G. Howes, “A prescription for the turbulent heating of astrophysical plasmas”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 409, no. 1. Oxford University Press (OUP), pp. L104–L108, Oct. 19, 2010. doi: 10.1111/j.1745-3933.2010.00958.x.  
  
G. G. Howes, “PREDICTION OF THE PROTON-TO-TOTAL TURBULENT HEATING IN THE SOLAR WIND”, *The Astrophysical Journal*, vol. 738, no. 1. American Astronomical Society, p. 40, Aug. 10, 2011. doi: 10.1088/0004-637x/738/1/40.  
  
G. G. Howes, “A dynamical model of plasma turbulence in the solar wind”, *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 373, no. 2041. The Royal Society, p. 20140145, May 13, 2015. doi: 10.1098/rsta.2014.0145.  
  
G. G. Howes, “THE DYNAMICAL GENERATION OF CURRENT SHEETS IN ASTROPHYSICAL PLASMA TURBULENCE”, *The Astrophysical Journal*, vol. 827, no. 2. American Astronomical Society, p. L28, Aug. 16, 2016. doi: 10.3847/2041-8205/827/2/l28.  
  
G. G. Howes, “A prospectus on kinetic heliophysics”, *Physics of Plasmas*, vol. 24, no. 5. AIP Publishing, p. 055907, May 2017. doi: 10.1063/1.4983993.  
  
G. G. Howes and S. Bourouaine, “The development of magnetic field line wander by plasma turbulence”, *Journal of Plasma Physics*, vol. 83, no. 4. Cambridge University Press (CUP), Aug. 2017. doi: 10.1017/s0022377817000617.  
  
G. G. Howes, D. J. Drake, K. D. Nielson, T. A. Carter, C. A. Kletzingand F. Skiff, “Toward Astrophysical Turbulence in the Laboratory”, *Physical Review Letters*, vol. 109, no. 25. American Physical Society (APS), Dec. 17, 2012. doi: 10.1103/physrevlett.109.255001.  
  
G. G. Howes, A. J. McCubbinand K. G. Klein, “Spatially localized particle energization by Landau damping in current sheets produced by strong Alfvén wave collisions”, *Journal of Plasma Physics*, vol. 84, no. 1. Cambridge University Press (CUP), Jan. 24, 2018. doi: 10.1017/s0022377818000053.  
  
G. G. Howes and K. D. Nielson, “Alfvén wave collisions, the fundamental building block of plasma turbulence. I. Asymptotic solution”, *Physics of Plasmas*, vol. 20, no. 7. AIP Publishing, p. 072302, Jul. 2013. doi: 10.1063/1.4812805.  
  
G. G. Howes, “Alfvén wave collisions, the fundamental building block of plasma turbulence. III. Theory for experimental design”, *Physics of Plasmas*, vol. 20, no. 7. AIP Publishing, p. 072304, Jul. 2013. doi: 10.1063/1.4812808.  
  
G. G. Howes, J. M. TenBargeand W. Dorland, “A weakened cascade model for turbulence in astrophysical plasmas”, *Physics of Plasmas*, vol. 18, no. 10. AIP Publishing, p. 102305, Oct. 2011. doi: 10.1063/1.3646400.  
  
K. G. Klein, G. G. Howesand J. M. TenBarge, “Diagnosing collisionless energy transfer using field–particle correlations: gyrokinetic turbulence”, *Journal of Plasma Physics*, vol. 83, no. 4. Cambridge University Press (CUP), Jul. 24, 2017. doi: 10.1017/s0022377817000563.  
  
T. C. Li, G. G. Howes, K. G. Kleinand J. M. TenBarge, “ENERGY DISSIPATION AND LANDAU DAMPING IN TWO- AND THREE-DIMENSIONAL PLASMA TURBULENCE”, *The Astrophysical Journal*, vol. 832, no. 2. American Astronomical Society, p. L24, Nov. 23, 2016. doi: 10.3847/2041-8205/832/2/l24.  
  
K. D. Nielson, G. G. Howesand W. Dorland, “Alfvén wave collisions, the fundamental building block of plasma turbulence. II. Numerical solution”, *Physics of Plasmas*, vol. 20, no. 7. AIP Publishing, p. 072303, Jul. 2013. doi: 10.1063/1.4812807.  
  
R. Numata, G. G. Howes, T. Tatsuno, M. Barnesand W. Dorland, “AstroGK: Astrophysical gyrokinetics code”, *Journal of Computational Physics*, vol. 229, no. 24. Elsevier BV, pp. 9347–9372, Dec. 2010. doi: 10.1016/j.jcp.2010.09.006.  
  
J. M. TenBarge, W. Daughton, H. Karimabadi, G. G. Howesand W. Dorland, “Collisionless reconnection in the large guide field regime: Gyrokinetic versus particle-in-cell simulations”, *Physics of Plasmas*, vol. 21, no. 2. AIP Publishing, p. 020708, Feb. 2014. doi: 10.1063/1.4867068.  
  
J. M. TenBarge and G. G. Howes, “Evidence of critical balance in kinetic Alfvén wave turbulence simulations”, *Physics of Plasmas*, vol. 19, no. 5. AIP Publishing, p. 055901, May 2012. doi: 10.1063/1.3693974.  
  
J. M. TenBarge, G. G. Howesand W. Dorland, “COLLISIONLESS DAMPING AT ELECTRON SCALES IN SOLAR WIND TURBULENCE”, *The Astrophysical Journal*, vol. 774, no. 2. American Astronomical Society, p. 139, Aug. 26, 2013. doi: 10.1088/0004-637x/774/2/139.  
  
J. M. TenBarge, G. G. Howes, W. Dorlandand G. W. Hammett, “An oscillating Langevin antenna for driving plasma turbulence simulations”, *Computer Physics Communications*, vol. 185, no. 2. Elsevier BV, pp. 578–589, Feb. 2014. doi: 10.1016/j.cpc.2013.10.022.  
  
J. M. TenBarge, J. J. Podesta, K. G. Kleinand G. G. Howes, “INTERPRETING MAGNETIC VARIANCE ANISOTROPY MEASUREMENTS IN THE SOLAR WIND”, *The Astrophysical Journal*, vol. 753, no. 2. American Astronomical Society, p. 107, Jun. 19, 2012. doi: 10.1088/0004-637x/753/2/107.  
  
J. L. Verniero and G. G. Howes, “The Alfvénic nature of energy transfer mediation in localized, strongly nonlinear Alfvén wavepacket collisions”, *Journal of Plasma Physics*, vol. 84, no. 1. Cambridge University Press (CUP), Jan. 30, 2018. doi: 10.1017/s0022377818000090.  
  
J. L. Verniero, G. G. Howesand K. G. Klein, “Nonlinear energy transfer and current sheet development in localized Alfvén wavepacket collisions in the strong turbulence limit”, *Journal of Plasma Physics*, vol. 84, no. 1. Cambridge University Press (CUP), Jan. 17, 2018. doi: 10.1017/s0022377817001003.  
  
C. Palenzuela, “Effects of the microphysical equation of state in the mergers of magnetized neutron stars with neutrino cooling”, *Physical Review D*, vol. 92, no. 4. American Physical Society (APS), Aug. 25, 2015. doi: 10.1103/physrevd.92.044045.  
  
S. Chang, F.-B. Tian, H. Luo, J. F. Doyleand B. Rousseau, “The Role of Finite Displacements in Vocal Fold Modeling”, *Journal of Biomechanical Engineering*, vol. 135, no. 11. ASME International, Oct. 01, 2013. doi: 10.1115/1.4025330.  
  
H. Luo, H. Dai, J. Songand J. Doyle, “Effect of pre-existing camber on fluid–structure interaction of cicada wings”, *51st AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition*. American Institute of Aeronautics and Astronautics, Jan. 05, 2013. doi: 10.2514/6.2013-952.  
  
H. Luo, H. Dai, S. S. Das, J. Songand J. Doyle, “Toward high-fidelity modeling of the fluid-structure interaction for insect wings”, *50th AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition*. American Institute of Aeronautics and Astronautics, Jan. 09, 2012. doi: 10.2514/6.2012-1212.  
  
H. Luo, B. Yin, H. Daiand J. Doyle, “A 3D Computational Study of the Flow-Structure Interaction in Flapping Flight”, *48th AIAA Aerospace Sciences Meeting Including the New Horizons Forum and Aerospace Exposition*. American Institute of Aeronautics and Astronautics, Jan. 04, 2010. doi: 10.2514/6.2010-556.  
  
F.-B. Tian, H. Luo, J. Songand X.-Y. Lu, “Force production and asymmetric deformation of a flexible flapping wing in forward flight”, *Journal of Fluids and Structures*, vol. 36. Elsevier BV, pp. 149–161, Jan. 2013. doi: 10.1016/j.jfluidstructs.2012.07.006.  
  
D. Meral and B. Urbanc, “Discrete Molecular Dynamics Study of Oligomer Formation by N-Terminally Truncated Amyloid β-Protein”, *Journal of Molecular Biology*, vol. 425, no. 12. Elsevier BV, pp. 2260–2275, Jun. 2013. doi: 10.1016/j.jmb.2013.03.010.  
  
S. Toal, D. Meral, D. Verbaro, B. Urbancand R. Schweitzer-Stenner, “pH-Independence of Trialanine and the Effects of Termini Blocking in Short Peptides: A Combined Vibrational, NMR, UVCD, and Molecular Dynamics Study”, *The Journal of Physical Chemistry B*, vol. 117, no. 14. American Chemical Society (ACS), pp. 3689–3706, Mar. 28, 2013. doi: 10.1021/jp310466b.  
  
E. Abdikamalov, “NEUTRINO-DRIVEN TURBULENT CONVECTION AND STANDING ACCRETION SHOCK INSTABILITY IN THREE-DIMENSIONAL CORE-COLLAPSE SUPERNOVAE”, *The Astrophysical Journal*, vol. 808, no. 1. American Astronomical Society, p. 70, Jul. 17, 2015. doi: 10.1088/0004-637x/808/1/70.  
  
J. Blackman, “Numerical relativity waveform surrogate model for generically precessing binary black hole mergers”, *Physical Review D*, vol. 96, no. 2. American Physical Society (APS), Jul. 31, 2017. doi: 10.1103/physrevd.96.024058.  
  
D. Clausen, A. L. Piroand C. D. Ott, “THE BLACK HOLE FORMATION PROBABILITY”, *The Astrophysical Journal*, vol. 799, no. 2. American Astronomical Society, p. 190, Jan. 28, 2015. doi: 10.1088/0004-637x/799/2/190.  
  
S. M. Couch and C. D. Ott, “THE ROLE OF TURBULENCE IN NEUTRINO-DRIVEN CORE-COLLAPSE SUPERNOVA EXPLOSIONS”, *The Astrophysical Journal*, vol. 799, no. 1. American Astronomical Society, p. 5, Jan. 09, 2015. doi: 10.1088/0004-637x/799/1/5.  
  
W. J. Engels, R. Freyand C. D. Ott, “Multivariate regression analysis of gravitational waves from rotating core collapse”, *Physical Review D*, vol. 90, no. 12. American Physical Society (APS), Dec. 08, 2014. doi: 10.1103/physrevd.90.124026.  
  
J. Lippuner and L. F. Roberts, “r-PROCESS LANTHANIDE PRODUCTION AND HEATING RATES IN KILONOVAE”, *The Astrophysical Journal*, vol. 815, no. 2. American Astronomical Society, p. 82, Dec. 11, 2015. doi: 10.1088/0004-637x/815/2/82.  
  
P. Mösta, “GRHydro: a new open-source general-relativistic magnetohydrodynamics code for the Einstein toolkit”, *Classical and Quantum Gravity*, vol. 31, no. 1. IOP Publishing, p. 015005, Nov. 15, 2013. doi: 10.1088/0264-9381/31/1/015005.  
  
C. D. Ott, “Massive Computation for Understanding Core-Collapse Supernova Explosions”, *Computing in Science & Engineering*, vol. 18, no. 5. Institute of Electrical and Electronics Engineers (IEEE), pp. 78–92, Sep. 2016. doi: 10.1109/mcse.2016.81.  
  
D. Radice, E. Abdikamalov, L. Rezzollaand C. D. Ott, “A new spherical harmonics scheme for multi-dimensional radiation transport I. Static matter configurations”, *Journal of Computational Physics*, vol. 242. Elsevier BV, pp. 648–669, Jun. 2013. doi: 10.1016/j.jcp.2013.01.048.  
  
D. Radice, S. M. Couchand C. D. Ott, “Implicit large eddy simulations of anisotropic weakly compressible turbulence with application to core-collapse supernovae”, *Computational Astrophysics and Cosmology*, vol. 2, no. 1. Springer Science and Business Media LLC, Aug. 21, 2015. doi: 10.1186/s40668-015-0011-0.  
  
D. Radice, F. Galeazzi, J. Lippuner, L. F. Roberts, C. D. Ottand L. Rezzolla, “Dynamical mass ejection from binary neutron star mergers”, *Monthly Notices of the Royal Astronomical Society*, vol. 460, no. 3. Oxford University Press (OUP), pp. 3255–3271, May 23, 2016. doi: 10.1093/mnras/stw1227.  
  
D. Radice, C. D. Ott, E. Abdikamalov, S. M. Couch, R. Haasand E. Schnetter, “NEUTRINO-DRIVEN CONVECTION IN CORE-COLLAPSE SUPERNOVAE: HIGH-RESOLUTION SIMULATIONS”, *The Astrophysical Journal*, vol. 820, no. 1. American Astronomical Society, p. 76, Mar. 22, 2016. doi: 10.3847/0004-637x/820/1/76.  
  
S. Richers, D. Kasen, E. O’Connor, R. Fernándezand C. D. Ott, “MONTE CARLO NEUTRINO TRANSPORT THROUGH REMNANT DISKS FROM NEUTRON STAR MERGERS”, *The Astrophysical Journal*, vol. 813, no. 1. American Astronomical Society, p. 38, Oct. 27, 2015. doi: 10.1088/0004-637x/813/1/38.  
  
S. Richers, C. D. Ott, E. Abdikamalov, E. O’Connorand C. Sullivan, “Equation of state effects on gravitational waves from rotating core collapse”, *Physical Review D*, vol. 95, no. 6. American Physical Society (APS), Mar. 29, 2017. doi: 10.1103/physrevd.95.063019.  
  
L. F. Roberts, C. D. Ott, R. Haas, E. P. O’Connor, P. Dienerand E. Schnetter, “GENERAL-RELATIVISTIC THREE-DIMENSIONAL MULTI-GROUP NEUTRINO RADIATION-HYDRODYNAMICS SIMULATIONS OF CORE-COLLAPSE SUPERNOVAE”, *The Astrophysical Journal*, vol. 831, no. 1. American Astronomical Society, p. 98, Oct. 28, 2016. doi: 10.3847/0004-637x/831/1/98.  
  
A. S. Schneider, L. F. Roberts, C. D. Ottand E. O’Connor, “Equation of state effects in the core collapse of a star”, *Physical Review C*, vol. 100, no. 5. American Physical Society (APS), Nov. 07, 2019. doi: 10.1103/physrevc.100.055802.  
  
J. Blackman, “Fast and Accurate Prediction of Numerical Relativity Waveforms from Binary Black Hole Coalescences Using Surrogate Models”, *Physical Review Letters*, vol. 115, no. 12. American Physical Society (APS), Sep. 18, 2015. doi: 10.1103/physrevlett.115.121102.  
  
L. E. Kidder, “SpECTRE: A task-based discontinuous Galerkin code for relativistic astrophysics”, *Journal of Computational Physics*, vol. 335. Elsevier BV, pp. 84–114, Apr. 2017. doi: 10.1016/j.jcp.2016.12.059.  
  
R. Smith, “Fast and accurate inference on gravitational waves from precessing compact binaries”, *Physical Review D*, vol. 94, no. 4. American Physical Society (APS), Aug. 15, 2016. doi: 10.1103/physrevd.94.044031.  
  
J. M. N. Djiokap, S. X. Hu, W.-C. Jiang, L.-Y. Pengand A. F. Starace, “Enhanced asymmetry in few-cycle attosecond pulse ionization of He in the vicinity of autoionizing resonances”, *New Journal of Physics*, vol. 14, no. 9. IOP Publishing, p. 095010, Sep. 13, 2012. doi: 10.1088/1367-2630/14/9/095010.  
  
W. E. East, V. Paschalidisand F. Pretorius, “ECCENTRIC MERGERS OF BLACK HOLES WITH SPINNING NEUTRON STARS”, *The Astrophysical Journal*, vol. 807, no. 1. American Astronomical Society, p. L3, Jun. 25, 2015. doi: 10.1088/2041-8205/807/1/l3.  
  
W. E. East, V. Paschalidisand F. Pretorius, “Equation of state effects and one-arm spiral instability in hypermassive neutron stars formed in eccentric neutron star mergers”, *Classical and Quantum Gravity*, vol. 33, no. 24. IOP Publishing, p. 244004, Dec. 01, 2016. doi: 10.1088/0264-9381/33/24/244004.  
  
W. E. East, V. Paschalidis, F. Pretoriusand S. L. Shapiro, “Relativistic simulations of eccentric binary neutron star mergers: One-arm spiral instability and effects of neutron star spin”, *Physical Review D*, vol. 93, no. 2. American Physical Society (APS), Jan. 08, 2016. doi: 10.1103/physrevd.93.024011.  
  
V. Paschalidis, W. E. East, F. Pretoriusand S. L. Shapiro, “One-arm spiral instability in hypermassive neutron stars formed by dynamical-capture binary neutron star mergers”, *Physical Review D*, vol. 92, no. 12. American Physical Society (APS), Dec. 30, 2015. doi: 10.1103/physrevd.92.121502.  
  
H. Che, M. L. Goldsteinand A. F. Viñas, “Bidirectional Energy Cascades and the Origin of Kinetic Alfvénic and Whistler Turbulence in the Solar Wind”, *Physical Review Letters*, vol. 112, no. 6. American Physical Society (APS), Feb. 11, 2014. doi: 10.1103/physrevlett.112.061101.  
  
W. A. Al-Saidi, H. Fengand K. A. Fichthorn, “Adsorption of Polyvinylpyrrolidone on Ag Surfaces: Insight into a Structure-Directing Agent”, *Nano Letters*, vol. 12, no. 2. American Chemical Society (ACS), pp. 997–1001, Jan. 04, 2012. doi: 10.1021/nl2041113.  
  
S. Akula, “Interpreting the first CMS and ATLAS SUSY results”, *Physics Letters B*, vol. 699, no. 5. Elsevier BV, pp. 377–382, May 2011. doi: 10.1016/j.physletb.2011.04.041.  
  
S. Akula, M. Liu, P. Nathand G. Peim, “Naturalness, supersymmetry and implications for LHC and dark matter”, *Physics Letters B*, vol. 709, no. 3. Elsevier BV, pp. 192–199, Mar. 2012. doi: 10.1016/j.physletb.2012.01.077.  
  
J. Walker and S. Boldyrev, “Magnetorotational dynamo action in the shearing box”, *Monthly Notices of the Royal Astronomical Society*, vol. 470, no. 3. Oxford University Press (OUP), pp. 2653–2658, Apr. 28, 2017. doi: 10.1093/mnras/stx1032.  
  
J. Walker, S. Boldyrevand N. F. Loureiro, “Influence of tearing instability on magnetohydrodynamic turbulence”, *Physical Review E*, vol. 98, no. 3. American Physical Society (APS), Sep. 24, 2018. doi: 10.1103/physreve.98.033209.  
  
J. Walker, G. Lesurand S. Boldyrev, “On the nature of magnetic turbulence in rotating, shearing flows”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 457, no. 1. Oxford University Press (OUP), pp. L39–L43, Jan. 05, 2016. doi: 10.1093/mnrasl/slv200.  
  
V. Zhdankin, J. Walker, S. Boldyrevand G. Lesur, “Universal small-scale structure in turbulence driven by magnetorotational instability”, *Monthly Notices of the Royal Astronomical Society*, vol. 467, no. 3. Oxford University Press (OUP), pp. 3620–3627, Feb. 14, 2017. doi: 10.1093/mnras/stx372.  
  
I. A. Jou, D. V. Melnikov, A. Nadtochiyand M. E. Gracheva, “Charged particle separation by an electrically tunable nanoporous membrane”, *Nanotechnology*, vol. 25, no. 14. IOP Publishing, p. 145201, Mar. 12, 2014. doi: 10.1088/0957-4484/25/14/145201.  
  
S. Hong and T. S. Rahman, “Rationale for the Higher Reactivity of Interfacial Sites in Methanol Decomposition on Au13/TiO2(110)”, *Journal of the American Chemical Society*, vol. 135, no. 20. American Chemical Society (ACS), pp. 7629–7635, May 09, 2013. doi: 10.1021/ja4010738.  
  
M. A. Ajaib, I. Gogoladze, Q. Shafiand C. S. Ün, “A predictive Yukawa unified SO(10) model: Higgs and sparticle masses”, *Journal of High Energy Physics*, vol. 2013, no. 7. Springer Science and Business Media LLC, Jul. 2013. doi: 10.1007/jhep07(2013)139.  
  
M. A. Ajaib, I. Gogoladze, Q. Shafiand C. S. Ün, “Split sfermion families, Yukawa unification and muon g − 2”, *Journal of High Energy Physics*, vol. 2014, no. 5. Springer Science and Business Media LLC, May 2014. doi: 10.1007/jhep05(2014)079.  
  
K. S. Babu, I. Gogoladze, Q. Shafiand C. S. Ün, “Muon, 125 GeV Higgs boson, and neutralino dark matter in a flavor symmetry-based MSSM”, *Physical Review D*, vol. 90, no. 11. American Physical Society (APS), Dec. 16, 2014. doi: 10.1103/physrevd.90.116002.  
  
D. A. Demir and C. S. Ün, “Stop on top: SUSY parameter regions and fine-tuning constraints”, *Physical Review D*, vol. 90, no. 9. American Physical Society (APS), Nov. 17, 2014. doi: 10.1103/physrevd.90.095015.  
  
I. Gogoladze, A. Mustafayev, Q. Shafiand C. S. Ün, “Yukawa unification and sparticle spectroscopy in gauge mediation models”, *Physical Review D*, vol. 91, no. 9. American Physical Society (APS), May 18, 2015. doi: 10.1103/physrevd.91.096005.  
  
I. Gogoladze, F. Nasir, Q. Shafiand C. S. Ün, “Nonuniversal gaugino masses and muon”, *Physical Review D*, vol. 90, no. 3. American Physical Society (APS), Aug. 11, 2014. doi: 10.1103/physrevd.90.035008.  
  
I. Gogoladze, Q. Shafiand C. S. Ün, “125 GeV Higgs boson from t-b-τ Yukawa unification”, *Journal of High Energy Physics*, vol. 2012, no. 7. Springer Science and Business Media LLC, Jul. 2012. doi: 10.1007/jhep07(2012)055.  
  
I. Gogoladze, Q. Shafiand C. S. Ün, “Higgs boson mass from t-b-τ Yukawa unification”, *Journal of High Energy Physics*, vol. 2012, no. 8. Springer Science and Business Media LLC, Aug. 2012. doi: 10.1007/jhep08(2012)028.  
  
S. Raza, Q. Shafiand C. S. Ün, “NLSP gluino and NLSP stop scenarios fromYukawa unification”, *Physical Review D*, vol. 92, no. 5. American Physical Society (APS), Sep. 09, 2015. doi: 10.1103/physrevd.92.055010.  
  
M. Banik, “Surface-Enhanced Raman Trajectories on a Nano-Dumbbell: Transition from Field to Charge Transfer Plasmons as the Spheres Fuse”, *ACS Nano*, vol. 6, no. 11. American Chemical Society (ACS), pp. 10343–10354, Oct. 29, 2012. doi: 10.1021/nn304277n.  
  
M. Banik, “Surface-Enhanced Raman Scattering of a Single Nanodumbbell: Dibenzyldithio-Linked Silver Nanospheres”, *The Journal of Physical Chemistry C*, vol. 116, no. 18. American Chemical Society (ACS), pp. 10415–10423, Apr. 30, 2012. doi: 10.1021/jp302013k.  
  
M. Banik, “Surface-Enhanced Raman Scattering of a Single Nanodumbbell: Dibenzyldithio-Linked Silver Nanospheres”, *The Journal of Physical Chemistry C*, vol. 116, no. 18. American Chemical Society (ACS), pp. 10415–10423, Apr. 30, 2012. doi: 10.1021/jp302013k.  
  
S. K. Pal, A. S. Mereshchenko, E. V. Butaeva, P. Z. El-Khouryand A. N. Tarnovsky, “Global sampling of the photochemical reaction paths of bromoform by ultrafast deep-UV through near-IR transient absorption and *ab initio* multiconfigurational calculations”, *The Journal of Chemical Physics*, vol. 138, no. 12. AIP Publishing, p. 124501, Mar. 28, 2013. doi: 10.1063/1.4789268.  
  
E. Altiere, D. P. Fahey, M. W. Noel, R. J. Smithand T. J. Carroll, “Dipole-dipole interaction between rubidium Rydberg atoms”, *Physical Review A*, vol. 84, no. 5. American Physical Society (APS), Nov. 28, 2011. doi: 10.1103/physreva.84.053431.  
  
A. Cheng, A. Hasenfratz, Y. Liu, G. Petropoulosand D. Schaich, “Finite size scaling of conformal theories in the presence of a near-marginal operator”, *Physical Review D*, vol. 90, no. 1. American Physical Society (APS), Jul. 23, 2014. doi: 10.1103/physrevd.90.014509.  
  
A. Cheng, A. Hasenfratz, Y. Liu, G. Petropoulosand D. Schaich, “Improving the continuum limit of gradient flow step scaling”, *Journal of High Energy Physics*, vol. 2014, no. 5. Springer Science and Business Media LLC, May 2014. doi: 10.1007/jhep05(2014)137.  
  
A. Cheng, A. Hasenfratz, G. Petropoulosand D. Schaich, “Scale-dependent mass anomalous dimension from Dirac eigenmodes”, *Journal of High Energy Physics*, vol. 2013, no. 7. Springer Science and Business Media LLC, Jul. 2013. doi: 10.1007/jhep07(2013)061.  
  
A. Hasenfratz, A. Cheng, G. Petropoulosand D. Schaich, “Reaching the Chiral Limit in Many Flavor Systems”, *Strong Coupling Gauge Theories in the LHC Perspective (SCGT12)*. WORLD SCIENTIFIC, Jan. 27, 2014. doi: 10.1142/9789814566254\_0004.  
  
J. Brunnemann and D. Rideout, “Oriented matroids—combinatorial structures underlying loop quantum gravity”, *Classical and Quantum Gravity*, vol. 27, no. 20. IOP Publishing, p. 205008, Sep. 08, 2010. doi: 10.1088/0264-9381/27/20/205008.  
  
D. Krioukov, M. Kitsak, R. S. Sinkovits, D. Rideout, D. Meyerand M. Boguñá, “Network Cosmology”, *Scientific Reports*, vol. 2, no. 1. Springer Science and Business Media LLC, Nov. 16, 2012. doi: 10.1038/srep00793.  
  
J. M. N. Djiokap, A. V. Meremianin, N. L. Manakov, S. X. Hu, L. B. Madsenand A. F. Starace, “Kinematical vortices in double photoionization of helium by attosecond pulses”, *Physical Review A*, vol. 96, no. 1. American Physical Society (APS), Jul. 07, 2017. doi: 10.1103/physreva.96.013405.  
  
J. M. N. Djiokap, A. V. Meremianin, N. L. Manakov, L. B. Madsen, S. X. Huand A. F. Starace, “Molecular Symmetry-Mixed Dichroism in Double Photoionization of ”, *Physical Review Letters*, vol. 123, no. 14. American Physical Society (APS), Oct. 02, 2019. doi: 10.1103/physrevlett.123.143202.  
  
J. M. N. Djiokap and A. F. Starace, “Doubly-excited state effects on two-photon double ionization of helium by time-delayed, oppositely circularly-polarized attosecond pulses”, *Journal of Optics*, vol. 19, no. 12. IOP Publishing, p. 124003, Oct. 30, 2017. doi: 10.1088/2040-8986/aa8fc0.  
  
J. M. Ngoko Djiokap, S. X. Hu, L. B. Madsen, N. L. Manakov, A. V. Meremianinand A. F. Starace, “Electron Vortices in Photoionization by Circularly Polarized Attosecond Pulses”, *Physical Review Letters*, vol. 115, no. 11. American Physical Society (APS), Sep. 10, 2015. doi: 10.1103/physrevlett.115.113004.  
  
J. M. Ngoko Djiokap, A. V. Meremianin, N. L. Manakov, S. X. Hu, L. B. Madsenand A. F. Starace, “Multistart spiral electron vortices in ionization by circularly polarized UV pulses”, *Physical Review A*, vol. 94, no. 1. American Physical Society (APS), Jul. 12, 2016. doi: 10.1103/physreva.94.013408.  
  
J. M. Ngoko Djiokap, A. V. Meremianin, N. L. Manakov, L. B. Madsen, S. X. Huand A. F. Starace, “Dynamical electron vortices in attosecond double photoionization of ”, *Physical Review A*, vol. 98, no. 6. American Physical Society (APS), Dec. 07, 2018. doi: 10.1103/physreva.98.063407.  
  
J. M. Ngoko Djiokap and A. F. Starace, “Origin of the multiphoton-regime harmonic-generation plateau structure”, *Physical Review A*, vol. 102, no. 1. American Physical Society (APS), Jul. 06, 2020. doi: 10.1103/physreva.102.013103.  
  
G. C. Bower, “THE PROPER MOTION OF THE GALACTIC CENTER PULSAR RELATIVE TO SAGITTARIUS A*”, The Astrophysical Journal, vol. 798, no. 2. American Astronomical Society, p. 120, Jan. 08, 2015. doi: 10.1088/0004-637x/798/2/120.*  
  
*C. D. Brinkerink, “ALMA and VLA measurements of frequency-dependent time lags in Sagittarius A*: evidence for a relativistic outflow”, *Astronomy & Astrophysics*, vol. 576. EDP Sciences, p. A41, Mar. 24, 2015. doi: 10.1051/0004-6361/201424783.  
  
C.-K. Chan, D. Psaltis, F. Özel, R. Narayanand A. Sa¸dowski, “THE POWER OF IMAGING: CONSTRAINING THE PLASMA PROPERTIES OF GRMHD SIMULATIONS USING EHT OBSERVATIONS OF Sgr A*”, The Astrophysical Journal, vol. 799, no. 1. American Astronomical Society, p. 1, Jan. 09, 2015. doi: 10.1088/0004-637x/799/1/1.*  
  
*J. Dexter, E. Agol, P. C. Fragileand J. C. McKinney, “Radiative Models of Sagittarius A* and M87 from Relativistic MHD Simulations”, *Journal of Physics: Conference Series*, vol. 372. IOP Publishing, p. 012023, Jul. 30, 2012. doi: 10.1088/1742-6596/372/1/012023.  
  
J. Dexter, B. Kelly, G. C. Bower, D. P. Marrone, J. Stoneand R. Plambeck, “An 8 h characteristic time-scale in submillimetre light curves of Sagittarius A*”, Monthly Notices of the Royal Astronomical Society, vol. 442, no. 3. Oxford University Press (OUP), pp. 2797–2808, Jun. 26, 2014. doi: 10.1093/mnras/stu1039.*  
  
*J. Dexter, J. C. McKinneyand E. Agol, “The size of the jet launching region in M87”, Monthly Notices of the Royal Astronomical Society, vol. 421, no. 2. Oxford University Press (OUP), pp. 1517–1528, Feb. 06, 2012. doi: 10.1111/j.1365-2966.2012.20409.x.*  
  
*J. Dexter, J. C. McKinney, S. Markoffand A. Tchekhovskoy, “Transient jet formation and state transitions from large-scale magnetic reconnection in black hole accretion discs”, Monthly Notices of the Royal Astronomical Society, vol. 440, no. 3. Oxford University Press (OUP), pp. 2185–2190, Mar. 28, 2014. doi: 10.1093/mnras/stu581.*  
  
*S. S. Doeleman, “Jet-Launching Structure Resolved Near the Supermassive Black Hole in M87”, Science, vol. 338, no. 6105. American Association for the Advancement of Science (AAAS), pp. 355–358, Oct. 19, 2012. doi: 10.1126/science.1224768.*  
  
*V. L. Fish, “IMAGING AN EVENT HORIZON: MITIGATION OF SCATTERING TOWARD SAGITTARIUS A*”, *The Astrophysical Journal*, vol. 795, no. 2. American Astronomical Society, p. 134, Oct. 22, 2014. doi: 10.1088/0004-637x/795/2/134.  
  
F. Foucart, M. Chandra, C. F. Gammieand E. Quataert, “Evolution of accretion discs around a kerr black hole using extended magnetohydrodynamics”, *Monthly Notices of the Royal Astronomical Society*, vol. 456, no. 2. Oxford University Press (OUP), pp. 1332–1345, Dec. 23, 2015. doi: 10.1093/mnras/stv2687.  
  
M. Inoue, “Greenland telescope project: Direct confirmation of black hole with sub‐millimeter VLBI”, *Radio Science*, vol. 49, no. 7. American Geophysical Union (AGU), pp. 564–571, Jul. 2014. doi: 10.1002/2014rs005450.  
  
T. Johannsen, “MASSES OF NEARBY SUPERMASSIVE BLACK HOLES WITH VERY LONG BASELINE INTERFEROMETRY”, *The Astrophysical Journal*, vol. 758, no. 1. American Astronomical Society, p. 30, Sep. 21, 2012. doi: 10.1088/0004-637x/758/1/30.  
  
M. D. Johnson, V. L. Fish, S. S. Doeleman, A. E. Broderick, J. F. C. Wardleand D. P. Marrone, “RELATIVE ASTROMETRY OF COMPACT FLARING STRUCTURES IN Sgr A\* WITH POLARIMETRIC VERY LONG BASELINE INTERFEROMETRY”, *The Astrophysical Journal*, vol. 794, no. 2. American Astronomical Society, p. 150, Oct. 06, 2014. doi: 10.1088/0004-637x/794/2/150.  
  
M. D. Johnson, “Resolved magnetic-field structure and variability near the event horizon of Sagittarius A*”, Science, vol. 350, no. 6265. American Association for the Advancement of Science (AAAS), pp. 1242–1245, Dec. 04, 2015. doi: 10.1126/science.aac7087.*  
  
*H. S. Krawczynski, “X-ray polarimetry with the Polarization Spectroscopic Telescope Array (PolSTAR)”, Astroparticle Physics, vol. 75. Elsevier BV, pp. 8–28, Feb. 2016. doi: 10.1016/j.astropartphys.2015.10.009.*  
  
*J.-P. Lasota, E. Gourgoulhon, M. Abramowicz, A. Tchekhovskoyand R. Narayan, “Extracting black-hole rotational energy: The generalized Penrose process”, Physical Review D, vol. 89, no. 2. American Physical Society (APS), Jan. 31, 2014. doi: 10.1103/physrevd.89.024041.*  
  
*R.-S. Lu, “IMAGING THE SUPERMASSIVE BLACK HOLE SHADOW AND JET BASE OF M87 WITH THE EVENT HORIZON TELESCOPE”, The Astrophysical Journal, vol. 788, no. 2. American Astronomical Society, p. 120, May 29, 2014. doi: 10.1088/0004-637x/788/2/120.*  
  
*R.-S. Lu, “FINE-SCALE STRUCTURE OF THE QUASAR 3C 279 MEASURED WITH 1.3 mm VERY LONG BASELINE INTERFEROMETRY”, The Astrophysical Journal, vol. 772, no. 1. American Astronomical Society, p. 13, Jun. 28, 2013. doi: 10.1088/0004-637x/772/1/13.*  
  
*R.-S. Lu, “RESOLVING THE INNER JET STRUCTURE OF 1924-292 WITH THE EVENT HORIZON TELESCOPE”, The Astrophysical Journal, vol. 757, no. 1. American Astronomical Society, p. L14, Sep. 04, 2012. doi: 10.1088/2041-8205/757/1/l14.*  
  
*J. C. McKinney, “Probing Black Hole Gravity”, Science, vol. 337, no. 6097. American Association for the Advancement of Science (AAAS), pp. 916–917, Aug. 24, 2012. doi: 10.1126/science.1227083.*  
  
*J. C. McKinney, L. Daiand M. J. Avara, “Efficiency of super-Eddington magnetically-arrested accretion”, Monthly Notices of the Royal Astronomical Society: Letters, vol. 454, no. 1. Oxford University Press (OUP), pp. L6–L10, Sep. 08, 2015. doi: 10.1093/mnrasl/slv115.*  
  
*J. C. McKinney, A. Tchekhovskoyand R. D. Blandford, “General relativistic magnetohydrodynamic simulations of magnetically choked accretion flows around black holes”, Monthly Notices of the Royal Astronomical Society, vol. 423, no. 4. Oxford University Press (OUP), pp. 3083–3117, Jun. 01, 2012. doi: 10.1111/j.1365-2966.2012.21074.x.*  
  
*J. C. McKinney, A. Tchekhovskoyand R. D. Blandford, “Alignment of Magnetized Accretion Disks and Relativistic Jets with Spinning Black Holes”, Science, vol. 339, no. 6115. American Association for the Advancement of Science (AAAS), pp. 49–52, Jan. 04, 2013. doi: 10.1126/science.1230811.*  
  
*J. C. McKinney, A. Tchekhovskoy, A. Sadowskiand R. Narayan, “Three-dimensional general relativistic radiation magnetohydrodynamical simulation of super-Eddington accretion, using a new code harmrad with M1 closure”, Monthly Notices of the Royal Astronomical Society, vol. 441, no. 4. Oxford University Press (OUP), pp. 3177–3208, May 30, 2014. doi: 10.1093/mnras/stu762.*  
  
*J. C. McKinney and D. A. Uzdensky, “A reconnection switch to trigger gamma-ray burst jet dissipation”, Monthly Notices of the Royal Astronomical Society, vol. 419, no. 1. Oxford University Press (OUP), pp. 573–607, Nov. 02, 2011. doi: 10.1111/j.1365-2966.2011.19721.x.*  
  
*R. F. Penna, A. Sądowski, A. K. Kulkarniand R. Narayan, “The Shakura-Sunyaev viscosity prescription with variable α (r)”, Monthly Notices of the Royal Astronomical Society, vol. 428, no. 3. Oxford University Press (OUP), pp. 2255–2274, Nov. 09, 2012. doi: 10.1093/mnras/sts185.*  
  
*R. F. Penna, A. Sądowskiand J. C. McKinney, “Thin-disc theory with a non-zero-torque boundary condition and comparisons with simulations”, Monthly Notices of the Royal Astronomical Society, vol. 420, no. 1. Oxford University Press (OUP), pp. 684–698, Dec. 15, 2011. doi: 10.1111/j.1365-2966.2011.20084.x.*  
  
*R. L. Plambeck, “PROBING THE PARSEC-SCALE ACCRETION FLOW OF 3C 84 WITH MILLIMETER WAVELENGTH POLARIMETRY”, The Astrophysical Journal, vol. 797, no. 1. American Astronomical Society, p. 66, Nov. 24, 2014. doi: 10.1088/0004-637x/797/1/66.*  
  
*D. Psaltis, R. Narayan, V. L. Fish, A. E. Broderick, A. Loeband S. S. Doeleman, “EVENT HORIZON TELESCOPE EVIDENCE FOR ALIGNMENT OF THE BLACK HOLE IN THE CENTER OF THE MILKY WAY WITH THE INNER STELLAR DISK”, The Astrophysical Journal, vol. 798, no. 1. American Astronomical Society, p. 15, Dec. 15, 2014. doi: 10.1088/0004-637x/798/1/15.*  
  
*H. R. Russell, A. C. Fabian, B. R. McNamaraand A. E. Broderick, “Inside the Bondi radius of M87”, Monthly Notices of the Royal Astronomical Society, vol. 451, no. 1. Oxford University Press (OUP), pp. 588–600, May 28, 2015. doi: 10.1093/mnras/stv954.*  
  
*A. Sądowski, R. Narayan, J. C. McKinneyand A. Tchekhovskoy, “Numerical simulations of super-critical black hole accretion flows in general relativity”, Monthly Notices of the Royal Astronomical Society, vol. 439, no. 1. Oxford University Press (OUP), pp. 503–520, Jan. 30, 2014. doi: 10.1093/mnras/stt2479.*  
  
*A. Sądowski, R. Narayan, A. Tchekhovskoyand Y. Zhu, “Semi-implicit scheme for treating radiation under M1 closure in general relativistic conservative fluid dynamics codes”, Monthly Notices of the Royal Astronomical Society, vol. 429, no. 4. Oxford University Press (OUP), pp. 3533–3550, Jan. 11, 2013. doi: 10.1093/mnras/sts632.*  
  
*R. V. Shcherbakov and J. C. McKinney, “SUBMILLIMETER QUASI-PERIODIC OSCILLATIONS IN MAGNETICALLY CHOKED ACCRETION FLOW MODELS OF SgrA*”, *The Astrophysical Journal*, vol. 774, no. 2. American Astronomical Society, p. L22, Aug. 23, 2013. doi: 10.1088/2041-8205/774/2/l22.  
  
R. V. Shcherbakov, R. F. Pennaand J. C. McKinney, “SAGITTARIUS A\* ACCRETION FLOW AND BLACK HOLE PARAMETERS FROM GENERAL RELATIVISTIC DYNAMICAL AND POLARIZED RADIATIVE MODELING”, *The Astrophysical Journal*, vol. 755, no. 2. American Astronomical Society, p. 133, Aug. 02, 2012. doi: 10.1088/0004-637x/755/2/133.  
  
R. V. Shcherbakov, R. F. Pennaand J. C. McKinney, “Constraining the Accretion Flow in Sgr A\* by General Relativistic Dynamical and Polarized Radiative Modeling”, *Proceedings of the International Astronomical Union*, vol. 8, no. S290. Cambridge University Press (CUP), pp. 309–310, Aug. 2012. doi: 10.1017/s1743921312020157.  
  
A. Shulevski, “The peculiar radio galaxy 4C 35.06: a case for recurrent AGN activity?”, *Astronomy & Astrophysics*, vol. 579. EDP Sciences, p. A27, Jun. 22, 2015. doi: 10.1051/0004-6361/201425416.  
  
R. D. Starr, C. E. Schlemm II, G. C. Ho, L. R. Nittler, R. E. Goldand S. C. Solomon, “Calibration of the MESSENGER X-Ray Spectrometer”, *Planetary and Space Science*, vol. 122. Elsevier BV, pp. 13–25, Mar. 2016. doi: 10.1016/j.pss.2016.01.003.  
  
A. Sądowski, R. Narayan, A. Tchekhovskoy, D. Abarca, Y. Zhuand J. C. McKinney, “Global simulations of axisymmetric radiative black hole accretion discs in general relativity with a mean-field magnetic dynamo”, *Monthly Notices of the Royal Astronomical Society*, vol. 447, no. 1. Oxford University Press (OUP), pp. 49–71, Dec. 12, 2014. doi: 10.1093/mnras/stu2387.  
  
A. Tchekhovskoy, J. C. McKinneyand R. Narayan, “General Relativistic Modeling of Magnetized Jets from Accreting Black Holes”, *Journal of Physics: Conference Series*, vol. 372. IOP Publishing, p. 012040, Jul. 30, 2012. doi: 10.1088/1742-6596/372/1/012040.  
  
L. Vertatschitsch, “R2DBE: A Wideband Digital Backend for the Event Horizon Telescope”, *Publications of the Astronomical Society of the Pacific*, vol. 127, no. 958. IOP Publishing, pp. 1226–1239, Dec. 2015. doi: 10.1086/684513.  
  
J. Wagner, “First 230 GHz VLBI fringes on 3C 279 using the APEX Telescope”, *Astronomy & Astrophysics*, vol. 581. EDP Sciences, p. A32, Aug. 27, 2015. doi: 10.1051/0004-6361/201423613.  
  
A. R. Whitney, “Demonstration of a 16 Gbps Station-1Broadband-RF VLBI System”, *Publications of the Astronomical Society of the Pacific*, vol. 125, no. 924. IOP Publishing, pp. 196–203, Feb. 2013. doi: 10.1086/669718.  
  
X. Yang and A. Hassanein, “Molecular dynamics simulation of deuterium trapping and bubble formation in tungsten”, *Journal of Nuclear Materials*, vol. 434, no. 1–3. Elsevier BV, pp. 1–6, Mar. 2013. doi: 10.1016/j.jnucmat.2012.10.045.  
  
X. Yang and A. Hassanein, “Molecular dynamics simulation of erosion and surface evolution of tungsten due to bombardment with deuterium and carbon in Tokamak fusion environments”, *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, vol. 308. Elsevier BV, pp. 80–87, Aug. 2013. doi: 10.1016/j.nimb.2013.05.012.  
  
W. Horton, M. Goniche, Y. Peysson, J. Decker, A. Ekedahland X. Litaudon, “Penetration of lower hybrid current drive waves in tokamaks”, *Physics of Plasmas*, vol. 20, no. 11. AIP Publishing, p. 112508, Nov. 2013. doi: 10.1063/1.4831981.  
  
M. Adeel Ajaib, I. Gogoladze, F. Nasirand Q. Shafi, “Revisiting mGMSB in light of a 125 GeV Higgs”, *Physics Letters B*, vol. 713, no. 4–5. Elsevier BV, pp. 462–468, Jul. 2012. doi: 10.1016/j.physletb.2012.06.036.  
  
J. Healy and P. Laguna, “Critical collapse of scalar fields beyond axisymmetry”, *General Relativity and Gravitation*, vol. 46, no. 5. Springer Science and Business Media LLC, Apr. 08, 2014. doi: 10.1007/s10714-014-1722-2.  
  
J. Healy, P. Lagunaand D. Shoemaker, “Decoding the final state in binary black hole mergers”, *Classical and Quantum Gravity*, vol. 31, no. 21. IOP Publishing, p. 212001, Oct. 16, 2014. doi: 10.1088/0264-9381/31/21/212001.  
  
K. Jani, J. Healy, J. A. Clark, L. London, P. Lagunaand D. Shoemaker, “Georgia tech catalog of gravitational waveforms”, *Classical and Quantum Gravity*, vol. 33, no. 20. IOP Publishing, p. 204001, Sep. 26, 2016. doi: 10.1088/0264-9381/33/20/204001.  
  
D. Shoemaker, K. Jani, L. Londonand L. Pekowsky, “Connecting Numerical Relativity and Data Analysis of Gravitational Wave Detectors”, *Gravitational Wave Astrophysics*. Springer International Publishing, pp. 245–258, Nov. 10, 2014. doi: 10.1007/978-3-319-10488-1\_21.  
  
H. Sotani, K. D. Kokkotas, P. Lagunaand C. F. Sopuerta, “Electromagnetic waves from neutron stars and black holes driven by polar gravitational perturbations”, *General Relativity and Gravitation*, vol. 46, no. 3. Springer Science and Business Media LLC, Feb. 21, 2014. doi: 10.1007/s10714-014-1675-5.  
  
E. D. Cubuk, W. L. Wang, K. Zhao, J. J. Vlassak, Z. Suoand E. Kaxiras, “Morphological Evolution of Si Nanowires upon Lithiation: A First-Principles Multiscale Model”, *Nano Letters*, vol. 13, no. 5. American Chemical Society (ACS), pp. 2011–2015, Apr. 02, 2013. doi: 10.1021/nl400132q.  
  
C. H. K. Chen, L. Leung, S. Boldyrev, B. A. Marucaand S. D. Bale, “Ion‐scale spectral break of solar wind turbulence at high and low beta”, *Geophysical Research Letters*, vol. 41, no. 22. American Geophysical Union (AGU), pp. 8081–8088, Nov. 25, 2014. doi: 10.1002/2014gl062009.  
  
J. Mason, S. Boldyrev, F. Cattaneoand J. C. Perez, “The statistics of a passive scalar in field-guided magnetohydrodynamic turbulence”, *Geophysical & Astrophysical Fluid Dynamics*, vol. 108, no. 6. Informa UK Limited, pp. 686–695, Oct. 13, 2014. doi: 10.1080/03091929.2014.964231.  
  
V. Zhdankin, S. Boldyrev, J. C. Perezand S. M. Tobias, “ENERGY DISSIPATION IN MAGNETOHYDRODYNAMIC TURBULENCE: COHERENT STRUCTURES OR “NANOFLARES”?”, *The Astrophysical Journal*, vol. 795, no. 2. American Astronomical Society, p. 127, Oct. 22, 2014. doi: 10.1088/0004-637x/795/2/127.  
  
V. Zhdankin, D. A. Uzdenskyand S. Boldyrev, “Temporal Intermittency of Energy Dissipation in Magnetohydrodynamic Turbulence”, *Physical Review Letters*, vol. 114, no. 6. American Physical Society (APS), Feb. 09, 2015. doi: 10.1103/physrevlett.114.065002.  
  
A. Alekseenko and C. Euler, “A Bhatnagar–Gross–Krook kinetic model with velocity-dependent collision frequency and corrected relaxation of moments”, *Continuum Mechanics and Thermodynamics*, vol. 28, no. 3. Springer Science and Business Media LLC, pp. 751–763, Jan. 15, 2015. doi: 10.1007/s00161-014-0407-0.  
  
A. Alekseenko, S. Gimelshein, T. Nguyenand P. Vedula, “Solution of non-continuum flows using BGK-type model with enforced relaxation of moments”, *AIP Conference Proceedings*. Author(s), 2016. doi: 10.1063/1.4967674.  
  
D. P. Fahey, T. J. Carrolland M. W. Noel, “Imaging the dipole-dipole energy exchange between ultracold rubidium Rydberg atoms”, *Physical Review A*, vol. 91, no. 6. American Physical Society (APS), Jun. 01, 2015. doi: 10.1103/physreva.91.062702.  
  
R. Feynman, “Quantum interference in the field ionization of Rydberg atoms”, *Physical Review A*, vol. 92, no. 4. American Physical Society (APS), Oct. 13, 2015. doi: 10.1103/physreva.92.043412.  
  
K. Ahmadi-Majlan, “Tuning metal-insulator behavior in LaTiO3/SrTiO3 heterostructures integrated directly on Si(100) through control of atomic layer thickness”, *Applied Physics Letters*, vol. 112, no. 19. AIP Publishing, p. 193104, May 07, 2018. doi: 10.1063/1.5018069.  
  
H. Chen, “Magnetically driven orbital-selective insulator–metal transition in double perovskite oxides”, *npj Quantum Materials*, vol. 3, no. 1. Springer Science and Business Media LLC, Nov. 08, 2018. doi: 10.1038/s41535-018-0131-2.  
  
H. Chen, D. P. Kumah, A. S. Disa, F. J. Walker, C. H. Ahnand S. Ismail-Beigi, “Modifying the Electronic Orbitals of Nickelate Heterostructures via Structural Distortions”, *Physical Review Letters*, vol. 110, no. 18. American Physical Society (APS), May 01, 2013. doi: 10.1103/physrevlett.110.186402.  
  
H. Chen and A. J. Millis, “Phase diagram ofas a function of chemical doping, epitaxial strain, and external pressure”, *Physical Review B*, vol. 94, no. 16. American Physical Society (APS), Oct. 03, 2016. doi: 10.1103/physrevb.94.165106.  
  
H. Chen and A. Millis, “Design of new Mott multiferroics via complete charge transfer: promising candidates for bulk photovoltaics”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Jul. 21, 2017. doi: 10.1038/s41598-017-06396-5.  
  
H. Chen, H. Park, A. J. Millisand C. A. Marianetti, “Charge transfer across transition-metal oxide interfaces: Emergent conductance and electronic structure”, *Physical Review B*, vol. 90, no. 24. American Physical Society (APS), Dec. 22, 2014. doi: 10.1103/physrevb.90.245138.  
  
X. Chen, “Interfacial Charge Engineering in Ferroelectric‐Controlled Mott Transistors”, *Advanced Materials*, vol. 29, no. 31. Wiley, p. 1701385, Jun. 19, 2017. doi: 10.1002/adma.201701385.  
  
E. I. Paredes Aulestia, “Pressure-induced enhancement of non-polar to polar transition temperature in metallic LiOsO3”, *Applied Physics Letters*, vol. 113, no. 1. AIP Publishing, p. 012902, Jul. 02, 2018. doi: 10.1063/1.5035133.  
  
J. J. Dudek, R. G. Edwards, P. Guoand C. E. Thomas, “Toward the excited isoscalar meson spectrum from lattice QCD”, *Physical Review D*, vol. 88, no. 9. American Physical Society (APS), Nov. 18, 2013. doi: 10.1103/physrevd.88.094505.  
  
A. Alekseenko and E. Josyula, “Deterministic solution of the spatially homogeneous Boltzmann equation using discontinuous Galerkin discretizations in the velocity space”, *Journal of Computational Physics*, vol. 272. Elsevier BV, pp. 170–188, Sep. 2014. doi: 10.1016/j.jcp.2014.03.031.  
  
R. Bosworth, A. Ketsdever, N. Gimelsheinand S. Gimelshein, “Determination of thermophoretic force on a particle in transitional flow”, *AIP Conference Proceedings*. AIP Publishing LLC, 2014. doi: 10.1063/1.4902611.  
  
A.-D. N. Celestine, V. Agrawaland B. Runnels, “Experimental and numerical investigation into mechanical degradation of polymers”, *Composites Part B: Engineering*, vol. 201. Elsevier BV, p. 108369, Nov. 2020. doi: 10.1016/j.compositesb.2020.108369.  
  
B. M. Cornella, S. F. Gimelshein, T. C. Lillyand A. D. Ketsdever, “Neutral gas heating via non-resonant optical lattices”, *Applied Physics Letters*, vol. 103, no. 19. AIP Publishing, p. 194103, Nov. 04, 2013. doi: 10.1063/1.4829918.  
  
N. Gimelshein, S. Gimelshein, T. Lillyand E. Moskovets, “Numerical Modeling of Ion Transport in an ESI-MS System”, *Journal of the American Society for Mass Spectrometry*, vol. 25, no. 5. American Chemical Society (ACS), pp. 820–831, Mar. 22, 2014. doi: 10.1007/s13361-014-0838-7.  
  
N. Gimelshein, S. Gimelshein, C. C. Pradzynski, T. Zeuchand U. Buck, “The temperature and size distribution of large water clusters from a non-equilibrium model”, *The Journal of Chemical Physics*, vol. 142, no. 24. AIP Publishing, p. 244305, Jun. 28, 2015. doi: 10.1063/1.4922312.  
  
S. Gimelshein, T. Lillyand E. Moskovets, “Numerical Analysis of Ion-Funnel Transmission Efficiency in an API-MS System with a Continuum/Microscopic Approach”, *Journal of the American Society for Mass Spectrometry*, vol. 26, no. 11. American Chemical Society (ACS), pp. 1911–1922, Aug. 05, 2015. doi: 10.1007/s13361-015-1214-y.  
  
J. G. Ribot, V. Agrawaland B. Runnels, “A new approach for phase field modeling of grain boundaries with strongly nonconvex energy”, *Modelling and Simulation in Materials Science and Engineering*, vol. 27, no. 8. IOP Publishing, p. 084007, Oct. 09, 2019. doi: 10.1088/1361-651x/ab47a0.  
  
J. S. Graul, B. M. Cornella, A. D. Ketsdever, T. C. Lillyand M. N. Shneider, “Experimentally observed field–gas interaction in intense optical lattices”, *Applied Physics Letters*, vol. 103, no. 24. AIP Publishing, p. 244106, Dec. 09, 2013. doi: 10.1063/1.4848781.  
  
J. S. Graul, S. F. Gimelsheinand T. C. Lilly, “Kinetic view of chirped optical lattice gas heating”, *AIP Conference Proceedings*. AIP Publishing LLC, 2014. doi: 10.1063/1.4902599.  
  
J. S. Graul, S. F. Gimelsheinand T. C. Lilly, “Numerical examination of optical lattice gas heating within realistic optical cavities”, *AIP Conference Proceedings*. AIP Publishing LLC, 2014. doi: 10.1063/1.4902598.  
  
J. S. Graul, S. F. Gimelsheinand T. C. Lilly, “Numerical prediction of optical lattice-induced gas heating within multipass optical cavities”, *Applied Physics B*, vol. 117, no. 1. Springer Science and Business Media LLC, pp. 353–361, May 05, 2014. doi: 10.1007/s00340-014-5842-x.  
  
J. S. Graul, S. F. Gimelsheinand T. C. Lilly, “Optical lattice gas heating simulation under application of intrapulse frequency chirping”, *Applied Physics B*, vol. 120, no. 3. Springer Science and Business Media LLC, pp. 573–579, Jul. 16, 2015. doi: 10.1007/s00340-015-6168-z.  
  
J. S. Graul and T. C. Lilly, “Coherent Rayleigh-Brillouin scattering as a flow diagnostic technique”, *AIP Conference Proceedings*. AIP Publishing LLC, 2014. doi: 10.1063/1.4902615.  
  
A. D. Ketsdever and S. Gimelshein, “A spacecraft’s own ambient environment: The role of simulation-based research”, *AIP Conference Proceedings*. AIP Publishing LLC, 2014. doi: 10.1063/1.4902754.  
  
J. K. Lefkowitz, M. Uddi, B. C. Windom, G. Louand Y. Ju, “In situ species diagnostics and kinetic study of plasma activated ethylene dissociation and oxidation in a low temperature flow reactor”, *Proceedings of the Combustion Institute*, vol. 35, no. 3. Elsevier BV, pp. 3505–3512, 2015. doi: 10.1016/j.proci.2014.08.001.  
  
C. A. Maldonado, A. D. Ketsdeverand S. F. Gimelshein, “Measured force on elongated bodies in a simulated low-Earth orbit environment”, *AIP Conference Proceedings*. AIP Publishing LLC, 2014. doi: 10.1063/1.4902740.  
  
B. Runnels and V. Agrawal, “Phase field disconnections: A continuum method for disconnection-mediated grain boundary motion”, *Scripta Materialia*, vol. 186. Elsevier BV, pp. 6–10, Sep. 2020. doi: 10.1016/j.scriptamat.2020.04.042.  
  
M. K. Shaffer, T. C. Lilly, B. V. Zhdanovand R. J. Knize, “In situ non-perturbative temperature measurement in a Cs alkali laser”, *Optics Letters*, vol. 40, no. 1. The Optical Society, p. 119, Dec. 24, 2014. doi: 10.1364/ol.40.000119.  
  
A. L. Ventura, A. D. Ketsdever, N. E. Gimelsheinand S. F. Gimelshein, “Experimental characterization of edge force on the Crookes radiometer”, *AIP Conference Proceedings*. AIP Publishing LLC, 2014. doi: 10.1063/1.4902613.  
  
S. H. Won, S. Nakane, C. B. Reuter, B. C. Windomand Y. Ju, “Effect of Ignition Chemistry on Turbulent Premixed Flames of n-Heptane and Toluene”, *53rd AIAA Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 03, 2015. doi: 10.2514/6.2015-0430.  
  
I. Wysong, S. Gimelshein, Y. Bondarand M. Ivanov, “Comparison of direct simulation Monte Carlo chemistry and vibrational models applied to oxygen shock measurements”, *Physics of Fluids*, vol. 26, no. 4. AIP Publishing, p. 043101, Apr. 2014. doi: 10.1063/1.4871023.  
  
D. Carmody, M. J. Puescheland P. W. Terry, “Gyrokinetic studies of microinstabilities in the reversed field pinch”, *Physics of Plasmas*, vol. 20, no. 5. AIP Publishing, p. 052110, May 2013. doi: 10.1063/1.4803509.  
  
L. C. Jarrott, “Visualizing fast electron energy transport into laser-compressed high-density fast-ignition targets”, *Nature Physics*, vol. 12, no. 5. Springer Science and Business Media LLC, pp. 499–504, Jan. 11, 2016. doi: 10.1038/nphys3614.  
  
J. Kim, C. McGuffey, B. Qiao, M. S. Wei, P. E. Grabowskiand F. N. Beg, “Varying stopping and self-focusing of intense proton beams as they heat solid density matter”, *Physics of Plasmas*, vol. 23, no. 4. AIP Publishing, p. 043104, Apr. 2016. doi: 10.1063/1.4945617.  
  
J. Kim, B. Qiao, C. McGuffey, M. S. Wei, P. E. Grabowskiand F. N. Beg, “Self-Consistent Simulation of Transport and Energy Deposition of Intense Laser-Accelerated Proton Beams in Solid-Density Matter”, *Physical Review Letters*, vol. 115, no. 5. American Physical Society (APS), Jul. 28, 2015. doi: 10.1103/physrevlett.115.054801.  
  
A. Sorokovikova, “Generation of Superponderomotive Electrons in Multipicosecond Interactions of Kilojoule Laser Beams with Solid-Density Plasmas”, *Physical Review Letters*, vol. 116, no. 15. American Physical Society (APS), Apr. 12, 2016. doi: 10.1103/physrevlett.116.155001.  
  
D. Wu, B. Qiao, C. McGuffey, X. T. Heand F. N. Beg, “Generation of high-energy mono-energetic heavy ion beams by radiation pressure acceleration of ultra-intense laser pulses”, *Physics of Plasmas*, vol. 21, no. 12. AIP Publishing, p. 123118, Dec. 2014. doi: 10.1063/1.4904402.  
  
C. Z. Xiao, Z. J. Liu, T. W. Huang, C. Y. Zheng, B. Qiaoand X. T. He, “Research on ponderomotive driven Vlasov–Poisson system in electron acoustic wave parametric region”, *Physics of Plasmas*, vol. 21, no. 3. AIP Publishing, p. 032107, Mar. 2014. doi: 10.1063/1.4867664.  
  
T. Yabuuchi, “Impact of extended preplasma on energy coupling in kilojoule energy relativistic laser interaction with cone wire targets relevant to fast ignition”, *New Journal of Physics*, vol. 15, no. 1. IOP Publishing, p. 015020, Jan. 25, 2013. doi: 10.1088/1367-2630/15/1/015020.  
  
L. Ingber, M. Pappaleporeand R. R. Stesiak, “Electroencephalographic field influence on calcium momentum waves”, *Journal of Theoretical Biology*, vol. 343. Elsevier BV, pp. 138–153, Feb. 2014. doi: 10.1016/j.jtbi.2013.11.002.  
  
A. E. Fraser, P. W. Terry, E. G. Zweibeland M. J. Pueschel, “Coupling of damped and growing modes in unstable shear flow”, *Physics of Plasmas*, vol. 24, no. 6. AIP Publishing, p. 062304, Jun. 2017. doi: 10.1063/1.4985322.  
  
M. J. Pueschel, G. Rossi, D. Told, P. W. Terry, F. Jenkoand T. A. Carter, “A basic plasma test for gyrokinetics: GDC turbulence in LAPD”, *Plasma Physics and Controlled Fusion*, vol. 59, no. 2. IOP Publishing, p. 024006, Jan. 17, 2017. doi: 10.1088/1361-6587/aa52e6.  
  
P. W. Terry, “Overview of gyrokinetic studies of finite-*β*microturbulence”, *Nuclear Fusion*, vol. 55, no. 10. IOP Publishing, p. 104011, Jun. 20, 2015. doi: 10.1088/0029-5515/55/10/104011.  
  
Z. R. Williams, M. J. Pueschel, P. W. Terryand T. Hauff, “Turbulence, transport, and zonal flows in the Madison symmetric torus reversed-field pinch”, *Physics of Plasmas*, vol. 24, no. 12. AIP Publishing, p. 122309, Dec. 2017. doi: 10.1063/1.5000252.  
  
Z. R. Williams, “Impact of resonant magnetic perturbations on zonal flows and microturbulence”, *Nuclear Fusion*, vol. 60, no. 9. IOP Publishing, p. 096004, Jul. 31, 2020. doi: 10.1088/1741-4326/ab9be7.  
  
Y. Yan and D. Blume, “Harmonically trapped Fermi gas: Temperature dependence of the Tan contact”, *Physical Review A*, vol. 88, no. 2. American Physical Society (APS), Aug. 27, 2013. doi: 10.1103/physreva.88.023616.  
  
Y. Yan and D. Blume, “Abnormal Superfluid Fraction of Harmonically Trapped Few-Fermion Systems”, *Physical Review Letters*, vol. 112, no. 23. American Physical Society (APS), Jun. 13, 2014. doi: 10.1103/physrevlett.112.235301.  
  
Y. Yan and D. Blume, “Temperature dependence of small harmonically trapped atom systems with Bose, Fermi, and Boltzmann statistics”, *Physical Review A*, vol. 90, no. 1. American Physical Society (APS), Jul. 21, 2014. doi: 10.1103/physreva.90.013620.  
  
Y. Yan and D. Blume, “Incorporating exact two-body propagators for zero-range interactions into-body Monte Carlo simulations”, *Physical Review A*, vol. 91, no. 4. American Physical Society (APS), Apr. 08, 2015. doi: 10.1103/physreva.91.043607.  
  
Y. Yan and D. Blume, “Path-Integral Monte Carlo Determination of the Fourth-Order Virial Coefficient for a Unitary Two-Component Fermi Gas with Zero-Range Interactions”, *Physical Review Letters*, vol. 116, no. 23. American Physical Society (APS), Jun. 07, 2016. doi: 10.1103/physrevlett.116.230401.  
  
X. Y. Yin and D. Blume, “Small two-component Fermi gases in a cubic box with periodic boundary conditions”, *Physical Review A*, vol. 87, no. 6. American Physical Society (APS), Jun. 10, 2013. doi: 10.1103/physreva.87.063609.  
  
X. Y. Yin and D. Blume, “Trapped unitary two-component Fermi gases with up to ten particles”, *Physical Review A*, vol. 92, no. 1. American Physical Society (APS), Jul. 06, 2015. doi: 10.1103/physreva.92.013608.  
  
H. Chen, “Evidence for Ultralow-Energy Vibrations in Large Organic Molecules”, *Nano Letters*, vol. 17, no. 8. American Chemical Society (ACS), pp. 4929–4933, Jul. 26, 2017. doi: 10.1021/acs.nanolett.7b01963.  
  
L. Huang, “Sequence of Silicon Monolayer Structures Grown on a Ru Surface: from a Herringbone Structure to Silicene”, *Nano Letters*, vol. 17, no. 2. American Chemical Society (ACS), pp. 1161–1166, Jan. 23, 2017. doi: 10.1021/acs.nanolett.6b04804.  
  
Y. Jiang, “Direct observation of Pt nanocrystal coalescence induced by electron-excitation-enhanced van der Waals interactions”, *Nano Research*, vol. 7, no. 3. Springer Science and Business Media LLC, pp. 308–314, Jan. 03, 2014. doi: 10.1007/s12274-013-0396-5.  
  
R. Ma, “Direct Four-Probe Measurement of Grain-Boundary Resistivity and Mobility in Millimeter-Sized Graphene”, *Nano Letters*, vol. 17, no. 9. American Chemical Society (ACS), pp. 5291–5296, Aug. 14, 2017. doi: 10.1021/acs.nanolett.7b01624.  
  
J. Ren, “Kondo Effect of Cobalt Adatoms on a Graphene Monolayer Controlled by Substrate-Induced Ripples”, *Nano Letters*, vol. 14, no. 7. American Chemical Society (ACS), pp. 4011–4015, Jun. 11, 2014. doi: 10.1021/nl501425n.  
  
G. Wang, “From bidirectional rectifier to polarity-controllable transistor in black phosphorus by dual gate modulation”, *2D Materials*, vol. 4, no. 2. IOP Publishing, p. 025056, Mar. 24, 2017. doi: 10.1088/2053-1583/aa6535.  
  
Y. Wang, “Monolayer PtSe2, a New Semiconducting Transition-Metal-Dichalcogenide, Epitaxially Grown by Direct Selenization of Pt”, *Nano Letters*, vol. 15, no. 6. American Chemical Society (ACS), pp. 4013–4018, May 27, 2015. doi: 10.1021/acs.nanolett.5b00964.  
  
W. D. Xiao, “Impact of heterocirculene molecular symmetry upon two-dimensional crystallization”, *Scientific Reports*, vol. 4, no. 1. Springer Science and Business Media LLC, Jun. 24, 2014. doi: 10.1038/srep05415.  
  
Y. Yao, “Graphene cover-promoted metal-catalyzed reactions”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 48. Proceedings of the National Academy of Sciences, pp. 17023–17028, Nov. 17, 2014. doi: 10.1073/pnas.1416368111.  
  
K. Yin, “Unsupported single-atom-thick copper oxide monolayers”, *2D Materials*, vol. 4, no. 1. IOP Publishing, p. 011001, Oct. 20, 2016. doi: 10.1088/2053-1583/4/1/011001.  
  
Y. Y. Zhang, R. Mishra, T. J. Pennycook, A. Y. Borisevich, S. J. Pennycookand S. T. Pantelides, “Oxygen Disorder, a Way to Accommodate Large Epitaxial Strains in Oxides”, *Advanced Materials Interfaces*, vol. 2, no. 18. Wiley, p. 1500344, Sep. 22, 2015. doi: 10.1002/admi.201500344.  
  
Y. Y. Zhang, Y.-L. Wang, L. Meng, S. B. Zhangand H.-J. Gao, “Thermally Controlled Adenine Dimer Chain Rotation on Cu(110): The Critical Role of van der Waals Interactions”, *The Journal of Physical Chemistry C*, vol. 118, no. 12. American Chemical Society (ACS), pp. 6278–6282, Mar. 18, 2014. doi: 10.1021/jp4118979.  
  
P. Gao, “High-Resolution Tracking Asymmetric Lithium Insertion and Extraction and Local Structure Ordering in SnS2”, *Nano Letters*, vol. 16, no. 9. American Chemical Society (ACS), pp. 5582–5588, Aug. 12, 2016. doi: 10.1021/acs.nanolett.6b02136.  
  
J. Pan, “Ferromagnetism and perfect spin filtering in transition-metal-doped graphyne nanoribbons”, *Physical Review B*, vol. 92, no. 20. American Physical Society (APS), Nov. 25, 2015. doi: 10.1103/physrevb.92.205429.  
  
Q. Qiao, “Direct observation of oxygen-vacancy-enhanced polarization in a SrTiO3-buffered ferroelectric BaTiO3 film on GaAs”, *Applied Physics Letters*, vol. 107, no. 20. AIP Publishing, p. 201604, Nov. 16, 2015. doi: 10.1063/1.4936159.  
  
L. Madeira, S. A. Vitiello, S. Gandolfiand K. E. Schmidt, “Vortex line in the unitary Fermi gas”, *Physical Review A*, vol. 93, no. 4. American Physical Society (APS), Apr. 06, 2016. doi: 10.1103/physreva.93.043604.  
  
D. Lonardoni, “Auxiliary field diffusion Monte Carlo calculations of light and medium-mass nuclei with local chiral interactions”, *Physical Review C*, vol. 97, no. 4. American Physical Society (APS), Apr. 24, 2018. doi: 10.1103/physrevc.97.044318.  
  
C. W. Hsu, B. G. DeLacy, S. G. Johnson, J. D. Joannopoulosand M. Soljačić, “Theoretical Criteria for Scattering Dark States in Nanostructured Particles”, *Nano Letters*, vol. 14, no. 5. American Chemical Society (ACS), pp. 2783–2788, May 07, 2014. doi: 10.1021/nl500340n.  
  
Y. Shen, D. Ye, I. Celanovic, S. G. Johnson, J. D. Joannopoulosand M. Soljačić, “Optical Broadband Angular Selectivity”, *Science*, vol. 343, no. 6178. American Association for the Advancement of Science (AAAS), pp. 1499–1501, Mar. 28, 2014. doi: 10.1126/science.1249799.  
  
A. Oganesov, G. Vahala, L. Vahala, J. Yepez, M. Soeand B. Zhang, “Unitary quantum lattice gas algorithm generated from the Dirac collision operator for 1D soliton–soliton collisions”, *Radiation Effects and Defects in Solids*, vol. 170, no. 1. Informa UK Limited, pp. 55–64, Jan. 02, 2015. doi: 10.1080/10420150.2014.988625.  
  
J. Adelman, “CMS computing operations during run 1”, *Journal of Physics: Conference Series*, vol. 513, no. 3. IOP Publishing, p. 032040, Jun. 11, 2014. doi: 10.1088/1742-6596/513/3/032040.  
  
J. Balcas, “Using the glideinWMS System as a Common Resource Provisioning Layer in CMS”, *Journal of Physics: Conference Series*, vol. 664, no. 6. IOP Publishing, p. 062031, Dec. 23, 2015. doi: 10.1088/1742-6596/664/6/062031.  
  
J. Balcas, “Using the glideinWMS System as a Common Resource Provisioning Layer in CMS”, *Journal of Physics: Conference Series*, vol. 664, no. 6. IOP Publishing, p. 062031, Dec. 23, 2015. doi: 10.1088/1742-6596/664/6/062031.  
  
S. Chatrchyan, “Search for resonances in the dijet mass spectrum from 7 TeV pp collisions at CMS”, *Physics Letters B*, vol. 704, no. 3. Elsevier BV, pp. 123–142, Oct. 2011. doi: 10.1016/j.physletb.2011.09.015.  
  
S. Chatrchyan, “Observation of a new boson at a mass of 125 GeV with the CMS experiment at the LHC”, *Physics Letters B*, vol. 716, no. 1. Elsevier BV, pp. 30–61, Sep. 2012. doi: 10.1016/j.physletb.2012.08.021.  
  
S. Chatrchyan, “Search for heavy lepton partners of neutrinos in proton–proton collisions in the context of the type III seesaw mechanism”, *Physics Letters B*, vol. 718, no. 2. Elsevier BV, pp. 348–368, Dec. 2012. doi: 10.1016/j.physletb.2012.10.070.  
  
S. Chatrchyan, “Searches for Higgs bosons in pp collisions at in the context of four-generation and fermiophobic models”, *Physics Letters B*, vol. 725, no. 1–3. Elsevier BV, pp. 36–59, Aug. 2013. doi: 10.1016/j.physletb.2013.06.043.  
  
S. Chatrchyan, “Measurement of the and ZZ production cross sections in pp collisions at ”, *Physics Letters B*, vol. 721, no. 4–5. Elsevier BV, pp. 190–211, Apr. 2013. doi: 10.1016/j.physletb.2013.03.027.  
  
S. Chatrchyan, “Search for a Higgs boson decaying into a Z and a photon in pp collisions at ”, *Physics Letters B*, vol. 726, no. 4–5. Elsevier BV, pp. 587–609, Nov. 2013. doi: 10.1016/j.physletb.2013.09.057.  
  
S. Chatrchyan, “Search for gluino mediated bottom- and top-squark production in multijet final states in pp collisions at 8 TeV”, *Physics Letters B*, vol. 725, no. 4–5. Elsevier BV, pp. 243–270, Oct. 2013. doi: 10.1016/j.physletb.2013.06.058.  
  
S. Chatrchyan, “Multiplicity and transverse momentum dependence of two- and four-particle correlations in pPb and PbPb collisions”, *Physics Letters B*, vol. 724, no. 4–5. Elsevier BV, pp. 213–240, Jul. 2013. doi: 10.1016/j.physletb.2013.06.028.  
  
S. Chatrchyan, “Search for heavy resonances in the W/Z-tagged dijet mass spectrum in pp collisions at 7 TeV”, *Physics Letters B*, vol. 723, no. 4–5. Elsevier BV, pp. 280–301, Jun. 2013. doi: 10.1016/j.physletb.2013.05.040.  
  
S. Chatrchyan, “Search for a non-standard-model Higgs boson decaying to a pair of new light bosons in four-muon final states”, *Physics Letters B*, vol. 726, no. 4–5. Elsevier BV, pp. 564–586, Nov. 2013. doi: 10.1016/j.physletb.2013.09.009.  
  
S. Chatrchyan, “Observation of long-range, near-side angular correlations in pPb collisions at the LHC”, *Physics Letters B*, vol. 718, no. 3. Elsevier BV, pp. 795–814, Jan. 2013. doi: 10.1016/j.physletb.2012.11.025.  
  
S. Chatrchyan, “Search for a narrow, spin-2 resonance decaying to a pair of Z bosons in the final state”, *Physics Letters B*, vol. 718, no. 4–5. Elsevier BV, pp. 1208–1228, Jan. 2013. doi: 10.1016/j.physletb.2012.11.063.  
  
S. Chatrchyan, “Search for flavor changing neutral currents in top quark decays in pp collisions at 7 TeV”, *Physics Letters B*, vol. 718, no. 4–5. Elsevier BV, pp. 1252–1272, Jan. 2013. doi: 10.1016/j.physletb.2012.12.045.  
  
S. Chatrchyan, “Search for baryon number violation in top-quark decays”, *Physics Letters B*, vol. 731. Elsevier BV, pp. 173–196, Apr. 2014. doi: 10.1016/j.physletb.2014.02.033.  
  
T. Chwalek, “No file left behind - monitoring transfer latencies in PhEDEx”, *Journal of Physics: Conference Series*, vol. 396, no. 3. IOP Publishing, p. 032089, Dec. 13, 2012. doi: 10.1088/1742-6596/396/3/032089.  
  
R. Kaselis, “CMS Data Transfer operations after the first years of LHC collisions”, *Journal of Physics: Conference Series*, vol. 396, no. 4. IOP Publishing, p. 042033, Dec. 13, 2012. doi: 10.1088/1742-6596/396/4/042033.  
  
V. Khachatryan, “Measurement of the charge ratio of atmospheric muons with the CMS detector”, *Physics Letters B*, vol. 692, no. 2. Elsevier BV, pp. 83–104, Aug. 2010. doi: 10.1016/j.physletb.2010.07.033.  
  
V. Khachatryan, “Search for supersymmetry in pp collisions at 7 TeV in events with jets and missing transverse energy”, *Physics Letters B*, vol. 698, no. 3. Elsevier BV, pp. 196–218, Apr. 2011. doi: 10.1016/j.physletb.2011.03.021.  
  
V. Khachatryan, “Search for microscopic black hole signatures at the Large Hadron Collider”, *Physics Letters B*, vol. 697, no. 5. Elsevier BV, pp. 434–453, Mar. 2011. doi: 10.1016/j.physletb.2011.02.032.  
  
V. Khachatryan, “Constraints on the Higgs boson width from off-shell production and decay to Z-boson pairs”, *Physics Letters B*, vol. 736. Elsevier BV, pp. 64–85, Sep. 2014. doi: 10.1016/j.physletb.2014.06.077.  
  
V. Khachatryan, “Search for stealth supersymmetry in events with jets, either photons or leptons, and low missing transverse momentum in pp collisions at 8 TeV”, *Physics Letters B*, vol. 743. Elsevier BV, pp. 503–525, Apr. 2015. doi: 10.1016/j.physletb.2015.03.017.  
  
V. Khachatryan, “Search for lepton-flavour-violating decays of the Higgs boson”, *Physics Letters B*, vol. 749. Elsevier BV, pp. 337–362, Oct. 2015. doi: 10.1016/j.physletb.2015.07.053.  
  
V. Khachatryan, “Constraints on the pMSSM, AMSB model and on other models from the search for long-lived charged particles in proton–proton collisions at $$\sqrt{s} =8\,\text {TeV} $$ s = 8 TeV”, *The European Physical Journal C*, vol. 75, no. 7. Springer Science and Business Media LLC, Jul. 2015. doi: 10.1140/epjc/s10052-015-3533-3.  
  
V. Khachatryan, “Search for a standard model Higgs boson produced in association with a top-quark pair and decaying to bottom quarks using a matrix element method”, *The European Physical Journal C*, vol. 75, no. 6. Springer Science and Business Media LLC, Jun. 2015. doi: 10.1140/epjc/s10052-015-3454-1.  
  
V. Khachatryan, “Searches for supersymmetry based on events with b jets and four W bosons in pp collisions at 8 TeV”, *Physics Letters B*, vol. 745. Elsevier BV, pp. 5–28, May 2015. doi: 10.1016/j.physletb.2015.04.002.  
  
V. Khachatryan, “Long-range two-particle correlations of strange hadrons with charged particles in pPb and PbPb collisions at LHC energies”, *Physics Letters B*, vol. 742. Elsevier BV, pp. 200–224, Mar. 2015. doi: 10.1016/j.physletb.2015.01.034.  
  
V. Khachatryan, “Measurements of differential and double-differential Drell–Yan cross sections in proton–proton collisions at $$\sqrt{s} = 8$$ s = 8  TeV TeV”, *The European Physical Journal C*, vol. 75, no. 4. Springer Science and Business Media LLC, Apr. 2015. doi: 10.1140/epjc/s10052-015-3364-2.  
  
V. Khachatryan, “Search for exotic decays of a Higgs boson into undetectable particles and one or more photons”, *Physics Letters B*, vol. 753. Elsevier BV, pp. 363–388, Feb. 2016. doi: 10.1016/j.physletb.2015.12.017.  
  
V. Khachatryan, “Search for heavy resonances decaying to two Higgs bosons in final states containing four b quarks”, *The European Physical Journal C*, vol. 76, no. 7. Springer Science and Business Media LLC, Jul. 2016. doi: 10.1140/epjc/s10052-016-4206-6.  
  
V. Khachatryan, “Search for supersymmetry in the multijet and missing transverse momentum final state in pp collisions at 13 TeV”, *Physics Letters B*, vol. 758. Elsevier BV, pp. 152–180, Jul. 2016. doi: 10.1016/j.physletb.2016.05.002.  
  
V. Khachatryan, “Search for exotic decays of a Higgs boson into undetectable particles and one or more photons”, *Physics Letters B*, vol. 753. Elsevier BV, pp. 363–388, Feb. 2016. doi: 10.1016/j.physletb.2015.12.017.  
  
V. Khachatryan, “A search for pair production of new light bosons decaying into muons”, *Physics Letters B*, vol. 752. Elsevier BV, pp. 146–168, Jan. 2016. doi: 10.1016/j.physletb.2015.10.067.  
  
V. Khachatryan, “Multiplicity and rapidity dependence of strange hadron production in pp, pPb, and PbPb collisions at the LHC”, *Physics Letters B*, vol. 768. Elsevier BV, pp. 103–129, May 2017. doi: 10.1016/j.physletb.2017.01.075.  
  
V. Khachatryan, “Evidence for collectivity in pp collisions at the LHC”, *Physics Letters B*, vol. 765. Elsevier BV, pp. 193–220, Feb. 2017. doi: 10.1016/j.physletb.2016.12.009.  
  
V. Khachatryan, “Search for supersymmetry in events with photons and missing transverse energy in pp collisions at 13 TeV”, *Physics Letters B*, vol. 769. Elsevier BV, pp. 391–412, Jun. 2017. doi: 10.1016/j.physletb.2017.04.005.  
  
V. Khachatryan, “Search for single production of a heavy vector-like T quark decaying to a Higgs boson and a top quark with a lepton and jets in the final state”, *Physics Letters B*, vol. 771. Elsevier BV, pp. 80–105, Aug. 2017. doi: 10.1016/j.physletb.2017.05.019.  
  
V. Khachatryan, “Search for heavy resonances decaying into a vector boson and a Higgs boson in final states with charged leptons, neutrinos, and b quarks”, *Physics Letters B*, vol. 768. Elsevier BV, pp. 137–162, May 2017. doi: 10.1016/j.physletb.2017.02.040.  
  
V. Khachatryan, “Search for new physics in same-sign dilepton events in proton–proton collisions at $$\sqrt{s} = 13\,\text {TeV} $$ s = 13 TeV”, *The European Physical Journal C*, vol. 76, no. 8. Springer Science and Business Media LLC, Aug. 2016. doi: 10.1140/epjc/s10052-016-4261-z.  
  
A. M. Sirunyan, “Constraints on anomalous Higgs boson couplings using production and decay information in the four-lepton final state”, *Physics Letters B*, vol. 775. Elsevier BV, pp. 1–24, Dec. 2017. doi: 10.1016/j.physletb.2017.10.021.  
  
J. Yao, A.-C. Lesage, B. G. Bodmann, F. Hussainand D. J. Kouri, “Inverse scattering theory: Inverse scattering series method for one dimensional non-compact support potential”, *Journal of Mathematical Physics*, vol. 55, no. 12. AIP Publishing, p. 123512, Dec. 2014. doi: 10.1063/1.4904725.  
  
J. Yao, A.-C. Lesage, B. G. Bodmann, F. Hussainand D. J. Kouri, “One dimensional acoustic direct nonlinear inversion using the Volterra inverse scattering series”, *Inverse Problems*, vol. 30, no. 7. IOP Publishing, p. 075006, Jun. 01, 2014. doi: 10.1088/0266-5611/30/7/075006.  
  
M. Aaboud, “Performance of the ATLAS Transition Radiation Tracker in Run 1 of the LHC: tracker properties”, *Journal of Instrumentation*, vol. 12, no. 5. IOP Publishing, pp. P05002–P05002, May 03, 2017. doi: 10.1088/1748-0221/12/05/p05002.  
  
M. Aaboud, “Measurement of the cross section for inclusive isolated-photon production in pp collisions at using the ATLAS detector”, *Physics Letters B*, vol. 770. Elsevier BV, pp. 473–493, Jul. 2017. doi: 10.1016/j.physletb.2017.04.072.  
  
R. D. Ball, “Parton distributions with LHC data”, *Nuclear Physics B*, vol. 867, no. 2. Elsevier BV, pp. 244–289, Feb. 2013. doi: 10.1016/j.nuclphysb.2012.10.003.  
  
G. Cowan, K. Cranmer, E. Grossand O. Vitells, “Asymptotic formulae for likelihood-based tests of new physics”, *The European Physical Journal C*, vol. 71, no. 2. Springer Science and Business Media LLC, Feb. 2011. doi: 10.1140/epjc/s10052-011-1554-0.  
  
J. Pumplin, D. R. Stump, J. Huston, H.-L. Lai, P. Nadolskyand W.-K. Tung, “New Generation of Parton Distributions with Uncertainties from Global QCD Analysis”, *Journal of High Energy Physics*, vol. 2002, no. 7. Springer Science and Business Media LLC, pp. 012–012, Jul. 04, 2002. doi: 10.1088/1126-6708/2002/07/012.  
  
E. Re, “Single-top Wt-channel production matched with parton showers using the POWHEG method”, *The European Physical Journal C*, vol. 71, no. 2. Springer Science and Business Media LLC, Feb. 2011. doi: 10.1140/epjc/s10052-011-1547-z.  
  
B. Cerutti, G. R. Werner, D. A. Uzdenskyand M. C. Begelman, “BEAMING AND RAPID VARIABILITY OF HIGH-ENERGY RADIATION FROM RELATIVISTIC PAIR PLASMA RECONNECTION”, *The Astrophysical Journal*, vol. 754, no. 2. American Astronomical Society, p. L33, Jul. 16, 2012. doi: 10.1088/2041-8205/754/2/l33.  
  
B. Cerutti, G. R. Werner, D. A. Uzdenskyand M. C. Begelman, “SIMULATIONS OF PARTICLE ACCELERATION BEYOND THE CLASSICAL SYNCHROTRON BURNOFF LIMIT IN MAGNETIC RECONNECTION: AN EXPLANATION OF THE CRAB FLARES”, *The Astrophysical Journal*, vol. 770, no. 2. American Astronomical Society, p. 147, Jun. 05, 2013. doi: 10.1088/0004-637x/770/2/147.  
  
B. Cerutti, G. R. Werner, D. A. Uzdenskyand M. C. Begelman, “THREE-DIMENSIONAL RELATIVISTIC PAIR PLASMA RECONNECTION WITH RADIATIVE FEEDBACK IN THE CRAB NEBULA”, *The Astrophysical Journal*, vol. 782, no. 2. American Astronomical Society, p. 104, Feb. 04, 2014. doi: 10.1088/0004-637x/782/2/104.  
  
B. Cerutti, G. R. Werner, D. A. Uzdenskyand M. C. Begelman, “Gamma-ray flares in the Crab Nebula: A case of relativistic reconnection?”, *Physics of Plasmas*, vol. 21, no. 5. AIP Publishing, p. 056501, May 2014. doi: 10.1063/1.4872024.  
  
K. Nalewajko, D. A. Uzdensky, B. Cerutti, G. R. Wernerand M. C. Begelman, “ON THE DISTRIBUTION OF PARTICLE ACCELERATION SITES IN PLASMOID-DOMINATED RELATIVISTIC MAGNETIC RECONNECTION”, *The Astrophysical Journal*, vol. 815, no. 2. American Astronomical Society, p. 101, Dec. 15, 2015. doi: 10.1088/0004-637x/815/2/101.  
  
G. R. Werner, A. A. Philippovand D. A. Uzdensky, “Particle acceleration in relativistic magnetic reconnection with strong inverse-Compton cooling in pair plasmas”, *Monthly Notices of the Royal Astronomical Society: Letters*, vol. 482, no. 1. Oxford University Press (OUP), pp. L60–L64, Aug. 25, 2018. doi: 10.1093/mnrasl/sly157.  
  
G. R. Werner and D. A. Uzdensky, “Nonthermal Particle Acceleration in 3D Relativistic Magnetic Reconnection in Pair Plasma”, *The Astrophysical Journal*, vol. 843, no. 2. American Astronomical Society, p. L27, Jul. 10, 2017. doi: 10.3847/2041-8213/aa7892.  
  
G. R. Werner, D. A. Uzdensky, M. C. Begelman, B. Ceruttiand K. Nalewajko, “Non-thermal particle acceleration in collisionless relativistic electron–proton reconnection”, *Monthly Notices of the Royal Astronomical Society*, vol. 473, no. 4. Oxford University Press (OUP), pp. 4840–4861, Sep. 28, 2017. doi: 10.1093/mnras/stx2530.  
  
S. Dhakal and R. Sureshkumar, “Uniaxial Extension of Surfactant Micelles: Counterion Mediated Chain Stiffening and a Mechanism of Rupture by Flow-Induced Energy Redistribution”, *ACS Macro Letters*, vol. 5, no. 1. American Chemical Society (ACS), pp. 108–111, Dec. 30, 2015. doi: 10.1021/acsmacrolett.5b00761.  
  
S. Dhakal and R. Sureshkumar, “Anomalous diffusion and stress relaxation in surfactant micelles”, *Physical Review E*, vol. 96, no. 1. American Physical Society (APS), Jul. 24, 2017. doi: 10.1103/physreve.96.012605.  
  
A. Sambasivam, S. Dhakaland R. Sureshkumar, “Structure and rheology of self-assembled aqueous suspensions of nanoparticles and wormlike micelles”, *Molecular Simulation*, vol. 44, no. 6. Informa UK Limited, pp. 485–493, Oct. 20, 2017. doi: 10.1080/08927022.2017.1387658.  
  
L. O. Baksmaty, H. Lu, C. J. Bolechand H. Pu, “A Bogoliubov–de Gennes study of trapped spin-imbalanced unitary Fermi gases”, *New Journal of Physics*, vol. 13, no. 5. IOP Publishing, p. 055014, May 25, 2011. doi: 10.1088/1367-2630/13/5/055014.  
  
L. Dong, L. Zhou, B. Wu, B. Ramachandhranand H. Pu, “Cavity-assisted dynamical spin-orbit coupling in cold atoms”, *Physical Review A*, vol. 89, no. 1. American Physical Society (APS), Jan. 24, 2014. doi: 10.1103/physreva.89.011602.  
  
L. Dong, C. Zhuand H. Pu, “Photon-Induced Spin-Orbit Coupling in Ultracold Atoms inside Optical Cavity”, *Atoms*, vol. 3, no. 2. MDPI AG, pp. 182–194, May 26, 2015. doi: 10.3390/atoms3020182.  
  
Y. Dong, L. Dong, M. Gongand H. Pu, “Dynamical phases in quenched spin–orbit-coupled degenerate Fermi gas”, *Nature Communications*, vol. 6, no. 1. Springer Science and Business Media LLC, Jan. 20, 2015. doi: 10.1038/ncomms7103.  
  
H. Hu, L. Jiang, H. Pu, Y. Chenand X.-J. Liu, “Universal Impurity-Induced Bound State in Topological Superfluids”, *Physical Review Letters*, vol. 110, no. 2. American Physical Society (APS), Jan. 10, 2013. doi: 10.1103/physrevlett.110.020401.  
  
H. Lu, L. O. Baksmaty, C. J. Bolechand H. Pu, “Expansion of 1D Polarized Superfluids: The Fulde-Ferrell-Larkin-Ovchinnikov State Reveals Itself”, *Physical Review Letters*, vol. 108, no. 22. American Physical Society (APS), May 29, 2012. doi: 10.1103/physrevlett.108.225302.  
  
B. Ramachandhran, H. Huand H. Pu, “Emergence of topological and strongly correlated ground states in trapped Rashba spin-orbit-coupled Bose gases”, *Physical Review A*, vol. 87, no. 3. American Physical Society (APS), Mar. 26, 2013. doi: 10.1103/physreva.87.033627.  
  
J. Zhang, H. Hu, X.-J. Liuand H. Pu, “FERMI GASES WITH SYNTHETIC SPIN–ORBIT COUPLING”, *Annual Review of Cold Atoms and Molecules*. WORLD SCIENTIFIC, pp. 81–143, Mar. 31, 2014. doi: 10.1142/9789814590174\_0002.  
  
H. Gou, B. L. Yonke, A. Epshteyn, D. Y. Kim, J. S. Smithand T. A. Strobel, “Pressure-induced polymerization of P(CN)3”, *The Journal of Chemical Physics*, vol. 142, no. 19. AIP Publishing, p. 194503, May 18, 2015. doi: 10.1063/1.4919640.  
  
J. Shaw, D. Monismith, Y. Zhang, D. Doerrand H. S. Chakraborty, “Ion survival in grazing collisions of with vicinal nanosurfaces as a probe for subband electronic structures”, *Physical Review A*, vol. 98, no. 5. American Physical Society (APS), Nov. 21, 2018. doi: 10.1103/physreva.98.052705.  
  
M. Sadjadi, B. Bhattarai, D. A. Drabold, M. F. Thorpeand M. Wilson, “Refining glass structure in two dimensions”, *Physical Review B*, vol. 96, no. 20. American Physical Society (APS), Nov. 10, 2017. doi: 10.1103/physrevb.96.201405.  
  
P. Giannakeas, L. Khaykovich, J.-M. Rostand C. H. Greene, “Nonadiabatic Molecular Association in Thermal Gases Driven by Radio-Frequency Pulses”, *Physical Review Letters*, vol. 123, no. 4. American Physical Society (APS), Jul. 24, 2019. doi: 10.1103/physrevlett.123.043204.  
  
K. M. Daily, R. E. Wootenand C. H. Greene, “Hyperspherical theory of the quantum Hall effect: The role of exceptional degeneracy”, *Physical Review B*, vol. 92, no. 12. American Physical Society (APS), Sep. 21, 2015. doi: 10.1103/physrevb.92.125427.  
  
B. Yan, R. E. Wooten, K. M. Dailyand C. H. Greene, “Hyperspherical Slater determinant approach to few-body fractional quantum Hall states”, *Annals of Physics*, vol. 380. Elsevier BV, pp. 188–205, May 2017. doi: 10.1016/j.aop.2017.03.004.  
  
N. A. Mehta and D. A. Levin, “Coarse graining of Ethylammonium Nitrate using Effective Field Coarse Graining Method”, *54th AIAA Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 02, 2016. doi: 10.2514/6.2016-0955.  
  
X. Wang, M. Zebarjadiand K. Esfarjani, “First principles calculations of solid-state thermionic transport in layered van der Waals heterostructures”, *Nanoscale*, vol. 8, no. 31. Royal Society of Chemistry (RSC), pp. 14695–14704, 2016. doi: 10.1039/c6nr02436j.  
  
D. J. Bernstein, T. Lafleur, J. Daligaultand S. D. Baalrud, “Friction force in strongly magnetized plasmas”, *Physical Review E*, vol. 102, no. 4. American Physical Society (APS), Oct. 06, 2020. doi: 10.1103/physreve.102.041201.  
  
N. R. Shaffer and S. D. Baalrud, “The Barkas effect in plasma transport”, *Physics of Plasmas*, vol. 26, no. 3. AIP Publishing, p. 032110, Mar. 2019. doi: 10.1063/1.5089140.  
  
N. R. Shaffer, S. K. Tiwariand S. D. Baalrud, “Pair correlation functions of strongly coupled two-temperature plasma”, *Physics of Plasmas*, vol. 24, no. 9. AIP Publishing, p. 092703, Sep. 2017. doi: 10.1063/1.4999185.  
  
S. K. Tiwari and S. D. Baalrud, “Reduction of electron heating by magnetizing ultracold neutral plasma”, *Physics of Plasmas*, vol. 25, no. 1. AIP Publishing, p. 013511, Jan. 2018. doi: 10.1063/1.5013320.  
  
D. M. Sussman, “Spatial distribution of entanglements in thin free-standing films”, *Physical Review E*, vol. 94, no. 1. American Physical Society (APS), Jul. 26, 2016. doi: 10.1103/physreve.94.012503.  
  
X. Wang, K. Esfarjaniand M. Zebarjadi, “First-Principles Calculation of Charge Transfer at the Silicon–Organic Interface”, *The Journal of Physical Chemistry C*, vol. 121, no. 29. American Chemical Society (ACS), pp. 15529–15537, Jul. 18, 2017. doi: 10.1021/acs.jpcc.7b03275.  
  
X. Wang, M. Zebarjadiand K. Esfarjani, “High-Performance Solid-State Thermionic Energy Conversion Based on 2D van der Waals Heterostructures: A First-Principles Study”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, Jun. 18, 2018. doi: 10.1038/s41598-018-27430-0.  
  
Z. Wang, Y. Xu, H. Puand K. R. A. Hazzard, “Number-conserving interacting fermion models with exact topological superconducting ground states”, *Physical Review B*, vol. 96, no. 11. American Physical Society (APS), Sep. 07, 2017. doi: 10.1103/physrevb.96.115110.  
  
L. Chen, H. Pu, Z.-Q. Yuand Y. Zhang, “Collective excitation of a trapped Bose-Einstein condensate with spin-orbit coupling”, *Physical Review A*, vol. 95, no. 3. American Physical Society (APS), Mar. 15, 2017. doi: 10.1103/physreva.95.033616.  
  
L. Yang and H. Pu, “Bose-Fermi mapping and a multibranch spin-chain model for strongly interacting quantum gases in one dimension: Dynamics and collective excitations”, *Physical Review A*, vol. 94, no. 3. American Physical Society (APS), Sep. 12, 2016. doi: 10.1103/physreva.94.033614.  
  
L. Yang and H. Pu, “One-body density matrix and momentum distribution of strongly interacting one-dimensional spinor quantum gases”, *Physical Review A*, vol. 95, no. 5. American Physical Society (APS), May 12, 2017. doi: 10.1103/physreva.95.051602.  
  
C. Zhu, L. Dongand H. Pu, “Effects of spin-orbit coupling on Jaynes-Cummings and Tavis-Cummings models”, *Physical Review A*, vol. 94, no. 5. American Physical Society (APS), Nov. 22, 2016. doi: 10.1103/physreva.94.053621.  
  
A. S. Kim and H.-J. Kim, “Dissipative Dynamics of Granular Materials”, *Granular Materials*. InTech, Sep. 06, 2017. doi: 10.5772/intechopen.69196.  
  
B. Wang, “Modern gyrokinetic particle-in-cell simulation of fusion plasmas on top supercomputers”, *The International Journal of High Performance Computing Applications*, vol. 33, no. 1. SAGE Publications, pp. 169–188, Jun. 29, 2017. doi: 10.1177/1094342017712059.  
  
S. Catterall and J. Giedt, “Real space renormalization group for twisted lattice N 𝒩 =4 super Yang-Mills”, *Journal of High Energy Physics*, vol. 2014, no. 11. Springer Science and Business Media LLC, Nov. 2014. doi: 10.1007/jhep11(2014)050.  
  
J. Giedt, “Anomalous dimensions on the lattice”, *International Journal of Modern Physics A*, vol. 31, no. 10. World Scientific Pub Co Pte Lt, p. 1630011, Apr. 06, 2016. doi: 10.1142/s0217751x16300118.  
  
D. Howarth and J. Giedt, “The sigma meson from lattice QCD with two-pion interpolating operators”, *International Journal of Modern Physics C*, vol. 28, no. 10. World Scientific Pub Co Pte Lt, p. 1750124, Oct. 2017. doi: 10.1142/s0129183117501248.  
  
M. G. Aartsen, “Measurement of the *νμ*

ν  
 μ  
   
   
   
 energy spectrum with IceCube-79”, <i>The European Physical Journal C</i>, vol. 77, no. 10. Springer Science and Business Media LLC, Oct. 2017. doi: 10.1140/epjc/s10052-017-5261-3.

M. G. Aartsen, “Search for neutrinos from decaying dark matter with IceCube”, *The European Physical Journal C*, vol. 78, no. 10. Springer Science and Business Media LLC, Oct. 2018. doi: 10.1140/epjc/s10052-018-6273-3.  
  
M. G. Aartsen, “Constraints on Minute-Scale Transient Astrophysical Neutrino Sources”, *Physical Review Letters*, vol. 122, no. 5. American Physical Society (APS), Feb. 06, 2019. doi: 10.1103/physrevlett.122.051102.  
  
M. G. Aartsen, “Neutrino oscillation studies with IceCube-DeepCore”, *Nuclear Physics B*, vol. 908. Elsevier BV, pp. 161–177, Jul. 2016. doi: 10.1016/j.nuclphysb.2016.03.028.  
  
M. G. Aartsen, “All-flavour search for neutrinos from dark matter annihilations in the Milky Way with IceCube/DeepCore”, *The European Physical Journal C*, vol. 76, no. 10. Springer Science and Business Media LLC, Sep. 28, 2016. doi: 10.1140/epjc/s10052-016-4375-3.  
  
M. G. Aartsen, “First search for dark matter annihilations in the Earth with the IceCube detector”, *The European Physical Journal C*, vol. 77, no. 2. Springer Science and Business Media LLC, Feb. 2017. doi: 10.1140/epjc/s10052-016-4582-y.  
  
M. G. Aartsen, “Search for annihilating dark matter in the Sun with 3 years of IceCube data”, *The European Physical Journal C*, vol. 77, no. 3. Springer Science and Business Media LLC, Mar. 2017. doi: 10.1140/epjc/s10052-017-4689-9.  
  
M. G. Aartsen, “Search for neutrinos from dark matter self-annihilations in the center of the Milky Way with 3 years of IceCube/DeepCore”, *The European Physical Journal C*, vol. 77, no. 9. Springer Science and Business Media LLC, Sep. 2017. doi: 10.1140/epjc/s10052-017-5213-y.  
  
M. G. Aartsen, “PINGU: a vision for neutrino and particle physics at the South Pole”, *Journal of Physics G: Nuclear and Particle Physics*, vol. 44, no. 5. IOP Publishing, p. 054006, Apr. 07, 2017. doi: 10.1088/1361-6471/44/5/054006.  
  
M. G. Aartsen, “Efficient propagation of systematic uncertainties from calibration to analysis with the SnowStorm method in IceCube”, *Journal of Cosmology and Astroparticle Physics*, vol. 2019, no. 10. IOP Publishing, pp. 048–048, Oct. 21, 2019. doi: 10.1088/1475-7516/2019/10/048.  
  
M. G. Aartsen, “Development of an analysis to probe the neutrino mass ordering with atmospheric neutrinos using three years of IceCube DeepCore data”, *The European Physical Journal C*, vol. 80, no. 1. Springer Science and Business Media LLC, Jan. 2020. doi: 10.1140/epjc/s10052-019-7555-0.  
  
M. G. Aartsen, “Neutrinos below 100 TeV from the southern sky employing refined veto techniques to IceCube data”, *Astroparticle Physics*, vol. 116. Elsevier BV, p. 102392, Mar. 2020. doi: 10.1016/j.astropartphys.2019.102392.  
  
N. Mehta and D. Levin, “Molecular Dynamics Electrospray Simulations of Coarse-Grained Ethylammonium Nitrate (EAN) and 1-Ethyl-3-Methylimidazolium Tetrafluoroborate (EMIM-BF4)”, *Aerospace*, vol. 5, no. 1. MDPI AG, p. 1, Dec. 28, 2017. doi: 10.3390/aerospace5010001.  
  
N. A. Mehta and D. A. Levin, “Comparison of two protic ionic liquid behaviors in the presence of an electric field using molecular dynamics”, *The Journal of Chemical Physics*, vol. 147, no. 23. AIP Publishing, p. 234505, Dec. 21, 2017. doi: 10.1063/1.5001827.  
  
S. S. Sawant, O. Tumuklu, V. Theofilisand D. A. Levin, “Analysis of Spanwise Homogeneous Perturbations in Laminar Hypersonic Shock-Boundary Layer Interactions”, *AIAA Scitech 2020 Forum*. American Institute of Aeronautics and Astronautics, Jan. 05, 2020. doi: 10.2514/6.2020-0108.  
  
T. N. Bernard, “Gyrokinetic continuum simulations of plasma turbulence in the Texas Helimak”, *Physics of Plasmas*, vol. 26, no. 4. AIP Publishing, p. 042301, Apr. 2019. doi: 10.1063/1.5085457.  
  
J. Juno, A. Hakim, J. TenBarge, E. Shiand W. Dorland, “Discontinuous Galerkin algorithms for fully kinetic plasmas”, *Journal of Computational Physics*, vol. 353. Elsevier BV, pp. 110–147, Jan. 2018. doi: 10.1016/j.jcp.2017.10.009.  
  
V. Skoutnev, A. Hakim, J. Junoand J. M. TenBarge, “Temperature-dependent Saturation of Weibel-type Instabilities in Counter-streaming Plasmas”, *The Astrophysical Journal*, vol. 872, no. 2. American Astronomical Society, p. L28, Feb. 21, 2019. doi: 10.3847/2041-8213/ab0556.  
  
A. Ashtekar and B. Gupt, “Quantum gravity in the sky: interplay between fundamental theory and observations”, *Classical and Quantum Gravity*, vol. 34, no. 1. IOP Publishing, p. 014002, Dec. 08, 2016. doi: 10.1088/1361-6382/34/1/014002.  
  
B. Bonga, B. Guptand N. Yokomizo, “Tensor perturbations during inflation in a spatially closed Universe”, *Journal of Cosmology and Astroparticle Physics*, vol. 2017, no. 5. IOP Publishing, pp. 021–021, May 10, 2017. doi: 10.1088/1475-7516/2017/05/021.  
  
M. Agathos, F. Zappa, S. Bernuzzi, A. Perego, M. Breschiand D. Radice, “Inferring prompt black-hole formation in neutron star mergers from gravitational-wave data”, *Physical Review D*, vol. 101, no. 4. American Physical Society (APS), Feb. 05, 2020. doi: 10.1103/physrevd.101.044006.  
  
S. Bernuzzi, “Accretion-induced prompt black hole formation in asymmetric neutron star mergers, dynamical ejecta, and kilonova signals”, *Monthly Notices of the Royal Astronomical Society*, vol. 497, no. 2. Oxford University Press (OUP), pp. 1488–1507, Jun. 27, 2020. doi: 10.1093/mnras/staa1860.  
  
M. Breschi, “Kilohertz gravitational waves from binary neutron star remnants: Time-domain model and constraints on extreme matter”, *Physical Review D*, vol. 100, no. 10. American Physical Society (APS), Nov. 14, 2019. doi: 10.1103/physrevd.100.104029.  
  
T. Dietrich, “CoRe database of binary neutron star merger waveforms”, *Classical and Quantum Gravity*, vol. 35, no. 24. IOP Publishing, pp. 24LT01, Nov. 13, 2018. doi: 10.1088/1361-6382/aaebc0.  
  
A. Endrizzi, “Thermodynamics conditions of matter in the neutrino decoupling region during neutron star mergers”, *The European Physical Journal A*, vol. 56, no. 1. Springer Science and Business Media LLC, Jan. 2020. doi: 10.1140/epja/s10050-019-00018-6.  
  
G. M. Fuller, A. Kusenko, D. Radiceand V. Takhistov, “Positrons and 511 keV Radiation as Tracers of Recent Binary Neutron Star Mergers”, *Physical Review Letters*, vol. 122, no. 12. American Physical Society (APS), Mar. 29, 2019. doi: 10.1103/physrevlett.122.121101.  
  
V. Nedora, S. Bernuzzi, D. Radice, A. Perego, A. Endrizziand N. Ortiz, “Spiral-wave Wind for the Blue Kilonova”, *The Astrophysical Journal*, vol. 886, no. 2. American Astronomical Society, p. L30, Nov. 27, 2019. doi: 10.3847/2041-8213/ab5794.  
  
A. Perego, S. Bernuzziand D. Radice, “Thermodynamics conditions of matter in neutron star mergers”, *The European Physical Journal A*, vol. 55, no. 8. Springer Science and Business Media LLC, Aug. 2019. doi: 10.1140/epja/i2019-12810-7.  
  
D. Radice, “General-relativistic Large-eddy Simulations of Binary Neutron Star Mergers”, *The Astrophysical Journal*, vol. 838, no. 1. American Astronomical Society, p. L2, Mar. 16, 2017. doi: 10.3847/2041-8213/aa6483.  
  
D. Radice, “Binary Neutron Star Merger Simulations with a Calibrated Turbulence Model”, *Symmetry*, vol. 12, no. 8. MDPI AG, p. 1249, Jul. 29, 2020. doi: 10.3390/sym12081249.  
  
D. Radice and L. Dai, “Multimessenger parameter estimation of GW170817”, *The European Physical Journal A*, vol. 55, no. 4. Springer Science and Business Media LLC, Apr. 2019. doi: 10.1140/epja/i2019-12716-4.  
  
D. Radice, A. Perego, S. Bernuzziand B. Zhang, “Long-lived remnants from binary neutron star mergers”, *Monthly Notices of the Royal Astronomical Society*, vol. 481, no. 3. Oxford University Press (OUP), pp. 3670–3682, Sep. 14, 2018. doi: 10.1093/mnras/sty2531.  
  
D. Radice, A. Perego, K. Hotokezaka, S. Bernuzzi, S. A. Frommand L. F. Roberts, “Viscous-dynamical Ejecta from Binary Neutron Star Mergers”, *The Astrophysical Journal*, vol. 869, no. 2. American Astronomical Society, p. L35, Dec. 19, 2018. doi: 10.3847/2041-8213/aaf053.  
  
D. Radice, A. Perego, K. Hotokezaka, S. A. Fromm, S. Bernuzziand L. F. Roberts, “Binary Neutron Star Mergers: Mass Ejection, Electromagnetic Counterparts, and Nucleosynthesis”, *The Astrophysical Journal*, vol. 869, no. 2. American Astronomical Society, p. 130, Dec. 19, 2018. doi: 10.3847/1538-4357/aaf054.  
  
L. Madeira, S. Gandolfi, K. E. Schmidtand V. S. Bagnato, “Vortices in low-density neutron matter and cold Fermi gases”, *Physical Review C*, vol. 100, no. 1. American Physical Society (APS), Jul. 08, 2019. doi: 10.1103/physrevc.100.014001.  
  
L. Madeira, A. Lovato, F. Pederivaand K. E. Schmidt, “Quantum Monte Carlo formalism for dynamical pions and nucleons”, *Physical Review C*, vol. 98, no. 3. American Physical Society (APS), Sep. 27, 2018. doi: 10.1103/physrevc.98.034005.  
  
N. Shulumba, O. Hellmanand A. J. Minnich, “Lattice Thermal Conductivity of Polyethylene Molecular Crystals from First-Principles Including Nuclear Quantum Effects”, *Physical Review Letters*, vol. 119, no. 18. American Physical Society (APS), Oct. 31, 2017. doi: 10.1103/physrevlett.119.185901.  
  
G. Bergner and S. Catterall, “Supersymmetry on the lattice”, *International Journal of Modern Physics A*, vol. 31, no. 22. World Scientific Pub Co Pte Lt, p. 1643005, Aug. 09, 2016. doi: 10.1142/s0217751x16430053.  
  
S. Catterall, “Supersymmetry on a Lattice”, *Journal of Physics: Conference Series*, vol. 640. IOP Publishing, p. 012050, Sep. 28, 2015. doi: 10.1088/1742-6596/640/1/012050.  
  
S. Catterall, “Fermion mass without symmetry breaking”, *Journal of High Energy Physics*, vol. 2016, no. 1. Springer Science and Business Media LLC, Jan. 2016. doi: 10.1007/jhep01(2016)121.  
  
V. Zhdankin, D. A. Uzdensky, G. R. Wernerand M. C. Begelman, “System-size Convergence of Nonthermal Particle Acceleration in Relativistic Plasma Turbulence”, *The Astrophysical Journal*, vol. 867, no. 1. American Astronomical Society, p. L18, Oct. 31, 2018. doi: 10.3847/2041-8213/aae88c.  
  
V. Zhdankin, D. A. Uzdensky, G. R. Wernerand M. C. Begelman, “Electron and Ion Energization in Relativistic Plasma Turbulence”, *Physical Review Letters*, vol. 122, no. 5. American Physical Society (APS), Feb. 08, 2019. doi: 10.1103/physrevlett.122.055101.  
  
V. Siddhu, “Maximum *a posteriori* probability estimates for quantum tomography”, *Physical Review A*, vol. 99, no. 1. American Physical Society (APS), Jan. 28, 2019. doi: 10.1103/physreva.99.012342.  
  
V. Siddhu and R. B. Griffiths, “Degradable quantum channels using pure-state to product-of-pure-state isometries”, *Physical Review A*, vol. 94, no. 5. American Physical Society (APS), Nov. 23, 2016. doi: 10.1103/physreva.94.052331.  
  
F. Foucart, M. Chandra, C. F. Gammie, E. Quataertand A. Tchekhovskoy, “How important is non-ideal physics in simulations of sub-Eddington accretion on to spinning black holes?”, *Monthly Notices of the Royal Astronomical Society*, vol. 470, no. 2. Oxford University Press (OUP), pp. 2240–2252, Jun. 03, 2017. doi: 10.1093/mnras/stx1368.  
  
X. Mu, “Redox Trimetallic Nanozyme with Neutral Environment Preference for Brain Injury”, *ACS Nano*. American Chemical Society (ACS), Feb. 15, 2019. doi: 10.1021/acsnano.8b08045.  
  
Y. Qiao, “Fluorescence enhancement of gold nanoclusters*via*Zn doping for biomedical applications”, *RSC Advances*, vol. 8, no. 14. Royal Society of Chemistry (RSC), pp. 7396–7402, 2018. doi: 10.1039/c7ra13072d.  
  
D. George and E. A. Huerta, “Deep Learning for real-time gravitational wave detection and parameter estimation: Results with Advanced LIGO data”, *Physics Letters B*, vol. 778. Elsevier BV, pp. 64–70, Mar. 2018. doi: 10.1016/j.physletb.2017.12.053.  
  
D. George, H. Shenand E. A. Huerta, “Classification and unsupervised clustering of LIGO data with Deep Transfer Learning”, *Physical Review D*, vol. 97, no. 10. American Physical Society (APS), May 21, 2018. doi: 10.1103/physrevd.97.101501.  
  
S. Habib and E. A. Huerta, “Characterization of numerical relativity waveforms of eccentric binary black hole mergers”, *Physical Review D*, vol. 100, no. 4. American Physical Society (APS), Aug. 09, 2019. doi: 10.1103/physrevd.100.044016.  
  
E. A. Huerta, “Enabling real-time multi-messenger astrophysics discoveries with deep learning”, *Nature Reviews Physics*, vol. 1, no. 10. Springer Science and Business Media LLC, pp. 600–608, Oct. 03, 2019. doi: 10.1038/s42254-019-0097-4.  
  
E. A. Huerta, “Physics of eccentric binary black hole mergers: A numerical relativity perspective”, *Physical Review D*, vol. 100, no. 6. American Physical Society (APS), Sep. 04, 2019. doi: 10.1103/physrevd.100.064003.  
  
E. A. Huerta, “Complete waveform model for compact binaries on eccentric orbits”, *Physical Review D*, vol. 95, no. 2. American Physical Society (APS), Jan. 31, 2017. doi: 10.1103/physrevd.95.024038.  
  
E. A. Huerta, “Eccentric, nonspinning, inspiral, Gaussian-process merger approximant for the detection and characterization of eccentric binary black hole mergers”, *Physical Review D*, vol. 97, no. 2. American Physical Society (APS), Jan. 24, 2018. doi: 10.1103/physrevd.97.024031.  
  
A. Khan, E. A. Huerta, S. Wang, R. Gruendl, E. Jenningsand H. Zheng, “Deep learning at scale for the construction of galaxy catalogs in the Dark Energy Survey”, *Physics Letters B*, vol. 795. Elsevier BV, pp. 248–258, Aug. 2019. doi: 10.1016/j.physletb.2019.06.009.  
  
A. Rebei, “Fusing numerical relativity and deep learning to detect higher-order multipole waveforms from eccentric binary black hole mergers”, *Physical Review D*, vol. 100, no. 4. American Physical Society (APS), Aug. 12, 2019. doi: 10.1103/physrevd.100.044025.  
  
S. G. Rosofsky and E. A. Huerta, “Artificial neural network subgrid models of 2D compressible magnetohydrodynamic turbulence”, *Physical Review D*, vol. 101, no. 8. American Physical Society (APS), Apr. 09, 2020. doi: 10.1103/physrevd.101.084024.  
  
W. Wei and E. A. Huerta, “Gravitational wave denoising of binary black hole mergers with deep learning”, *Physics Letters B*, vol. 800. Elsevier BV, p. 135081, Jan. 2020. doi: 10.1016/j.physletb.2019.135081.  
  
W. Wei, “Deep transfer learning for star cluster classification: I. application to the PHANGS–*HST* survey”, *Monthly Notices of the Royal Astronomical Society*, vol. 493, no. 3. Oxford University Press (OUP), pp. 3178–3193, Feb. 04, 2020. doi: 10.1093/mnras/staa325.  
  
J. Rantaharju, C. Picaand F. Sannino, “Ideal walking dynamics via a gauged NJL model”, *Physical Review D*, vol. 96, no. 1. American Physical Society (APS), Jul. 25, 2017. doi: 10.1103/physrevd.96.014512.  
  
J. A. Gomez, M. Degroote, J. Zhao, Y. Qiuand G. E. Scuseria, “Spin polynomial similarity transformation for repulsive Hamiltonians: interpolating between coupled cluster and spin-projected unrestricted Hartree–Fock”, *Physical Chemistry Chemical Physics*, vol. 19, no. 33. Royal Society of Chemistry (RSC), pp. 22385–22394, 2017. doi: 10.1039/c7cp04075j.  
  
S. Lee and L. Lindsay, “Hydrodynamic phonon drift and second sound in a (20,20) single-wall carbon nanotube”, *Physical Review B*, vol. 95, no. 18. American Physical Society (APS), May 18, 2017. doi: 10.1103/physrevb.95.184304.  
  
X. Li and S. Lee, “Role of hydrodynamic viscosity on phonon transport in suspended graphene”, *Physical Review B*, vol. 97, no. 9. American Physical Society (APS), Mar. 30, 2018. doi: 10.1103/physrevb.97.094309.  
  
C. Alexandrou, “Proton and neutron electromagnetic form factors from lattice QCD”, *Physical Review D*, vol. 100, no. 1. American Physical Society (APS), Jul. 25, 2019. doi: 10.1103/physrevd.100.014509.  
  
C. Lauer, “Investigating volume effects for *Nf* = 2 twisted clover fermions at the physical point”, *Proceedings of The 36th Annual International Symposium on Lattice Field Theory — PoS(LATTICE2018)*. Sissa Medialab, May 29, 2019. doi: 10.22323/1.334.0314.  
  
Z. Dai, “Surface buckling of black phosphorus: Determination, origin, and influence on electronic structure”, *Physical Review Materials*, vol. 1, no. 7. American Physical Society (APS), Dec. 29, 2017. doi: 10.1103/physrevmaterials.1.074003.  
  
Z. Dai, “Crystal structure reconstruction in the surface monolayer of the quantum spin liquid candidate *α*-RuCl3”, *2D Materials*, vol. 7, no. 3. IOP Publishing, p. 035004, May 01, 2020. doi: 10.1088/2053-1583/ab7e0e.  
  
W. Jin, “Phase transition and electronic structure evolution of induced by W substitution”, *Physical Review B*, vol. 98, no. 14. American Physical Society (APS), Oct. 31, 2018. doi: 10.1103/physrevb.98.144114.  
  
G. Yin, J.-X. Yu, Y. Liu, R. K. Lake, J. Zangand K. L. Wang, “Planar Hall Effect in Antiferromagnetic MnTe Thin Films”, *Physical Review Letters*, vol. 122, no. 10. American Physical Society (APS), Mar. 13, 2019. doi: 10.1103/physrevlett.122.106602.  
  
J.-X. Yu, “Three Jahn-Teller States of Matter in Spin-Crossover System Mn(taa)”, *Physical Review Letters*, vol. 124, no. 22. American Physical Society (APS), Jun. 03, 2020. doi: 10.1103/physrevlett.124.227201.  
  
J.-X. Yu, G. Christouand H.-P. Cheng, “Analysis of Exchange Interactions in Dimers of Mn3 Single-Molecule Magnets, and Their Sensitivity to External Pressure”, *The Journal of Physical Chemistry C*, vol. 124, no. 27. American Chemical Society (ACS), pp. 14768–14774, Jun. 03, 2020. doi: 10.1021/acs.jpcc.0c02213.  
  
J.-X. Yu, M. Dalyand J. Zang, “Thermally driven topology in frustrated systems”, *Physical Review B*, vol. 99, no. 10. American Physical Society (APS), Mar. 27, 2019. doi: 10.1103/physrevb.99.104431.  
  
J.-X. Yu and J. Zang, “Giant perpendicular magnetic anisotropy in Fe/III-V nitride thin films”, *Science Advances*, vol. 4, no. 3. American Association for the Advancement of Science (AAAS), Mar. 02, 2018. doi: 10.1126/sciadv.aar7814.  
  
B. Kloss and Y. Bar Lev, “Spin transport in a long-range-interacting spin chain”, *Physical Review A*, vol. 99, no. 3. American Physical Society (APS), Mar. 14, 2019. doi: 10.1103/physreva.99.032114.  
  
B. Kloss, Y. B. Levand D. Reichman, “Time-dependent variational principle in matrix-product state manifolds: Pitfalls and potential”, *Physical Review B*, vol. 97, no. 2. American Physical Society (APS), Jan. 26, 2018. doi: 10.1103/physrevb.97.024307.  
  
D. J. Luitz, Y. Bar Levand A. Lazarides, “Absence of dynamical localization in interacting driven systems”, *SciPost Physics*, vol. 3, no. 4. Stichting SciPost, Oct. 25, 2017. doi: 10.21468/scipostphys.3.4.029.  
  
L. Gao, “Mega-Gauss Plasma Jet Creation Using a Ring of Laser Beams”, *The Astrophysical Journal*, vol. 873, no. 2. American Astronomical Society, p. L11, Mar. 08, 2019. doi: 10.3847/2041-8213/ab07bd.  
  
Y. Núñez Fernández and K. Hallberg, “Solving the Multi-site and Multi-orbital Dynamical Mean Field Theory Using Density Matrix Renormalization”, *Frontiers in Physics*, vol. 6. Frontiers Media SA, Feb. 26, 2018. doi: 10.3389/fphy.2018.00013.  
  
Y. Núñez-Fernández, G. Kotliarand K. Hallberg, “Emergent low-energy bound states in the two-orbital Hubbard model”, *Physical Review B*, vol. 97, no. 12. American Physical Society (APS), Mar. 30, 2018. doi: 10.1103/physrevb.97.121113.  
  
D. M. Sussman, M. Paoluzzi, M. Cristina Marchettiand M. Lisa Manning, “Anomalous glassy dynamics in simple models of dense biological tissue”, *EPL (Europhysics Letters)*, vol. 121, no. 3. IOP Publishing, p. 36001, Feb. 01, 2018. doi: 10.1209/0295-5075/121/36001.  
  
A. Bazavov, S. Catterall, R. G. Jhaand J. Unmuth-Yockey, “Tensor renormalization group study of the non-Abelian Higgs model in two dimensions”, *Physical Review D*, vol. 99, no. 11. American Physical Society (APS), Jun. 24, 2019. doi: 10.1103/physrevd.99.114507.  
  
N. Butt, S. Catterall, Y. Meurice, R. Sakaiand J. Unmuth-Yockey, “Tensor network formulation of the massless Schwinger model with staggered fermions”, *Physical Review D*, vol. 101, no. 9. American Physical Society (APS), May 26, 2020. doi: 10.1103/physrevd.101.094509.  
  
N. Butt, S. Catteralland D. Schaich, “ invariant Higgs-Yukawa model with reduced staggered fermions”, *Physical Review D*, vol. 98, no. 11. American Physical Society (APS), Dec. 26, 2018. doi: 10.1103/physrevd.98.114514.  
  
S. Catterall and N. Butt, “Simulations of lattice gauge theory with dynamical reduced staggered fermions”, *Physical Review D*, vol. 99, no. 1. American Physical Society (APS), Jan. 14, 2019. doi: 10.1103/physrevd.99.014505.  
  
S. Catterall, J. Laihoand J. Unmuth-Yockey, “Kähler-Dirac fermions on Euclidean dynamical triangulations”, *Physical Review D*, vol. 98, no. 11. American Physical Society (APS), Dec. 11, 2018. doi: 10.1103/physrevd.98.114503.  
  
J. Giedt, S. Catterall, P. Damgaardand D. Schaich, “S-duality in lattice super Yang-Mills”, *Proceedings of 34th annual International Symposium on Lattice Field Theory — PoS(LATTICE2016)*. Sissa Medialab, Dec. 27, 2016. doi: 10.22323/1.256.0209.  
  
R. G. Jha, S. Catterall, D. Schaichand T. Wiseman, “Testing the holographic principle using lattice simulations”, *EPJ Web of Conferences*, vol. 175. EDP Sciences, p. 08004, 2018. doi: 10.1051/epjconf/201817508004.  
  
A. D. Chien, A. A. Holmes, M. Otten, C. J. Umrigar, S. Sharmaand P. M. Zimmerman, “Excited States of Methylene, Polyenes, and Ozone from Heat-Bath Configuration Interaction”, *The Journal of Physical Chemistry A*, vol. 122, no. 10. American Chemical Society (ACS), pp. 2714–2722, Feb. 23, 2018. doi: 10.1021/acs.jpca.8b01554.  
  
B. Xu, T. Feng, Z. Li, S. T. Pantelidesand Y. Wu, “Constructing Highly Porous Thermoelectric Monoliths with High-Performance and Improved Portability from Solution-Synthesized Shape-Controlled Nanocrystals”, *Nano Letters*, vol. 18, no. 6. American Chemical Society (ACS), pp. 4034–4039, May 28, 2018. doi: 10.1021/acs.nanolett.8b01691.  
  
B. Xu, T. Feng, Z. Li, L. Zhou, S. T. Pantelidesand Y. Wu, “Creating Zipper‐Like van der Waals Gap Discontinuity in Low‐Temperature‐Processed Nanostructured PbBi 2 *n* Te 1+3 *n* : Enhanced Phonon Scattering and Improved Thermoelectric Performance”, *Angewandte Chemie International Edition*, vol. 57, no. 34. Wiley, pp. 10938–10943, Jul. 19, 2018. doi: 10.1002/anie.201805890.  
  
S. S. Tayal and O. Zatsarinny, “Electron-impact excitation of forbidden and allowed transitions in Fe ii”, *Physical Review A*, vol. 98, no. 1. American Physical Society (APS), Jul. 11, 2018. doi: 10.1103/physreva.98.012706.  
  
Y. Lu, P. Kilian, F. Guo, H. Liand E. Liang, “Time-step dependent force interpolation scheme for suppressing numerical Cherenkov instability in relativistic particle-in-cell simulations”, *Journal of Computational Physics*, vol. 413. Elsevier BV, p. 109388, Jul. 2020. doi: 10.1016/j.jcp.2020.109388.  
  
Y. Lu, “MPRAD: A Monte Carlo and ray-tracing code for the proton radiography in high-energy-density plasma experiments”, *Review of Scientific Instruments*, vol. 90, no. 12. AIP Publishing, p. 123503, Dec. 01, 2019. doi: 10.1063/1.5123392.  
  
Y. Lu, “Modeling hydrodynamics, magnetic fields, and synthetic radiographs for high-energy-density plasma flows in shock-shear targets”, *Physics of Plasmas*, vol. 27, no. 1. AIP Publishing, p. 012303, Jan. 2020. doi: 10.1063/1.5126149.  
  
Y. Lu, “Numerical simulation of magnetized jet creation using a hollow ring of laser beams”, *Physics of Plasmas*, vol. 26, no. 2. AIP Publishing, p. 022902, Feb. 2019. doi: 10.1063/1.5050924.  
  
A. M. Sirunyan, “A search for pair production of new light bosons decaying into muons in proton-proton collisions at 13  TeV”, *Physics Letters B*, vol. 796. Elsevier BV, pp. 131–154, Sep. 2019. doi: 10.1016/j.physletb.2019.07.013.  
  
A. M. Sirunyan, “Evidence for light-by-light scattering and searches for axion-like particles in ultraperipheral PbPb collisions at ”, *Physics Letters B*, vol. 797. Elsevier BV, p. 134826, Oct. 2019. doi: 10.1016/j.physletb.2019.134826.  
  
A. M. Sirunyan, “Measurement of meson production in pp and PbPb collisions at TeV”, *Physics Letters B*, vol. 796. Elsevier BV, pp. 168–190, Sep. 2019. doi: 10.1016/j.physletb.2019.07.014.  
  
A. M. Sirunyan, “Search for anomalous electroweak production of vector boson pairs in association with two jets in proton-proton collisions at 13 TeV”, *Physics Letters B*, vol. 798. Elsevier BV, p. 134985, Nov. 2019. doi: 10.1016/j.physletb.2019.134985.  
  
A. M. Sirunyan, “Search for an exotic decay of the Higgs boson to a pair of light pseudoscalars in the final state with two muons and two b quarks in pp collisions at 13 TeV”, *Physics Letters B*, vol. 795. Elsevier BV, pp. 398–423, Aug. 2019. doi: 10.1016/j.physletb.2019.06.021.  
  
A. M. Sirunyan, “Pseudorapidity distributions of charged hadrons in xenon-xenon collisions at ”, *Physics Letters B*, vol. 799. Elsevier BV, p. 135049, Dec. 2019. doi: 10.1016/j.physletb.2019.135049.  
  
A. M. Sirunyan, “Search for dark matter in events with a leptoquark and missing transverse momentum in proton-proton collisions at 13 TeV”, *Physics Letters B*, vol. 795. Elsevier BV, pp. 76–99, Aug. 2019. doi: 10.1016/j.physletb.2019.05.046.  
  
A. M. Sirunyan, “Performance of missing transverse momentum reconstruction in proton-proton collisions at √*s* = 13 TeV using the CMS detector”, *Journal of Instrumentation*, vol. 14, no. 7. IOP Publishing, pp. P07004–P07004, Jul. 04, 2019. doi: 10.1088/1748-0221/14/07/p07004.  
  
A. M. Sirunyan, “Search for a standard model-like Higgs boson in the mass range between 70 and 110 GeV in the diphoton final state in proton-proton collisions at and 13 TeV”, *Physics Letters B*, vol. 793. Elsevier BV, pp. 320–347, Jun. 2019. doi: 10.1016/j.physletb.2019.03.064.  
  
A. M. Sirunyan, “Search for an L − L gauge boson using Z → 4μ events in proton-proton collisions at TeV”, *Physics Letters B*, vol. 792. Elsevier BV, pp. 345–368, May 2019. doi: 10.1016/j.physletb.2019.01.072.  
  
A. M. Sirunyan, “Search for invisible decays of a Higgs boson produced through vector boson fusion in proton-proton collisions at ”, *Physics Letters B*, vol. 793. Elsevier BV, pp. 520–551, Jun. 2019. doi: 10.1016/j.physletb.2019.04.025.  
  
A. M. Sirunyan, “An embedding technique to determine ττ backgrounds in proton-proton collision data”, *Journal of Instrumentation*, vol. 14, no. 6. IOP Publishing, pp. P06032–P06032, Jun. 21, 2019. doi: 10.1088/1748-0221/14/06/p06032.  
  
A. M. Sirunyan, “Non-Gaussian elliptic-flow fluctuations in PbPb collisions at ”, *Physics Letters B*, vol. 789. Elsevier BV, pp. 643–665, Feb. 2019. doi: 10.1016/j.physletb.2018.11.063.  
  
A. M. Sirunyan, “Combined measurements of Higgs boson couplings in proton–proton collisions at $$\sqrt{s}=13\,\text {Te}\text {V} $$”, *The European Physical Journal C*, vol. 79, no. 5. Springer Science and Business Media LLC, May 2019. doi: 10.1140/epjc/s10052-019-6909-y.  
  
A. M. Sirunyan, “Measurement and interpretation of differential cross sections for Higgs boson production at ”, *Physics Letters B*, vol. 792. Elsevier BV, pp. 369–396, May 2019. doi: 10.1016/j.physletb.2019.03.059.  
  
A. M. Sirunyan, “Measurement of electroweak WZ boson production and search for new physics in WZ + two jets events in pp collisions at ”, *Physics Letters B*, vol. 795. Elsevier BV, pp. 281–307, Aug. 2019. doi: 10.1016/j.physletb.2019.05.042.  
  
A. M. Sirunyan, “Search for supersymmetric partners of electrons and muons in proton–proton collisions at ”, *Physics Letters B*, vol. 790. Elsevier BV, pp. 140–166, Mar. 2019. doi: 10.1016/j.physletb.2019.01.005.  
  
A. M. Sirunyan, “Measurement of nuclear modification factors of ϒ(1S), ϒ(2S), and ϒ(3S) mesons in PbPb collisions at TeV”, *Physics Letters B*, vol. 790. Elsevier BV, pp. 270–293, Mar. 2019. doi: 10.1016/j.physletb.2019.01.006.  
  
A. M. Sirunyan, “Search for a W′ boson decaying to a τ lepton and a neutrino in proton-proton collisions at ”, *Physics Letters B*, vol. 792. Elsevier BV, pp. 107–131, May 2019. doi: 10.1016/j.physletb.2019.01.069.  
  
A. M. Sirunyan, “Measurements of properties of the Higgs boson decaying to a W boson pair in pp collisions at $\sqrt{s} = 13\ \text{Te}\mspace{-1mu}\text{V}$”, *Physics Letters B*, vol. 791. Elsevier BV, pp. 96–129, Apr. 2019. doi: 10.1016/j.physletb.2018.12.073.  
  
A. M. Sirunyan, “Observation of prompt J/ψ meson elliptic flow in high-multiplicity pPb collisions at TeV”, *Physics Letters B*, vol. 791. Elsevier BV, pp. 172–194, Apr. 2019. doi: 10.1016/j.physletb.2019.02.018.  
  
A. M. Sirunyan, “Measurement of prompt ψ(2S) production cross sections in proton–lead and proton–proton collisions at ”, *Physics Letters B*, vol. 790. Elsevier BV, pp. 509–532, Mar. 2019. doi: 10.1016/j.physletb.2019.01.058.  
  
A. M. Sirunyan, “Measurement of the single top quark and antiquark production cross sections in the t channel and their ratio in proton-proton collisions at ”, *Physics Letters B*, vol. 800. Elsevier BV, p. 135042, Jan. 2020. doi: 10.1016/j.physletb.2019.135042.  
  
A. M. Sirunyan, “Observation of nuclear modifications in W± boson production in pPb collisions at ”, *Physics Letters B*, vol. 800. Elsevier BV, p. 135048, Jan. 2020. doi: 10.1016/j.physletb.2019.135048.  
  
A. M. Sirunyan, “Search for light pseudoscalar boson pairs produced from decays of the 125 GeV Higgs boson in final states with two muons and two nearby tracks in pp collisions at ”, *Physics Letters B*, vol. 800. Elsevier BV, p. 135087, Jan. 2020. doi: 10.1016/j.physletb.2019.135087.  
  
A. M. Sirunyan, “Search for long-lived particles using nonprompt jets and missing transverse momentum with proton-proton collisions at ”, *Physics Letters B*, vol. 797. Elsevier BV, p. 134876, Oct. 2019. doi: 10.1016/j.physletb.2019.134876.  
  
A. M. Sirunyan, “Combination of CMS searches for heavy resonances decaying to pairs of bosons or leptons”, *Physics Letters B*, vol. 798. Elsevier BV, p. 134952, Nov. 2019. doi: 10.1016/j.physletb.2019.134952.  
  
A. M. Sirunyan, “Search for Higgs and Z boson decays to J/ψ or Y pairs in the four-muon final state in proton-proton collisions at ”, *Physics Letters B*, vol. 797. Elsevier BV, p. 134811, Oct. 2019. doi: 10.1016/j.physletb.2019.134811.  
  
A. M. Sirunyan, “Search for MSSM Higgs bosons decaying to μ+μ− in proton-proton collisions at ”, *Physics Letters B*, vol. 798. Elsevier BV, p. 134992, Nov. 2019. doi: 10.1016/j.physletb.2019.134992.  
  
A. M. Sirunyan, “Performance of the reconstruction and identification of high-momentum muons in proton-proton collisions at √*s* = 13 TeV”, *Journal of Instrumentation*, vol. 15, no. 2. IOP Publishing, pp. P02027–P02027, Feb. 28, 2020. doi: 10.1088/1748-0221/15/02/p02027.  
  
A. M. Sirunyan, “Combined search for supersymmetry with photons in proton-proton collisions at TeV”, *Physics Letters B*, vol. 801. Elsevier BV, p. 135183, Feb. 2020. doi: 10.1016/j.physletb.2019.135183.  
  
A. M. Sirunyan, “Running of the top quark mass from proton-proton collisions at ”, *Physics Letters B*, vol. 803. Elsevier BV, p. 135263, Apr. 2020. doi: 10.1016/j.physletb.2020.135263.  
  
A. M. Sirunyan, “Production of baryons in proton-proton and lead-lead collisions at ”, *Physics Letters B*, vol. 803. Elsevier BV, p. 135328, Apr. 2020. doi: 10.1016/j.physletb.2020.135328.  
  
A. M. Sirunyan, “Study of excited states decaying to in proton-proton collisions at ”, *Physics Letters B*, vol. 803. Elsevier BV, p. 135345, Apr. 2020. doi: 10.1016/j.physletb.2020.135345.  
  
A. M. Sirunyan, “Observation of the decay in proton-proton collisions at ”, *Physics Letters B*, vol. 802. Elsevier BV, p. 135203, Mar. 2020. doi: 10.1016/j.physletb.2020.135203.  
  
A. M. Sirunyan, “Combination of searches for heavy resonances decaying to WW, WZ, ZZ, WH, and ZH boson pairs in proton–proton collisions at and 13 TeV”, *Physics Letters B*, vol. 774. Elsevier BV, pp. 533–558, Nov. 2017. doi: 10.1016/j.physletb.2017.09.083.  
  
Y. Quan and W. E. Pickett, “A maximally particle-hole asymmetric spectrum emanating from a semi-Dirac point”, *Journal of Physics: Condensed Matter*, vol. 30, no. 7. IOP Publishing, p. 075501, Jan. 23, 2018. doi: 10.1088/1361-648x/aaa521.  
  
O. Jansen, T. Wang, D. J. Stark, E. d’Humières, T. Toncianand A. V. Arefiev, “Leveraging extreme laser-driven magnetic fields for gamma-ray generation and pair production”, *Plasma Physics and Controlled Fusion*, vol. 60, no. 5. IOP Publishing, p. 054006, Mar. 19, 2018. doi: 10.1088/1361-6587/aab222.  
  
M. Murakami, A. Arefievand M. A. Zosa, “Generation of ultrahigh field by micro-bubble implosion”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, May 24, 2018. doi: 10.1038/s41598-018-25594-3.  
  
M. Fernando, D. Neilsen, H. Lim, E. Hirschmannand H. Sundar, “Massively Parallel Simulations of Binary Black Hole Intermediate-Mass-Ratio Inspirals”, *SIAM Journal on Scientific Computing*, vol. 41, no. 2. Society for Industrial & Applied Mathematics (SIAM), pp. C97–C138, Jan. 2019. doi: 10.1137/18m1196972.  
  
A. Hasenfratz, C. Rebbiand O. Witzel, “Testing Fermion Universality at a Conformal Fixed Point”, *EPJ Web of Conferences*, vol. 175. EDP Sciences, p. 03006, 2018. doi: 10.1051/epjconf/201817503006.  
  
A. Hasenfratz, C. Rebbiand O. Witzel, “Determination of the N*f*=12 step scaling function using Möbius domain wall fermions”, *Proceedings of The 36th Annual International Symposium on Lattice Field Theory — PoS(LATTICE2018)*. Sissa Medialab, May 29, 2019. doi: 10.22323/1.334.0306.  
  
A. Hasenfratz, C. Rebbiand O. Witzel, “Nonperturbative determination of β functions for SU(3) gauge theories with 10 and 12 fundamental flavors using domain wall fermions”, *Physics Letters B*, vol. 798. Elsevier BV, p. 134937, Nov. 2019. doi: 10.1016/j.physletb.2019.134937.  
  
P. Titum, J. T. Iosue, J. R. Garrison, A. V. Gorshkovand Z.-X. Gong, “Probing Ground-State Phase Transitions through Quench Dynamics”, *Physical Review Letters*, vol. 123, no. 11. American Physical Society (APS), Sep. 11, 2019. doi: 10.1103/physrevlett.123.115701.  
  
M. Brown, K. Gelberand M. Mebratu, “Taylor State Merging at SSX: Experiment and Simulation”, *Plasma*, vol. 3, no. 1. MDPI AG, pp. 27–37, Mar. 17, 2020. doi: 10.3390/plasma3010004.  
  
O. I. Malyi, M. T. Yeung, K. R. Poeppelmeier, C. Perssonand A. Zunger, “Spontaneous Non-stoichiometry and Ordering in Degenerate but Gapped Transparent Conductors”, *Matter*, vol. 1, no. 1. Elsevier BV, pp. 280–294, Jul. 2019. doi: 10.1016/j.matt.2019.05.014.  
  
Z. Wang, Q. Liu, J.-W. Luoand A. Zunger, “Digging for topological property in disordered alloys: the emergence of Weyl semimetal phase and sequential band inversions in PbSe–SnSe alloys”, *Materials Horizons*, vol. 6, no. 10. Royal Society of Chemistry (RSC), pp. 2124–2134, 2019. doi: 10.1039/c9mh00574a.  
  
Z. Wang, J.-W. Luoand A. Zunger, “Alloy theory with atomic resolution for Rashba or topological systems”, *Physical Review Materials*, vol. 3, no. 4. American Physical Society (APS), Apr. 26, 2019. doi: 10.1103/physrevmaterials.3.044605.  
  
L. Yuan, Q. Liu, X. Zhang, J.-W. Luo, S.-S. Liand A. Zunger, “Uncovering and tailoring hidden Rashba spin–orbit splitting in centrosymmetric crystals”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, Feb. 22, 2019. doi: 10.1038/s41467-019-08836-4.  
  
T. Wang, Z. Gong, K. Chinand A. Arefiev, “Impact of ion dynamics on laser-driven electron acceleration and gamma-ray emission in structured targets at ultra-high laser intensities”, *Plasma Physics and Controlled Fusion*, vol. 61, no. 8. IOP Publishing, p. 084004, Jun. 21, 2019. doi: 10.1088/1361-6587/ab2499.  
  
T. Wang, T. Toncian, M. S. Weiand A. V. Arefiev, “Structured targets for detection of Megatesla-level magnetic fields through Faraday rotation of XFEL beams”, *Physics of Plasmas*, vol. 26, no. 1. AIP Publishing, p. 013105, Jan. 2019. doi: 10.1063/1.5066109.  
  
J. Li, “Ionization injection of highly-charged copper ions for laser driven acceleration from ultra-thin foils”, *Scientific Reports*, vol. 9, no. 1. Springer Science and Business Media LLC, Jan. 24, 2019. doi: 10.1038/s41598-018-37085-6.  
  
P. P. Dholabhai, “Atomic-scale structure of misfit dislocations in CeO2/MgO heterostructures and thermodynamic stability of dopant–defect complexes at the heterointerface”, *Physical Chemistry Chemical Physics*, vol. 21, no. 37. Royal Society of Chemistry (RSC), pp. 20878–20891, 2019. doi: 10.1039/c9cp03727f.  
  
A. A. Kaptanoglu, K. D. Morgan, C. J. Hansenand S. L. Brunton, “Characterizing magnetized plasmas with dynamic mode decomposition”, *Physics of Plasmas*, vol. 27, no. 3. AIP Publishing, p. 032108, Mar. 2020. doi: 10.1063/1.5138932.  
  
D. Matsunami, L. Pogosian, A. Saurabhand T. Vachaspati, “Decay of Cosmic String Loops due to Particle Radiation”, *Physical Review Letters*, vol. 122, no. 20. American Physical Society (APS), May 20, 2019. doi: 10.1103/physrevlett.122.201301.  
  
S. Hajinazar, A. Thorn, E. D. Sandoval, S. Kharabadzeand A. N. Kolmogorov, “MAISE: Construction of neural network interatomic models and evolutionary structure optimization”, *Computer Physics Communications*, vol. 259. Elsevier BV, p. 107679, Feb. 2021. doi: 10.1016/j.cpc.2020.107679.  
  
A. Thorn, J. Rojas-Nunez, S. Hajinazar, S. E. Baltazarand A. N. Kolmogorov, “Toward *ab Initio* Ground States of Gold Clusters via Neural Network Modeling”, *The Journal of Physical Chemistry C*, vol. 123, no. 50. American Chemical Society (ACS), pp. 30088–30098, Nov. 25, 2019. doi: 10.1021/acs.jpcc.9b08517.  
  
M. Murakami, J. J. Honrubia, K. Weichman, A. V. Arefievand S. V. Bulanov, “Generation of megatesla magnetic fields by intense-laser-driven microtube implosions”, *Scientific Reports*, vol. 10, no. 1. Springer Science and Business Media LLC, Oct. 06, 2020. doi: 10.1038/s41598-020-73581-4.  
  
K. Weichman, A. P. L. Robinson, M. Murakamiand A. V. Arefiev, “Strong surface magnetic field generation in relativistic short pulse laser–plasma interaction with an applied seed magnetic field”, *New Journal of Physics*, vol. 22, no. 11. IOP Publishing, p. 113009, Nov. 01, 2020. doi: 10.1088/1367-2630/abc496.  
  
W. Vigilante, O. Lopezand J. Fung, “Brownian dynamics simulations of sphere clusters in optical tweezers”, *Optics Express*, vol. 28, no. 24. Optica Publishing Group, p. 36131, Nov. 13, 2020. doi: 10.1364/oe.409078.  
  
J. Wolcott-Green, Z. Haimanand G. L. Bryan, “Suppression of **H2**-cooling in protogalaxies aided by trapped Ly*α* cooling radiation”, *Monthly Notices of the Royal Astronomical Society*, vol. 500, no. 1. Oxford University Press (OUP), pp. 138–144, Oct. 09, 2020. doi: 10.1093/mnras/staa3057.  
  
J. Blackman, “A Surrogate model of gravitational waveforms from numerical relativity simulations of precessing binary black hole mergers”, *Physical Review D*, vol. 95, no. 10. American Physical Society (APS), May 17, 2017. doi: 10.1103/physrevd.95.104023.  
  
A. Bohé, “Improved effective-one-body model of spinning, nonprecessing binary black holes for the era of gravitational-wave astrophysics with advanced detectors”, *Physical Review D*, vol. 95, no. 4. American Physical Society (APS), Feb. 17, 2017. doi: 10.1103/physrevd.95.044028.  
  
A. Bohn, “What does a binary black hole merger look like?”, *Classical and Quantum Gravity*, vol. 32, no. 6. IOP Publishing, p. 065002, Feb. 23, 2015. doi: 10.1088/0264-9381/32/6/065002.  
  
K. Chakravarti, “Systematic effects from black hole-neutron star waveform model uncertainties on the neutron star equation of state”, *Physical Review D*, vol. 99, no. 2. American Physical Society (APS), Jan. 31, 2019. doi: 10.1103/physrevd.99.024049.  
  
T. Chu, “On the accuracy and precision of numerical waveforms: effect of waveform extraction methodology”, *Classical and Quantum Gravity*, vol. 33, no. 16. IOP Publishing, p. 165001, Jul. 14, 2016. doi: 10.1088/0264-9381/33/16/165001.  
  
M. B. Deaton, “BLACK HOLE-NEUTRON STAR MERGERS WITH A HOT NUCLEAR EQUATION OF STATE: OUTFLOW AND NEUTRINO-COOLED DISK FOR A LOW-MASS, HIGH-SPIN CASE”, *The Astrophysical Journal*, vol. 776, no. 1. American Astronomical Society, p. 47, Sep. 24, 2013. doi: 10.1088/0004-637x/776/1/47.  
  
M. B. Deaton, “Elastic scattering in general relativistic ray tracing for neutrinos”, *Physical Review D*, vol. 98, no. 10. American Physical Society (APS), Nov. 14, 2018. doi: 10.1103/physrevd.98.103014.  
  
M. D. Duez, F. Foucart, L. E. Kidder, C. D. Ottand S. A. Teukolsky, “Equation of state effects in black hole–neutron star mergers”, *Classical and Quantum Gravity*, vol. 27, no. 11. IOP Publishing, p. 114106, May 10, 2010. doi: 10.1088/0264-9381/27/11/114106.  
  
R. Fernández, A. Tchekhovskoy, E. Quataert, F. Foucartand D. Kasen, “Long-term GRMHD simulations of neutron star merger accretion discs: implications for electromagnetic counterparts”, *Monthly Notices of the Royal Astronomical Society*, vol. 482, no. 3. Oxford University Press (OUP), pp. 3373–3393, Oct. 30, 2018. doi: 10.1093/mnras/sty2932.  
  
F. Foucart, “First direct comparison of nondisrupting neutron star-black hole and binary black hole merger simulations”, *Physical Review D*, vol. 88, no. 6. American Physical Society (APS), Sep. 09, 2013. doi: 10.1103/physrevd.88.064017.  
  
F. Foucart, “Black-hole–neutron-star mergers at realistic mass ratios: Equation of state and spin orientation effects”, *Physical Review D*, vol. 87, no. 8. American Physical Society (APS), Apr. 02, 2013. doi: 10.1103/physrevd.87.084006.  
  
F. Foucart, “Dynamical ejecta from precessing neutron star-black hole mergers with a hot, nuclear-theory based equation of state”, *Classical and Quantum Gravity*, vol. 34, no. 4. IOP Publishing, p. 044002, Jan. 20, 2017. doi: 10.1088/1361-6382/aa573b.  
  
F. Foucart, “Gravitational waveforms from spectral Einstein code simulations: Neutron star-neutron star and low-mass black hole-neutron star binaries”, *Physical Review D*, vol. 99, no. 4. American Physical Society (APS), Feb. 11, 2019. doi: 10.1103/physrevd.99.044008.  
  
F. Foucart, M. D. Duez, L. E. Kidder, R. Nguyen, H. P. Pfeifferand M. A. Scheel, “Evaluating radiation transport errors in merger simulations using a Monte Carlo algorithm”, *Physical Review D*, vol. 98, no. 6. American Physical Society (APS), Sep. 11, 2018. doi: 10.1103/physrevd.98.063007.  
  
F. Foucart, M. D. Duez, L. E. Kidder, M. A. Scheel, B. Szilagyiand S. A. Teukolsky, “Black hole-neutron star mergers forblack holes”, *Physical Review D*, vol. 85, no. 4. American Physical Society (APS), Feb. 07, 2012. doi: 10.1103/physrevd.85.044015.  
  
F. Foucart, M. D. Duez, L. E. Kidderand S. A. Teukolsky, “Black hole-neutron star mergers: Effects of the orientation of the black hole spin”, *Physical Review D*, vol. 83, no. 2. American Physical Society (APS), Jan. 06, 2011. doi: 10.1103/physrevd.83.024005.  
  
F. Foucart, T. Hindererand S. Nissanke, “Remnant baryon mass in neutron star-black hole mergers: Predictions for binary neutron star mimickers and rapidly spinning black holes”, *Physical Review D*, vol. 98, no. 8. American Physical Society (APS), Oct. 23, 2018. doi: 10.1103/physrevd.98.081501.  
  
F. Foucart, “Post-merger evolution of a neutron star-black hole binary with neutrino transport”, *Physical Review D*, vol. 91, no. 12. American Physical Society (APS), Jun. 11, 2015. doi: 10.1103/physrevd.91.124021.  
  
C. J. Handmer, B. Szilágyiand J. Winicour, “Spectral Cauchy characteristic extraction of strain, news and gravitational radiation flux”, *Classical and Quantum Gravity*, vol. 33, no. 22. IOP Publishing, p. 225007, Oct. 21, 2016. doi: 10.1088/0264-9381/33/22/225007.  
  
D. A. Hemberger, “Final spin and radiated energy in numerical simulations of binary black holes with equal masses and equal, aligned or antialigned spins”, *Physical Review D*, vol. 88, no. 6. American Physical Society (APS), Sep. 05, 2013. doi: 10.1103/physrevd.88.064014.  
  
D. A. Hemberger, “Dynamical excision boundaries in spectral evolutions of binary black hole spacetimes”, *Classical and Quantum Gravity*, vol. 30, no. 11. IOP Publishing, p. 115001, Apr. 25, 2013. doi: 10.1088/0264-9381/30/11/115001.  
  
K. Henriksson, F. Foucart, L. E. Kidderand S. A. Teukolsky, “Initial data for high-compactness black hole–neutron star binaries”, *Classical and Quantum Gravity*, vol. 33, no. 10. IOP Publishing, p. 105009, Apr. 19, 2016. doi: 10.1088/0264-9381/33/10/105009.  
  
T. Hinderer, “Periastron advance in spinning black hole binaries: comparing effective-one-body and numerical relativity”, *Physical Review D*, vol. 88, no. 8. American Physical Society (APS), Oct. 04, 2013. doi: 10.1103/physrevd.88.084005.  
  
I. Hinder, “Error-analysis and comparison to analytical models of numerical waveforms produced by the NRAR Collaboration”, *Classical and Quantum Gravity*, vol. 31, no. 2. IOP Publishing, p. 025012, Jan. 21, 2013. doi: 10.1088/0264-9381/31/2/025012.  
  
J. Lange, “Parameter estimation method that directly compares gravitational wave observations to numerical relativity”, *Physical Review D*, vol. 96, no. 10. American Physical Society (APS), Nov. 22, 2017. doi: 10.1103/physrevd.96.104041.  
  
A. Le Tiec, “Periastron advance in spinning black hole binaries: Gravitational self-force from numerical relativity”, *Physical Review D*, vol. 88, no. 12. American Physical Society (APS), Dec. 09, 2013. doi: 10.1103/physrevd.88.124027.  
  
G. Lovelace, “Massive disc formation in the tidal disruption of a neutron star by a nearly extremal black hole”, *Classical and Quantum Gravity*, vol. 30, no. 13. IOP Publishing, p. 135004, Jun. 03, 2013. doi: 10.1088/0264-9381/30/13/135004.  
  
G. Lovelace, “Modeling the source of GW150914 with targeted numerical-relativity simulations”, *Classical and Quantum Gravity*, vol. 33, no. 24. IOP Publishing, p. 244002, Nov. 18, 2016. doi: 10.1088/0264-9381/33/24/244002.  
  
G. Lovelace, “Nearly extremal apparent horizons in simulations of merging black holes”, *Classical and Quantum Gravity*, vol. 32, no. 6. IOP Publishing, p. 065007, Feb. 26, 2015. doi: 10.1088/0264-9381/32/6/065007.  
  
I. MacDonald, “Suitability of hybrid gravitational waveforms for unequal-mass binaries”, *Physical Review D*, vol. 87, no. 2. American Physical Society (APS), Jan. 04, 2013. doi: 10.1103/physrevd.87.024009.  
  
A. H. Mroué, H. P. Pfeiffer, L. E. Kidderand S. A. Teukolsky, “Measuring orbital eccentricity and periastron advance in quasicircular black hole simulations”, *Physical Review D*, vol. 82, no. 12. American Physical Society (APS), Dec. 08, 2010. doi: 10.1103/physrevd.82.124016.  
  
A. H. Mroué, “Catalog of 174 Binary Black Hole Simulations for Gravitational Wave Astronomy”, *Physical Review Letters*, vol. 111, no. 24. American Physical Society (APS), Dec. 11, 2013. doi: 10.1103/physrevlett.111.241104.  
  
M. Okounkova, M. A. Scheeland S. A. Teukolsky, “Numerical black hole initial data and shadows in dynamical Chern–Simons gravity”, *Classical and Quantum Gravity*, vol. 36, no. 5. IOP Publishing, p. 054001, Feb. 04, 2019. doi: 10.1088/1361-6382/aafcdf.  
  
M. Okounkova, L. C. Stein, M. A. Scheeland D. A. Hemberger, “Numerical binary black hole mergers in dynamical Chern-Simons gravity: Scalar field”, *Physical Review D*, vol. 96, no. 4. American Physical Society (APS), Aug. 16, 2017. doi: 10.1103/physrevd.96.044020.  
  
S. Ossokine, L. E. Kidderand H. P. Pfeiffer, “Precession-tracking coordinates for simulations of compact-object binaries”, *Physical Review D*, vol. 88, no. 8. American Physical Society (APS), Oct. 22, 2013. doi: 10.1103/physrevd.88.084031.  
  
Y. Pan, “Inspiral-merger-ringdown multipolar waveforms of nonspinning black-hole binaries using the effective-one-body formalism”, *Physical Review D*, vol. 84, no. 12. American Physical Society (APS), Dec. 27, 2011. doi: 10.1103/physrevd.84.124052.  
  
Y. Pan, “Effective-one-body waveforms calibrated to numerical relativity simulations: Coalescence of nonprecessing, spinning, equal-mass black holes”, *Physical Review D*, vol. 81, no. 8. American Physical Society (APS), Apr. 20, 2010. doi: 10.1103/physrevd.81.084041.  
  
Y. Pan, “Stability of nonspinning effective-one-body model in approximating two-body dynamics and gravitational-wave emission”, *Physical Review D*, vol. 89, no. 6. American Physical Society (APS), Mar. 05, 2014. doi: 10.1103/physrevd.89.061501.  
  
Y. Pan, “Inspiral-merger-ringdown waveforms of spinning, precessing black-hole binaries in the effective-one-body formalism”, *Physical Review D*, vol. 89, no. 8. American Physical Society (APS), Apr. 02, 2014. doi: 10.1103/physrevd.89.084006.  
  
M. A. Scheel, “Improved methods for simulating nearly extremal binary black holes”, *Classical and Quantum Gravity*, vol. 32, no. 10. IOP Publishing, p. 105009, Apr. 28, 2015. doi: 10.1088/0264-9381/32/10/105009.  
  
B. Szilágyi, “Approaching the Post-Newtonian Regime with Numerical Relativity: A Compact-Object Binary Simulation Spanning 350 Gravitational-Wave Cycles”, *Physical Review Letters*, vol. 115, no. 3. American Physical Society (APS), Jul. 16, 2015. doi: 10.1103/physrevlett.115.031102.  
  
N. Tacik, “Initial data for black hole–neutron star binaries, with rotating stars”, *Classical and Quantum Gravity*, vol. 33, no. 22. IOP Publishing, p. 225012, Oct. 25, 2016. doi: 10.1088/0264-9381/33/22/225012.  
  
N. W. Taylor, “Comparing gravitational waveform extrapolation to Cauchy-characteristic extraction in binary black hole simulations”, *Physical Review D*, vol. 88, no. 12. American Physical Society (APS), Dec. 03, 2013. doi: 10.1103/physrevd.88.124010.  
  
N. W. Taylor, L. E. Kidderand S. A. Teukolsky, “Spectral methods for the wave equation in second-order form”, *Physical Review D*, vol. 82, no. 2. American Physical Society (APS), Jul. 28, 2010. doi: 10.1103/physrevd.82.024037.  
  
V. Varma, S. E. Field, M. A. Scheel, J. Blackman, L. E. Kidderand H. P. Pfeiffer, “Surrogate model of hybridized numerical relativity binary black hole waveforms”, *Physical Review D*, vol. 99, no. 6. American Physical Society (APS), Mar. 27, 2019. doi: 10.1103/physrevd.99.064045.  
  
K.-H. Chu, J. Colditz, M. Malik, T. Yatesand B. Primack, “Identifying Key Target Audiences for Public Health Campaigns: Leveraging Machine Learning in the Case of Hookah Tobacco Smoking”, *Journal of Medical Internet Research*, vol. 21, no. 7. JMIR Publications Inc., p. e12443, Jul. 08, 2019. doi: 10.2196/12443.  
  
K.-H. Chu, J. Colditz, J. Sidani, M. Zimmerand B. Primack, “Re-evaluating standards of human subjects protection for sensitive health data in social media networks”, *Social Networks*, vol. 67. Elsevier BV, pp. 41–46, Oct. 2021. doi: 10.1016/j.socnet.2019.10.010.  
  
J. E. Sidani, “I wake up and hit the JUUL: Analyzing Twitter for JUUL nicotine effects and dependence”, *Drug and Alcohol Dependence*, vol. 204. Elsevier BV, p. 107500, Nov. 2019. doi: 10.1016/j.drugalcdep.2019.06.005.  
  
J. E. Sidani, J. B. Colditz, E. L. Barrett, K. Chu, A. E. Jamesand B. A. Primack, “JUUL on Twitter: Analyzing Tweets About Use of a New Nicotine Delivery System”, *Journal of School Health*, vol. 90, no. 2. Wiley, pp. 135–142, Dec. 11, 2019. doi: 10.1111/josh.12858.  
  
R. Ranganathan, S. Rokkam, T. Desaiand P. Keblinski, “Generation of amorphous carbon models using liquid quench method: A reactive molecular dynamics study”, *Carbon*, vol. 113. Elsevier BV, pp. 87–99, Mar. 2017. doi: 10.1016/j.carbon.2016.11.024.  
  
M. Makaremi, K. D. Jordan, G. D. Guthrieand E. M. Myshakin, “Multiphase Monte Carlo and Molecular Dynamics Simulations of Water and CO2 Intercalation in Montmorillonite and Beidellite”, *The Journal of Physical Chemistry C*, vol. 119, no. 27. American Chemical Society (ACS), pp. 15112–15124, Jun. 26, 2015. doi: 10.1021/acs.jpcc.5b01754.  
  
E. M. Myshakin, M. Makaremi, V. N. Romanov, K. D. Jordanand G. D. Guthrie, “Molecular Dynamics Simulations of Turbostratic Dry and Hydrated Montmorillonite with Intercalated Carbon Dioxide”, *The Journal of Physical Chemistry A*, vol. 118, no. 35. American Chemical Society (ACS), pp. 7454–7468, May 06, 2014. doi: 10.1021/jp500221w.  
  
D. R. Monismith, “Incorporating parallelism and high performance computing into computer science courses”, *2015 IEEE Frontiers in Education Conference (FIE)*. IEEE, Oct. 2015. doi: 10.1109/fie.2015.7344410.  
  
G. Cao, S. Wang, M. Hwang, A. Padmanabhan, Z. Zhangand K. Soltani, “A scalable framework for spatiotemporal analysis of location-based social media data”, *Computers, Environment and Urban Systems*, vol. 51. Elsevier BV, pp. 70–82, May 2015. doi: 10.1016/j.compenvurbsys.2015.01.002.  
  
Y. Fan, Y. Liu, S. Wang, D. Tarboton, A. Yildirimand N. Wilkins-Diehr, “Accelerating TauDEM as a Scalable Hydrological Terrain Analysis Service on XSEDE”, *Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment*. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616510.  
  
Z. Gong, W. Tangand J.-C. Thill, “Parallelization of ensemble neural networks for spatial land-use modeling”, *Proceedings of the 5th ACM SIGSPATIAL International Workshop on Location-Based Social Networks*. ACM, Nov. 06, 2012. doi: 10.1145/2442796.2442808.  
  
P. Riteau, “A cloud computing approach to on-demand and scalable cybergis analytics”, *Proceedings of the 5th ACM workshop on Scientific cloud computing*. ACM, Jun. 23, 2014. doi: 10.1145/2608029.2608032.  
  
W. Tang, W. Fengand M. Jia, “Massively parallel spatial point pattern analysis: Ripley’s K function accelerated using graphics processing units”, *International Journal of Geographical Information Science*, vol. 29, no. 3. Informa UK Limited, pp. 412–439, Feb. 13, 2015. doi: 10.1080/13658816.2014.976569.  
  
W. Tang and M. Jia, “Global Sensitivity Analysis of a Large Agent-Based Model of Spatial Opinion Exchange: A Heterogeneous Multi-GPU Acceleration Approach”, *Annals of the Association of American Geographers*, vol. 104, no. 3. Informa UK Limited, pp. 485–509, Apr. 29, 2014. doi: 10.1080/00045608.2014.892342.  
  
W. Tang, S. Wang, D. A. Bennettand Y. Liu, “Agent-based modeling within a cyberinfrastructure environment: a service-oriented computing approach”, *International Journal of Geographical Information Science*, vol. 25, no. 9. Informa UK Limited, pp. 1323–1346, Sep. 2011. doi: 10.1080/13658816.2011.585342.  
  
C. Youn, “Leveraging XSEDE HPC resources to address computational challenges with high-resolution topography data”, *Proceedings of the 2014 Annual Conference on Extreme Science and Engineering Discovery Environment*. ACM, Jul. 13, 2014. doi: 10.1145/2616498.2616564.  
  
D. A. Bennett, W. Tangand S. Wang, “Toward an understanding of provenance in complex land use dynamics”, *Journal of Land Use Science*, vol. 6, no. 2–3. Informa UK Limited, pp. 211–230, Jun. 2011. doi: 10.1080/1747423x.2011.558598.  
  
R. K. Meentemeyer, W. Tang, M. A. Dorning, J. B. Vogler, N. J. Cunniffeand D. A. Shoemaker, “FUTURES: Multilevel Simulations of Emerging Urban–Rural Landscape Structure Using a Stochastic Patch-Growing Algorithm”, *Annals of the Association of American Geographers*, vol. 103, no. 4. Informa UK Limited, pp. 785–807, Jul. 2013. doi: 10.1080/00045608.2012.707591.  
  
A. Padmanabhan, “FluMapper”, *Proceedings of the Conference on Extreme Science and Engineering Discovery Environment: Gateway to Discovery*. ACM, Jul. 22, 2013. doi: 10.1145/2484762.2484821.  
  
A. Padmanabhan, “Integration of science gateways”, *Proceedings of the Conference on Extreme Science and Engineering Discovery Environment: Gateway to Discovery*. ACM, Jul. 22, 2013. doi: 10.1145/2484762.2484808.  
  
W. Tang, D. A. Bennettand S. Wang, “A parallel agent-based model of land use opinions”, *Journal of Land Use Science*, vol. 6, no. 2–3. Informa UK Limited, pp. 121–135, Jun. 2011. doi: 10.1080/1747423x.2011.558597.  
  
W. Tang and W. Feng, “Parallel map projection of vector-based big spatial data: Coupling cloud computing with graphics processing units”, *Computers, Environment and Urban Systems*, vol. 61. Elsevier BV, pp. 187–197, Jan. 2017. doi: 10.1016/j.compenvurbsys.2014.01.001.  
  
Y. Zhao, A. Padmanabhanand S. Wang, “A parallel computing approach to viewshed analysis of large terrain data using graphics processing units”, *International Journal of Geographical Information Science*, vol. 27, no. 2. Informa UK Limited, pp. 363–384, Feb. 2013. doi: 10.1080/13658816.2012.692372.  
  
I.-H. Kim and M.-H. Tsou, “Enabling Digital Earth simulation models using cloud computing or grid computing – two approaches supporting high-performance GIS simulation frameworks”, *International Journal of Digital Earth*, vol. 6, no. 4. Informa UK Limited, pp. 383–403, Apr. 17, 2013. doi: 10.1080/17538947.2013.783125.  
  
C. Shen, “Network patterns and social architecture in Massively Multiplayer Online Games: Mapping the social world of *EverQuest II*”, *New Media & Society*, vol. 16, no. 4. SAGE Publications, pp. 672–691, Jun. 18, 2013. doi: 10.1177/1461444813489507.  
  
C. Shen, P. Mongeand D. Williams, “Virtual Brokerage and Closure”, *Communication Research*, vol. 41, no. 4. SAGE Publications, pp. 459–480, Aug. 03, 2012. doi: 10.1177/0093650212455197.  
  
C. Shen, P. Mongeand D. Williams, “The evolution of social ties online: A longitudinal study in a massively multiplayer online game”, *Journal of the Association for Information Science and Technology*, vol. 65, no. 10. Wiley, pp. 2127–2137, Apr. 04, 2014. doi: 10.1002/asi.23129.  
  
A. CHINCO, A. D. CLARK‐JOSEPHand M. YE, “Sparse Signals in the Cross‐Section of Returns”, *The Journal of Finance*, vol. 74, no. 1. Wiley, pp. 449–492, Nov. 14, 2018. doi: 10.1111/jofi.12733.  
  
M. Ye, “Who Provides Liquidity and When: An Analysis of Price vs. Speed Competition on Liquidity and Welfare”, *SSRN Electronic Journal*. Elsevier BV, 2017. doi: 10.2139/ssrn.2902984.  
  
R. M. Bond, “A 61-million-person experiment in social influence and political mobilization”, *Nature*, vol. 489, no. 7415. Springer Science and Business Media LLC, pp. 295–298, Sep. 2012. doi: 10.1038/nature11421.  
  
N. A. Christakis and J. H. Fowler, “Friendship and natural selection”, *Proceedings of the National Academy of Sciences*, vol. 111, no. supplement\_3. Proceedings of the National Academy of Sciences, pp. 10796–10801, Jul. 14, 2014. doi: 10.1073/pnas.1400825111.  
  
M. Regenwetter, “Heterogeneity and parsimony in intertemporal choice.”, *Decision*, vol. 5, no. 2. American Psychological Association (APA), pp. 63–94, Apr. 2018. doi: 10.1037/dec0000069.  
  
A. K.-Y. Leung and D. Cohen, “Within- and between-culture variation: Individual differences and the cultural logics of honor, face, and dignity cultures.”, *Journal of Personality and Social Psychology*, vol. 100, no. 3. American Psychological Association (APA), pp. 507–526, Mar. 2011. doi: 10.1037/a0022151.  
  
R. Whalen, Y. Huang, C. Tanis, A. Sawant, B. Uzziand N. Contractor, “Citation Distance”, *Proceedings of the 25th International Conference Companion on World Wide Web - WWW ’16 Companion*. ACM Press, 2016. doi: 10.1145/2872518.2890515.  
  
M. Solaimani, S. Salam, A. M. Mustafa, L. Khan, P. T. Brandtand B. Thuraisingham, “Near real-time atrocity event coding”, *2016 IEEE Conference on Intelligence and Security Informatics (ISI)*. IEEE, Sep. 2016. doi: 10.1109/isi.2016.7745457.  
  
A. Eldawy, L. Niu, D. Haynesand Z. Su, “Large Scale Analytics of Vector+Raster Big Spatial Data”, *Proceedings of the 25th ACM SIGSPATIAL International Conference on Advances in Geographic Information Systems*. ACM, Nov. 07, 2017. doi: 10.1145/3139958.3140042.  
  
B. E. Bagozzi, “The Prevalence and Severity of Underreporting Bias in Machine- and Human-Coded Data”, *Political Science Research and Methods*, vol. 7, no. 3. Cambridge University Press (CUP), pp. 641–649, Mar. 05, 2018. doi: 10.1017/psrm.2018.11.  
  
M. Solaimani, S. Salam, L. Khan, P. T. Brandtand V. D’Orazio, “APART: Automatic Political Actor Recommendation in Real-time”, *Social, Cultural, and Behavioral Modeling*. Springer International Publishing, pp. 342–348, 2017. doi: 10.1007/978-3-319-60240-0\_42.  
  
H. Kim, “UTDEventData: An R package to access political event data”, *Journal of Open Source Software*, vol. 4, no. 36. The Open Journal, p. 1322, Apr. 22, 2019. doi: 10.21105/joss.01322.  
  
E. Shook, D. D. Vento, A. Zoncaand J. Wang, “GISandbox”, *Proceedings of the Practice and Experience on Advanced Research Computing*. ACM, Jul. 22, 2018. doi: 10.1145/3219104.3219150.  
  
J. R. Haber, “Sorting Schools: A Computational Analysis of Charter School Identities and Stratification”, *Sociology of Education*, vol. 94, no. 1. SAGE Publications, pp. 43–64, Sep. 01, 2020. doi: 10.1177/0038040720953218.  
  
A. K. Gunasekaran, M. B. Imani, L. Khan, C. Grant, P. T. Brandtand J. S. Holmes, “SPERG: Scalable Political Event Report Geoparsing in Big Data”, *2018 IEEE International Conference on Intelligence and Security Informatics (ISI)*. IEEE, Nov. 2018. doi: 10.1109/isi.2018.8587373.  
  
Y. Liang, K. Jabr, C. Grant, J. Irvineand A. Halterman, “New Techniques for Coding Political Events across Languages”, *2018 IEEE International Conference on Information Reuse and Integration (IRI)*. IEEE, Jul. 2018. doi: 10.1109/iri.2018.00020.  
  
K. Lee and M.-P. Kwan, “The Effects of GPS-Based Buffer Size on the Association between Travel Modes and Environmental Contexts”, *ISPRS International Journal of Geo-Information*, vol. 8, no. 11. MDPI AG, p. 514, Nov. 13, 2019. doi: 10.3390/ijgi8110514.  
  
M. Cai, M. Del Negro, E. Herbst, E. Matlin, R. Sarfatiand F. Schorfheide, “Online Estimation of DSGE Models”, *SSRN Electronic Journal*. Elsevier BV, 2019. doi: 10.2139/ssrn.3426004.  
  
S. K. Ramadugu, Y.-H. Chung, E. J. Fuentes, K. G. Riceand C. J. Margulis, “In Silico Prediction of the 3D Structure of Trimeric Asialoglycoprotein Receptor Bound to Triantennary Oligosaccharide”, *Journal of the American Chemical Society*, vol. 132, no. 26. American Chemical Society (ACS), pp. 9087–9095, Jun. 11, 2010. doi: 10.1021/ja1021766.  
  
S. K. Ramadugu, Z. Li, H. K. Kashyapand C. J. Margulis, “The Role of Glu41 in the Binding of Dimannose to P51G-m4-CVN”, *Biochemistry*, vol. 53, no. 9. American Chemical Society (ACS), pp. 1477–1484, Feb. 24, 2014. doi: 10.1021/bi4014159.  
  
A. Danner, A. Breslow, J. Baskinand D. Wilikofsky, “Hybrid MPI/GPU interpolation for grid DEM construction”, *Proceedings of the 20th International Conference on Advances in Geographic Information Systems*. ACM, Nov. 06, 2012. doi: 10.1145/2424321.2424360.  
  
W. Chen and E. Deelman, “Workflow overhead analysis and optimizations”, *Proceedings of the 6th workshop on Workflows in support of large-scale science*. ACM, Nov. 14, 2011. doi: 10.1145/2110497.2110500.  
  
W. Chen, E. Deelmanand R. Sakellariou, “Imbalance optimization in scientific workflows”, *Proceedings of the 27th international ACM conference on International conference on supercomputing*. ACM, Jun. 10, 2013. doi: 10.1145/2464996.2467270.  
  
M. Becker, W. C.-W. Huang, H. Batelaan, E. J. Smytheand F. Capasso, “Measurement of the ultrafast temporal response of a plasmonic antenna”, *Annalen der Physik*, vol. 525, no. 1–2. Wiley, pp. L6–L11, Oct. 05, 2012. doi: 10.1002/andp.201200206.  
  
W. C.-W. Huang, R. Bach, P. Beierleand H. Batelaan, “A low-power optical electron switch”, *Journal of Physics D: Applied Physics*, vol. 47, no. 8. IOP Publishing, p. 085102, Feb. 03, 2014. doi: 10.1088/0022-3727/47/8/085102.  
  
W. C.-W. Huang and H. Batelaan, “Dynamics Underlying the Gaussian Distribution of the Classical Harmonic Oscillator in Zero-Point Radiation”, *Journal of Computational Methods in Physics*, vol. 2013. Hindawi Limited, pp. 1–19, Oct. 07, 2013. doi: 10.1155/2013/308538.  
  
W. C.-W. Huang and H. Batelaan, “Discrete Excitation Spectrum of a Classical Harmonic Oscillator in Zero-Point Radiation”, *Foundations of Physics*, vol. 45, no. 3. Springer Science and Business Media LLC, pp. 333–353, Jan. 21, 2015. doi: 10.1007/s10701-015-9866-9.  
  
J. Urbanic and T. Maiden, “Evaluating the Wide Area Classroom after 10,500 HPC Students”, *2018 IEEE/ACM Workshop on Education for High-Performance Computing (EduHPC)*. IEEE, Nov. 2018. doi: 10.1109/eduhpc.2018.00009.  
  
R. E. Beattie, W. Henke, M. F. Campa, T. C. Hazen, L. R. McAlileyand J. H. Campbell, “Variation in microbial community structure correlates with heavy-metal contamination in soils decades after mining ceased”, *Soil Biology and Biochemistry*, vol. 126. Elsevier BV, pp. 57–63, Nov. 2018. doi: 10.1016/j.soilbio.2018.08.011.  
  
C. H. Bock, “A comparison of UP-PCR and RAPD markers to study genetic diversity of*Fusicladium effusum*(G. Winter), cause of pecan scab”, *Forest Pathology*, vol. 44, no. 4. Wiley, pp. 266–275, Feb. 26, 2014. doi: 10.1111/efp.12090.  
  
A. Snedden, J. Coughlin, L. A. Phillips, G. Mathewsand I.-S. Suh, “Star formation and gas phase history of the cosmic web”, *Monthly Notices of the Royal Astronomical Society*, vol. 455, no. 3. Oxford University Press (OUP), pp. 2804–2825, Nov. 25, 2015. doi: 10.1093/mnras/stv2421.  
  
A. Snedden, L. A. Phillips, G. J. Mathews, J. Coughlin, I.-S. Suhand A. Bhattacharya, “A new multi-scale structure finding algorithm to identify cosmological structure”, *Journal of Computational Physics*, vol. 299. Elsevier BV, pp. 92–97, Oct. 2015. doi: 10.1016/j.jcp.2015.07.004.  
  
V. U. Chimalgi, M. R. K. Nishatand S. S. Ahmed, “Nonlinear polarization and efficiency droop in hexagonal InGaN/GaN disk-in-wire LEDs”, *Superlattices and Microstructures*, vol. 84. Elsevier BV, pp. 91–98, Aug. 2015. doi: 10.1016/j.spmi.2015.04.034.  
  
F. M. Besem, R. E. Kielb, P. Galpin, L. Zoriand N. L. Key, “Mistuned Forced Response Predictions of an Embedded Rotor in a Multistage Compressor”, *Journal of Turbomachinery*, vol. 138, no. 6. ASME International, Feb. 09, 2016. doi: 10.1115/1.4032164.  
  
F. M. Besem, R. E. Kielband N. L. Key, “Forced Response Sensitivity of a Mistuned Rotor From an Embedded Compressor Stage”, *Journal of Turbomachinery*, vol. 138, no. 3. ASME International, Nov. 17, 2015. doi: 10.1115/1.4031866.  
  
S. Hegde, Z. Mao, T. Pan, L. Zori, R. Campregherand R. Kielb, “Separation of Up and Downstream Forced Response Excitations of an Embedded Compressor Rotor”, *Journal of Turbomachinery*, vol. 141, no. 9. ASME International, Aug. 01, 2019. doi: 10.1115/1.4044212.  
  
J. Li, N. Aye-Addo, R. Kielband N. Key, “Mistuned Higher-Order Mode Forced Response of an Embedded Compressor Rotor—Part II: Mistuned Forced Response Prediction”, *Journal of Turbomachinery*, vol. 140, no. 3. ASME International, Dec. 20, 2017. doi: 10.1115/1.4038519.  
  
J. Li, N. Aye-Addo, R. Kielband N. Key, “Mistuned Higher-Order Mode Forced Response of an Embedded Compressor Rotor: Part II — Mistuned Forced Response Prediction”, *Volume 7B: Structures and Dynamics*. American Society of Mechanical Engineers, Jun. 26, 2017. doi: 10.1115/gt2017-64647.  
  
J. Li, N. Aye-Addo, N. Kormanik III, D. Matthews, N. Keyand R. Kielb, “Mistuned Higher-Order Mode Forced Response of an Embedded Compressor Rotor: Part I — Steady and Unsteady Aerodynamics”, *Volume 7B: Structures and Dynamics*. American Society of Mechanical Engineers, Jun. 26, 2017. doi: 10.1115/gt2017-64633.  
  
J. Li and R. E. Kielb, “Effects of Blade Count Ratio on Aerodynamic Forcing and Mode Excitability”, *Volume 7B: Structures and Dynamics*. American Society of Mechanical Engineers, Jun. 15, 2015. doi: 10.1115/gt2015-43304.  
  
J. Li and R. Kielb, “Forcing Superposition and Decomposition of an Embedded Compressor Rotor”, *Volume 7B: Structures and Dynamics*. American Society of Mechanical Engineers, Jun. 26, 2017. doi: 10.1115/gt2017-64657.  
  
Z. Mao, S. Hegde, T. Pan, R. E. Kielb, L. Zoriand R. Campregher, “Influence of Rotor-Stator Interaction and Reflecting Boundary Conditions on Compressor Forced Response”, *Volume 2A: Turbomachinery*. American Society of Mechanical Engineers, Jun. 11, 2018. doi: 10.1115/gt2018-75232.  
  
Z. Mao and R. E. Kielb, “Interaction of Concurrent Forced Response and Flutter Phenomena in a Compressor Stage”, *Volume 7B: Structures and Dynamics*. American Society of Mechanical Engineers, Jun. 26, 2017. doi: 10.1115/gt2017-63376.  
  
E. Coulter, R. Knepperand J. Fischer, “Programmable Education Infrastructure: Cloud resources as HPC Education Environments”, *The Journal of Computational Science Education*, vol. 10, no. 1. The Shodor Education Foundation, Inc., pp. 107–107, Jan. 2019. doi: 10.22369/issn.2153-4136/10/1/18.  
  
J. M. Lowe, J. Fischer, S. Sudarshan, G. Turner, C. A. Stewartand D. Y. Hancock, “High Availability on Jetstream”, *Proceedings of the 9th Workshop on Scientific Cloud Computing*. ACM, Jun. 11, 2018. doi: 10.1145/3217880.3217884.  
  
S. Sarajlic, J. Chastang, S. Marru, J. Fischerand M. Lowe, “Scaling JupyterHub Using Kubernetes on Jetstream Cloud”, *Proceedings of the Practice and Experience on Advanced Research Computing*. ACM, Jul. 22, 2018. doi: 10.1145/3219104.3229249.  
  
L. Liao, C. W. Ingram, J. Bacsa, Z. J. Zhangand T. Dinadayalane, “A hydrogen bonded Co(ii) coordination complex and a triply interpenetrating 3-D manganese(ii) coordination polymer from diaza crown ether with dibenzoate sidearms”, *CrystEngComm*, vol. 18, no. 14. Royal Society of Chemistry (RSC), pp. 2425–2436, 2016. doi: 10.1039/c6ce00360e.  
  
A. Xu and S. Q. Yang, “Customer Relationship Management as an Imperative for Academic Libraries”, *Advances in Marketing, Customer Relationship Management, and E-Services*. IGI Global, pp. 44–77, 2015. doi: 10.4018/978-1-4666-6547-7.ch003.  
  
D. B. Larkins and J. Dinan, “Extending a Message Passing Runtime to Support Partitioned, Global Logical Address Spaces”, *2016 First International Workshop on Communication Optimizations in HPC (COMHPC)*. IEEE, Nov. 2016. doi: 10.1109/comhpc.2016.007.  
  
D. Haynes, A. Jokelaand S. Manson, “IPUMS-Terra: integrated big heterogeneous spatiotemporal data analysis system”, *Journal of Geographical Systems*, vol. 20, no. 4. Springer Science and Business Media LLC, pp. 343–361, Sep. 06, 2018. doi: 10.1007/s10109-018-0277-2.  
  
M. J. Abdolhosseini Qomi, “Combinatorial molecular optimization of cement hydrates”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, Sep. 24, 2014. doi: 10.1038/ncomms5960.  
  
M. J. Abdolhosseini Qomi, F.-J. Ulmand R. J.-M. Pellenq, “Evidence on the Dual Nature of Aluminum in the Calcium-Silicate-Hydrates Based on Atomistic Simulations”, *Journal of the American Ceramic Society*. Wiley, p. n/a–n/a, Jan. 2012. doi: 10.1111/j.1551-2916.2011.05058.x.  
  
J. A. Abell, N. Orbović, D. B. McCallenand B. Jeremic, “Earthquake soil-structure interaction of nuclear power plants, differences in response to 3-D, 3 × 1-D, and 1-D excitations”, *Earthquake Engineering & Structural Dynamics*, vol. 47, no. 6. Wiley, pp. 1478–1495, Feb. 26, 2018. doi: 10.1002/eqe.3026.  
  
A. Acevedo, L. Brodskyand R. Andino, “Mutational and fitness landscapes of an RNA virus revealed through population sequencing”, *Nature*, vol. 505, no. 7485. Springer Science and Business Media LLC, pp. 686–690, Nov. 27, 2013. doi: 10.1038/nature12861.  
  
J. B. Addison, “Reversible Assembly of β-Sheet Nanocrystals within Caddisfly Silk”, *Biomacromolecules*, vol. 15, no. 4. American Chemical Society (ACS), pp. 1269–1275, Mar. 13, 2014. doi: 10.1021/bm401822p.  
  
J. L. Adelman and M. Grabe, “Simulating rare events using a weighted ensemble-based string method”, *The Journal of Chemical Physics*, vol. 138, no. 4. AIP Publishing, p. 044105, Jan. 28, 2013. doi: 10.1063/1.4773892.  
  
E. Afgan, “The Galaxy platform for accessible, reproducible and collaborative biomedical analyses: 2016 update”, *Nucleic Acids Research*, vol. 44, no. W1. Oxford University Press (OUP), pp. W3–W10, May 02, 2016. doi: 10.1093/nar/gkw343.  
  
E. Afgan, “Genomics Virtual Laboratory: A Practical Bioinformatics Workbench for the Cloud”, *PLOS ONE*, vol. 10, no. 10. Public Library of Science (PLoS), p. e0140829, Oct. 26, 2015. doi: 10.1371/journal.pone.0140829.  
  
Z. Ahmad, T. Xie, C. Maheshwari, J. C. Grossmanand V. Viswanathan, “Machine Learning Enabled Computational Screening of Inorganic Solid Electrolytes for Suppression of Dendrite Formation in Lithium Metal Anodes”, *ACS Central Science*, vol. 4, no. 8. American Chemical Society (ACS), pp. 996–1006, Aug. 10, 2018. doi: 10.1021/acscentsci.8b00229.  
  
M. J. Alam, M. A. H. Samee, M. Rabbiand M. S. Rahman, “Minimum-Layer Upward Drawings of Trees”, *Journal of Graph Algorithms and Applications*, vol. 14, no. 2. Journal of Graph Algorithms and Applications, pp. 245–267, 2010. doi: 10.7155/jgaa.00206.  
  
A. Alavi, M. Ruffalo, A. Parvangada, Z. Huangand Z. Bar-Joseph, “A web server for comparative analysis of single-cell RNA-seq data”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Nov. 13, 2018. doi: 10.1038/s41467-018-07165-2.  
  
R. Alhadeff and A. Warshel, “Reexamining the origin of the directionality of myosin V”, *Proceedings of the National Academy of Sciences*, vol. 114, no. 39. Proceedings of the National Academy of Sciences, pp. 10426–10431, Sep. 11, 2017. doi: 10.1073/pnas.1711214114.  
  
S. I. Allec, N. V. Ilaweand B. M. Wong, “Unusual Bandgap Oscillations in Template-Directed π-Conjugated Porphyrin Nanotubes”, *The Journal of Physical Chemistry Letters*, vol. 7, no. 13. American Chemical Society (ACS), pp. 2362–2367, Jun. 10, 2016. doi: 10.1021/acs.jpclett.6b01020.  
  
M. AlQuraishi, G. Koytiger, A. Jenney, G. MacBeathand P. K. Sorger, “A multiscale statistical mechanical framework integrates biophysical and genomic data to assemble cancer networks”, *Nature Genetics*, vol. 46, no. 12. Springer Science and Business Media LLC, pp. 1363–1371, Nov. 02, 2014. doi: 10.1038/ng.3138.  
  
M. AlQuraishi and H. H. McAdams, “Direct inference of protein–DNA interactions using compressed sensing methods”, *Proceedings of the National Academy of Sciences*, vol. 108, no. 36. Proceedings of the National Academy of Sciences, pp. 14819–14824, Aug. 08, 2011. doi: 10.1073/pnas.1106460108.  
  
M. AlQuraishi and H. H. McAdams, “Three enhancements to the inference of statistical protein-DNA potentials”, *Proteins: Structure, Function, and Bioinformatics*, vol. 81, no. 3. Wiley, pp. 426–442, Nov. 12, 2012. doi: 10.1002/prot.24201.  
  
M. AlQuraishi, S. Tangand X. Xia, “An affinity-structure database of helix-turn-helix: DNA complexes with a universal coordinate system”, *BMC Bioinformatics*, vol. 16, no. 1. Springer Science and Business Media LLC, Nov. 19, 2015. doi: 10.1186/s12859-015-0819-2.  
  
A. M. Amarante, “Modeling the coverage of an AFM tip by enzymes and its application in nanobiosensors”, *Journal of Molecular Graphics and Modelling*, vol. 53. Elsevier BV, pp. 100–104, Sep. 2014. doi: 10.1016/j.jmgm.2014.07.009.  
  
T. A. Ameen, H. Ilatikhameneh, J. Z. Huang, M. Povolotskyi, R. Rahmanand G. Klimeck, “Combination of Equilibrium and Nonequilibrium Carrier Statistics Into an Atomistic Quantum Transport Model for Tunneling Heterojunctions”, *IEEE Transactions on Electron Devices*, vol. 64, no. 6. Institute of Electrical and Electronics Engineers (IEEE), pp. 2512–2518, Jun. 2017. doi: 10.1109/ted.2017.2690626.  
  
R. M. Anderson, D. F. Yancey, L. Zhang, S. T. Chill, G. Henkelmanand R. M. Crooks, “A Theoretical and Experimental Approach for Correlating Nanoparticle Structure and Electrocatalytic Activity”, *Accounts of Chemical Research*, vol. 48, no. 5. American Chemical Society (ACS), pp. 1351–1357, May 04, 2015. doi: 10.1021/acs.accounts.5b00125.  
  
R. M. Anderson, L. Zhang, J. A. Loussaert, A. I. Frenkel, G. Henkelmanand R. M. Crooks, “An Experimental and Theoretical Investigation of the Inversion of Pd@Pt Core@Shell Dendrimer-Encapsulated Nanoparticles”, *ACS Nano*, vol. 7, no. 10. American Chemical Society (ACS), pp. 9345–9353, Oct. 02, 2013. doi: 10.1021/nn4040348.  
  
R. M. Anderson, L. Zhang, D. Wu, S. R. Brankovic, G. Henkelmanand R. M. Crooks, “A Theoretical and Experimental In-Situ Electrochemical Infrared Spectroscopy Study of Adsorbed CO on Pt Dendrimer-Encapsulated Nanoparticles”, *Journal of The Electrochemical Society*, vol. 163, no. 4. The Electrochemical Society, pp. H3061–H3065, Dec. 04, 2015. doi: 10.1149/2.0061604jes.  
  
S. S. An, D. L. Jamesand S. Marschner, “Motion-driven concatenative synthesis of cloth sounds”, *ACM Transactions on Graphics*, vol. 31, no. 4. Association for Computing Machinery (ACM), pp. 1–10, Jul. 2012. doi: 10.1145/2185520.2185598.  
  
D. Antipov, N. Hartwick, M. Shen, M. Raiko, A. Lapidusand P. A. Pevzner, “plasmidSPAdes: assembling plasmids from whole genome sequencing data”, *Bioinformatics*. Oxford University Press (OUP), p. btw493, Jul. 27, 2016. doi: 10.1093/bioinformatics/btw493.  
  
E. Aprile, “Physics reach of the XENON1T dark matter experiment.”, *Journal of Cosmology and Astroparticle Physics*, vol. 2016, no. 4. IOP Publishing, pp. 027–027, Apr. 14, 2016. doi: 10.1088/1475-7516/2016/04/027.  
  
M. Aravena, “Large gas reservoirs and free–free emission in two lensed star-forming galaxies at z = 2.7”, *Monthly Notices of the Royal Astronomical Society*, vol. 433, no. 1. Oxford University Press (OUP), pp. 498–505, May 21, 2013. doi: 10.1093/mnras/stt741.  
  
P. G. Arias, H. G. Im, P. Narayananand A. Trouvé, “A computational study of non-premixed flame extinction by water spray”, *Proceedings of the Combustion Institute*, vol. 33, no. 2. Elsevier BV, pp. 2591–2597, Jan. 2011. doi: 10.1016/j.proci.2010.07.043.  
  
P. G. Arias, “Dynamics of flow–soot interaction in wrinkled non-premixed ethylene–air flames”, *Combustion Theory and Modelling*, vol. 19, no. 5. Informa UK Limited, pp. 568–586, Aug. 17, 2015. doi: 10.1080/13647830.2015.1067331.  
  
M. V. Arnoni, “Infections Caused by Fusarium Species in Pediatric Cancer Patients and Review of Published Literature”, *Mycopathologia*, vol. 183, no. 6. Springer Science and Business Media LLC, pp. 941–949, Mar. 21, 2018. doi: 10.1007/s11046-018-0257-6.  
  
E. K. Asciutto, M. Dang, S. S. Pochapsky, J. D. Maduraand T. C. Pochapsky, “Experimentally Restrained Molecular Dynamics Simulations for Characterizing the Open States of Cytochrome P450cam”, *Biochemistry*, vol. 50, no. 10. American Chemical Society (ACS), pp. 1664–1671, Feb. 08, 2011. doi: 10.1021/bi101820d.  
  
V. Babin, C. Rolandand C. Sagui, “The α-sheet: A missing-in-action secondary structure?”, *Proteins: Structure, Function, and Bioinformatics*, vol. 79, no. 3. Wiley, pp. 937–946, Jan. 03, 2011. doi: 10.1002/prot.22935.  
  
M. L. Baker, J. Zhang, S. J. Ludtkeand W. Chiu, “Cryo-EM of macromolecular assemblies at near-atomic resolution”, *Nature Protocols*, vol. 5, no. 10. Springer Science and Business Media LLC, pp. 1697–1708, Sep. 30, 2010. doi: 10.1038/nprot.2010.126.  
  
N. Balci, A. M. Isenbergand M. S. Jolly, “Turbulence in vertically averaged convection”, *Physica D: Nonlinear Phenomena*, vol. 376–377. Elsevier BV, pp. 216–227, Aug. 2018. doi: 10.1016/j.physd.2018.02.005.  
  
J. R. Baltzer, R. J. Adrianand X. Wu, “Structural organization of large and very large scales in turbulent pipe flow simulation”, *Journal of Fluid Mechanics*, vol. 720. Cambridge University Press (CUP), pp. 236–279, Feb. 27, 2013. doi: 10.1017/jfm.2012.642.  
  
V. Bansal, “Accurate detection and genotyping of SNPs utilizing population sequencing data”, *Genome Research*, vol. 20, no. 4. Cold Spring Harbor Laboratory, pp. 537–545, Feb. 11, 2010. doi: 10.1101/gr.100040.109.  
  
A. Baranova, J. Bode, G. Manyamand M. Emelianenko, “An efficient algorithm for systematic analysis of nucleotide strings suitable for siRNA design”, *BMC Research Notes*, vol. 4, no. 1. Springer Science and Business Media LLC, May 27, 2011. doi: 10.1186/1756-0500-4-168.  
  
L. N. Barbosa, “Molecular identification and phylogenetic analysis of*Bothrops insularis*bacterial and fungal microbiota”, *Journal of Toxicology and Environmental Health, Part A*, vol. 81, no. 6. Informa UK Limited, pp. 142–153, Jan. 10, 2018. doi: 10.1080/15287394.2017.1395581.  
  
L. Baroudi, M. Kawajiand T. Lee, “Effects of initial conditions on the simulation of inertial coalescence of two drops”, *Computers & Mathematics with Applications*, vol. 67, no. 2. Elsevier BV, pp. 282–289, Feb. 2014. doi: 10.1016/j.camwa.2013.05.002.  
  
C. L. Barrett, C. DeBoever, K. Jepsen, C. C. Saenz, D. A. Carsonand K. A. Frazer, “Systematic transcriptome analysis reveals tumor-specific isoforms for ovarian cancer diagnosis and therapy”, *Proceedings of the National Academy of Sciences*, vol. 112, no. 23. Proceedings of the National Academy of Sciences, May 26, 2015. doi: 10.1073/pnas.1508057112.  
  
C. L. Barrett, “Transcriptome Sequencing of Tumor Subpopulations Reveals a Spectrum of Therapeutic Options for Squamous Cell Lung Cancer”, *PLoS ONE*, vol. 8, no. 3. Public Library of Science (PLoS), p. e58714, Mar. 20, 2013. doi: 10.1371/journal.pone.0058714.  
  
L. Bartlett and E. F. Connor, “Exogenous phytohormones and the induction of plant galls by insects”, *Arthropod-Plant Interactions*. Springer Science and Business Media LLC, Jun. 05, 2014. doi: 10.1007/s11829-014-9309-0.  
  
N. K. Batmanghelich, A. Saeedi, M. Cho, R. S. J. Esteparand P. Golland, “Generative Method to Discover Genetically Driven Image Biomarkers”, *Lecture Notes in Computer Science*. Springer International Publishing, pp. 30–42, 2015. doi: 10.1007/978-3-319-19992-4\_3.  
  
N. K. Batmanghelich, B. Taskarand C. Davatzikos, “Generative-Discriminative Basis Learning for Medical Imaging”, *IEEE Transactions on Medical Imaging*, vol. 31, no. 1. Institute of Electrical and Electronics Engineers (IEEE), pp. 51–69, Jan. 2012. doi: 10.1109/tmi.2011.2162961.  
  
L. Bauerdick, “Using Xrootd to Federate Regional Storage”, *Journal of Physics: Conference Series*, vol. 396, no. 4. IOP Publishing, p. 042009, Dec. 13, 2012. doi: 10.1088/1742-6596/396/4/042009.  
  
L. A. T. Bauerdick, “Xrootd Monitoring for the CMS Experiment”, *Journal of Physics: Conference Series*, vol. 396, no. 4. IOP Publishing, p. 042058, Dec. 13, 2012. doi: 10.1088/1742-6596/396/4/042058.  
  
D. J. Beard, “Intracranial Pressure Elevation Reduces Flow through Collateral Vessels and the Penetrating Arterioles they Supply. a Possible Explanation for ‘Collateral Failure’ and Infarct Expansion after Ischemic Stroke”, *Journal of Cerebral Blood Flow & Metabolism*, vol. 35, no. 5. SAGE Publications, pp. 861–872, Feb. 11, 2015. doi: 10.1038/jcbfm.2015.2.  
  
Y. Bekenstein, “Thermal Doping by Vacancy Formation in Copper Sulfide Nanocrystal Arrays”, *Nano Letters*, vol. 14, no. 3. American Chemical Society (ACS), pp. 1349–1353, Feb. 27, 2014. doi: 10.1021/nl4043642.  
  
M. Belgin, G. Backand C. J. Ribbens, “Applicability of Pattern-based sparse matrix representation for real applications”, *Procedia Computer Science*, vol. 1, no. 1. Elsevier BV, pp. 203–211, May 2010. doi: 10.1016/j.procs.2010.04.023.  
  
M. Belgin, G. Backand C. J. Ribbens, “Operation Stacking for Ensemble Computations With Variable Convergence”, *The International Journal of High Performance Computing Applications*, vol. 24, no. 2. SAGE Publications, pp. 194–212, Nov. 03, 2009. doi: 10.1177/1094342009347892.  
  
R. E. Bell, “Widespread Persistent Thickening of the East Antarctic Ice Sheet by Freezing from the Base”, *Science*, vol. 331, no. 6024. American Association for the Advancement of Science (AAAS), pp. 1592–1595, Mar. 25, 2011. doi: 10.1126/science.1200109.  
  
J. P. Bergfield, H. M. Heitzer, C. Van Dyck, T. J. Marksand M. A. Ratner, “Harnessing Quantum Interference in Molecular Dielectric Materials”, *ACS Nano*, vol. 9, no. 6. American Chemical Society (ACS), pp. 6412–6418, Jun. 04, 2015. doi: 10.1021/acsnano.5b02042.  
  
J. J. Berg and G. Coop, “A Population Genetic Signal of Polygenic Adaptation”, *PLoS Genetics*, vol. 10, no. 8. Public Library of Science (PLoS), p. e1004412, Aug. 07, 2014. doi: 10.1371/journal.pgen.1004412.  
  
N. P. Bethel and M. Grabe, “Atomistic insight into lipid translocation by a TMEM16 scramblase”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 49. Proceedings of the National Academy of Sciences, pp. 14049–14054, Nov. 21, 2016. doi: 10.1073/pnas.1607574113.  
  
M. Béthermin, “A UNIFIED EMPIRICAL MODEL FOR INFRARED GALAXY COUNTS BASED ON THE OBSERVED PHYSICAL EVOLUTION OF DISTANT GALAXIES”, *The Astrophysical Journal*, vol. 757, no. 2. American Astronomical Society, p. L23, Sep. 11, 2012. doi: 10.1088/2041-8205/757/2/l23.  
  
G. Bhatia, “A Covering Method for Detecting Genetic Associations between Rare Variants and Common Phenotypes”, *PLoS Computational Biology*, vol. 6, no. 10. Public Library of Science (PLoS), p. e1000954, Oct. 14, 2010. doi: 10.1371/journal.pcbi.1000954.  
  
K. Bi, D. Vanderpool, S. Singhal, T. Linderoth, C. Moritzand J. M. Good, “Transcriptome-based exon capture enables highly cost-effective comparative genomic data collection at moderate evolutionary scales”, *BMC Genomics*, vol. 13, no. 1. Springer Science and Business Media LLC, p. 403, 2012. doi: 10.1186/1471-2164-13-403.  
  
R. L. Birke, V. Znamenskiyand J. R. Lombardi, “A charge-transfer surface enhanced Raman scattering model from time-dependent density functional theory calculations on a Ag10-pyridine complex”, *The Journal of Chemical Physics*, vol. 132, no. 21. AIP Publishing, p. 214707, Jun. 07, 2010. doi: 10.1063/1.3431210.  
  
C. G. Bischak, S. Longhi, D. M. Snead, S. Costanzo, E. Terrerand C. H. Londergan, “Probing Structural Transitions in the Intrinsically Disordered C-Terminal Domain of the Measles Virus Nucleoprotein by Vibrational Spectroscopy of Cyanylated Cysteines”, *Biophysical Journal*, vol. 99, no. 5. Elsevier BV, pp. 1676–1683, Sep. 2010. doi: 10.1016/j.bpj.2010.06.060.  
  
J. M. Blacktop, “Augmented Cocaine Seeking in Response to Stress or CRF Delivered into the Ventral Tegmental Area Following Long-Access Self-Administration Is Mediated by CRF Receptor Type 1 But Not CRF Receptor Type 2”, *Journal of Neuroscience*, vol. 31, no. 31. Society for Neuroscience, pp. 11396–11403, Aug. 03, 2011. doi: 10.1523/jneurosci.1393-11.2011.  
  
A. M. Blázquez-Medela, “Osteoprotegerin is associated with cardiovascular risk in hypertension and/or diabetes”, *European Journal of Clinical Investigation*, vol. 42, no. 5. Wiley, pp. 548–556, Nov. 04, 2011. doi: 10.1111/j.1365-2362.2011.02619.x.  
  
A. M. Blázquez-Medela, “Increased plasma soluble endoglin levels as an indicator of cardiovascular alterations in hypertensive and diabetic patients”, *BMC Medicine*, vol. 8, no. 1. Springer Science and Business Media LLC, Dec. 2010. doi: 10.1186/1741-7015-8-86.  
  
A. M. Blázquez-Medela, “Hypertension and Hyperglycemia Synergize to Cause Incipient Renal Tubular Alterations Resulting in Increased NGAL Urinary Excretion in Rats”, *PLoS ONE*, vol. 9, no. 8. Public Library of Science (PLoS), p. e105988, Aug. 22, 2014. doi: 10.1371/journal.pone.0105988.  
  
A. M. Blázquez-Medela, “Increased Klk9 Urinary Excretion Is Associated to Hypertension-Induced Cardiovascular Damage and Renal Alterations”, *Medicine*, vol. 94, no. 41. Ovid Technologies (Wolters Kluwer Health), p. e1617, Oct. 2015. doi: 10.1097/md.0000000000001617.  
  
A. M. Blázquez-Medela, “Increased Klk9 Urinary Excretion Is Associated to Hypertension-Induced Cardiovascular Damage and Renal Alterations”, *Medicine*, vol. 94, no. 41. Ovid Technologies (Wolters Kluwer Health), p. e1617, Oct. 2015. doi: 10.1097/md.0000000000001617.  
  
A. M. Blazquez-Medela, “ABCC6 deficiency is associated with activation of BMP signaling in liver and kidney”, *FEBS Open Bio*, vol. 5, no. 1. Wiley, pp. 257–263, Jan. 2015. doi: 10.1016/j.fob.2015.03.009.  
  
V. Bondarenko, D. D. Mowrey, T. S. Tillman, E. Seyoum, Y. Xuand P. Tang, “NMR structures of the human α7 nAChR transmembrane domain and associated anesthetic binding sites”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1838, no. 5. Elsevier BV, pp. 1389–1395, May 2014. doi: 10.1016/j.bbamem.2013.12.018.  
  
A. M. Borland, “Engineering crassulacean acid metabolism to improve water-use efficiency”, *Trends in Plant Science*, vol. 19, no. 5. Elsevier BV, pp. 327–338, May 2014. doi: 10.1016/j.tplants.2014.01.006.  
  
A. Borner, Z. Liand D. A. Levin, “Modeling of an ionic liquid electrospray using molecular dynamics with constraints”, *The Journal of Chemical Physics*, vol. 136, no. 12. AIP Publishing, p. 124507, Mar. 28, 2012. doi: 10.1063/1.3696006.  
  
A. Borner, Z. Liand D. A. Levin, “Prediction of Fundamental Properties of Ionic Liquid Electrospray Thrusters using Molecular Dynamics”, *The Journal of Physical Chemistry B*, vol. 117, no. 22. American Chemical Society (ACS), pp. 6768–6781, May 29, 2013. doi: 10.1021/jp402092e.  
  
K. I. Boström, “Matrix Gla protein limits pulmonary arteriovenous malformations in ALK1 deficiency”, *European Respiratory Journal*, vol. 45, no. 3. European Respiratory Society (ERS), pp. 849–852, Jan. 22, 2015. doi: 10.1183/09031936.00114714.  
  
M. S. Bothwell, “SPT 0538–50: PHYSICAL CONDITIONS IN THE INTERSTELLAR MEDIUM OF A STRONGLY LENSED DUSTY STAR-FORMING GALAXY AT*z*= 2.8”, *The Astrophysical Journal*, vol. 779, no. 1. American Astronomical Society, p. 67, Nov. 26, 2013. doi: 10.1088/0004-637x/779/1/67.  
  
J. L. Bouvard, D. K. Francis, M. A. Tschopp, E. B. Marin, D. J. Bammannand M. F. Horstemeyer, “An internal state variable material model for predicting the time, thermomechanical, and stress state dependence of amorphous glassy polymers under large deformation”, *International Journal of Plasticity*, vol. 42. Elsevier BV, pp. 168–193, Mar. 2013. doi: 10.1016/j.ijplas.2012.10.005.  
  
J. L. Bouvard, D. K. Ward, D. Hossain, E. B. Marin, D. J. Bammannand M. F. Horstemeyer, “A general inelastic internal state variable model for amorphous glassy polymers”, *Acta Mechanica*, vol. 213, no. 1–2. Springer Science and Business Media LLC, pp. 71–96, Jun. 19, 2010. doi: 10.1007/s00707-010-0349-y.  
  
C. E. Bradburne, “Temporal Transcriptional Response during Infection of Type II Alveolar Epithelial Cells with Francisella tularensis Live Vaccine Strain (LVS) Supports a General Host Suppression and Bacterial Uptake by Macropinocytosis”, *Journal of Biological Chemistry*, vol. 288, no. 15. Elsevier BV, pp. 10780–10791, Apr. 2013. doi: 10.1074/jbc.m112.362178.  
  
G. Bratzel and M. J. Buehler, “Sequence-structure correlations in silk: Poly-Ala repeat of N. clavipes MaSp1 is naturally optimized at a critical length scale”, *Journal of the Mechanical Behavior of Biomedical Materials*, vol. 7. Elsevier BV, pp. 30–40, Mar. 2012. doi: 10.1016/j.jmbbm.2011.07.012.  
  
G. Bratzel and M. J. Buehler, “Molecular mechanics of silk nanostructures under varied mechanical loading”, *Biopolymers*, vol. 97, no. 6. Wiley, pp. 408–417, Oct. 24, 2011. doi: 10.1002/bip.21729.  
  
G. Bratzel, Z. Qinand M. J. Buehler, “Viscoelastic relaxation time and structural evolution during length contraction of spider silk protein nanostructures”, *MRS Communications*, vol. 3, no. 3. Springer Science and Business Media LLC, pp. 185–190, Sep. 2013. doi: 10.1557/mrc.2013.33.  
  
S. C. Bresler, “ALK Mutations Confer Differential Oncogenic Activation and Sensitivity to ALK Inhibition Therapy in Neuroblastoma”, *Cancer Cell*, vol. 26, no. 5. Elsevier BV, pp. 682–694, Nov. 2014. doi: 10.1016/j.ccell.2014.09.019.  
  
R. C. Brower, G. T. Flemingand H. Neuberger, “Lattice radial quantization: 3D Ising”, *Physics Letters B*, vol. 721, no. 4–5. Elsevier BV, pp. 299–305, Apr. 2013. doi: 10.1016/j.physletb.2013.03.009.  
  
M. Brylinski and W. P. Feinstein, “eFindSite: Improved prediction of ligand binding sites in protein models using meta-threading, machine learning and auxiliary ligands”, *Journal of Computer-Aided Molecular Design*, vol. 27, no. 6. Springer Science and Business Media LLC, pp. 551–567, Jun. 2013. doi: 10.1007/s10822-013-9663-5.  
  
M. J. Buehler, “Materials by design—A perspective from atoms to structures”, *MRS Bulletin*, vol. 38, no. 2. Springer Science and Business Media LLC, pp. 169–176, Feb. 2013. doi: 10.1557/mrs.2013.26.  
  
C. C. Bueno, “Nanobiosensor for Diclofop Detection Based on Chemically Modified AFM Probes”, *IEEE Sensors Journal*, vol. 14, no. 5. Institute of Electrical and Electronics Engineers (IEEE), pp. 1467–1475, May 2014. doi: 10.1109/jsen.2014.2301997.  
  
J. Bulava, “Excited states in lattice QCD with the stochastic LapH method”, *EPJ Web of Conferences*, vol. 73. EDP Sciences, p. 03018, 2014. doi: 10.1051/epjconf/20147303018.  
  
J. Bulava, B. Fahy, B. Hörz, K. J. Juge, C. Morningstarand C. H. Wong, “I= 1 and I= 2 π–π scattering phase shifts from Nf= 2 + 1 lattice QCD”, *Nuclear Physics B*, vol. 910. Elsevier BV, pp. 842–867, Sep. 2016. doi: 10.1016/j.nuclphysb.2016.07.024.  
  
S. P. Burton and Z. F. Burton, “The σ enigma: Bacterial σ factors, archaeal TFB and eukaryotic TFIIB are homologs”, *Transcription*, vol. 5, no. 4. Informa UK Limited, p. e967599, Aug. 08, 2014. doi: 10.4161/21541264.2014.967599.  
  
K. Cai, “Molecular Russian dolls”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Dec. 10, 2018. doi: 10.1038/s41467-018-07673-1.  
  
C. Calero, C. Knorowskiand A. Travesset, “Determination of anharmonic free energy contributions: Low temperature phases of the Lennard-Jones system”, *The Journal of Chemical Physics*, vol. 144, no. 12. AIP Publishing, p. 124102, Mar. 22, 2016. doi: 10.1063/1.4944069.  
  
M. S. Campbell, “MAKER-P: A Tool Kit for the Rapid Creation, Management, and Quality Control of Plant Genome Annotations    ”, *Plant Physiology*, vol. 164, no. 2. Oxford University Press (OUP), pp. 513–524, Dec. 04, 2013. doi: 10.1104/pp.113.230144.  
  
M. B. Cannell, C. H. T. Kong, M. S. Imtiazand D. R. Laver, “Control of Sarcoplasmic Reticulum Ca2+ Release by Stochastic RyR Gating within a 3D Model of the Cardiac Dyad and Importance of Induction Decay for CICR Termination”, *Biophysical Journal*, vol. 104, no. 10. Elsevier BV, pp. 2149–2159, May 2013. doi: 10.1016/j.bpj.2013.03.058.  
  
A. R. Carson, “Effective filtering strategies to improve data quality from population-based whole exome sequencing studies”, *BMC Bioinformatics*, vol. 15, no. 1. Springer Science and Business Media LLC, May 02, 2014. doi: 10.1186/1471-2105-15-125.  
  
G. Ceder, S. P. Ongand Y. Wang, “Predictive modeling and design rules for solid electrolytes”, *MRS Bulletin*, vol. 43, no. 10. Springer Science and Business Media LLC, pp. 746–751, Oct. 2018. doi: 10.1557/mrs.2018.210.  
  
J. N. Chadwick and D. L. James, “Animating fire with sound”, *ACM Transactions on Graphics*, vol. 30, no. 4. Association for Computing Machinery (ACM), pp. 1–8, Jul. 2011. doi: 10.1145/2010324.1964979.  
  
J. N. Chadwick, C. Zhengand D. L. James, “Precomputed acceleration noise for improved rigid-body sound”, *ACM Transactions on Graphics*, vol. 31, no. 4. Association for Computing Machinery (ACM), pp. 1–9, Jul. 2012. doi: 10.1145/2185520.2185599.  
  
M. Chaker-Margot, M. Hunziker, J. Barandun, B. D. Dilland S. Klinge, “Stage-specific assembly events of the 6-MDa small-subunit processome initiate eukaryotic ribosome biogenesis”, *Nature Structural & Molecular Biology*, vol. 22, no. 11. Springer Science and Business Media LLC, pp. 920–923, Oct. 19, 2015. doi: 10.1038/nsmb.3111.  
  
L. P. Chamorro, “Turbulence effects on a full-scale 2.5 MW horizontal-axis wind turbine under neutrally stratified conditions”, *Wind Energy*, vol. 18, no. 2. Wiley, pp. 339–349, Jan. 14, 2014. doi: 10.1002/we.1700.  
  
N. W. Chaney, J. D. Herman, P. M. Reedand E. F. Wood, “Flood and drought hydrologic monitoring: the role of model parameter uncertainty”, *Hydrology and Earth System Sciences*, vol. 19, no. 7. Copernicus GmbH, pp. 3239–3251, Jul. 24, 2015. doi: 10.5194/hess-19-3239-2015.  
  
N. W. Chaney, J. D. Herman, P. M. Reedand E. F. Wood, “Flood and drought hydrologic monitoring: the role of model parameter uncertainty”, *Hydrology and Earth System Sciences*, vol. 19, no. 7. Copernicus GmbH, pp. 3239–3251, Jul. 24, 2015. doi: 10.5194/hess-19-3239-2015.  
  
N. W. Chaney, J. D. Herman, P. M. Reedand E. F. Wood, “Flood and drought hydrologic monitoring: the role of model parameter uncertainty”, *Hydrology and Earth System Sciences*, vol. 19, no. 7. Copernicus GmbH, pp. 3239–3251, Jul. 24, 2015. doi: 10.5194/hess-19-3239-2015.  
  
N. W. Chaney, P. Metcalfeand E. F. Wood, “HydroBlocks: a field‐scale resolving land surface model for application over continental extents”, *Hydrological Processes*, vol. 30, no. 20. Wiley, pp. 3543–3559, Aug. 19, 2016. doi: 10.1002/hyp.10891.  
  
N. W. Chaney, J. K. Roundy, J. E. Herrera-Estradaand E. F. Wood, “High-resolution modeling of the spatial heterogeneity of soil moisture: Applications in network design”, *Water Resources Research*, vol. 51, no. 1. American Geophysical Union (AGU), pp. 619–638, Jan. 2015. doi: 10.1002/2013wr014964.  
  
N. W. Chaney, “POLARIS: A 30-meter probabilistic soil series map of the contiguous United States”, *Geoderma*, vol. 274. Elsevier BV, pp. 54–67, Jul. 2016. doi: 10.1016/j.geoderma.2016.03.025.  
  
N. W. Chaney, “POLARIS: A 30-meter probabilistic soil series map of the contiguous United States”, *Geoderma*, vol. 274. Elsevier BV, pp. 54–67, Jul. 2016. doi: 10.1016/j.geoderma.2016.03.025.  
  
H. J. Changlani, N. M. Tubmanand T. L. Hughes, “Charge density waves in disordered media circumventing the Imry-Ma argument”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Aug. 24, 2016. doi: 10.1038/srep31897.  
  
S.-W. Chang and M. J. Buehler, “Molecular biomechanics of collagen molecules”, *Materials Today*, vol. 17, no. 2. Elsevier BV, pp. 70–76, Mar. 2014. doi: 10.1016/j.mattod.2014.01.019.  
  
S.-W. Chang, B. P. Flynn, J. W. Rubertiand M. J. Buehler, “Molecular mechanism of force induced stabilization of collagen against enzymatic breakdown”, *Biomaterials*, vol. 33, no. 15. Elsevier BV, pp. 3852–3859, May 2012. doi: 10.1016/j.biomaterials.2012.02.001.  
  
S.-W. Chang, A. K. Nairand M. J. Buehler, “Nanoindentation study of size effects in nickel–graphene nanocomposites”, *Philosophical Magazine Letters*, vol. 93, no. 4. Informa UK Limited, pp. 196–203, Apr. 2013. doi: 10.1080/09500839.2012.759293.  
  
S.-W. Chang, S. J. Shefelbineand M. J. Buehler, “Structural and Mechanical Differences between Collagen Homo- and Heterotrimers: Relevance for the Molecular Origin of Brittle Bone Disease”, *Biophysical Journal*, vol. 102, no. 3. Elsevier BV, pp. 640–648, Feb. 2012. doi: 10.1016/j.bpj.2011.11.3999.  
  
S. Chauhan, “ZKSCAN3 Is a Master Transcriptional Repressor of Autophagy”, *Molecular Cell*, vol. 50, no. 1. Elsevier BV, pp. 16–28, Apr. 2013. doi: 10.1016/j.molcel.2013.01.024.  
  
C.-T. Chen, S. Ghosh, C. Malla Reddyand M. J. Buehler, “Molecular mechanics of elastic and bendable caffeine co-crystals”, *Physical Chemistry Chemical Physics*, vol. 16, no. 26. Royal Society of Chemistry (RSC), p. 13165, 2014. doi: 10.1039/c3cp55117b.  
  
C. H. Chen, A. Khan, J. J.-T. Huangand M. B. Ulmschneider, “Mechanisms of Membrane Pore Formation by Amyloidogenic Peptides in Amyotrophic Lateral Sclerosis”, *Chemistry - A European Journal*, vol. 22, no. 29. Wiley, pp. 9958–9961, Jun. 16, 2016. doi: 10.1002/chem.201601765.  
  
C. H. Chen, “Simulation-Guided Rational *de Novo* Design of a Small Pore-Forming Antimicrobial Peptide”, *Journal of the American Chemical Society*, vol. 141, no. 12. American Chemical Society (ACS), pp. 4839–4848, Mar. 06, 2019. doi: 10.1021/jacs.8b11939.  
  
C. Chen and T. M. Taha, “A communication reduction approach to iteratively solve large sparse linear systems on a GPGPU cluster”, *Cluster Computing*, vol. 17, no. 2. Springer Science and Business Media LLC, pp. 327–337, Jun. 22, 2013. doi: 10.1007/s10586-013-0279-2.  
  
C. H. Chen, G. Wiedman, A. Khanand M. B. Ulmschneider, “Absorption and folding of melittin onto lipid bilayer membranes via unbiased atomic detail microsecond molecular dynamics simulation”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1838, no. 9. Elsevier BV, pp. 2243–2249, Sep. 2014. doi: 10.1016/j.bbamem.2014.04.012.  
  
H. Chen, W. Chen, C. Liu, L. Zhang, J. Suand X. Zhou, “Relational Network for Knowledge Discovery through Heterogeneous Biomedical and Clinical Features”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Jul. 18, 2016. doi: 10.1038/srep29915.  
  
K.-J. Chen, V. Bromm, A. Heger, M. Jeonand S. Woosley, “COSMOLOGICAL IMPACT OF POPULATION III BINARIES”, *The Astrophysical Journal*, vol. 802, no. 1. American Astronomical Society, p. 13, Mar. 16, 2015. doi: 10.1088/0004-637x/802/1/13.  
  
L. Chen, “Large-scale ruminant genome sequencing provides insights into their evolution and distinct traits”, *Science*, vol. 364, no. 6446. American Association for the Advancement of Science (AAAS), Jun. 21, 2019. doi: 10.1126/science.aav6202.  
  
W. Chen and J. K. Shen, “Effects of system net charge and electrostatic truncation on all-atom constant pH molecular dynamics”, *Journal of Computational Chemistry*, vol. 35, no. 27. Wiley, pp. 1986–1996, Aug. 21, 2014. doi: 10.1002/jcc.23713.  
  
W. Chen, J. A. Wallace, Z. Yueand J. K. Shen, “Introducing Titratable Water to All-Atom Molecular Dynamics at Constant pH”, *Biophysical Journal*, vol. 105, no. 4. Elsevier BV, pp. L15–L17, Aug. 2013. doi: 10.1016/j.bpj.2013.06.036.  
  
W.-Y. Chen, J. Zhang, H. Geng, Z. Du, T. Nakadaiand R. G. Roeder, “A TAF4 coactivator function for E proteins that involves enhanced TFIID binding”, *Genes & Development*, vol. 27, no. 14. Cold Spring Harbor Laboratory, pp. 1596–1609, Jul. 15, 2013. doi: 10.1101/gad.216192.113.  
  
T. D. Chheda, “Structure and elasticity of phlogopite under compression: Geophysical implications”, *Physics of the Earth and Planetary Interiors*, vol. 233. Elsevier BV, pp. 1–12, Aug. 2014. doi: 10.1016/j.pepi.2014.05.004.  
  
S. T. Chill, “EON: software for long time simulations of atomic scale systems”, *Modelling and Simulation in Materials Science and Engineering*, vol. 22, no. 5. IOP Publishing, p. 055002, May 16, 2014. doi: 10.1088/0965-0393/22/5/055002.  
  
H. D. Cho, O. Kwonand S. P. Midkiff, “HDArray: Parallel Array Interface for Distributed Heterogeneous Devices”, *Languages and Compilers for Parallel Computing*. Springer International Publishing, pp. 176–184, 2019. doi: 10.1007/978-3-030-34627-0\_13.  
  
E. J. Choi, K. Min, K.-I. Nishikawaand C. R. Choi, “A study of the early-stage evolution of relativistic electron-ion shock using three-dimensional particle-in-cell simulations”, *Physics of Plasmas*, vol. 21, no. 7. AIP Publishing, p. 072905, Jul. 2014. doi: 10.1063/1.4890479.  
  
J. Choi, A. Dotter, C. Conroy, M. Cantiello, B. Paxtonand B. D. Johnson, “MESA ISOCHRONES AND STELLAR TRACKS (MIST). I. SOLAR-SCALED MODELS”, *The Astrophysical Journal*, vol. 823, no. 2. American Astronomical Society, p. 102, May 26, 2016. doi: 10.3847/0004-637x/823/2/102.  
  
C.-C. Chou and M. J. Buehler, “Molecular Mechanics of Disulfide Bonded Alpha-Helical Protein Filaments”, *BioNanoScience*, vol. 3, no. 1. Springer Science and Business Media LLC, pp. 85–94, Nov. 28, 2012. doi: 10.1007/s12668-012-0065-2.  
  
C.-C. Chou and M. J. Buehler, “Structure and Mechanical Properties of Human Trichocyte Keratin Intermediate Filament Protein”, *Biomacromolecules*, vol. 13, no. 11. American Chemical Society (ACS), pp. 3522–3532, Oct. 03, 2012. doi: 10.1021/bm301254u.  
  
A. Choudhury, “New insights into the structure, chemistry, and properties of Cu4SnS4”, *Journal of Solid State Chemistry*, vol. 253. Elsevier BV, pp. 192–201, Sep. 2017. doi: 10.1016/j.jssc.2017.05.033.  
  
G. Chuai, “Deciphering relationship between microhomology and in-frame mutation occurrence in human CRISPR-based gene knockout”, *Molecular Therapy - Nucleic Acids*, vol. 5. Elsevier BV, p. e323, 2016. doi: 10.1038/mtna.2016.35.  
  
R. I. Citron, H. Gendaand S. Ida, “Formation of Phobos and Deimos via a giant impact”, *Icarus*, vol. 252. Elsevier BV, pp. 334–338, May 2015. doi: 10.1016/j.icarus.2015.02.011.  
  
J. Cohen, “Molecular Phylogenetics, Molecular Evolution, and Patterns of Clade Support in Lithospermum (Boraginaceae) and Related Taxa”, *Systematic Botany*, vol. 37, no. 2. American Society of Plant Taxonomists, 2012. doi: 10.1600/03634412x635539.  
  
J. I. Cohen, “A phylogenetic analysis of morphological and molecular characters of Boraginaceae: evolutionary relationships, taxonomy, and patterns of character evolution”, *Cladistics*, vol. 30, no. 2. Wiley, pp. 139–169, Jul. 10, 2013. doi: 10.1111/cla.12036.  
  
J. I. Cohen, “Floral evolution in*Lithospermum*(Boraginaceae): independent origins of similar flower types”, *Botanical Journal of the Linnean Society*, vol. 180, no. 2. Oxford University Press (OUP), pp. 213–228, Dec. 23, 2015. doi: 10.1111/boj.12368.  
  
T. X. Collaboration, “Exclusion of leptophilic dark matter models using XENON100 electronic recoil data”, *Science*, vol. 349, no. 6250. American Association for the Advancement of Science (AAAS), pp. 851–854, Aug. 21, 2015. doi: 10.1126/science.aab2069.  
  
K. W. Connington, T. Leeand J. F. Morris, “Interaction of fluid interfaces with immersed solid particles using the lattice Boltzmann method for liquid–gas–particle systems”, *Journal of Computational Physics*, vol. 283. Elsevier BV, pp. 453–477, Feb. 2015. doi: 10.1016/j.jcp.2014.11.044.  
  
E. F. Connor, L. Bartlett, S. O’Toole, S. Byrd, K. Biskarand J. Orozco, “The mechanism of gall induction makes galls red”, *Arthropod-Plant Interactions*, vol. 6, no. 4. Springer Science and Business Media LLC, pp. 489–495, Jul. 11, 2012. doi: 10.1007/s11829-012-9210-7.  
  
C. M. Cooper, L. ‐N . Moresiand A. Lenardic, “Effects of continental configuration on mantle heat loss”, *Geophysical Research Letters*, vol. 40, no. 11. American Geophysical Union (AGU), pp. 2647–2651, Jun. 10, 2013. doi: 10.1002/grl.50547.  
  
P. J. Coskren, “Functional consequences of age-related morphologic changes to pyramidal neurons of the rhesus monkey prefrontal cortex”, *Journal of Computational Neuroscience*, vol. 38, no. 2. Springer Science and Business Media LLC, pp. 263–283, Dec. 20, 2014. doi: 10.1007/s10827-014-0541-5.  
  
J. W. Coughlin, G. J. Mathews, L. A. Phillips, A. P. Sneddenand I.-S. Suh, “Probing Time-dependent Dark Energy with the Flux Power Spectrum of the Ly*α* Forest”, *The Astrophysical Journal*, vol. 874, no. 1. American Astronomical Society, p. 11, Mar. 15, 2019. doi: 10.3847/1538-4357/ab04f9.  
  
K. N. Crabtree, M. R. Talipov, O. Martinez, G. D. O’Connor, S. L. Khursanand M. C. McCarthy, “Detection and Structure of HOON: Microwave Spectroscopy Reveals an O-O Bond Exceeding 1.9 A”, *Science*, vol. 342, no. 6164. American Association for the Advancement of Science (AAAS), pp. 1354–1357, Dec. 12, 2013. doi: 10.1126/science.1244180.  
  
S. W. Cranford and M. J. Buehler, *Biomateriomics*. Springer Netherlands, 2012. doi: 10.1007/978-94-007-1611-7.  
  
S. W. Cranford, N. M. Pugnoand M. J. Buehler, “Silk and Web Synergy: The Merging of Material and Structural Performance”, *Biotechnology of Silk*. Springer Netherlands, pp. 219–268, Sep. 20, 2013. doi: 10.1007/978-94-007-7119-2\_12.  
  
S. W. Cranford, A. Tarakanova, N. M. Pugnoand M. J. Buehler, “Nonlinear material behaviour of spider silk yields robust webs”, *Nature*, vol. 482, no. 7383. Springer Science and Business Media LLC, pp. 72–76, Feb. 2012. doi: 10.1038/nature10739.  
  
T. T. Creyts, “Freezing of ridges and water networks preserves the Gamburtsev Subglacial Mountains for millions of years”, *Geophysical Research Letters*, vol. 41, no. 22. American Geophysical Union (AGU), pp. 8114–8122, Nov. 17, 2014. doi: 10.1002/2014gl061491.  
  
L. Croitor, “Polymeric Luminescent Zn(II) and Cd(II) Dicarboxylates Decorated by Oxime Ligands: Tuning the Dimensionality and Adsorption Capacity”, *Crystal Growth & Design*, vol. 14, no. 8. American Chemical Society (ACS), pp. 3935–3948, Jul. 23, 2014. doi: 10.1021/cg5005402.  
  
L. Croitor, E. B. Coropceanu, A. E. Masunov, H. J. Rivera-Jacquez, A. V. Simineland M. S. Fonari, “Mechanism of Nonlinear Optical Enhancement and Supramolecular Isomerism in 1D Polymeric Zn(II) and Cd(II) Sulfates with Pyridine-4-aldoxime Ligands”, *The Journal of Physical Chemistry C*, vol. 118, no. 17. American Chemical Society (ACS), pp. 9217–9227, Apr. 18, 2014. doi: 10.1021/jp5007395.  
  
S. B. Cronan, K. D. Keyand A. A. Vaughn, “Beyond the dichotomy: Modernizing stigma categorization.”, *Stigma and Health*, vol. 1, no. 4. American Psychological Association (APA), pp. 225–243, Nov. 2016. doi: 10.1037/sah0000031.  
  
A. M. Crotty, “Molecular Packing in Organic Solar Cell Materials: Insights from the Emission Line Shapes of P3HT/PCBM Polymer Blend Nanoparticles”, *The Journal of Physical Chemistry C*, vol. 118, no. 34. American Chemical Society (ACS), pp. 19975–19984, Aug. 18, 2014. doi: 10.1021/jp5040932.  
  
J. Cui, “Comprehensive characterization of the genomic alterations in human gastric cancer”, *International Journal of Cancer*, vol. 137, no. 1. Wiley, pp. 86–95, Dec. 03, 2014. doi: 10.1002/ijc.29352.  
  
W. Cui, J. Shi, H. Liu, C. Luand H. Wang, “Novel high-pressure crystal structures of boron trifluoride”, *Journal of Physics and Chemistry of Solids*, vol. 75, no. 10. Elsevier BV, pp. 1094–1098, Oct. 2014. doi: 10.1016/j.jpcs.2014.03.013.  
  
W. Cui, “Hydrogen segregation and its roles in structural stability and metallization: silane under pressure”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, Aug. 12, 2015. doi: 10.1038/srep13039.  
  
N. Dahl and M. Xue, “Prediction of the 14 June 2010 Oklahoma City Extreme Precipitation and Flooding Event in a Multiphysics Multi-Initial-Conditions Storm-Scale Ensemble Forecasting System”, *Weather and Forecasting*, vol. 31, no. 4. American Meteorological Society, pp. 1215–1246, Jul. 12, 2016. doi: 10.1175/waf-d-15-0116.1.  
  
A. Damsgaard, D. L. Egholm, J. A. Piotrowski, S. Tulaczyk, N. K. Larsenand K. Tylmann, “Discrete element modeling of subglacial sediment deformation”, *Journal of Geophysical Research: Earth Surface*, vol. 118, no. 4. American Geophysical Union (AGU), pp. 2230–2242, Oct. 18, 2013. doi: 10.1002/2013jf002830.  
  
A. Damsgaard, D. L. Egholm, J. A. Piotrowski, S. Tulaczyk, N. K. Larsenand C. F. Brædstrup, “A new methodology to simulate subglacial deformation of water-saturated granular material”, *The Cryosphere*, vol. 9, no. 6. Copernicus GmbH, pp. 2183–2200, Nov. 20, 2015. doi: 10.5194/tc-9-2183-2015.  
  
A. Das, “Digital imaging of root traits (DIRT): a high-throughput computing and collaboration platform for field-based root phenomics”, *Plant Methods*, vol. 11, no. 1. Springer Science and Business Media LLC, Nov. 02, 2015. doi: 10.1186/s13007-015-0093-3.  
  
I. Das, “Influence of persistent wind scour on the surface mass balance of Antarctica”, *Nature Geoscience*, vol. 6, no. 5. Springer Science and Business Media LLC, pp. 367–371, Mar. 31, 2013. doi: 10.1038/ngeo1766.  
  
A. Dasmahapatra and P. Kroll, “Computational study of impact of composition, density, and temperature on thermal conductivity of amorphous silicon boron nitride”, *Journal of the American Ceramic Society*, vol. 101, no. 8. Wiley, pp. 3489–3497, Feb. 19, 2018. doi: 10.1111/jace.15470.  
  
A. Dasmahapatra and P. Kroll, “Modeling amorphous silicon nitride: A comparative study of empirical potentials”, *Computational Materials Science*, vol. 148. Elsevier BV, pp. 165–175, Jun. 2018. doi: 10.1016/j.commatsci.2017.12.008.  
  
P. Das, B. Murrayand G. Belfort, “Alzheimer’s Protective A2T Mutation Changes the Conformational Landscape of the Aβ1–42 Monomer Differently Than Does the A2V Mutation”, *Biophysical Journal*, vol. 108, no. 3. Elsevier BV, pp. 738–747, Feb. 2015. doi: 10.1016/j.bpj.2014.12.013.  
  
I. Davidi, “Hierarchical Structures of Polystyrene-*block*-poly(2-vinylpyridine)/Palladium–Pincer Surfactants: Effect of Weak Surfactant–Polymer Interactions on the Morphological Behavior”, *Macromolecules*, vol. 47, no. 16. American Chemical Society (ACS), pp. 5774–5783, Aug. 06, 2014. doi: 10.1021/ma5010343.  
  
B. L. Davis and M. I. Hussein, “Nanophononic Metamaterial: Thermal Conductivity Reduction by Local Resonance”, *Physical Review Letters*, vol. 112, no. 5. American Physical Society (APS), Feb. 07, 2014. doi: 10.1103/physrevlett.112.055505.  
  
C. DeBoever, “Transcriptome Sequencing Reveals Potential Mechanism of Cryptic 3’ Splice Site Selection in SF3B1-mutated Cancers”, *PLOS Computational Biology*, vol. 11, no. 3. Public Library of Science (PLoS), p. e1004105, Mar. 13, 2015. doi: 10.1371/journal.pcbi.1004105.  
  
C. DeBoever, “Whole Transcriptome Sequencing Enables Discovery and Analysis of Viruses in Archived Primary Central Nervous System Lymphomas”, *PLoS ONE*, vol. 8, no. 9. Public Library of Science (PLoS), p. e73956, Sep. 04, 2013. doi: 10.1371/journal.pone.0073956.  
  
M. Deininger, “Curing CML with imatinib—a dream come true?”, *Nature Reviews Clinical Oncology*, vol. 8, no. 3. Springer Science and Business Media LLC, pp. 127–128, Feb. 01, 2011. doi: 10.1038/nrclinonc.2011.17.  
  
Q. Deng and Y. Chen, “A COARSE-GRAINED ATOMISTIC METHOD FOR 3D DYNAMIC FRACTURE SIMULATION”, *International Journal for Multiscale Computational Engineering*, vol. 11, no. 3. Begell House, pp. 227–237, 2013. doi: 10.1615/intjmultcompeng.2013005442.  
  
R. B. de Oliveira, “Ketamine anesthesia helps preserve neuronal viability”, *Journal of Neuroscience Methods*, vol. 189, no. 2. Elsevier BV, pp. 230–232, Jun. 2010. doi: 10.1016/j.jneumeth.2010.03.029.  
  
R. B. de Oliveira, “Pacemaker currents in mouse locus coeruleus neurons”, *Neuroscience*, vol. 170, no. 1. Elsevier BV, pp. 166–177, Sep. 2010. doi: 10.1016/j.neuroscience.2010.06.028.  
  
H. C. DePaoli, A. M. Borland, G. A. Tuskan, J. C. Cushmanand X. Yang, “Synthetic biology as it relates to CAM photosynthesis: challenges and opportunities”, *Journal of Experimental Botany*, vol. 65, no. 13. Oxford University Press (OUP), pp. 3381–3393, Feb. 24, 2014. doi: 10.1093/jxb/eru038.  
  
P. Deshlahra, R. T. Carrand E. Iglesia, “Ionic and Covalent Stabilization of Intermediates and Transition States in Catalysis by Solid Acids”, *Journal of the American Chemical Society*, vol. 136, no. 43. American Chemical Society (ACS), pp. 15229–15247, Oct. 21, 2014. doi: 10.1021/ja506149c.  
  
P. Deshlahra, R. T. Carr, S.-H. Chaiand E. Iglesia, “Mechanistic Details and Reactivity Descriptors in Oxidation and Acid Catalysis of Methanol”, *ACS Catalysis*, vol. 5, no. 2. American Chemical Society (ACS), pp. 666–682, Dec. 24, 2014. doi: 10.1021/cs501599y.  
  
P. Deshlahra and E. Iglesia, “Methanol Oxidative Dehydrogenation on Oxide Catalysts: Molecular and Dissociative Routes and Hydrogen Addition Energies as Descriptors of Reactivity”, *The Journal of Physical Chemistry C*, vol. 118, no. 45. American Chemical Society (ACS), pp. 26115–26129, Nov. 05, 2014. doi: 10.1021/jp507922u.  
  
F. A. L. de Souza, A. R. Ambrozio, E. S. Souza, D. F. Cipriano, W. L. Scopeland J. C. C. Freitas, “NMR Spectral Parameters in Graphene, Graphite, and Related Materials: Ab Initio Calculations and Experimental Results”, *The Journal of Physical Chemistry C*, vol. 120, no. 48. American Chemical Society (ACS), pp. 27707–27716, Nov. 23, 2016. doi: 10.1021/acs.jpcc.6b10042.  
  
F. DiMaio, J. Zhang, W. Chiuand D. Baker, “Cryo-EM model validation using independent map reconstructions”, *Protein Science*, vol. 22, no. 6. Wiley, pp. 865–868, May 25, 2013. doi: 10.1002/pro.2267.  
  
L. S. Dimas, G. H. Bratzel, I. Eylonand M. J. Buehler, “Tough Composites Inspired by Mineralized Natural Materials: Computation, 3D printing, and Testing”, *Advanced Functional Materials*, vol. 23, no. 36. Wiley, pp. 4629–4638, Jun. 17, 2013. doi: 10.1002/adfm.201300215.  
  
L. S. Dimas and M. J. Buehler, “Modeling and additive manufacturing of bio-inspired composites with tunable fracture mechanical properties”, *Soft Matter*, vol. 10, no. 25. Royal Society of Chemistry (RSC), p. 4436, 2014. doi: 10.1039/c3sm52890a.  
  
T. C. Dinadayalane and J. Leszczynski, “Comparative Theoretical Study on the Positional Preference for Functionalization of Two OH and SH Groups with (5,5) Armchair SWCNT”, *The Journal of Physical Chemistry C*, vol. 117, no. 27. American Chemical Society (ACS), pp. 14441–14450, Jul. 01, 2013. doi: 10.1021/jp404592u.  
  
T. C. Dinadayalane, J. S. Murray, M. C. Concha, P. Politzerand J. Leszczynski, “Reactivities of Sites on (5,5) Single-Walled Carbon Nanotubes with and without a Stone-Wales Defect”, *Journal of Chemical Theory and Computation*, vol. 6, no. 4. American Chemical Society (ACS), pp. 1351–1357, Mar. 10, 2010. doi: 10.1021/ct900669t.  
  
J. Ding, W. Hu, E. Paekand D. Mitlin, “Review of Hybrid Ion Capacitors: From Aqueous to Lithium to Sodium”, *Chemical Reviews*, vol. 118, no. 14. American Chemical Society (ACS), pp. 6457–6498, Jun. 28, 2018. doi: 10.1021/acs.chemrev.8b00116.  
  
Y. Ding, “GeauxDock: A novel approach for mixed-resolution ligand docking using a descriptor-based force field”, *Journal of Computational Chemistry*, vol. 36, no. 27. Wiley, pp. 2013–2026, Aug. 06, 2015. doi: 10.1002/jcc.24031.  
  
X. Dong, N. E. Hudson, C. Luand T. A. Springer, “Structural determinants of integrin β-subunit specificity for latent TGF-β”, *Nature Structural & Molecular Biology*, vol. 21, no. 12. Springer Science and Business Media LLC, pp. 1091–1096, Nov. 10, 2014. doi: 10.1038/nsmb.2905.  
  
X. Dong, “αVβ3 Integrin Crystal Structures and Their Functional Implications”, *Biochemistry*, vol. 51, no. 44. American Chemical Society (ACS), pp. 8814–8828, Oct. 29, 2012. doi: 10.1021/bi300734n.  
  
K. M. Dorn, J. D. Fankhauser, D. L. Wyseand M. D. Marks, “*De novo*assembly of the pennycress (*Thlaspi arvense*) transcriptome provides tools for the development of a winter cover crop and biodiesel feedstock”, *The Plant Journal*, vol. 75, no. 6. Wiley, pp. 1028–1038, Aug. 14, 2013. doi: 10.1111/tpj.12267.  
  
A. Dotter, “MESA ISOCHRONES AND STELLAR TRACKS (MIST) 0: METHODS FOR THE CONSTRUCTION OF STELLAR ISOCHRONES”, *The Astrophysical Journal Supplement Series*, vol. 222, no. 1. American Astronomical Society, p. 8, Jan. 14, 2016. doi: 10.3847/0067-0049/222/1/8.  
  
N. R. Douglas, “Dual Action of ATP Hydrolysis Couples Lid Closure to Substrate Release into the Group II Chaperonin Chamber”, *Cell*, vol. 144, no. 2. Elsevier BV, pp. 240–252, Jan. 2011. doi: 10.1016/j.cell.2010.12.017.  
  
S. Draguta, “New acentric materials constructed from aminopyridines and 4-nitrophenol”, *CrystEngComm*, vol. 15, no. 23. Royal Society of Chemistry (RSC), p. 4700, 2013. doi: 10.1039/c3ce40291f.  
  
J. W. Driver, D. K. Jamison, K. Uppulury, A. R. Rogers, A. B. Kolomeiskyand M. R. Diehl, “Productive Cooperation among Processive Motors Depends Inversely on Their Mechanochemical Efficiency”, *Biophysical Journal*, vol. 101, no. 2. Elsevier BV, pp. 386–395, Jul. 2011. doi: 10.1016/j.bpj.2011.05.067.  
  
J. W. Driver, A. R. Rogers, D. K. Jamison, R. K. Das, A. B. Kolomeiskyand M. R. Diehl, “Coupling between motor proteins determines dynamic behaviors of motor protein assemblies”, *Physical Chemistry Chemical Physics*, vol. 12, no. 35. Royal Society of Chemistry (RSC), p. 10398, 2010. doi: 10.1039/c0cp00117a.  
  
C. Duan, Q. Wang, Z. Tangand J. Wu, “The study of an extended hierarchy equation of motion in the spin-boson model: The cutoff function of the sub-Ohmic spectral density”, *The Journal of Chemical Physics*, vol. 147, no. 16. AIP Publishing, p. 164112, Oct. 28, 2017. doi: 10.1063/1.4997669.  
  
D. H. E. Dubin, “Cyclotron waves in a non-neutral plasma column”, *Physics of Plasmas*, vol. 20, no. 4. AIP Publishing, p. 042120, Apr. 2013. doi: 10.1063/1.4802101.  
  
G.-J. Du, “Epigallocatechin Gallate (EGCG) Is the Most Effective Cancer Chemopreventive Polyphenol in Green Tea”, *Nutrients*, vol. 4, no. 11. MDPI AG, pp. 1679–1691, Nov. 08, 2012. doi: 10.3390/nu4111679.  
  
J. R. Duke and N. Ananth, “Simulating Excited State Dynamics in Systems with Multiple Avoided Crossings Using Mapping Variable Ring Polymer Molecular Dynamics”, *The Journal of Physical Chemistry Letters*, vol. 6, no. 21. American Chemical Society (ACS), pp. 4219–4223, Oct. 09, 2015. doi: 10.1021/acs.jpclett.5b01957.  
  
R. E. Duke, O. N. Starovoytov, J.-P. Piquemaland G. A. Cisneros, “GEM\*: A Molecular Electronic Density-Based Force Field for Molecular Dynamics Simulations”, *Journal of Chemical Theory and Computation*, vol. 10, no. 4. American Chemical Society (ACS), pp. 1361–1365, Mar. 03, 2014. doi: 10.1021/ct500050p.  
  
M. Dupré, L. Hsuand B. Kanté, “On the design of random metasurface based devices”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, May 08, 2018. doi: 10.1038/s41598-018-25488-4.  
  
M. Dupré, J. Park, L. Hsu, A. Ndaoand B. Kanté, “Towards Random Metasurface based Devices”, *Conference on Lasers and Electro-Optics*. OSA, 2018. doi: 10.1364/cleo\_qels.2018.fth4j.7.  
  
T. Duque, M. A. H. Samee, M. Kazemian, H. N. Pham, M. H. Brodskyand S. Sinha, “Simulations of Enhancer Evolution Provide Mechanistic Insights into Gene Regulation”, *Molecular Biology and Evolution*, vol. 31, no. 1. Oxford University Press (OUP), pp. 184–200, Oct. 04, 2013. doi: 10.1093/molbev/mst170.  
  
J. Dutil, J. L. Colon-Colon, J. L. Matta, R. Sutphenand M. Echenique, “Identification of the prevalent BRCA1 and BRCA2 mutations in the female population of Puerto Rico”, *Cancer Genetics*, vol. 205, no. 5. Elsevier BV, pp. 242–248, May 2012. doi: 10.1016/j.cancergen.2012.04.002.  
  
I. Dutta, P. Kumarand M. S. Bakir, “Interface-related reliability challenges in 3-D interconnect systems with through-silicon vias”, *JOM*, vol. 63, no. 10. Springer Science and Business Media LLC, pp. 70–77, Oct. 2011. doi: 10.1007/s11837-011-0179-y.  
  
T. Dvir, L. Fink, R. Asor, Y. Schilt, A. Steinarand U. Raviv, “Charged membranes under confinement induced by polymer-, salt-, or ionic liquid solutions”, *Soft Matter*, vol. 9, no. 44. Royal Society of Chemistry (RSC), p. 10640, 2013. doi: 10.1039/c3sm51916c.  
  
S. R. Eichten, “Epigenetic and Genetic Influences on DNA Methylation Variation in Maize Populations”, *The Plant Cell*, vol. 25, no. 8. Oxford University Press (OUP), pp. 2783–2797, Aug. 2013. doi: 10.1105/tpc.113.114793.  
  
S. R. Eichten, “Spreading of Heterochromatin Is Limited to Specific Families of Maize Retrotransposons”, *PLoS Genetics*, vol. 8, no. 12. Public Library of Science (PLoS), p. e1003127, Dec. 13, 2012. doi: 10.1371/journal.pgen.1003127.  
  
S. R. Eichten, “Heritable Epigenetic Variation among Maize Inbreds”, *PLoS Genetics*, vol. 7, no. 11. Public Library of Science (PLoS), p. e1002372, Nov. 17, 2011. doi: 10.1371/journal.pgen.1002372.  
  
Ş. Ekesan and D. M. York, “Framework for Conducting and Analyzing Crystal Simulations of Nucleic Acids to Aid in Modern Force Field Evaluation”, *The Journal of Physical Chemistry B*, vol. 123, no. 22. American Chemical Society (ACS), pp. 4611–4624, Apr. 19, 2019. doi: 10.1021/acs.jpcb.8b11923.  
  
C. E. Ekuma, “Metal-insulator transition in a weakly interacting disordered electron system”, *Physical Review B*, vol. 92, no. 20. American Physical Society (APS), Nov. 25, 2015. doi: 10.1103/physrevb.92.201114.  
  
S. C. Epstein, A. R. Huff, E. S. Winesett, C. H. Londerganand L. K. Charkoudian, “Tracking carrier protein motions with Raman spectroscopy”, *Nature Communications*, vol. 10, no. 1. Springer Science and Business Media LLC, May 20, 2019. doi: 10.1038/s41467-019-10184-2.  
  
I. Errea, “High-Pressure Hydrogen Sulfide from First Principles: A Strongly Anharmonic Phonon-Mediated Superconductor”, *Physical Review Letters*, vol. 114, no. 15. American Physical Society (APS), Apr. 16, 2015. doi: 10.1103/physrevlett.114.157004.  
  
M. C. Estep, “Allopolyploidy, diversification, and the Miocene grassland expansion”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 42. Proceedings of the National Academy of Sciences, pp. 15149–15154, Oct. 06, 2014. doi: 10.1073/pnas.1404177111.  
  
B. Ewen-Campen, N. Shaner, K. A. Panfilio, Y. Suzuki, S. Rothand C. G. Extavour, “The maternal and early embryonic transcriptome of the milkweed bug Oncopeltus fasciatus”, *BMC Genomics*, vol. 12, no. 1. Springer Science and Business Media LLC, Jan. 25, 2011. doi: 10.1186/1471-2164-12-61.  
  
A. Fakhari and T. Lee, “Multiple-relaxation-time lattice Boltzmann method for immiscible fluids at high Reynolds numbers”, *Physical Review E*, vol. 87, no. 2. American Physical Society (APS), Feb. 15, 2013. doi: 10.1103/physreve.87.023304.  
  
C. E. Faller, K. A. Reilly, R. D. Hills Jr.and O. Guvench, “Peptide Backbone Sampling Convergence with the Adaptive Biasing Force Algorithm”, *The Journal of Physical Chemistry B*, vol. 117, no. 2. American Chemical Society (ACS), pp. 518–526, Jan. 02, 2013. doi: 10.1021/jp309741j.  
  
D. Fang and G. A. Cisneros, “Alternative Pathway for the Reaction Catalyzed by DNA Dealkylase AlkB from Ab Initio QM/MM Calculations”, *Journal of Chemical Theory and Computation*, vol. 10, no. 11. American Chemical Society (ACS), pp. 5136–5148, Oct. 09, 2014. doi: 10.1021/ct500572t.  
  
E. Faraggi and A. Kloczkowski, “A global machine learning based scoring function for protein structure prediction”, *Proteins: Structure, Function, and Bioinformatics*, vol. 82, no. 5. Wiley, pp. 752–759, Nov. 22, 2013. doi: 10.1002/prot.24454.  
  
E. Faraggi, T. Zhang, Y. Yang, L. Kurganand Y. Zhou, “SPINE X: Improving protein secondary structure prediction by multistep learning coupled with prediction of solvent accessible surface area and backbone torsion angles”, *Journal of Computational Chemistry*, vol. 33, no. 3. Wiley, pp. 259–267, Nov. 02, 2011. doi: 10.1002/jcc.21968.  
  
S. Farokhirad, T. Leeand J. F. Morris, “Effects of Inertia and Viscosity on Single Droplet Deformation in Confined Shear Flow”, *Communications in Computational Physics*, vol. 13, no. 3. Global Science Press, pp. 706–724, Mar. 2013. doi: 10.4208/cicp.431011.260112s.  
  
W. P. Feinstein and M. Brylinski, “*e*FindSite: Enhanced Fingerprint-Based Virtual Screening Against Predicted Ligand Binding Sites in Protein Models”, *Molecular Informatics*, vol. 33, no. 2. Wiley, pp. 135–150, Feb. 2014. doi: 10.1002/minf.201300143.  
  
D. Feng, A. N. Chernikovand N. P. Chrisochoides, “Two-level locality-aware parallel Delaunay image-to-mesh conversion”, *Parallel Computing*, vol. 59. Elsevier BV, pp. 60–70, Nov. 2016. doi: 10.1016/j.parco.2016.01.007.  
  
X. Feng, J. Zhang, G. Gao, H. Liuand H. Wang, “Compressed sodalite-like MgH6 as a potential high-temperature superconductor”, *RSC Advances*, vol. 5, no. 73. Royal Society of Chemistry (RSC), pp. 59292–59296, 2015. doi: 10.1039/c5ra11459d.  
  
Y. Feng, “Chesapeake Bay nitrogen fluxes derived from a land‐estuarine ocean biogeochemical modeling system: Model description, evaluation, and nitrogen budgets”, *Journal of Geophysical Research: Biogeosciences*, vol. 120, no. 8. American Geophysical Union (AGU), pp. 1666–1695, Aug. 2015. doi: 10.1002/2015jg002931.  
  
C. Fernandes-Cerqueira, “Concerted Action of ANP and Dopamine D1-Receptor to Regulate Sodium Homeostasis in Nephrotic Syndrome”, *BioMed Research International*, vol. 2013. Hindawi Limited, pp. 1–8, 2013. doi: 10.1155/2013/397391.  
  
F. Ferraccioli, C. A. Finn, T. A. Jordan, R. E. Bell, L. M. Andersonand D. Damaske, “East Antarctic rifting triggers uplift of the Gamburtsev Mountains”, *Nature*, vol. 479, no. 7373. Springer Science and Business Media LLC, pp. 388–392, Nov. 2011. doi: 10.1038/nature10566.  
  
S. P. Ficklin, “Tripal: a construction toolkit for online genome databases”, *Database*, vol. 2011, no. 0. Oxford University Press (OUP), pp. bar044–bar044, Sep. 29, 2011. doi: 10.1093/database/bar044.  
  
S. W. Finefrock, “Measurement of Thermal Conductivity of PbTe Nanocrystal Coated Glass Fibers by the 3ω Method”, *Nano Letters*, vol. 13, no. 11. American Chemical Society (ACS), pp. 5006–5012, Oct. 28, 2013. doi: 10.1021/nl400558u.  
  
M. T. M. Finn, C. L. Smithand M. R. Nash, “Open-Ended Measurement of Whole-Body Movement: A Feasibility Study”, *The Quantitative Methods for Psychology*, vol. 14, no. 1. The Quantitative Methods for Psychology, pp. 38–54, Feb. 01, 2018. doi: 10.20982/tqmp.14.1.p038.  
  
G. Fisher, C. M. Thomson, R. Stroek, C. M. Czekster, J. S. Hirschiand R. G. da Silva, “Allosteric Activation Shifts the Rate-Limiting Step in a Short-Form ATP Phosphoribosyltransferase”, *Biochemistry*, vol. 57, no. 29. American Chemical Society (ACS), pp. 4357–4367, Jun. 25, 2018. doi: 10.1021/acs.biochem.8b00559.  
  
F. FITMAWATI, R. FAUZIAH, I. HAYATI, N. SOFIYANTI, E. INOUEand D. D. MATRA, “Phylogenetic analysis of Mangifera from central region of Sumatra using trnL-F intergenic spacer”, *Biodiversitas Journal of Biological Diversity*, vol. 18, no. 3. UNS Solo, pp. 1035–1040, Jul. 12, 2017. doi: 10.13057/biodiv/d180322.  
  
J. C. Flores-Canales, M. Vargas-Uribe, A. S. Ladokhinand M. Kurnikova, “Membrane Association of the Diphtheria Toxin Translocation Domain Studied by Coarse-Grained Simulations and Experiment”, *The Journal of Membrane Biology*, vol. 248, no. 3. Springer Science and Business Media LLC, pp. 529–543, Feb. 04, 2015. doi: 10.1007/s00232-015-9771-3.  
  
L. Forer, “Cloudflow - enabling faster biomedical pipelines with MapReduce and Spark”, *Scalable Computing: Practice and Experience*, vol. 17, no. 2. Scalable Computing: Practice and Experience, May 01, 2016. doi: 10.12694/scpe.v17i2.1159.  
  
D. A. Fox, P. Larsson, R. H. Lo, B. M. Kroncke, P. M. Kassonand L. Columbus, “Structure of the Neisserial Outer Membrane Protein Opa60: Loop Flexibility Essential to Receptor Recognition and Bacterial Engulfment”, *Journal of the American Chemical Society*, vol. 136, no. 28. American Chemical Society (ACS), pp. 9938–9946, May 19, 2014. doi: 10.1021/ja503093y.  
  
D. K. Francis, J. L. Bouvard, Y. Hammiand M. F. Horstemeyer, “Formulation of a damage internal state variable model for amorphous glassy polymers”, *International Journal of Solids and Structures*, vol. 51, no. 15–16. Elsevier BV, pp. 2765–2776, Aug. 2014. doi: 10.1016/j.ijsolstr.2014.03.025.  
  
W. R. Francis, L. M. Christianson, R. Kiko, M. L. Powers, N. C. Shanerand S. H. D Haddock, “A comparison across non-model animals suggests an optimal sequencing depth for de novo transcriptome assembly”, *BMC Genomics*, vol. 14, no. 1. Springer Science and Business Media LLC, p. 167, 2013. doi: 10.1186/1471-2164-14-167.  
  
K. A. Frazer, “Decoding the human genome”, *Genome Research*, vol. 22, no. 9. Cold Spring Harbor Laboratory, pp. 1599–1601, Sep. 2012. doi: 10.1101/gr.146175.112.  
  
N. Freas, P. Newtonand J. Perozich, “Analysis of nucleotide diphosphate sugar dehydrogenases reveals family and group‐specific relationships”, *FEBS Open Bio*, vol. 6, no. 1. Wiley, pp. 77–89, Jan. 2016. doi: 10.1002/2211-5463.12022.  
  
P. Fretwell, “Bedmap2: improved ice bed, surface and thickness datasets for Antarctica”, *[]*. Copernicus GmbH, Oct. 11, 2012. doi: 10.5194/tcd-6-4305-2012.  
  
C. Fu, B. M. Wong, K. N. Bozhilovand J. Guo, “Solid state lithiation–delithiation of sulphur in sub-nano confinement: a new concept for designing lithium–sulphur batteries”, *Chemical Science*, vol. 7, no. 2. Royal Society of Chemistry (RSC), pp. 1224–1232, 2016. doi: 10.1039/c5sc03419a.  
  
I. Fuentes-Calvo, A. M. Blázquez-Medela, N. Eleno, E. Santos, J. M. López-Novoaand C. Martínez-Salgado, “H-Ras isoform modulates extracellular matrix synthesis, proliferation, and migration in fibroblasts”, *American Journal of Physiology-Cell Physiology*, vol. 302, no. 4. American Physiological Society, pp. C686–C697, Feb. 15, 2012. doi: 10.1152/ajpcell.00103.2011.  
  
I. Fuentes-Calvo, A. M. Blázquez-Medela, E. Santos, J. M. López-Novoaand C. Martínez-Salgado, “Analysis of K-Ras Nuclear Expression in Fibroblasts and Mesangial Cells”, *PLoS ONE*, vol. 5, no. 1. Public Library of Science (PLoS), p. e8703, Jan. 14, 2010. doi: 10.1371/journal.pone.0008703.  
  
A. Furmanchuk, O. Isayev, T. C. Dinadayalaneand J. Leszczynski, “Car–Parrinello Molecular Dynamics Simulations of Tensile Tests on Si⟨001⟩ Nanowires”, *The Journal of Physical Chemistry C*, vol. 115, no. 25. American Chemical Society (ACS), pp. 12283–12292, Jun. 07, 2011. doi: 10.1021/jp201948g.  
  
F. Furtado, “Chemical Composition and Bioactivity of Essential Oil from Blepharocalyx salicifolius”, *International Journal of Molecular Sciences*, vol. 19, no. 1. MDPI AG, p. 33, Jan. 04, 2018. doi: 10.3390/ijms19010033.  
  
C. S. Gaines, T. J. Gieseand D. M. York, “Cleaning Up Mechanistic Debris Generated by Twister Ribozymes Using Computational RNA Enzymology”, *ACS Catalysis*, vol. 9, no. 7. American Chemical Society (ACS), pp. 5803–5815, May 22, 2019. doi: 10.1021/acscatal.9b01155.  
  
K. S. Gajula, “High-throughput mutagenesis reveals functional determinants for DNA targeting by activation-induced deaminase”, *Nucleic Acids Research*, vol. 42, no. 15. Oxford University Press (OUP), pp. 9964–9975, Jul. 26, 2014. doi: 10.1093/nar/gku689.  
  
B. D. Galloway, E. Sasmazand B. Padak, “Binding of SO3 to fly ash components: CaO, MgO, Na2O and K2O”, *Fuel*, vol. 145. Elsevier BV, pp. 79–83, Apr. 2015. doi: 10.1016/j.fuel.2014.12.046.  
  
G. Gao, R. Hoffmann, N. W. Ashcroft, H. Liu, A. Bergaraand Y. Ma, “Theoretical study of the ground-state structures and properties of niobium hydrides under pressure”, *Physical Review B*, vol. 88, no. 18. American Physical Society (APS), Nov. 12, 2013. doi: 10.1103/physrevb.88.184104.  
  
Y. Gao, Y. Zhangand B. Xu, “Confined Water-Assistant Thermal Response of a Graphene Oxide Heterostructure and Its Enabled Mechanical Sensors for Load Sensing and Mode Differentiation”, *ACS Applied Materials & Interfaces*, vol. 11, no. 21. American Chemical Society (ACS), pp. 19596–19604, May 06, 2019. doi: 10.1021/acsami.9b02629.  
  
H. Garcia Garces, R. T. Cordeiroand E. Bagagli, “PRP8 intein in dermatophytes: Evolution and species identification”, *Medical Mycology*, vol. 56, no. 6. Oxford University Press (OUP), pp. 746–758, Dec. 08, 2017. doi: 10.1093/mmy/myx102.  
  
H. Garcia Garces, “Molecular identification and phylogenetical analysis of dermatophyte fungi from Latin America”, *Mycoses*, vol. 59, no. 12. Wiley, pp. 787–797, Jul. 19, 2016. doi: 10.1111/myc.12532.  
  
R. García-Rodríguez and H. Liu, “Mechanistic Study of the Synthesis of CdSe Nanocrystals: Release of Selenium”, *Journal of the American Chemical Society*, vol. 134, no. 3. American Chemical Society (ACS), pp. 1400–1403, Jan. 12, 2012. doi: 10.1021/ja209246z.  
  
S. García, L. Zhang, G. W. Piburn, G. Henkelmanand S. M. Humphrey, “Microwave Synthesis of Classically Immiscible Rhodium–Silver and Rhodium–Gold Alloy Nanoparticles: Highly Active Hydrogenation Catalysts”, *ACS Nano*, vol. 8, no. 11. American Chemical Society (ACS), pp. 11512–11521, Nov. 10, 2014. doi: 10.1021/nn504746u.  
  
R. N. Garner, J. C. Gallucci, K. R. Dunbarand C. Turro, “[Ru(bpy)2(5-cyanouracil)2]2+ as a Potential Light-Activated Dual-Action Therapeutic Agent”, *Inorganic Chemistry*, vol. 50, no. 19. American Chemical Society (ACS), pp. 9213–9215, Aug. 31, 2011. doi: 10.1021/ic201615u.  
  
R. N. Garner, L. E. Joyceand C. Turro, “Effect of Electronic Structure on the Photoinduced Ligand Exchange of Ru(II) Polypyridine Complexes”, *Inorganic Chemistry*, vol. 50, no. 10. American Chemical Society (ACS), pp. 4384–4391, Apr. 19, 2011. doi: 10.1021/ic102482c.  
  
S. Garrison-Kimmel, M. Boylan-Kolchin, J. S. Bullockand E. N. Kirby, “Too big to fail in the Local Group”, *Monthly Notices of the Royal Astronomical Society*, vol. 444, no. 1. Oxford University Press (OUP), pp. 222–236, Aug. 13, 2014. doi: 10.1093/mnras/stu1477.  
  
S. Garrison-Kimmel, M. Boylan-Kolchin, J. S. Bullockand K. Lee, “ELVIS: Exploring the Local Volume in Simulations”, *Monthly Notices of the Royal Astronomical Society*, vol. 438, no. 3. Oxford University Press (OUP), pp. 2578–2596, Jan. 14, 2014. doi: 10.1093/mnras/stt2377.  
  
T. E. Gartner III, T. H. Epps IIIand A. Jayaraman, “Leveraging Gibbs Ensemble Molecular Dynamics and Hybrid Monte Carlo/Molecular Dynamics for Efficient Study of Phase Equilibria”, *Journal of Chemical Theory and Computation*, vol. 12, no. 11. American Chemical Society (ACS), pp. 5501–5510, Oct. 21, 2016. doi: 10.1021/acs.jctc.6b00575.  
  
M. Gaspari, M. Ruszkowskiand S. P. Oh, “Chaotic cold accretion on to black holes”, *Monthly Notices of the Royal Astronomical Society*, vol. 432, no. 4. Oxford University Press (OUP), pp. 3401–3422, May 17, 2013. doi: 10.1093/mnras/stt692.  
  
A. Gautieri, M. I. Pate, S. Vesentini, A. Redaelliand M. J. Buehler, “Hydration and distance dependence of intermolecular shearing between collagen molecules in a model microfibril”, *Journal of Biomechanics*, vol. 45, no. 12. Elsevier BV, pp. 2079–2083, Aug. 2012. doi: 10.1016/j.jbiomech.2012.05.047.  
  
A. Gautieri, S. Vesentini, A. Redaelliand M. J. Buehler, “Hierarchical Structure and Nanomechanics of Collagen Microfibrils from the Atomistic Scale Up”, *Nano Letters*, vol. 11, no. 2. American Chemical Society (ACS), pp. 757–766, Feb. 09, 2011. doi: 10.1021/nl103943u.  
  
B. Geng, Q. Xue, X. Zheng, G. Liu, Y. Renand H. Dong, “The effect of wing flexibility on sound generation of flapping wings”, *Bioinspiration & Biomimetics*, vol. 13, no. 1. IOP Publishing, p. 016010, Dec. 13, 2017. doi: 10.1088/1748-3190/aa8447.  
  
C. D. Gheewala, J. S. Hirschi, W.-H. Lee, D. W. Paley, M. J. Vetticattand T. H. Lambert, “Asymmetric Induction via a Helically Chiral Anion: Enantioselective Pentacarboxycyclopentadiene Brønsted Acid-Catalyzed Inverse-Electron-Demand Diels–Alder Cycloaddition of Oxocarbenium Ions”, *Journal of the American Chemical Society*, vol. 140, no. 10. American Chemical Society (ACS), pp. 3523–3527, Feb. 27, 2018. doi: 10.1021/jacs.8b00260.  
  
T. Giesa, G. Bratzeland M. J. Buehler, “Modeling and Simulation of Hierarchical Protein Materials”, *Nano and Cell Mechanics*. John Wiley & Sons, Ltd, pp. 389–409, Dec. 11, 2012. doi: 10.1002/9781118482568.ch15.  
  
T. Giesa and M. J. Buehler, “Nanoconfinement and the Strength of Biopolymers”, *Annual Review of Biophysics*, vol. 42, no. 1. Annual Reviews, pp. 651–673, May 06, 2013. doi: 10.1146/annurev-biophys-083012-130345.  
  
T. Giesa, N. M. Pugno, J. Y. Wong, D. L. Kaplanand M. J. Buehler, “What’s Inside the Box? - Length-Scales that Govern Fracture Processes of Polymer Fibers”, *Advanced Materials*, vol. 26, no. 3. Wiley, pp. 412–417, Nov. 11, 2013. doi: 10.1002/adma.201303323.  
  
S. A. Goff, “The iPlant Collaborative: Cyberinfrastructure for Plant Biology”, *Frontiers in Plant Science*, vol. 2. Frontiers Media SA, 2011. doi: 10.3389/fpls.2011.00034.  
  
R. Golovchak, “Medium range order and structural relaxation in As–Se network glasses through FSDP analysis”, *Materials Chemistry and Physics*, vol. 153. Elsevier BV, pp. 432–442, Mar. 2015. doi: 10.1016/j.matchemphys.2015.01.037.  
  
M. A. Gómez-Marcos, A. M. Blázquez-Medela, L. Gamella-Pozuelo, J. I. Recio-Rodriguez, L. García-Ortizand C. Martínez-Salgado, “Serum Superoxide Dismutase Is Associated with Vascular Structure and Function in Hypertensive and Diabetic Patients”, *Oxidative Medicine and Cellular Longevity*, vol. 2016. Hindawi Limited, pp. 1–8, 2016. doi: 10.1155/2016/9124676.  
  
T. Goto, “Magnetism and Faraday Rotation in Oxygen-Deficient Polycrystalline and Single-Crystal Iron-Substituted Strontium Titanate”, *Physical Review Applied*, vol. 7, no. 2. American Physical Society (APS), Feb. 08, 2017. doi: 10.1103/physrevapplied.7.024006.  
  
C.-H. Gow, C. Guo, D. Wang, Q. Huand J. Zhang, “Differential involvement of E2A-corepressor interactions in distinct leukemogenic pathways”, *Nucleic Acids Research*, vol. 42, no. 1. Oxford University Press (OUP), pp. 137–152, Sep. 21, 2013. doi: 10.1093/nar/gkt855.  
  
L. Grabill and A. Riemann, “Conformational Impact on Amino Acid-Surface π–π Interactions on a (7,7) Single-Walled Carbon Nanotube: A Molecular Mechanics Approach”, *The Journal of Physical Chemistry A*, vol. 122, no. 6. American Chemical Society (ACS), pp. 1713–1726, Feb. 01, 2018. doi: 10.1021/acs.jpca.7b11716.  
  
F. Gravina, “Role of mitochondria in contraction and pacemaking in the mouse uterus”, *British Journal of Pharmacology*, vol. 161, no. 6. Wiley, pp. 1375–1390, Jul. 07, 2010. doi: 10.1111/j.1476-5381.2010.00949.x.  
  
T. R. Greve, “SUBMILLIMETER OBSERVATIONS OF MILLIMETER BRIGHT GALAXIES DISCOVERED BY THE SOUTH POLE TELESCOPE”, *The Astrophysical Journal*, vol. 756, no. 1. American Astronomical Society, p. 101, Aug. 20, 2012. doi: 10.1088/0004-637x/756/1/101.  
  
G. Gronau, “A review of combined experimental and computational procedures for assessing biopolymer structure–process–property relationships”, *Biomaterials*, vol. 33, no. 33. Elsevier BV, pp. 8240–8255, Nov. 2012. doi: 10.1016/j.biomaterials.2012.06.054.  
  
B. Gullberg, “The nature of the [C ii] emission in dusty star-forming galaxies from the SPT survey”, *Monthly Notices of the Royal Astronomical Society*, vol. 449, no. 3. Oxford University Press (OUP), pp. 2883–2900, Apr. 03, 2015. doi: 10.1093/mnras/stv372.  
  
C. Guo, C.-H. Gow, Y. Li, A. Gardner, S. Khanand J. Zhang, “Regulated Clearance of Histone Deacetylase 3 Protects Independent Formation of Nuclear Receptor Corepressor Complexes”, *Journal of Biological Chemistry*, vol. 287, no. 15. Elsevier BV, pp. 12111–12120, Apr. 2012. doi: 10.1074/jbc.m111.327023.  
  
C. Guo, “The Optimal Corepressor Function of Nuclear Receptor Corepressor (NCoR) for Peroxisome Proliferator-activated Receptor γ Requires G Protein Pathway Suppressor 2”, *Journal of Biological Chemistry*, vol. 290, no. 6. Elsevier BV, pp. 3666–3679, Feb. 2015. doi: 10.1074/jbc.m114.598797.  
  
S. A. Guralp, I. H. Gubbuk, S. Kucukkolbasiand E. Gulari, “Universal cell capture by immobilized antimicrobial peptide plantaricin”, *Biochemical Engineering Journal*, vol. 101. Elsevier BV, pp. 18–22, Sep. 2015. doi: 10.1016/j.bej.2015.04.018.  
  
S. A. Guralp, Y. E. Murgha, J.-M. Rouillardand E. Gulari, “From Design to Screening: A New Antimicrobial Peptide Discovery Pipeline”, *PLoS ONE*, vol. 8, no. 3. Public Library of Science (PLoS), p. e59305, Mar. 19, 2013. doi: 10.1371/journal.pone.0059305.  
  
A. E. Gururaj, “Access to the Nucleus and Functional Association with c-Myc Is Required for the Full Oncogenic Potential of ΔEGFR/EGFRvIII”, *Journal of Biological Chemistry*, vol. 288, no. 5. Elsevier BV, pp. 3428–3438, Feb. 2013. doi: 10.1074/jbc.m112.399352.  
  
X.-K. Gu and E. Nikolla, “Fundamental Insights into High-Temperature Water Electrolysis Using Ni-Based Electrocatalysts”, *The Journal of Physical Chemistry C*, vol. 119, no. 48. American Chemical Society (ACS), pp. 26980–26988, Nov. 18, 2015. doi: 10.1021/acs.jpcc.5b07814.  
  
B. Hanson, V. Pryamitsynand V. Ganesan, “Mechanisms Underlying Ionic Mobilities in Nanocomposite Polymer Electrolytes”, *ACS Macro Letters*, vol. 2, no. 11. American Chemical Society (ACS), pp. 1001–1005, Oct. 24, 2013. doi: 10.1021/mz400234m.  
  
A. Harbuzariu, “Modelling heme-mediated brain injury associated with cerebral malaria in human brain cortical organoids”, *Scientific Reports*, vol. 9, no. 1. Springer Science and Business Media LLC, Dec. 16, 2019. doi: 10.1038/s41598-019-55631-8.  
  
O. Harismendy, “Population sequencing of two endocannabinoid metabolic genes identifies rare and common regulatory variants associated with extreme obesity and metabolite level”, *Genome Biology*, vol. 11, no. 11. Springer Science and Business Media LLC, p. R118, 2010. doi: 10.1186/gb-2010-11-11-r118.  
  
O. Harismendy, “9p21 DNA variants associated with coronary artery disease impair interferon-γ signalling response”, *Nature*, vol. 470, no. 7333. Springer Science and Business Media LLC, pp. 264–268, Feb. 2011. doi: 10.1038/nature09753.  
  
O. Harismendy, “Evaluation of ultra-deep targeted sequencing for personalized breast cancer care”, *Breast Cancer Research*, vol. 15, no. 6. Springer Science and Business Media LLC, Dec. 2013. doi: 10.1186/bcr3584.  
  
O. Harismendy, “Detection of low prevalence somatic mutations in solid tumors with ultra-deep targeted sequencing”, *Genome Biology*, vol. 12, no. 12. Springer Science and Business Media LLC, p. R124, 2011. doi: 10.1186/gb-2011-12-12-r124.  
  
R. M. Harris, H. Kao, J. M. Alarcon, H. A. Hofmannand A. A. Fenton, “Hippocampal transcriptomic responses to enzyme‐mediated cellular dissociation”, *Hippocampus*, vol. 29, no. 9. Wiley, pp. 876–882, May 14, 2019. doi: 10.1002/hipo.23095.  
  
J. D. Hartman, S. Monaco, B. Schatschneiderand G. J. O. Beran, “Fragment-based 13C nuclear magnetic resonance chemical shift predictions in molecular crystals: An alternative to planewave methods”, *The Journal of Chemical Physics*, vol. 143, no. 10. AIP Publishing, p. 102809, Sep. 14, 2015. doi: 10.1063/1.4922649.  
  
J. D. Hartman, T. J. Neubauer, B. G. Caulkins, L. J. Muellerand G. J. O. Beran, “Converging nuclear magnetic shielding calculations with respect to basis and system size in protein systems”, *Journal of Biomolecular NMR*, vol. 62, no. 3. Springer Science and Business Media LLC, pp. 327–340, May 21, 2015. doi: 10.1007/s10858-015-9947-2.  
  
S. C. Harvey, “The scrunchworm hypothesis: Transitions between A-DNA and B-DNA provide the driving force for genome packaging in double-stranded DNA bacteriophages”, *Journal of Structural Biology*, vol. 189, no. 1. Elsevier BV, pp. 1–8, Jan. 2015. doi: 10.1016/j.jsb.2014.11.012.  
  
M. Hasan, İ. E. Büyüktahtakınand E. Elamin, “A multi-criteria ranking algorithm (MCRA) for determining breast cancer therapy”, *Omega*, vol. 82. Elsevier BV, pp. 83–101, Jan. 2019. doi: 10.1016/j.omega.2017.12.005.  
  
J. J. Hasbestan and I. Senocak, “A short note on the use of the red–black tree in Cartesian adaptive mesh refinement algorithms”, *Journal of Computational Physics*, vol. 351. Elsevier BV, pp. 473–477, Dec. 2017. doi: 10.1016/j.jcp.2017.09.056.  
  
S. Haschke, “Direct oxygen isotope effect identifies the rate-determining step of electrocatalytic OER at an oxidic surface”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Nov. 01, 2018. doi: 10.1038/s41467-018-07031-1.  
  
S. Haseen and P. Kroll, “Paving the way for cristobalite TiO2 and GeO2 attainable under moderate tensile stress: A DFT study of transformation paths and activation barriers in cristobalite-rutile transformations of MO2 (M = Si, Ge, Ti)”, *Computational Materials Science*, vol. 170. Elsevier BV, p. 109170, Dec. 2019. doi: 10.1016/j.commatsci.2019.109170.  
  
N. Hayashi, “Reverse-Phase Protein Array for Prediction of Patients at Low Risk of Developing Bone Metastasis From Breast Cancer”, *The Oncologist*, vol. 19, no. 9. Oxford University Press (OUP), pp. 909–914, Aug. 12, 2014. doi: 10.1634/theoncologist.2014-0099.  
  
G. J. Herschlag, S. Mitranand G. Lin, “A consistent hierarchy of generalized kinetic equation approximations to the master equation applied to surface catalysis”, *The Journal of Chemical Physics*, vol. 142, no. 23. AIP Publishing, p. 234703, Jun. 21, 2015. doi: 10.1063/1.4922515.  
  
X. He, M. A. H. Samee, C. Blattiand S. Sinha, “Thermodynamics-Based Models of Transcriptional Regulation by Enhancers: The Roles of Synergistic Activation, Cooperative Binding and Short-Range Repression”, *PLoS Computational Biology*, vol. 6, no. 9. Public Library of Science (PLoS), p. e1000935, Sep. 16, 2010. doi: 10.1371/journal.pcbi.1000935.  
  
Y. D. Hezaveh, “PROSPECTS FOR MEASURING THE MASS OF BLACK HOLES AT HIGH REDSHIFTS WITH RESOLVED KINEMATICS USING GRAVITATIONAL LENSING”, *The Astrophysical Journal*, vol. 791, no. 2. American Astronomical Society, p. L41, Aug. 08, 2014. doi: 10.1088/2041-8205/791/2/l41.  
  
Y. D. Hezaveh, “DETECTION OF LENSING SUBSTRUCTURE USING ALMA OBSERVATIONS OF THE DUSTY GALAXY SDP.81”, *The Astrophysical Journal*, vol. 823, no. 1. American Astronomical Society, p. 37, May 19, 2016. doi: 10.3847/0004-637x/823/1/37.  
  
Y. D. Hezaveh and G. P. Holder, “EFFECTS OF STRONG GRAVITATIONAL LENSING ON MILLIMETER-WAVE GALAXY NUMBER COUNTS”, *The Astrophysical Journal*, vol. 734, no. 1. American Astronomical Society, p. 52, May 24, 2011. doi: 10.1088/0004-637x/734/1/52.  
  
Y. D. Hezaveh, “ALMA OBSERVATIONS OF SPT-DISCOVERED, STRONGLY LENSED, DUSTY, STAR-FORMING GALAXIES”, *The Astrophysical Journal*, vol. 767, no. 2. American Astronomical Society, p. 132, Apr. 04, 2013. doi: 10.1088/0004-637x/767/2/132.  
  
Y. D. Hezaveh, D. P. Marroneand G. P. Holder, “SIZE BIAS AND DIFFERENTIAL LENSING OF STRONGLY LENSED, DUSTY GALAXIES IDENTIFIED IN WIDE-FIELD SURVEYS”, *The Astrophysical Journal*, vol. 761, no. 1. American Astronomical Society, p. 20, Nov. 20, 2012. doi: 10.1088/0004-637x/761/1/20.  
  
Y. D. Hezaveh, P. J. Marshalland R. D. Blandford, “PROBING THE INNER KILOPARSEC OF MASSIVE GALAXIES WITH STRONG GRAVITATIONAL LENSING”, *The Astrophysical Journal*, vol. 799, no. 2. American Astronomical Society, p. L22, Jan. 27, 2015. doi: 10.1088/2041-8205/799/2/l22.  
  
Y. Hezaveh, K. Vanderlinde, G. Holderand T. de Haan, “LENSING NOISE IN MILLIMETER-WAVE GALAXY CLUSTER SURVEYS”, *The Astrophysical Journal*, vol. 772, no. 2. American Astronomical Society, p. 121, Jul. 15, 2013. doi: 10.1088/0004-637x/772/2/121.  
  
J. C. Hill and A. Condron, “Subtropical iceberg scours and meltwater routing in the deglacial western North Atlantic”, *Nature Geoscience*, vol. 7, no. 11. Springer Science and Business Media LLC, pp. 806–810, Oct. 12, 2014. doi: 10.1038/ngeo2267.  
  
A. Ho, J. McCleanand S. P. Ong, “The Promise and Challenges of Quantum Computing for Energy Storage”, *Joule*, vol. 2, no. 5. Elsevier BV, pp. 810–813, May 2018. doi: 10.1016/j.joule.2018.04.021.  
  
E. C. Hodkinson, “Heritability of ECG Biomarkers in the Netherlands Twin Registry Measured from Holter ECGs”, *Frontiers in Physiology*, vol. 7. Frontiers Media SA, Apr. 29, 2016. doi: 10.3389/fphys.2016.00154.  
  
M. Holzmann, R. C. Clay, M. A. Morales, N. M. Tubman, D. M. Ceperleyand C. Pierleoni, “Theory of finite size effects for electronic quantum Monte Carlo calculations of liquids and solids”, *Physical Review B*, vol. 94, no. 3. American Physical Society (APS), Jul. 12, 2016. doi: 10.1103/physrevb.94.035126.  
  
N. Horst and A. Travesset, “Prediction of binary nanoparticle superlattices from soft potentials”, *The Journal of Chemical Physics*, vol. 144, no. 1. AIP Publishing, p. 014502, Jan. 07, 2016. doi: 10.1063/1.4939238.  
  
D. Hossain, M. A. Tschopp, D. K. Ward, J. L. Bouvard, P. Wangand M. F. Horstemeyer, “Molecular dynamics simulations of deformation mechanisms of amorphous polyethylene”, *Polymer*, vol. 51, no. 25. Elsevier BV, pp. 6071–6083, Nov. 2010. doi: 10.1016/j.polymer.2010.10.009.  
  
M. F. Hrycyk, H. Garcia Garces, S. de M. G. Bosco, S. L. de Oliveira, S. A. Marquesand E. Bagagli, “Ecology of Paracoccidioides brasiliensis, P. lutzii and related species: infection in armadillos, soil occurrence and mycological aspects”, *Medical Mycology*. Oxford University Press (OUP), Jan. 06, 2018. doi: 10.1093/mmy/myx142.  
  
M.-X. Huang, “MEG source imaging method using fast L1 minimum-norm and its applications to signals with brain noise and human resting-state source amplitude images”, *NeuroImage*, vol. 84. Elsevier BV, pp. 585–604, Jan. 2014. doi: 10.1016/j.neuroimage.2013.09.022.  
  
W. Huang, “Multidomain architecture of estrogen receptor reveals interfacial cross-talk between its DNA-binding and ligand-binding domains”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Aug. 30, 2018. doi: 10.1038/s41467-018-06034-2.  
  
Y. Huang, Y. Chen, T. Cheng, L.-W. Wangand W. A. Goddard III, “Identification of the Selective Sites for Electrochemical Reduction of CO to C2+ Products on Copper Nanoparticles by Combining Reactive Force Fields, Density Functional Theory, and Machine Learning”, *ACS Energy Letters*, vol. 3, no. 12. American Chemical Society (ACS), pp. 2983–2988, Nov. 08, 2018. doi: 10.1021/acsenergylett.8b01933.  
  
J. A. Hummel, A. Stacy, M. Jeon, A. Oliveriand V. Bromm, “The first stars: formation under X-ray feedback”, *Monthly Notices of the Royal Astronomical Society*, vol. 453, no. 4. Oxford University Press (OUP), pp. 4137–4148, Sep. 15, 2015. doi: 10.1093/mnras/stv1902.  
  
D. R. Hummer, J. D. Kubicki, P. R. C. Kentand P. J. Heaney, “Single-Site and Monolayer Surface Hydration Energy of Anatase and Rutile Nanoparticles Using Density Functional Theory”, *The Journal of Physical Chemistry C*, vol. 117, no. 49. American Chemical Society (ACS), pp. 26084–26090, Nov. 27, 2013. doi: 10.1021/jp408345v.  
  
F. Hussain, R. G. Dutta, S. K. Jha, C. J. Langmeadand S. Jha, “Parameter discovery for stochastic biological models against temporal behavioral specifications using an SPRT based Metric for simulated annealing”, *2012 IEEE 2nd International Conference on Computational Advances in Bio and medical Sciences (ICCABS)*. IEEE, Feb. 2012. doi: 10.1109/iccabs.2012.6182640.  
  
F. Hussain, C. J. Langmead, Q. Mi, J. Dutta-Moscato, Y. Vodovotzand S. K. Jha, “Parameter discovery for stochastic computational models in systems biology using Bayesian model checking”, *2014 IEEE 4th International Conference on Computational Advances in Bio and Medical Sciences (ICCABS)*. IEEE, Jun. 2014. doi: 10.1109/iccabs.2014.6863925.  
  
M. I. Hussein and H. Honarvar, “Resonant Thermal Transport in Nanophononic Metamaterials”, *Handbook of Materials Modeling*. Springer International Publishing, pp. 1–21, 2018. doi: 10.1007/978-3-319-50257-1\_17-1.  
  
S. Hu, “CD30 expression defines a novel subgroup of diffuse large B-cell lymphoma with favorable prognosis and distinct gene expression signature: a report from the International DLBCL Rituximab-CHOP Consortium Program Study”, *Blood*, vol. 121, no. 14. American Society of Hematology, pp. 2715–2724, Apr. 04, 2013. doi: 10.1182/blood-2012-10-461848.  
  
J. A. Ice, “Genetics of Sjögren’s syndrome in the genome-wide association era”, *Journal of Autoimmunity*, vol. 39, no. 1–2. Elsevier BV, pp. 57–63, Aug. 2012. doi: 10.1016/j.jaut.2012.01.008.  
  
J. C. M. Ierich, “A Computational Protein Structure Refinement of the Yeast Acetohydroxyacid Synthase”, *Journal of the Brazilian Chemical Society*. Sociedade Brasileira de Quimica (SBQ), 2015. doi: 10.5935/0103-5053.20150144.  
  
H. Ilatikhameneh, Y. Tan, B. Novakovic, G. Klimeck, R. Rahmanand J. Appenzeller, “Tunnel Field-Effect Transistors in 2-D Transition Metal Dichalcogenide Materials”, *IEEE Journal on Exploratory Solid-State Computational Devices and Circuits*, vol. 1. Institute of Electrical and Electronics Engineers (IEEE), pp. 12–18, Dec. 2015. doi: 10.1109/jxcdc.2015.2423096.  
  
N. V. Ilawe, J. A. Zimmermanand B. M. Wong, “Breaking Badly: DFT-D2 Gives Sizeable Errors for Tensile Strengths in Palladium-Hydride Solids”, *Journal of Chemical Theory and Computation*, vol. 11, no. 11. American Chemical Society (ACS), pp. 5426–5435, Oct. 13, 2015. doi: 10.1021/acs.jctc.5b00653.  
  
M. S. Imtiaz, “Calcium Oscillations and Pacemaking”, *Advances in Experimental Medicine and Biology*. Springer Netherlands, pp. 511–520, 2012. doi: 10.1007/978-94-007-2888-2\_22.  
  
M. S. Imtiaz, S. K. Mohammed, F. Deebaand K. A. Wahid, “Tri-Scan: A Three Stage Color Enhancement Tool for Endoscopic Images”, *Journal of Medical Systems*, vol. 41, no. 6. Springer Science and Business Media LLC, May 20, 2017. doi: 10.1007/s10916-017-0738-z.  
  
M. S. Imtiaz, P.-Y. von der Weid, D. R. Laverand D. F. van Helden, “SR Ca2+ store refill—a key factor in cardiac pacemaking”, *Journal of Molecular and Cellular Cardiology*, vol. 49, no. 3. Elsevier BV, pp. 412–426, Sep. 2010. doi: 10.1016/j.yjmcc.2010.03.015.  
  
M. S. Imtiaz and K. A. Wahid, “Image enhancement and space-variant color reproduction method for endoscopic images using adaptive sigmoid function”, *2014 36th Annual International Conference of the IEEE Engineering in Medicine and Biology Society*. IEEE, Aug. 2014. doi: 10.1109/embc.2014.6944477.  
  
M. S. Imtiaz and K. A. Wahid, “Color Enhancement in Endoscopic Images Using Adaptive Sigmoid Function and Space Variant Color Reproduction”, *Computational and Mathematical Methods in Medicine*, vol. 2015. Hindawi Limited, pp. 1–19, 2015. doi: 10.1155/2015/607407.  
  
J. Irvin, A. J. Ropelewskiand J. Perozich, “*In silico* analysis of heme oxygenase structural homologues identifies group‐specific conservations”, *FEBS Open Bio*, vol. 7, no. 10. Wiley, pp. 1480–1498, Sep. 04, 2017. doi: 10.1002/2211-5463.12275.  
  
R. Iyyamperumal, L. Zhang, G. Henkelmanand R. M. Crooks, “Efficient Electrocatalytic Oxidation of Formic Acid Using Au@Pt Dendrimer-Encapsulated Nanoparticles”, *Journal of the American Chemical Society*, vol. 135, no. 15. American Chemical Society (ACS), pp. 5521–5524, Apr. 08, 2013. doi: 10.1021/ja4010305.  
  
S. Siebert, “Differential Gene Expression in the Siphonophore Nanomia bijuga (Cnidaria) Assessed with Multiple Next-Generation Sequencing Workflows”, *PLoS ONE*, vol. 6, no. 7. Public Library of Science (PLoS), p. e22953, Jul. 29, 2011. doi: 10.1371/journal.pone.0022953.  
  
C. Jain, L. M. Rodriguez-R, A. M. Phillippy, K. T. Konstantinidisand S. Aluru, “High throughput ANI analysis of 90K prokaryotic genomes reveals clear species boundaries”, *Nature Communications*, vol. 9, no. 1. Springer Science and Business Media LLC, Nov. 30, 2018. doi: 10.1038/s41467-018-07641-9.  
  
N. Jena, Dimple, S. D. Behereand A. De Sarkar, “Strain-Induced Optimization of Nanoelectromechanical Energy Harvesting and Nanopiezotronic Response in a MoS2 Monolayer Nanosheet”, *The Journal of Physical Chemistry C*, vol. 121, no. 17. American Chemical Society (ACS), pp. 9181–9190, Apr. 19, 2017. doi: 10.1021/acs.jpcc.7b01970.  
  
E. M. Jennings, J. S. Morris, R. J. Carroll, G. C. Manyamand V. Baladandayuthapani, “Bayesian methods for expression-based integration of various types of genomics data”, *EURASIP Journal on Bioinformatics and Systems Biology*, vol. 2013, no. 1. Springer Science and Business Media LLC, Sep. 21, 2013. doi: 10.1186/1687-4153-2013-13.  
  
M. Jeon, V. Bromm, A. H. Pawlikand M. Milosavljević, “The first galaxies: simulating their feedback-regulated assembly”, *Monthly Notices of the Royal Astronomical Society*, vol. 452, no. 2. Oxford University Press (OUP), pp. 1152–1170, Jul. 14, 2015. doi: 10.1093/mnras/stv1353.  
  
M. Jeon, A. H. Pawlik, V. Brommand M. Milosavljević, “Recovery from Population III supernova explosions and the onset of second-generation star formation”, *Monthly Notices of the Royal Astronomical Society*, vol. 444, no. 4. Oxford University Press (OUP), pp. 3288–3300, Nov. 11, 2014. doi: 10.1093/mnras/stu1980.  
  
M. Jeon, A. H. Pawlik, V. Brommand M. Milosavljević, “Radiative feedback from high-mass X-ray binaries on the formation of the first galaxies and early reionization”, *Monthly Notices of the Royal Astronomical Society*, vol. 440, no. 4. Oxford University Press (OUP), pp. 3778–3796, Apr. 17, 2014. doi: 10.1093/mnras/stu444.  
  
M. Jeon, “THE FIRST GALAXIES: ASSEMBLY WITH BLACK HOLE FEEDBACK”, *The Astrophysical Journal*, vol. 754, no. 1. American Astronomical Society, p. 34, Jul. 03, 2012. doi: 10.1088/0004-637x/754/1/34.  
  
Z. Jiang, K. Klyukinand V. Alexandrov, “Ab Initio Metadynamics Study of the VO2+/VO2+ Redox Reaction Mechanism at the Graphite Edge/Water Interface”, *ACS Applied Materials & Interfaces*, vol. 10, no. 24. American Chemical Society (ACS), pp. 20621–20626, May 29, 2018. doi: 10.1021/acsami.8b05864.  
  
H. Ji and Y. Li, “Reusing Random Walks in Monte Carlo Methods for Linear Systems”, *Procedia Computer Science*, vol. 9. Elsevier BV, pp. 383–392, 2012. doi: 10.1016/j.procs.2012.04.041.  
  
H. Ji, M. Mascagniand Y. Li, “Convergence Analysis of Markov Chain Monte Carlo Linear Solvers Using Ulam–von Neumann Algorithm”, *SIAM Journal on Numerical Analysis*, vol. 51, no. 4. Society for Industrial & Applied Mathematics (SIAM), pp. 2107–2122, Jan. 2013. doi: 10.1137/130904867.  
  
G. Jindal, D. Mondaland A. Warshel, “Exploring the Drug Resistance of HCV Protease”, *The Journal of Physical Chemistry B*, vol. 121, no. 28. American Chemical Society (ACS), pp. 6831–6840, Jul. 05, 2017. doi: 10.1021/acs.jpcb.7b04562.  
  
G. Jindal, B. Ramachandran, R. P. Boraand A. Warshel, “Exploring the Development of Ground-State Destabilization and Transition-State Stabilization in Two Directed Evolution Paths of Kemp Eliminases”, *ACS Catalysis*, vol. 7, no. 5. American Chemical Society (ACS), pp. 3301–3305, Apr. 07, 2017. doi: 10.1021/acscatal.7b00171.  
  
G. Jindal and A. Warshel, “Misunderstanding the preorganization concept can lead to confusions about the origin of enzyme catalysis”, *Proteins: Structure, Function, and Bioinformatics*, vol. 85, no. 12. Wiley, pp. 2157–2161, Sep. 30, 2017. doi: 10.1002/prot.25381.  
  
M. Johnson, Y. Jung, D. T. Dawson IIand M. Xue, “Comparison of Simulated Polarimetric Signatures in Idealized Supercell Storms Using Two-Moment Bulk Microphysics Schemes in WRF”, *Monthly Weather Review*, vol. 144, no. 3. American Meteorological Society, pp. 971–996, Feb. 16, 2016. doi: 10.1175/mwr-d-15-0233.1.  
  
M. N. R. Johnson, C. H. Londerganand L. K. Charkoudian, “Probing the Phosphopantetheine Arm Conformations of Acyl Carrier Proteins Using Vibrational Spectroscopy”, *Journal of the American Chemical Society*, vol. 136, no. 32. American Chemical Society (ACS), pp. 11240–11243, Aug. 04, 2014. doi: 10.1021/ja505442h.  
  
C. S. Jones and P. Cessi, “Interbasin Transport of the Meridional Overturning Circulation”, *Journal of Physical Oceanography*, vol. 46, no. 4. American Meteorological Society, pp. 1157–1169, Apr. 2016. doi: 10.1175/jpo-d-15-0197.1.  
  
Y. Joo, “Effect of Dipolar Molecule Structure on the Mechanism of Graphene-Enhanced Raman Scattering”, *The Journal of Physical Chemistry C*, vol. 120, no. 25. American Chemical Society (ACS), pp. 13815–13824, Jun. 17, 2016. doi: 10.1021/acs.jpcc.6b04098.  
  
R. Jungmann, M. S. Avendaño, J. B. Woehrstein, M. Dai, W. M. Shihand P. Yin, “Multiplexed 3D cellular super-resolution imaging with DNA-PAINT and Exchange-PAINT”, *Nature Methods*, vol. 11, no. 3. Springer Science and Business Media LLC, pp. 313–318, Feb. 02, 2014. doi: 10.1038/nmeth.2835.  
  
M.-C. Jung, C.-J. Kang, B. I. Minand K.-W. Lee, “Electronic structures and phonon spectra in boronitride superconductors LaBN (, Pt)”, *Physical Review B*, vol. 87, no. 14. American Physical Society (APS), Apr. 18, 2013. doi: 10.1103/physrevb.87.144509.  
  
A. Kalinowski, “Interfacial binding and aggregation of lamin A tail domains associated with Hutchinson–Gilford progeria syndrome”, *Biophysical Chemistry*, vol. 195. Elsevier BV, pp. 43–48, Dec. 2014. doi: 10.1016/j.bpc.2014.08.005.  
  
C.-J. Kang, K.-H. Ahn, K.-W. Leeand B. Il Min, “Electron and Phonon Band-Structure Calculations for the Antipolar SrPt3P Antiperovskite Superconductor: Evidence of Low-Energy Two-Dimensional Phonons”, *Journal of the Physical Society of Japan*, vol. 82, no. 5. Physical Society of Japan, p. 053703, May 15, 2013. doi: 10.7566/jpsj.82.053703.  
  
C.-J. Kang, H. C. Choi, K. Kimand B. I. Min, “Topological Properties and the Dynamical Crossover from Mixed-Valence to Kondo-Lattice Behavior in the Golden Phase of SmS”, *Physical Review Letters*, vol. 114, no. 16. American Physical Society (APS), Apr. 22, 2015. doi: 10.1103/physrevlett.114.166404.  
  
C.-J. Kang, “Electronic Structure of: Is it a Topological Insulator or Not?”, *Physical Review Letters*, vol. 116, no. 11. American Physical Society (APS), Mar. 17, 2016. doi: 10.1103/physrevlett.116.116401.  
  
C.-J. Kang, J. Kim, K. Kim, J. Kang, J. D. Denlingerand B. I. Min, “Band Symmetries of Mixed-Valence Topological Insulator: SmB6”, *Journal of the Physical Society of Japan*, vol. 84, no. 2. Physical Society of Japan, p. 024722, Feb. 15, 2015. doi: 10.7566/jpsj.84.024722.  
  
C.-J. Kang, K. Kimand B. I. Min, “Phonon softening and superconductivity triggered by spin-orbit coupling in simple-cubic-polonium crystals”, *Physical Review B*, vol. 86, no. 5. American Physical Society (APS), Aug. 20, 2012. doi: 10.1103/physrevb.86.054115.  
  
C.-J. Kang and B. I. Min, “Ferroelectric instability and topological crystalline insulating nature in PbPo”, *Physical Review B*, vol. 93, no. 4. American Physical Society (APS), Jan. 13, 2016. doi: 10.1103/physrevb.93.041104.  
  
I. M. Kaplow, J. L. MacIsaac, S. M. Mah, L. M. McEwen, M. S. Koborand H. B. Fraser, “A pooling-based approach to mapping genetic variants associated with DNA methylation”, *Genome Research*, vol. 25, no. 6. Cold Spring Harbor Laboratory, pp. 907–917, Apr. 24, 2015. doi: 10.1101/gr.183749.114.  
  
A. Kapusta and C. Feschotte, “Volatile evolution of long noncoding RNA repertoires: mechanisms and biological implications”, *Trends in Genetics*, vol. 30, no. 10. Elsevier BV, pp. 439–452, Oct. 2014. doi: 10.1016/j.tig.2014.08.004.  
  
A. Kapusta, “Transposable Elements Are Major Contributors to the Origin, Diversification, and Regulation of Vertebrate Long Noncoding RNAs”, *PLoS Genetics*, vol. 9, no. 4. Public Library of Science (PLoS), p. e1003470, Apr. 25, 2013. doi: 10.1371/journal.pgen.1003470.  
  
V. S. Karra, “Modeling the formation of collagen-mimetic triple helices and microfibrils”, *No Publisher Supplied*, 2017, doi: 10.7282/T3959MQW.  
  
M. Kazemian, “Evidence for Deep Regulatory Similarities in Early Developmental Programs across Highly Diverged Insects”, *Genome Biology and Evolution*, vol. 6, no. 9. Oxford University Press (OUP), pp. 2301–2320, Aug. 29, 2014. doi: 10.1093/gbe/evu184.  
  
S. Keten and M. J. Buehler, “Atomistic model of the spider silk nanostructure”, *Applied Physics Letters*, vol. 96, no. 15. AIP Publishing, p. 153701, Apr. 12, 2010. doi: 10.1063/1.3385388.  
  
S. Keten and M. J. Buehler, “Nanostructure and molecular mechanics of spider dragline silk protein assemblies”, *Journal of The Royal Society Interface*, vol. 7, no. 53. The Royal Society, pp. 1709–1721, Jun. 02, 2010. doi: 10.1098/rsif.2010.0149.  
  
S. Keten, C.-C. Chou, A. C. T. van Duinand M. J. Buehler, “Tunable nanomechanics of protein disulfide bonds in redox microenvironments”, *Journal of the Mechanical Behavior of Biomedical Materials*, vol. 5, no. 1. Elsevier BV, pp. 32–40, Jan. 2012. doi: 10.1016/j.jmbbm.2011.08.017.  
  
S. Keten, Z. Xu, B. Ihleand M. J. Buehler, “Nanoconfinement controls stiffness, strength and mechanical toughness of β-sheet crystals in silk”, *Nature Materials*, vol. 9, no. 4. Springer Science and Business Media LLC, pp. 359–367, Mar. 14, 2010. doi: 10.1038/nmat2704.  
  
T. H. Khan, S. K. Mohammed, M. S. Imtiazand K. A. Wahid, “Color reproduction and processing algorithm based on real-time mapping for endoscopic images”, *SpringerPlus*, vol. 5, no. 1. Springer Science and Business Media LLC, Jan. 06, 2016. doi: 10.1186/s40064-015-1612-4.  
  
T. Khan, R. Shrestha, M. S. Imtiazand K. A. Wahid, “Colour‐reproduction algorithm for transmitting variable video frames and its application to capsule endoscopy”, *Healthcare Technology Letters*, vol. 2, no. 2. Institution of Engineering and Technology (IET), pp. 52–57, Feb. 05, 2015. doi: 10.1049/htl.2014.0086.  
  
E. Khatami, E. Perepelitsky, M. Rigoland B. S. Shastry, “Linked-cluster expansion for the Green’s function of the infinite-Hubbard model”, *Physical Review E*, vol. 89, no. 6. American Physical Society (APS), Jun. 02, 2014. doi: 10.1103/physreve.89.063301.  
  
J. I. Khudyakov, C. D. Champagne, L. Preeyanon, R. M. Ortizand D. E. Crocker, “Muscle transcriptome response to ACTH administration in a free-ranging marine mammal”, *Physiological Genomics*, vol. 47, no. 8. American Physiological Society, pp. 318–330, Aug. 2015. doi: 10.1152/physiolgenomics.00030.2015.  
  
J. I. Khudyakov, L. Preeyanon, C. D. Champagne, R. M. Ortizand D. E. Crocker, “Transcriptome analysis of northern elephant seal (Mirounga angustirostris) muscle tissue provides a novel molecular resource and physiological insights”, *BMC Genomics*, vol. 16, no. 1. Springer Science and Business Media LLC, Feb. 08, 2015. doi: 10.1186/s12864-015-1253-6.  
  
K. Kianfar, S. M. T. Fatemi Ghomiand A. Oroojlooy Jadid, “Study of stochastic sequence-dependent flexible flow shop via developing a dispatching rule and a hybrid GA”, *Engineering Applications of Artificial Intelligence*, vol. 25, no. 3. Elsevier BV, pp. 494–506, Apr. 2012. doi: 10.1016/j.engappai.2011.12.004.  
  
D. H. Kim, “Interplay betweenand Festates in charge-orderedFeO(, Tm, Lu)”, *Physical Review B*, vol. 87, no. 18. American Physical Society (APS), May 10, 2013. doi: 10.1103/physrevb.87.184409.  
  
D. H. Kim, “Correlation between Mn and Ru valence states and magnetic phases in”, *Physical Review B*, vol. 91, no. 7. American Physical Society (APS), Feb. 17, 2015. doi: 10.1103/physrevb.91.075113.  
  
H. Kim, C.-J. Kang, K. Kim, J. H. Shimand B. I. Min, “Phonon softenings and the charge density wave instability in(element)”, *Physical Review B*, vol. 91, no. 16. American Physical Society (APS), Apr. 24, 2015. doi: 10.1103/physrevb.91.165130.  
  
H. Kim, C.-J. Kang, K. Kim, J. H. Shimand B. I. Min, “Suppression of the charge density wave instability in(= La, Er) due to large spin-orbit coupling”, *Physical Review B*, vol. 93, no. 12. American Physical Society (APS), Mar. 09, 2016. doi: 10.1103/physrevb.93.125116.  
  
J. Kim, “Termination-dependent surface in-gap states in a potential mixed-valent topological insulator:”, *Physical Review B*, vol. 90, no. 7. American Physical Society (APS), Aug. 18, 2014. doi: 10.1103/physrevb.90.075131.  
  
R. E. Kim, S. Kang, B. F. Spencer, H. Ozerand I. L. Al-Qadi, “Stochastic Analysis of Energy Dissipation of a Half-Car Model on Nondeformable Rough Pavement”, *Journal of Transportation Engineering, Part B: Pavements*, vol. 143, no. 4. American Society of Civil Engineers (ASCE), Dec. 2017. doi: 10.1061/jpeodx.0000014.  
  
S. Kim, K. Kim, C.-J. Kangand B. I. Min, “Pressure-induced phonon softenings and the structural and magnetic transitions in CrO”, *Physical Review B*, vol. 85, no. 9. American Physical Society (APS), Mar. 19, 2012. doi: 10.1103/physrevb.85.094106.  
  
S. Kim, K. Kim, C.-J. Kangand B. I. Min, “Correlation-assisted phonon softening and the orbital-selective Peierls transition in VO”, *Physical Review B*, vol. 87, no. 19. American Physical Society (APS), May 06, 2013. doi: 10.1103/physrevb.87.195106.  
  
Y. Kim, C. S. Glosterand W. E. Alexander, “An acceleration framework for synthetic aperture radar algorithms”, *SPIE Proceedings*. SPIE, Apr. 28, 2017. doi: 10.1117/12.2261397.  
  
C. N. Kingsley, J. C. Bierma, V. Phamand R. W. Martin, “γS-Crystallin Proteins from the Antarctic Nototheniid Toothfish: A Model System for Investigating Differential Resistance to Chemical and Thermal Denaturation”, *The Journal of Physical Chemistry B*, vol. 118, no. 47. American Chemical Society (ACS), pp. 13544–13553, Nov. 18, 2014. doi: 10.1021/jp509134d.  
  
C. N. Kingsley, “Preferential and Specific Binding of Human αB-Crystallin to a Cataract-Related Variant of γS-Crystallin”, *Structure*, vol. 21, no. 12. Elsevier BV, pp. 2221–2227, Dec. 2013. doi: 10.1016/j.str.2013.09.017.  
  
K. M. Knee, D. R. Goulet, J. Zhang, B. Chen, W. Chiuand J. A. King, “The group II chaperonin Mm-Cpn binds and refolds human γD crystallin”, *Protein Science*, vol. 20, no. 1. Wiley, pp. 30–41, Dec. 23, 2010. doi: 10.1002/pro.531.  
  
A. Komuravelli, A. Gurfinkeland S. Chaki, “SMT-Based Model Checking for Recursive Programs”, *Computer Aided Verification*. Springer International Publishing, pp. 17–34, 2014. doi: 10.1007/978-3-319-08867-9\_2.  
  
P. Kondikoppa, C.-H. Chiu, C. Cui, L. Xueand S.-J. Park, “Network-aware scheduling of mapreduce framework ondistributed clusters over high speed networks”, *Proceedings of the 2012 workshop on Cloud services, federation, and the 8th open cirrus summit*. ACM, Sep. 21, 2012. doi: 10.1145/2378975.2378985.  
  
J. Kowalke, “Structural Insight into Layered Silicon Hydrogen Phosphates Containing [SiO 6 ] Octahedra Prepared by Different Reaction Routes”, *European Journal of Inorganic Chemistry*, vol. 2019, no. 6. Wiley, pp. 828–836, Jan. 22, 2019. doi: 10.1002/ejic.201801321.  
  
E. G. Kratz, A. R. Walker, L. Lagardère, F. Lipparini, J.-P. Piquemaland G. Andrés Cisneros, “LICHEM: A QM/MM program for simulations with multipolar and polarizable force fields”, *Journal of Computational Chemistry*, vol. 37, no. 11. Wiley, pp. 1019–1029, Jan. 18, 2016. doi: 10.1002/jcc.24295.  
  
B. J. Kreakie, Y. Fanand T. H. Keitt, “Enhanced Migratory Waterfowl Distribution Modeling by Inclusion of Depth to Water Table Data”, *PLoS ONE*, vol. 7, no. 1. Public Library of Science (PLoS), p. e30142, Jan. 17, 2012. doi: 10.1371/journal.pone.0030142.  
  
J. D. Kubicki, M. Aryanpour, L. Kabalanand Q. Zhu, “Quantum mechanical calculations on FeOH nanoparticles”, *Geoderma*, vol. 189–190. Elsevier BV, pp. 236–242, Nov. 2012. doi: 10.1016/j.geoderma.2012.05.016.  
  
H. Kumar, D. Er, L. Dong, J. Liand V. B. Shenoy, “Elastic Deformations in 2D van der waals Heterostructures and their Impact on Optoelectronic Properties: Predictions from a Multiscale Computational Approach”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, Jun. 16, 2015. doi: 10.1038/srep10872.  
  
P. Kumar and I. Dutta, “Influence of electric current on diffusionally accommodated sliding at hetero-interfaces”, *Acta Materialia*, vol. 59, no. 5. Elsevier BV, pp. 2096–2108, Mar. 2011. doi: 10.1016/j.actamat.2010.12.011.  
  
P. Kumar and I. Dutta, “Effect of substrate surface on electromigration-induced sliding at hetero-interfaces”, *Journal of Physics D: Applied Physics*, vol. 46, no. 15. IOP Publishing, p. 155303, Mar. 18, 2013. doi: 10.1088/0022-3727/46/15/155303.  
  
P. Kumar, I. Duttaand M. S. Bakir, “Interfacial Effects During Thermal Cycling of Cu-Filled Through-Silicon Vias (TSV)”, *Journal of Electronic Materials*, vol. 41, no. 2. Springer Science and Business Media LLC, pp. 322–335, Aug. 10, 2011. doi: 10.1007/s11664-011-1726-6.  
  
P. Kumar, Z. Huang, I. Dutta, R. Sidhu, M. Renavikarand R. Mahajan, “Fracture of Sn-Ag-Cu Solder Joints on Cu Substrates. II: Fracture Mechanism Map”, *Journal of Electronic Materials*, vol. 41, no. 2. Springer Science and Business Media LLC, pp. 412–424, Nov. 17, 2011. doi: 10.1007/s11664-011-1806-7.  
  
P. Kunal, “Microwave-Assisted Synthesis of Pd*x*Au100–*x*Alloy Nanoparticles: A Combined Experimental and Theoretical Assessment of Synthetic and Compositional Effects upon Catalytic Reactivity”, *ACS Catalysis*, vol. 6, no. 8. American Chemical Society (ACS), pp. 4882–4893, Jun. 27, 2016. doi: 10.1021/acscatal.6b01014.  
  
R. Labib, “Improving daylighting in existing classrooms using laser cut panels”, *Lighting Research & Technology*, vol. 45, no. 5. SAGE Publications, pp. 585–598, Dec. 21, 2012. doi: 10.1177/1477153512471366.  
  
R. Labib, “Trade-off method to assess the interaction between light shelves and complex ceiling forms for optimized daylighting performance”, *Advances in Building Energy Research*, vol. 9, no. 2. Informa UK Limited, pp. 224–237, Mar. 03, 2015. doi: 10.1080/17512549.2015.1014838.  
  
H. Lamm and R. F. Lebed, “True muonium (*μ*+*μ*−) on the light front”, *Journal of Physics G: Nuclear and Particle Physics*, vol. 41, no. 12. IOP Publishing, p. 125003, Nov. 10, 2014. doi: 10.1088/0954-3899/41/12/125003.  
  
J. R. LASKY, D. L. DES MARAIS, J. K. McKAY, J. H. RICHARDS, T. E. JUENGERand T. H. KEITT, “Characterizing genomic variation of*Arabidopsis thaliana*: the roles of geography and climate”, *Molecular Ecology*, vol. 21, no. 22. Wiley, pp. 5512–5529, Aug. 01, 2012. doi: 10.1111/j.1365-294x.2012.05709.x.  
  
D. Lau, K. Broderick, M. J. Buehlerand O. Büyüköztürk, “A robust nanoscale experimental quantification of fracture energy in a bilayer material system”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 33. Proceedings of the National Academy of Sciences, pp. 11990–11995, Aug. 05, 2014. doi: 10.1073/pnas.1402893111.  
  
D. R. Laver, C. H. T. Kong, M. S. Imtiazand M. B. Cannell, “Termination of calcium-induced calcium release by induction decay: An emergent property of stochastic channel gating and molecular scale architecture”, *Journal of Molecular and Cellular Cardiology*, vol. 54. Elsevier BV, pp. 98–100, Jan. 2013. doi: 10.1016/j.yjmcc.2012.10.009.  
  
M. Law, “Automated Update, Revision, and Quality Control of the Maize Genome Annotations Using MAKER-P Improves the B73 RefGen\_v3 Gene Models and Identifies New Genes  ”, *Plant Physiology*, vol. 167, no. 1. Oxford University Press (OUP), pp. 25–39, Nov. 10, 2014. doi: 10.1104/pp.114.245027.  
  
B. J. Lawson, “Multiple Fermi surfaces in superconducting Nb-doped”, *Physical Review B*, vol. 94, no. 4. American Physical Society (APS), Jul. 25, 2016. doi: 10.1103/physrevb.94.041114.  
  
D. Lazzati and A. Heger, “THE INTERPLAY BETWEEN CHEMISTRY AND NUCLEATION IN THE FORMATION OF CARBONACEOUS DUST IN SUPERNOVA EJECTA”, *The Astrophysical Journal*, vol. 817, no. 2. American Astronomical Society, p. 134, Jan. 27, 2016. doi: 10.3847/0004-637x/817/2/134.  
  
V. R. Lecoustre, “Direct numerical simulations of non-premixed ethylene–air flames: Local flame extinction criterion”, *Combustion and Flame*, vol. 161, no. 11. Elsevier BV, pp. 2933–2950, Nov. 2014. doi: 10.1016/j.combustflame.2014.05.016.  
  
H. J. Lee, “NMR Structure of a Heterodimeric SAM:SAM Complex: Characterization and Manipulation of EphA2 Binding Reveal New Cellular Functions of SHIP2”, *Structure*, vol. 20, no. 1. Elsevier BV, pp. 41–55, Jan. 2012. doi: 10.1016/j.str.2011.11.013.  
  
M. Lee, V. Kolevand A. Warshel, “Validating a Coarse-Grained Voltage Activation Model by Comparing Its Performance to the Results of Monte Carlo Simulations”, *The Journal of Physical Chemistry B*, vol. 121, no. 50. American Chemical Society (ACS), pp. 11284–11291, Dec. 11, 2017. doi: 10.1021/acs.jpcb.7b09530.  
  
S.-H. Lee, “Parvalbumin-Positive Basket Cells Differentiate among Hippocampal Pyramidal Cells”, *Neuron*, vol. 82, no. 5. Elsevier BV, pp. 1129–1144, Jun. 2014. doi: 10.1016/j.neuron.2014.03.034.  
  
S.-J. Lee, B. Olsen, P. H. Schlesingerand N. A. Baker, “Characterization of Perfluorooctylbromide-Based Nanoemulsion Particles Using Atomistic Molecular Dynamics Simulations”, *The Journal of Physical Chemistry B*, vol. 114, no. 31. American Chemical Society (ACS), pp. 10086–10096, Jul. 16, 2010. doi: 10.1021/jp103228c.  
  
S.-J. Lee, P. H. Schlesinger, S. A. Wickline, G. M. Lanzaand N. A. Baker, “Interaction of Melittin Peptides with Perfluorocarbon Nanoemulsion Particles”, *The Journal of Physical Chemistry B*, vol. 115, no. 51. American Chemical Society (ACS), pp. 15271–15279, Dec. 06, 2011. doi: 10.1021/jp209543c.  
  
S.-J. Lee, P. H. Schlesinger, S. A. Wickline, G. M. Lanzaand N. A. Baker, “Simulation of fusion-mediated nanoemulsion interactions with model lipid bilayers”, *Soft Matter*, vol. 8, no. 26. Royal Society of Chemistry (RSC), p. 7024, 2012. doi: 10.1039/c2sm25847a.  
  
T.-J. Lee, “Arabidopsis thaliana Chromosome 4 Replicates in Two Phases That Correlate with Chromatin State”, *PLoS Genetics*, vol. 6, no. 6. Public Library of Science (PLoS), p. e1000982, Jun. 10, 2010. doi: 10.1371/journal.pgen.1000982.  
  
W. Lee, S. A. Mann, M. J. Windley, M. S. Imtiaz, J. I. Vandenbergand A. P. Hill, “In silico assessment of kinetics and state dependent binding properties of drugs causing acquired LQTS”, *Progress in Biophysics and Molecular Biology*, vol. 120, no. 1–3. Elsevier BV, pp. 89–99, Jan. 2016. doi: 10.1016/j.pbiomolbio.2015.12.005.  
  
S. Lehtola, N. M. Tubman, K. B. Whaleyand M. Head-Gordon, “Cluster decomposition of full configuration interaction wave functions: A tool for chemical interpretation of systems with strong correlation”, *The Journal of Chemical Physics*, vol. 147, no. 15. AIP Publishing, p. 154105, Oct. 21, 2017. doi: 10.1063/1.4996044.  
  
C. J. Lessard, “Identification of IRF8, TMEM39A, and IKZF3-ZPBP2 as Susceptibility Loci for Systemic Lupus Erythematosus in a Large-Scale Multiracial Replication Study”, *The American Journal of Human Genetics*, vol. 90, no. 4. Elsevier BV, pp. 648–660, Apr. 2012. doi: 10.1016/j.ajhg.2012.02.023.  
  
H. Liang, M. Ashour‐Abdalla, R. Richard, D. Schriver, M. El‐Alaouiand R. J. Walker, “Contrasting electron acceleration processes during two substorms”, *Journal of Geophysical Research: Space Physics*, vol. 119, no. 7. American Geophysical Union (AGU), pp. 5382–5400, Jul. 2014. doi: 10.1002/2013ja019721.  
  
W. Liang, “Tough Germanium Nanoparticles under Electrochemical Cycling”, *ACS Nano*, vol. 7, no. 4. American Chemical Society (ACS), pp. 3427–3433, Mar. 12, 2013. doi: 10.1021/nn400330h.  
  
M. D. J. Libardo, “Phagosomal Copper-Promoted Oxidative Attack on Intracellular *Mycobacterium tuberculosis*”, *ACS Infectious Diseases*, vol. 4, no. 11. American Chemical Society (ACS), pp. 1623–1634, Aug. 24, 2018. doi: 10.1021/acsinfecdis.8b00171.  
  
F. Libonati, A. K. Nair, L. Verganiand M. J. Buehler, “Fracture mechanics of hydroxyapatite single crystals under geometric confinement”, *Journal of the Mechanical Behavior of Biomedical Materials*, vol. 20. Elsevier BV, pp. 184–191, Apr. 2013. doi: 10.1016/j.jmbbm.2012.12.005.  
  
F. Libonati, A. K. Nair, L. Verganiand M. J. Buehler, “Mechanics of collagen–hydroxyapatite model nanocomposites”, *Mechanics Research Communications*, vol. 58. Elsevier BV, pp. 17–23, Jun. 2014. doi: 10.1016/j.mechrescom.2013.08.008.  
  
D. Li, “Anomalous optical and electronic properties of dense sodium”, *Physics Letters A*, vol. 374, no. 43. Elsevier BV, pp. 4458–4464, Sep. 2010. doi: 10.1016/j.physleta.2010.08.079.  
  
P. V. Lidsky, R. Andinoand I. M. Rouzine, “Variability in viral pathogenesis: modeling the dynamic of acute and persistent infections”, *Current Opinion in Virology*, vol. 23. Elsevier BV, pp. 120–124, Apr. 2017. doi: 10.1016/j.coviro.2017.05.001.  
  
D. F. Li, P. Zhang, J. Yanand H. Y. Liu, “Melting curve of lithium from quantum molecular-dynamics simulations”, *EPL (Europhysics Letters)*, vol. 95, no. 5. IOP Publishing, p. 56004, Aug. 17, 2011. doi: 10.1209/0295-5075/95/56004.  
  
H. Li, O. Y. Gnedin, N. Y. Gnedin, X. Meng, V. A. Semenovand A. V. Kravtsov, “STAR CLUSTER FORMATION IN COSMOLOGICAL SIMULATIONS. I. PROPERTIES OF YOUNG CLUSTERS”, *The Astrophysical Journal*, vol. 834, no. 1. American Astronomical Society, p. 69, Jan. 03, 2017. doi: 10.3847/1538-4357/834/1/69.  
  
H. Li, J. A. Ice, C. J. Lessardand K. L. Sivils, “Interferons in Sjögren’s Syndrome: Genes, Mechanisms, and Effects”, *Frontiers in Immunology*, vol. 4. Frontiers Media SA, 2013. doi: 10.3389/fimmu.2013.00290.  
  
J. Li, “Hot-electron generation from laser–pre-plasma interactions in cone-guided fast ignition”, *Physics of Plasmas*, vol. 20, no. 5. AIP Publishing, p. 052706, May 2013. doi: 10.1063/1.4807040.  
  
J. Li, “ß-Adrenergic Stimulation Increases RyR2 Activity via Intracellular Ca2+ and Mg2+ Regulation”, *PLoS ONE*, vol. 8, no. 3. Public Library of Science (PLoS), p. e58334, Mar. 22, 2013. doi: 10.1371/journal.pone.0058334.  
  
J. Li, B. Zhao, H. Liand J. Zheng, “Study of flux limiter using Fokker–Planck and fluid simulations of planar laser-driven ablation”, *Plasma Physics and Controlled Fusion*, vol. 52, no. 8. IOP Publishing, p. 085008, Jun. 30, 2010. doi: 10.1088/0741-3335/52/8/085008.  
  
N. Y. C. Lin, S. Goyal, X. Cheng, R. N. Zia, F. A. Escobedoand I. Cohen, “Far-from-equilibrium sheared colloidal liquids: Disentangling relaxation, advection, and shear-induced diffusion”, *Physical Review E*, vol. 88, no. 6. American Physical Society (APS), Dec. 18, 2013. doi: 10.1103/physreve.88.062309.  
  
N. Lin, Y. Zhu, R. Fanand M. Xiong, “A quadratically regularized functional canonical correlation analysis for identifying the global structure of pleiotropy with NGS data”, *PLOS Computational Biology*, vol. 13, no. 10. Public Library of Science (PLoS), p. e1005788, Oct. 17, 2017. doi: 10.1371/journal.pcbi.1005788.  
  
S. Lin, “Predictive modelling-based design and experiments for synthesis and spinning of bioinspired silk fibres”, *Nature Communications*, vol. 6, no. 1. Springer Science and Business Media LLC, May 28, 2015. doi: 10.1038/ncomms7892.  
  
Y. Lin, J. Yuan, M. Kolmogorov, M. W. Shen, M. Chaissonand P. A. Pevzner, “Assembly of long error-prone reads using de Bruijn graphs”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 52. Proceedings of the National Academy of Sciences, Dec. 12, 2016. doi: 10.1073/pnas.1604560113.  
  
Q. Li, “Genetic Perturbation of the Maize Methylome”, *The Plant Cell*, vol. 26, no. 12. Oxford University Press (OUP), pp. 4602–4616, Dec. 2014. doi: 10.1105/tpc.114.133140.  
  
Q. Li, “RNA-directed DNA methylation enforces boundaries between heterochromatin and euchromatin in the maize genome”, *Proceedings of the National Academy of Sciences*, vol. 112, no. 47. Proceedings of the National Academy of Sciences, pp. 14728–14733, Nov. 09, 2015. doi: 10.1073/pnas.1514680112.  
  
Q. Li, H. Liu, D. Zhou, W. Zheng, Z. Wuand Y. Ma, “A novel low compressible and superhard carbon nitride: Body-centered tetragonal CN2”, *Physical Chemistry Chemical Physics*, vol. 14, no. 37. Royal Society of Chemistry (RSC), p. 13081, 2012. doi: 10.1039/c2cp41694h.  
  
Q. Li, “Examining the Causes and Consequences of Context-Specific Differential DNA Methylation in Maize”, *Plant Physiology*, vol. 168, no. 4. Oxford University Press (OUP), pp. 1262–1274, Apr. 13, 2015. doi: 10.1104/pp.15.00052.  
  
Q. Li, “Structural and Mechanical Properties of Platinum Carbide”, *Inorganic Chemistry*, vol. 53, no. 11. American Chemical Society (ACS), pp. 5797–5802, May 15, 2014. doi: 10.1021/ic5006133.  
  
B. Liu, “An integrative and applicable phylogenetic footprinting framework for cis-regulatory motifs identification in prokaryotic genomes”, *BMC Genomics*, vol. 17, no. 1. Springer Science and Business Media LLC, Aug. 09, 2016. doi: 10.1186/s12864-016-2982-x.  
  
C. Liu, J. Su, F. Yang, K. Wei, J. Maand X. Zhou, “Compound signature detection on LINCS L1000 big data”, *Molecular BioSystems*, vol. 11, no. 3. Royal Society of Chemistry (RSC), pp. 714–722, 2015. doi: 10.1039/c4mb00677a.  
  
C. Liu, J. Su, F. Yang, K. Wei, J. Maand X. Zhou, “Compound signature detection on LINCS L1000 big data”, *Molecular BioSystems*, vol. 11, no. 3. Royal Society of Chemistry (RSC), pp. 714–722, 2015. doi: 10.1039/c4mb00677a.  
  
D. Liu, Q. Chenand Y. Wang, “A Sixth Order Accuracy Solution to a System of Nonlinear Differential Equations with Coupled Compact Method”, *Journal of Computational Engineering*, vol. 2013. Hindawi Limited, pp. 1–10, Dec. 04, 2013. doi: 10.1155/2013/432192.  
  
D. L. Yifan Wang, “Spectral Element Simulation of Reaction-Diffusion System in the Neuromuscular Junction”, *Journal of Applied & Computational Mathematics*, vol. 2, no. 4. OMICS Publishing Group, 2013. doi: 10.4172/2168-9679.1000136.  
  
D. Liu and Y. Zheng, “Modal Spectral Element Solutions to Incompressible Flows over Particles of Complex Shape”, *Journal of Computational Engineering*, vol. 2014. Hindawi Limited, pp. 1–11, Apr. 30, 2014. doi: 10.1155/2014/768538.  
  
H. Y. Liu, J. A. Abell, A. Diambraand F. Pisanò, “Modelling the cyclic ratcheting of sands through memory-enhanced bounding surface plasticity”, *Géotechnique*, vol. 69, no. 9. Thomas Telford Ltd., pp. 783–800, Sep. 2019. doi: 10.1680/jgeot.17.p.307.  
  
H. Liu, W. Cuiand Y. Ma, “Hybrid functional study rationalizes the simple cubic phase of calcium at high pressures”, *The Journal of Chemical Physics*, vol. 137, no. 18. AIP Publishing, p. 184502, Nov. 14, 2012. doi: 10.1063/1.4765326.  
  
H. Liu, E. R. Hernández, J. Yanand Y. Ma, “Anomalous Melting Behavior of Solid Hydrogen at High Pressures”, *The Journal of Physical Chemistry C*, vol. 117, no. 22. American Chemical Society (ACS), pp. 11873–11877, May 24, 2013. doi: 10.1021/jp403885h.  
  
H. Liu, Q. Li, L. Zhuand Y. Ma, “Superhard and superconductive polymorphs of diamond-like BC3”, *Physics Letters A*, vol. 375, no. 3. Elsevier BV, pp. 771–774, Jan. 2011. doi: 10.1016/j.physleta.2010.12.034.  
  
H. Liu, Q. Li, L. Zhuand Y. Ma, “Superhard polymorphs of diamond-like”, *Solid State Communications*, vol. 151, no. 9. Elsevier BV, pp. 716–719, May 2011. doi: 10.1016/j.ssc.2011.02.013.  
  
H. Liu and Y. Ma, “Proton or Deuteron Transfer in Phase IV of Solid Hydrogen and Deuterium”, *Physical Review Letters*, vol. 110, no. 2. American Physical Society (APS), Jan. 09, 2013. doi: 10.1103/physrevlett.110.025903.  
  
H. Liu, J. Tseand Y. Ma, “Robust Diffusive Proton Motions in Phase IV of Solid Hydrogen”, *The Journal of Physical Chemistry C*, vol. 118, no. 22. American Chemical Society (ACS), pp. 11902–11905, May 27, 2014. doi: 10.1021/jp503409p.  
  
H. Liu, J. S. Tseand W. J. Nellis, “The electrical conductivity of Al2O3 under shock-compression”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, Aug. 04, 2015. doi: 10.1038/srep12823.  
  
H. Liu, H. Wangand Y. Ma, “Quasi-Molecular and Atomic Phases of Dense Solid Hydrogen”, *The Journal of Physical Chemistry C*, vol. 116, no. 16. American Chemical Society (ACS), pp. 9221–9226, Apr. 12, 2012. doi: 10.1021/jp301596v.  
  
H. Liu, Y. Yaoand D. D. Klug, “Stable structures of He andat high pressure”, *Physical Review B*, vol. 91, no. 1. American Physical Society (APS), Jan. 07, 2015. doi: 10.1103/physrevb.91.014102.  
  
H. Liu, L. Zhu, W. Cuiand Y. Ma, “Room-temperature structures of solid hydrogen at high pressures”, *The Journal of Chemical Physics*, vol. 137, no. 7. AIP Publishing, p. 074501, Aug. 21, 2012. doi: 10.1063/1.4745186.  
  
J. Liu, P. S. Ayyaswamy, D. M. Eckmannand R. Radhakrishnan, “Modelling of binding free energy of targeted nanocarriers to cell surface”, *Heat and Mass Transfer*, vol. 50, no. 3. Springer Science and Business Media LLC, pp. 315–321, Dec. 14, 2013. doi: 10.1007/s00231-013-1274-0.  
  
Q. Liu, “*Striga hermonthicaMAX2*restores branching but not theVeryLowFluenceResponse in the*Arabidopsis thaliana max2*mutant”, *New Phytologist*, vol. 202, no. 2. Wiley, pp. 531–541, Jan. 31, 2014. doi: 10.1111/nph.12692.  
  
T. Liu, P. Singh, J. T. Jenkins, A. Jagota, M. Bykhovskaiaand C.-Y. Hui, “A continuum model of docking of synaptic vesicle to plasma membrane”, *Journal of The Royal Society Interface*, vol. 12, no. 102. The Royal Society, p. 20141119, Jan. 2015. doi: 10.1098/rsif.2014.1119.  
  
X. H. Liu, F. Fan, H. Yang, S. Zhang, J. Y. Huangand T. Zhu, “Self-Limiting Lithiation in Silicon Nanowires”, *ACS Nano*, vol. 7, no. 2. American Chemical Society (ACS), pp. 1495–1503, Jan. 03, 2013. doi: 10.1021/nn305282d.  
  
Y. Liu, “First-principles study on the structural and electronic properties of metallic HfH2 under pressure”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, Jun. 22, 2015. doi: 10.1038/srep11381.  
  
X. Li, “Structure of Ribosomal Silencing Factor Bound to Mycobacterium tuberculosis Ribosome”, *Structure*, vol. 23, no. 10. Elsevier BV, pp. 1858–1865, Oct. 2015. doi: 10.1016/j.str.2015.07.014.  
  
Y. Li, “MOMCMC: An efficient Monte Carlo method for multi-objective sampling over real parameter space”, *Computers & Mathematics with Applications*, vol. 64, no. 11. Elsevier BV, pp. 3542–3556, Dec. 2012. doi: 10.1016/j.camwa.2012.09.003.  
  
Y. Li, “CONFORMATIONAL SAMPLING IN TEMPLATE-FREE PROTEIN LOOP STRUCTURE MODELING: AN OVERVIEW”, *Computational and Structural Biotechnology Journal*, vol. 5, no. 6. Elsevier BV, p. e201302003, Feb. 2013. doi: 10.5936/csbj.201302003.  
  
Y. Li and J. P. Conte, “Effects of seismic isolation on the seismic response of a California high-speed rail prototype bridge with soil-structure and track-structure interactions”, *Earthquake Engineering & Structural Dynamics*, vol. 45, no. 15. Wiley, pp. 2415–2434, Jul. 04, 2016. doi: 10.1002/eqe.2770.  
  
Y. Li, J. Hao, H. Liu, Y. Liand Y. Ma, “The metallization and superconductivity of dense hydrogen sulfide”, *The Journal of Chemical Physics*, vol. 140, no. 17. AIP Publishing, p. 174712, May 07, 2014. doi: 10.1063/1.4874158.  
  
Y. Li, J. Hao, H. Liu, J. S. Tse, Y. Wangand Y. Ma, “Pressure-stabilized superconductive yttrium hydrides”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, May 05, 2015. doi: 10.1038/srep09948.  
  
Y. Li, H. Liu, I. Rataand E. Jakobsson, “Building a Knowledge-Based Statistical Potential by Capturing High-Order Inter-residue Interactions and its Applications in Protein Secondary Structure Assessment”, *Journal of Chemical Information and Modeling*, vol. 53, no. 2. American Chemical Society (ACS), pp. 500–508, Feb. 04, 2013. doi: 10.1021/ci300207x.  
  
Y. Li, X. Shi, Y. Liang, J. Xie, Y. Zhangand Q. Ma, “RNA-TVcurve: a Web server for RNA secondary structure comparison based on a multi-scale similarity of its triple vector curve representation”, *BMC Bioinformatics*, vol. 18, no. 1. Springer Science and Business Media LLC, Jan. 21, 2017. doi: 10.1186/s12859-017-1481-7.  
  
C. H. Londergan, R. Baskin, C. G. Bischak, K. W. Hoffman, D. M. Sneadand C. Reynoso, “Dynamic Asymmetry and the Role of the Conserved Active-Site Thiol in Rabbit Muscle Creatine Kinase”, *Biochemistry*, vol. 54, no. 1. American Chemical Society (ACS), pp. 83–95, Nov. 06, 2014. doi: 10.1021/bi5008063.  
  
W. Lopez, J. Ramachandran, A. Alsamarah, Y. Luo, A. L. Harrisand J. E. Contreras, “Mechanism of gating by calcium in connexin hemichannels”, *Proceedings of the National Academy of Sciences*, vol. 113, no. 49. Proceedings of the National Academy of Sciences, Nov. 21, 2016. doi: 10.1073/pnas.1609378113.  
  
B. C. Low and F. Fang, “Cylindrical Taylor states conserving total absolute magnetic helicity”, *Physics of Plasmas*, vol. 21, no. 9. AIP Publishing, p. 092116, Sep. 2014. doi: 10.1063/1.4896246.  
  
R. A. Luettich Jr., “Introduction to special section on The U.S. IOOS Coastal and Ocean Modeling Testbed”, *Journal of Geophysical Research: Oceans*, vol. 118, no. 12. American Geophysical Union (AGU), pp. 6319–6328, Dec. 2013. doi: 10.1002/2013jc008939.  
  
M. Lu, M. Zhangand H. Liu, “Predicted two-dimensional electrides: Lithium–carbon monolayer sheet”, *Physics Letters A*, vol. 379, no. 39. Elsevier BV, pp. 2511–2514, Oct. 2015. doi: 10.1016/j.physleta.2015.07.023.  
  
L. Luna-Zurita, “Complex Interdependence Regulates Heterotypic Transcription Factor Distribution and Coordinates Cardiogenesis”, *Cell*, vol. 164, no. 5. Elsevier BV, pp. 999–1014, Feb. 2016. doi: 10.1016/j.cell.2016.01.004.  
  
L. Luo, L. Zhang, G. Henkelmanand R. M. Crooks, “Unusual Activity Trend for CO Oxidation on Pd*x*Au140–*x*@Pt Core@Shell Nanoparticle Electrocatalysts”, *The Journal of Physical Chemistry Letters*, vol. 6, no. 13. American Chemical Society (ACS), pp. 2562–2568, Jun. 19, 2015. doi: 10.1021/acs.jpclett.5b00985.  
  
S.-X. Luo, J. S. Cannon, B. L. H. Taylor, K. M. Engle, K. N. Houkand R. H. Grubbs, “Z-Selective Cross-Metathesis and Homodimerization of 3*E*-1,3-Dienes: Reaction Optimization, Computational Analysis, and Synthetic Applications”, *Journal of the American Chemical Society*, vol. 138, no. 42. American Chemical Society (ACS), pp. 14039–14046, Oct. 17, 2016. doi: 10.1021/jacs.6b08387.  
  
X. Luo, “Predicting Two-Dimensional Boron–Carbon Compounds by the Global Optimization Method”, *Journal of the American Chemical Society*, vol. 133, no. 40. American Chemical Society (ACS), pp. 16285–16290, Sep. 19, 2011. doi: 10.1021/ja2072753.  
  
Y. Luo, A. R. Rossiand A. L. Harris, “Computational Studies of Molecular Permeation through Connexin26 Channels”, *Biophysical Journal*, vol. 110, no. 3. Elsevier BV, pp. 584–599, Feb. 2016. doi: 10.1016/j.bpj.2015.11.3528.  
  
S. Lu, Y. Wang, H. Liu, M.-. sheng . Miaoand Y. Ma, “Self-assembled ultrathin nanotubes on diamond (100) surface”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, Apr. 16, 2014. doi: 10.1038/ncomms4666.  
  
S. Lu, M. Wu, H. Liu, J. S. Tseand B. Yang, “Prediction of novel crystal structures and superconductivity of compressed HBr”, *RSC Advances*, vol. 5, no. 57. Royal Society of Chemistry (RSC), pp. 45812–45816, 2015. doi: 10.1039/c5ra06998j.  
  
K. Maeda, T. Colonius, A. D. Maxwell, W. Kreiderand M. R. Bailey, “Modeling and numerical simulation of the bubble cloud dynamics in an ultrasound field for burst wave lithotripsy”, *The Journal of the Acoustical Society of America*, vol. 144, no. 3. Acoustical Society of America (ASA), pp. 1780–1780, Sep. 2018. doi: 10.1121/1.5067866.  
  
K. Maeda, A. D. Maxwell, T. Colonius, W. Kreiderand M. R. Bailey, “Energy shielding by cavitation bubble clouds in burst wave lithotripsy”, *The Journal of the Acoustical Society of America*, vol. 144, no. 5. Acoustical Society of America (ASA), pp. 2952–2961, Nov. 2018. doi: 10.1121/1.5079641.  
  
N. A. Mahynski, S. K. Kumarand A. Z. Panagiotopoulos, “Tuning polymer architecture to manipulate the relative stability of different colloid crystal morphologies”, *Soft Matter*, vol. 11, no. 25. Royal Society of Chemistry (RSC), pp. 5146–5153, 2015. doi: 10.1039/c5sm00631g.  
  
N. A. Mahynski, S. K. Kumarand A. Z. Panagiotopoulos, “Relative stability of the FCC and HCP polymorphs with interacting polymers”, *Soft Matter*, vol. 11, no. 2. Royal Society of Chemistry (RSC), pp. 280–289, 2015. doi: 10.1039/c4sm02191f.  
  
N. A. Mahynski, A. Z. Panagiotopoulos, D. Mengand S. K. Kumar, “Stabilizing colloidal crystals by leveraging void distributions”, *Nature Communications*, vol. 5, no. 1. Springer Science and Business Media LLC, Jul. 21, 2014. doi: 10.1038/ncomms5472.  
  
N. A. Mahynski, L. Rovigatti, C. N. Likosand A. Z. Panagiotopoulos, “Bottom-Up Colloidal Crystal Assembly with a Twist”, *ACS Nano*, vol. 10, no. 5. American Chemical Society (ACS), pp. 5459–5467, May 04, 2016. doi: 10.1021/acsnano.6b01854.  
  
J. Ma, “STELLAR MASSES AND STAR FORMATION RATES OF LENSED, DUSTY, STAR-FORMING GALAXIES FROM THE SPT SURVEY”, *The Astrophysical Journal*, vol. 812, no. 1. American Astronomical Society, p. 88, Oct. 09, 2015. doi: 10.1088/0004-637x/812/1/88.  
  
I. Makarevitch, “Genomic Distribution of Maize Facultative Heterochromatin Marked by Trimethylation of H3K27”, *The Plant Cell*, vol. 25, no. 3. Oxford University Press (OUP), pp. 780–793, Mar. 01, 2013. doi: 10.1105/tpc.112.106427.  
  
L. Makowski, “X-ray solution scattering studies of the structural diversity intrinsic to protein ensembles”, *Biopolymers*, vol. 95, no. 8. Wiley, pp. 531–542, Apr. 01, 2011. doi: 10.1002/bip.21631.  
  
K. Makwana, H. Li, F. Guoand X. Li, “Dissipation and particle energization in moderate to low beta turbulent plasma via PIC simulations”, *Journal of Physics: Conference Series*, vol. 837. IOP Publishing, p. 012004, May 30, 2017. doi: 10.1088/1742-6596/837/1/012004.  
  
J. W. Malcom, K. M. Hernandez, R. Likos, T. Wayne, M. A. Leiboldand T. E. Juenger, “Extensive cross‐environment fitness variation lies along few axes of genetic variation in the model alga,*Chlamydomonas reinhardtii*”, *New Phytologist*, vol. 205, no. 2. Wiley, pp. 841–851, Sep. 29, 2014. doi: 10.1111/nph.13063.  
  
C. Mangold, S. Neogiand D. Donadio, “Optimal thickness of silicon membranes to achieve maximum thermoelectric efficiency: A first principles study”, *Applied Physics Letters*, vol. 109, no. 5. AIP Publishing, p. 053902, Aug. 2016. doi: 10.1063/1.4960197.  
  
J. R. Mantsch, D. A. Baker, D. Funk, A. D. Lêand Y. Shaham, “Stress-Induced Reinstatement of Drug Seeking: 20 Years of Progress”, *Neuropsychopharmacology*, vol. 41, no. 1. Springer Science and Business Media LLC, pp. 335–356, May 15, 2015. doi: 10.1038/npp.2015.142.  
  
V. H. Man, C. Rolandand C. Sagui, “Structural Determinants of Polyglutamine Protofibrils and Crystallites”, *ACS Chemical Neuroscience*, vol. 6, no. 4. American Chemical Society (ACS), pp. 632–645, Jan. 30, 2015. doi: 10.1021/cn500358g.  
  
G. S. Manyali, R. Warmbierand A. Quandt, “Computational study of the structural, electronic and optical properties of M2N2(NH): M=C, Si, Ge, Sn”, *Computational Materials Science*, vol. 79. Elsevier BV, pp. 710–714, Nov. 2013. doi: 10.1016/j.commatsci.2013.07.038.  
  
G. S. Manyali, R. Warmbierand A. Quandt, “First-principles studies of the structural, electronic and optical properties of dinitrides CN2, SiN2 and GeN2”, *Computational Materials Science*, vol. 95. Elsevier BV, pp. 706–711, Dec. 2014. doi: 10.1016/j.commatsci.2014.07.003.  
  
G. S. Manyali, R. Warmbierand A. Quandt, “First-principles study of Si3N2”, *Computational Materials Science*, vol. 96. Elsevier BV, pp. 140–145, Jan. 2015. doi: 10.1016/j.commatsci.2014.08.051.  
  
G. S. Manyali, R. Warmbier, A. Quandtand J. E. Lowther, “Ab initio study of elastic properties of super hard and graphitic structures of C3N4”, *Computational Materials Science*, vol. 69. Elsevier BV, pp. 299–303, Mar. 2013. doi: 10.1016/j.commatsci.2012.11.039.  
  
G. Manyam, A. Birerdincand A. Baranova, “KPP: KEGG Pathway Painter”, *BMC Systems Biology*, vol. 9, no. S2. Springer Science and Business Media LLC, Apr. 15, 2015. doi: 10.1186/1752-0509-9-s2-s3.  
  
G. Manyam, C. Ivan, G. A. Calinand K. R. Coombes, “targetHub: a programmable interface for miRNA–gene interactions”, *Bioinformatics*, vol. 29, no. 20. Oxford University Press (OUP), pp. 2657–2658, Sep. 06, 2013. doi: 10.1093/bioinformatics/btt439.  
  
G. Manyam, M. A. Payton, J. A. Roth, L. V. Abruzzoand K. R. Coombes, “Relax with CouchDB — Into the non-relational DBMS era of bioinformatics”, *Genomics*, vol. 100, no. 1. Elsevier BV, pp. 1–7, Jul. 2012. doi: 10.1016/j.ygeno.2012.05.006.  
  
Q. Ma, “Understanding the commonalities and differences in genomic organizations across closely related bacteria from an energy perspective”, *Science China Life Sciences*, vol. 57, no. 11. Springer Science and Business Media LLC, pp. 1121–1130, Sep. 18, 2014. doi: 10.1007/s11427-014-4734-y.  
  
A. E. Marras, “Cation-Activated Avidity for Rapid Reconfiguration of DNA Nanodevices”, *ACS Nano*, vol. 12, no. 9. American Chemical Society (ACS), pp. 9484–9494, Aug. 31, 2018. doi: 10.1021/acsnano.8b04817.  
  
S. Marras, “A Review of Element-Based Galerkin Methods for Numerical Weather Prediction: Finite Elements, Spectral Elements, and Discontinuous Galerkin”, *Archives of Computational Methods in Engineering*, vol. 23, no. 4. Springer Science and Business Media LLC, pp. 673–722, May 19, 2015. doi: 10.1007/s11831-015-9152-1.  
  
D. R. Martin, J. E. Forsmoand D. V. Matyushov, “Complex Dynamics of Water in Protein Confinement”, *The Journal of Physical Chemistry B*, vol. 122, no. 13. American Chemical Society (ACS), pp. 3418–3425, Dec. 05, 2017. doi: 10.1021/acs.jpcb.7b10448.  
  
D. Martizzi, C.-A. Faucher-Giguèreand E. Quataert, “Supernova feedback in an inhomogeneous interstellar medium”, *Monthly Notices of the Royal Astronomical Society*, vol. 450, no. 1. Oxford University Press (OUP), pp. 504–522, Apr. 17, 2015. doi: 10.1093/mnras/stv562.  
  
D. Martizzi, D. Fielding, C.-A. Faucher-Giguèreand E. Quataert, “Supernova feedback in a local vertically stratified medium: interstellar turbulence and galactic winds”, *Monthly Notices of the Royal Astronomical Society*, vol. 459, no. 3. Oxford University Press (OUP), pp. 2311–2326, Apr. 06, 2016. doi: 10.1093/mnras/stw745.  
  
D. D. Matra, T. Kozaki, K. Ishii, R. Poerwantoand E. Inoue, “De novo transcriptome assembly of mangosteen ( Garcinia mangostana L.) fruit”, *Genomics Data*, vol. 10. Elsevier BV, pp. 35–37, Dec. 2016. doi: 10.1016/j.gdata.2016.09.003.  
  
C. Mauney, M. Buongiorno Nardelliand D. Lazzati, “FORMATION AND PROPERTIES OF ASTROPHYSICAL CARBONACEOUS DUST. I. AB-INITIO CALCULATIONS OF THE CONFIGURATION AND BINDING ENERGIES OF SMALL CARBON CLUSTERS”, *The Astrophysical Journal*, vol. 800, no. 1. American Astronomical Society, p. 30, Feb. 05, 2015. doi: 10.1088/0004-637x/800/1/30.  
  
C. Mauney, M. Buongiorno Nardelliand D. Lazzati, “FORMATION AND PROPERTIES OF ASTROPHYSICAL CARBONACEOUS DUST. I. AB-INITIO CALCULATIONS OF THE CONFIGURATION AND BINDING ENERGIES OF SMALL CARBON CLUSTERS”, *The Astrophysical Journal*, vol. 800, no. 1. American Astronomical Society, p. 30, Feb. 05, 2015. doi: 10.1088/0004-637x/800/1/30.  
  
C. Mauney, M. Buongiorno Nardelliand D. Lazzati, “FORMATION AND PROPERTIES OF ASTROPHYSICAL CARBONACEOUS DUST. I. AB-INITIO CALCULATIONS OF THE CONFIGURATION AND BINDING ENERGIES OF SMALL CARBON CLUSTERS”, *The Astrophysical Journal*, vol. 800, no. 1. American Astronomical Society, p. 30, Feb. 05, 2015. doi: 10.1088/0004-637x/800/1/30.  
  
C. Mauney, M. Buongiorno Nardelliand D. Lazzati, “FORMATION AND PROPERTIES OF ASTROPHYSICAL CARBONACEOUS DUST. I. AB-INITIO CALCULATIONS OF THE CONFIGURATION AND BINDING ENERGIES OF SMALL CARBON CLUSTERS”, *The Astrophysical Journal*, vol. 800, no. 1. American Astronomical Society, p. 30, Feb. 05, 2015. doi: 10.1088/0004-637x/800/1/30.  
  
C. Mauney, M. Buongiorno Nardelliand D. Lazzati, “FORMATION AND PROPERTIES OF ASTROPHYSICAL CARBONACEOUS DUST. I. AB-INITIO CALCULATIONS OF THE CONFIGURATION AND BINDING ENERGIES OF SMALL CARBON CLUSTERS”, *The Astrophysical Journal*, vol. 800, no. 1. American Astronomical Society, p. 30, Feb. 05, 2015. doi: 10.1088/0004-637x/800/1/30.  
  
X. Ma, “Engineering Complex, Layered Metal Oxides: High-Performance Nickelate Oxide Nanostructures for Oxygen Exchange and Reduction”, *ACS Catalysis*, vol. 5, no. 7. American Chemical Society (ACS), pp. 4013–4019, Jun. 05, 2015. doi: 10.1021/acscatal.5b00756.  
  
X. Ma, “Engineering Complex, Layered Metal Oxides: High-Performance Nickelate Oxide Nanostructures for Oxygen Exchange and Reduction”, *ACS Catalysis*, vol. 5, no. 7. American Chemical Society (ACS), pp. 4013–4019, Jun. 05, 2015. doi: 10.1021/acscatal.5b00756.  
  
E. McCartney-Melstad, M. Gidişand H. B. Shaffer, “Population Genomics of the Foothill Yellow-Legged Frog (*Rana boylii*) and RADseq Parameter Choice for Large-Genome Organisms”, *[]*. Cold Spring Harbor Laboratory, Sep. 10, 2017. doi: 10.1101/186635.  
  
R. T. McLaughlin, M. R. Diehland A. B. Kolomeisky, “Collective dynamics of processive cytoskeletal motors”, *Soft Matter*, vol. 12, no. 1. Royal Society of Chemistry (RSC), pp. 14–21, 2016. doi: 10.1039/c5sm01609f.  
  
J. S. Medlin, J. I. Cohenand D. L. Beck, “Vector potential and population dynamics for Amblyomma inornatum”, *Ticks and Tick-borne Diseases*, vol. 6, no. 4. Elsevier BV, pp. 463–472, Jun. 2015. doi: 10.1016/j.ttbdis.2015.03.014.  
  
J. E. Medvedeva, D. B. Buchholzand R. P. H. Chang, “Recent Advances in Understanding the Structure and Properties of Amorphous Oxide Semiconductors”, *Advanced Electronic Materials*, vol. 3, no. 9. Wiley, p. 1700082, Aug. 07, 2017. doi: 10.1002/aelm.201700082.  
  
N. I. Medvedeva, D. C. Van Akenand J. E. Medvedeva, “First-principles study of phosphorus embrittlement in austenitic steels with κ-carbide precipitates”, *Computational Materials Science*, vol. 138. Elsevier BV, pp. 105–110, Oct. 2017. doi: 10.1016/j.commatsci.2017.06.027.  
  
D. Mehra, M. S. Imtiaz, D. F. van Helden, B. C. Knollmannand D. R. Laver, “Multiple Modes of Ryanodine Receptor 2 Inhibition by Flecainide”, *Molecular Pharmacology*, vol. 86, no. 6. American Society for Pharmacology & Experimental Therapeutics (ASPET), pp. 696–706, Oct. 01, 2014. doi: 10.1124/mol.114.094623.  
  
S. R. Mehrotra, S. Kim, T. Kubis, M. Povolotskyi, M. S. Lundstromand G. Klimeck, “Engineering Nanowire n-MOSFETs at <formula formulatype=”inline”><tex Notation=“TeX”>$L\_{g}&amp;lt;8~{\rm nm}$</tex></formula>”, *IEEE Transactions on Electron Devices*, vol. 60, no. 7. Institute of Electrical and Electronics Engineers (IEEE), pp. 2171–2177, Jul. 2013. doi: 10.1109/ted.2013.2263806.  
  
N. A. Mehta and D. A. Levin, “Molecular Dynamics Studies of Nitrogen collision on Graphene and Quartz Surfaces”, *54th AIAA Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 02, 2016. doi: 10.2514/6.2016-0502.  
  
N. A. Mehta, D. A. Levinand A. van Duin, “Molecular Dynamics Studies of Thermal Accommodation on Carbon Surfaces”, *11th AIAA/ASME Joint Thermophysics and Heat Transfer Conference*. American Institute of Aeronautics and Astronautics, Jun. 13, 2014. doi: 10.2514/6.2014-2681.  
  
C. Meldgin, U. Ray, P. Russ, D. Chen, D. M. Ceperleyand B. DeMarco, “Probing the Bose glass–superfluid transition using quantum quenches of disorder”, *Nature Physics*, vol. 12, no. 7. Springer Science and Business Media LLC, pp. 646–649, Mar. 14, 2016. doi: 10.1038/nphys3695.  
  
E. Melnic, “Robust Packing Patterns and Luminescence Quenching in Mononuclear [Cu(II)(*phen*)2] Sulfates”, *The Journal of Physical Chemistry C*, vol. 118, no. 51. American Chemical Society (ACS), pp. 30087–30100, Dec. 11, 2014. doi: 10.1021/jp5085845.  
  
X. Meng, “Discovery of Fe2P-Type Ti(Zr/Hf)2O6 Photocatalysts toward Water Splitting”, *Chemistry of Materials*, vol. 28, no. 5. American Chemical Society (ACS), pp. 1335–1342, Feb. 23, 2016. doi: 10.1021/acs.chemmater.5b04256.  
  
G. Mera, “Metal-catalyst-free access to multiwalled carbon nanotubes/silica nanocomposites (MWCNT/SiO2) from a single-source precursor”, *Dalton Transactions*, vol. 48, no. 29. Royal Society of Chemistry (RSC), pp. 11018–11033, 2019. doi: 10.1039/c9dt01783f.  
  
A. Mesgarnejad, A. Imanianand A. Karma, “Phase-field models for fatigue crack growth”, *Theoretical and Applied Fracture Mechanics*, vol. 103. Elsevier BV, p. 102282, Oct. 2019. doi: 10.1016/j.tafmec.2019.102282.  
  
P. A. Meyer, “Data publication with the structural biology data grid supports live analysis”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Mar. 07, 2016. doi: 10.1038/ncomms10882.  
  
Y. Miao, S. E. Nicholsand J. A. McCammon, “Mapping of Allosteric Druggable Sites in Activation-Associated Conformers of the M2 Muscarinic Receptor”, *Chemical Biology & Drug Design*, vol. 83, no. 2. Wiley, pp. 237–246, Oct. 30, 2013. doi: 10.1111/cbdd.12233.  
  
T. Ming, B. Jin, J. Song, H. Luo, R. Duand Y. Ding, “3D computational models explain muscle activation patterns and energetic functions of internal structures in fish swimming”, *[]*. Cold Spring Harbor Laboratory, Feb. 20, 2019. doi: 10.1101/556126.  
  
D. D. L. Minh, “Implicit ligand theory: Rigorous binding free energies and thermodynamic expectations from molecular docking”, *The Journal of Chemical Physics*, vol. 137, no. 10. AIP Publishing, p. 104106, Sep. 13, 2012. doi: 10.1063/1.4751284.  
  
D. D. L. Minh and J. D. Chodera, “Estimating equilibrium ensemble averages using multiple time slices from driven nonequilibrium processes: Theory and application to free energies, moments, and thermodynamic length in single-molecule pulling experiments”, *The Journal of Chemical Physics*, vol. 134, no. 2. AIP Publishing, p. 024111, Jan. 14, 2011. doi: 10.1063/1.3516517.  
  
D. D. L. Minh and L. Makowski, “Wide-Angle X-Ray Solution Scattering for Protein-Ligand Binding: Multivariate Curve Resolution with Bayesian Confidence Intervals”, *Biophysical Journal*, vol. 104, no. 4. Elsevier BV, pp. 873–883, Feb. 2013. doi: 10.1016/j.bpj.2012.12.019.  
  
D. D. L. Minh and D. L. (Paul) . Minh, “Understanding the Hastings Algorithm”, *Communications in Statistics - Simulation and Computation*, vol. 44, no. 2. Informa UK Limited, pp. 332–349, Aug. 13, 2014. doi: 10.1080/03610918.2013.777455.  
  
D. L. (Paul) . Minh, D. D. L. Minhand A. L. Nguyen, “Regenerative Markov Chain Monte Carlo for Any Distribution”, *Communications in Statistics - Simulation and Computation*, vol. 41, no. 9. Informa UK Limited, pp. 1745–1760, Oct. 2012. doi: 10.1080/03610918.2011.615433.  
  
D. D. L. Minh, D. L. (Paul) . Minhand A. L. Nguyen, “Layer Sampling”, *Communications in Statistics - Simulation and Computation*, vol. 45, no. 1. Informa UK Limited, pp. 73–100, Jun. 23, 2014. doi: 10.1080/03610918.2013.854907.  
  
S. Mirarab, N. Nguyen, S. Guo, L.-S. Wang, J. Kimand T. Warnow, “PASTA: Ultra-Large Multiple Sequence Alignment for Nucleotide and Amino-Acid Sequences”, *Journal of Computational Biology*, vol. 22, no. 5. Mary Ann Liebert Inc, pp. 377–386, May 2015. doi: 10.1089/cmb.2014.0156.  
  
S. Mirarab and T. Warnow, “FASTSP: linear time calculation of alignment accuracy”, *Bioinformatics*, vol. 27, no. 23. Oxford University Press (OUP), pp. 3250–3258, Oct. 07, 2011. doi: 10.1093/bioinformatics/btr553.  
  
R. Mirzaeifar, Z. Qinand M. J. Buehler, “Tensile strength of carbyne chains in varied chemical environments and structural lengths”, *Nanotechnology*, vol. 25, no. 37. IOP Publishing, p. 371001, Aug. 22, 2014. doi: 10.1088/0957-4484/25/37/371001.  
  
M. Misiura, Q. Wang, M. S. Cheungand A. B. Kolomeisky, “Theoretical Investigations of the Role of Mutations in Dynamics of Kinesin Motor Proteins”, *The Journal of Physical Chemistry B*, vol. 122, no. 17. American Chemical Society (ACS), pp. 4653–4661, Apr. 09, 2018. doi: 10.1021/acs.jpcb.8b00830.  
  
S. Mitran, “Continuum-kinetic-microscopic model of lung clearance due to core-annular fluid entrainment”, *Journal of Computational Physics*, vol. 244. Elsevier BV, pp. 193–211, Jul. 2013. doi: 10.1016/j.jcp.2013.01.037.  
  
L. M. Mocanu, “EXTRAGALACTIC MILLIMETER-WAVE POINT-SOURCE CATALOG, NUMBER COUNTS AND STATISTICS FROM 771 deg2OF THE SPT-SZ SURVEY”, *The Astrophysical Journal*, vol. 779, no. 1. American Astronomical Society, p. 61, Nov. 25, 2013. doi: 10.1088/0004-637x/779/1/61.  
  
S. L. Moffitt, “Probing the Unique Role of Gallium in Amorphous Oxide Semiconductors through Structure–Property Relationships”, *Advanced Electronic Materials*, vol. 3, no. 10. Wiley, p. 1700189, Sep. 2017. doi: 10.1002/aelm.201700189.  
  
H. Mohimani, “Automated Genome Mining of Ribosomal Peptide Natural Products”, *ACS Chemical Biology*, vol. 9, no. 7. American Chemical Society (ACS), pp. 1545–1551, May 23, 2014. doi: 10.1021/cb500199h.  
  
H. Mohimani, S. Kimand P. A. Pevzner, “A New Approach to Evaluating Statistical Significance of Spectral Identifications”, *Journal of Proteome Research*, vol. 12, no. 4. American Chemical Society (ACS), pp. 1560–1568, Mar. 08, 2013. doi: 10.1021/pr300453t.  
  
H. Mohimani, W.-T. Liu, R. D. Kersten, B. S. Moore, P. C. Dorresteinand P. A. Pevzner, “NRPquest: Coupling Mass Spectrometry and Genome Mining for Nonribosomal Peptide Discovery”, *Journal of Natural Products*, vol. 77, no. 8. American Chemical Society (ACS), pp. 1902–1909, Aug. 12, 2014. doi: 10.1021/np500370c.  
  
H. Mohimani, “Cycloquest: Identification of Cyclopeptides via Database Search of Their Mass Spectra against Genome Databases”, *Journal of Proteome Research*, vol. 10, no. 10. American Chemical Society (ACS), pp. 4505–4512, Sep. 07, 2011. doi: 10.1021/pr200323a.  
  
H. Mohimani, “Multiplex De Novo Sequencing of Peptide Antibiotics”, *Journal of Computational Biology*, vol. 18, no. 11. Mary Ann Liebert Inc, pp. 1371–1381, Nov. 2011. doi: 10.1089/cmb.2011.0158.  
  
H. Mohimani and P. A. Pevzner, “Dereplication, sequencing and identification of peptidic natural products: from genome mining to peptidogenomics to spectral networks”, *Natural Product Reports*, vol. 33, no. 1. Royal Society of Chemistry (RSC), pp. 73–86, 2016. doi: 10.1039/c5np00050e.  
  
H. Mohimani, Y.-L. Yang, W.-T. Liu, P.-W. Hsieh, P. C. Dorresteinand P. A. Pevzner, “Sequencing cyclic peptides by multistage mass spectrometry”, *PROTEOMICS*, vol. 11, no. 18. Wiley, pp. 3642–3650, Aug. 09, 2011. doi: 10.1002/pmic.201000697.  
  
D. Mondal and A. Warshel, “EF-Tu and EF-G are activated by allosteric effects”, *Proceedings of the National Academy of Sciences*, vol. 115, no. 13. Proceedings of the National Academy of Sciences, pp. 3386–3391, Mar. 12, 2018. doi: 10.1073/pnas.1800054115.  
  
M. Mookherjee, “High-pressure elasticity of sodium majorite garnet, Na2MgSi5O12”, *American Mineralogist*, vol. 99, no. 11–12. Mineralogical Society of America, pp. 2416–2423, Nov. 01, 2014. doi: 10.2138/am-2014-4956.  
  
M. Mookherjee, H. Kepplerand C. E. Manning, “Aluminum speciation in aqueous fluids at deep crustal pressure and temperature”, *Geochimica et Cosmochimica Acta*, vol. 133. Elsevier BV, pp. 128–141, May 2014. doi: 10.1016/j.gca.2014.02.016.  
  
M. Mookherjee and D. Mainprice, “Unusually large shear wave anisotropy for chlorite in subduction zone settings”, *Geophysical Research Letters*, vol. 41, no. 5. American Geophysical Union (AGU), pp. 1506–1513, Mar. 11, 2014. doi: 10.1002/2014gl059334.  
  
M. Mookherjee and J. Tsuchiya, “Elasticity of superhydrous phase, B, Mg10Si3O14(OH)4”, *Physics of the Earth and Planetary Interiors*, vol. 238. Elsevier BV, pp. 42–50, Jan. 2015. doi: 10.1016/j.pepi.2014.10.010.  
  
J. J. Moore and C. Kesselman, “A resiliency model for high performance infrastructure based on logical encapsulation”, *Proceedings of the 21st international symposium on High-Performance Parallel and Distributed Computing*. ACM, Jun. 18, 2012. doi: 10.1145/2287076.2287118.  
  
M. Moradi, V. Babin, C. Rolandand C. Sagui, “A classical molecular dynamics investigation of the free energy and structure of short polyproline conformers”, *The Journal of Chemical Physics*, vol. 133, no. 12. AIP Publishing, p. 125104, Sep. 28, 2010. doi: 10.1063/1.3481087.  
  
M. Moradi, V. Babin, C. Rolandand C. Sagui, “Reaction path ensemble of the B–Z-DNA transition: a comprehensive atomistic study”, *Nucleic Acids Research*, vol. 41, no. 1. Oxford University Press (OUP), pp. 33–43, Oct. 25, 2012. doi: 10.1093/nar/gks1003.  
  
M. Moradi, V. Babin, C. Rolandand C. Sagui, “Are Long-Range Structural Correlations Behind the Aggregration Phenomena of Polyglutamine Diseases?”, *PLoS Computational Biology*, vol. 8, no. 4. Public Library of Science (PLoS), p. e1002501, Apr. 26, 2012. doi: 10.1371/journal.pcbi.1002501.  
  
M. Moradi, V. Babin, C. Saguiand C. Roland, “PPII Propensity of Multiple-Guest Amino Acids in a Proline-Rich Environment”, *The Journal of Physical Chemistry B*, vol. 115, no. 26. American Chemical Society (ACS), pp. 8645–8656, Jun. 14, 2011. doi: 10.1021/jp203874f.  
  
M. Moradi, V. Babin, C. Saguiand C. Roland, “A Statistical Analysis of the PPII Propensity of Amino Acid Guests in Proline-Rich Peptides”, *Biophysical Journal*, vol. 100, no. 4. Elsevier BV, pp. 1083–1093, Feb. 2011. doi: 10.1016/j.bpj.2010.12.3742.  
  
M. Moradi, V. Babin, C. Saguiand C. Roland, “Recipes for Free Energy Calculations in Biomolecular Systems”, *Methods in Molecular Biology*. Humana Press, pp. 313–337, Aug. 18, 2012. doi: 10.1007/978-1-62703-017-5\_12.  
  
M. Moradi, C. Saguiand C. Roland, “Investigating rare events with nonequilibrium work measurements. II. Transition and reaction rates”, *The Journal of Chemical Physics*, vol. 140, no. 3. AIP Publishing, p. 034115, Jan. 21, 2014. doi: 10.1063/1.4861056.  
  
M. Moradi, C. Saguiand C. Roland, “Investigating rare events with nonequilibrium work measurements. I. Nonequilibrium transition path probabilities”, *The Journal of Chemical Physics*, vol. 140, no. 3. AIP Publishing, p. 034114, Jan. 21, 2014. doi: 10.1063/1.4861055.  
  
C. Morningstar, “Lattice QCD Study of Excited Hadron Resonances”, *Acta Physica Polonica B Proceedings Supplement*, vol. 9, no. 3. Jagiellonian University, p. 421, 2016. doi: 10.5506/aphyspolbsupp.9.421.  
  
L. Moshe, “Modulating the structure and interactions of lipid–peptide complexes by varying membrane composition and solution conditions”, *Soft Matter*, vol. 9, no. 29. Royal Society of Chemistry (RSC), p. 7117, 2013. doi: 10.1039/c3sm00105a.  
  
P. Motter, K. Sood, E. Jessupand B. Norris, “Lighthouse”, *Proceedings of the 3rd International Workshop on Software Engineering for High Performance Computing in Computational Science and Engineering*. ACM, Nov. 15, 2015. doi: 10.1145/2830168.2830169.  
  
F. Moucka, D. Bratkoand A. Luzar, “Electrolyte pore/solution partitioning by expanded grand canonical ensemble Monte Carlo simulation”, *The Journal of Chemical Physics*, vol. 142, no. 12. AIP Publishing, p. 124705, Mar. 27, 2015. doi: 10.1063/1.4914461.  
  
Q. Mou, C. J. Benmoreand J. L. Yarger, “*X-ray Intermolecular Structure Factor*(*XISF*): separation of intra- and intermolecular interactions from total X-ray scattering data”, *Journal of Applied Crystallography*, vol. 48, no. 3. International Union of Crystallography (IUCr), pp. 950–952, May 09, 2015. doi: 10.1107/s1600576715005518.  
  
D. D. Mowrey, “Open-Channel Structures of the Human Glycine Receptor α1 Full-Length Transmembrane Domain”, *Structure*, vol. 21, no. 10. Elsevier BV, pp. 1897–1904, Oct. 2013. doi: 10.1016/j.str.2013.07.014.  
  
V. Mozhayskiy, B. Miller, K.-L. Maand I. Tagkopoulos, “A scalable multi-scale framework for parallel simulation and visualization of microbial evolution”, *Proceedings of the 2011 TeraGrid Conference: Extreme Digital Discovery*. ACM, Jul. 18, 2011. doi: 10.1145/2016741.2016749.  
  
C. L. Muhich, B. D. Ehrhart, I. Al-Shankiti, B. J. Ward, C. B. Musgraveand A. W. Weimer, “A review and perspective of efficient hydrogen generation via solar thermal water splitting”, *Wiley Interdisciplinary Reviews: Energy and Environment*, vol. 5, no. 3. Wiley, pp. 261–287, May 21, 2015. doi: 10.1002/wene.174.  
  
C. L. Muhich, “Predicting the solar thermochemical water splitting ability and reaction mechanism of metal oxides: a case study of the hercynite family of water splitting cycles”, *Energy & Environmental Science*, vol. 8, no. 12. Royal Society of Chemistry (RSC), pp. 3687–3699, 2015. doi: 10.1039/c5ee01979f.  
  
C. L. Muhich, “Efficient Generation of H 2 by Splitting Water with an Isothermal Redox Cycle”, *Science*, vol. 341, no. 6145. American Association for the Advancement of Science (AAAS), pp. 540–542, Aug. 02, 2013. doi: 10.1126/science.1239454.  
  
S. Mukherjee, R. Alhadeffand A. Warshel, “Simulating the dynamics of the mechanochemical cycle of myosin-V”, *Proceedings of the National Academy of Sciences*, vol. 114, no. 9. Proceedings of the National Academy of Sciences, pp. 2259–2264, Feb. 13, 2017. doi: 10.1073/pnas.1700318114.  
  
S. Mukherjee and A. Warshel, “The FOF1 ATP synthase: from atomistic three-dimensional structure to the rotary-chemical function”, *Photosynthesis Research*, vol. 134, no. 1. Springer Science and Business Media LLC, pp. 1–15, Jul. 03, 2017. doi: 10.1007/s11120-017-0411-x.  
  
G. M. Mullen, L. Zhang, E. J. Evans Jr., T. Yan, G. Henkelmanand C. B. Mullins, “Oxygen and Hydroxyl Species Induce Multiple Reaction Pathways for the Partial Oxidation of Allyl Alcohol on Gold”, *Journal of the American Chemical Society*, vol. 136, no. 17. American Chemical Society (ACS), pp. 6489–6498, Apr. 16, 2014. doi: 10.1021/ja502347d.  
  
G. M. Mullen, L. Zhang, E. J. Evans, T. Yan, G. Henkelmanand C. B. Mullins, “Control of selectivity in allylic alcohol oxidation on gold surfaces: the role of oxygen adatoms and hydroxyl species”, *Physical Chemistry Chemical Physics*, vol. 17, no. 6. Royal Society of Chemistry (RSC), pp. 4730–4738, 2015. doi: 10.1039/c4cp04739g.  
  
D. J. Muñoz, K. Kratter, V. Springeland L. Hernquist, “Planet–disc interaction on a freely moving mesh”, *Monthly Notices of the Royal Astronomical Society*, vol. 445, no. 4. Oxford University Press (OUP), pp. 3475–3495, Oct. 29, 2014. doi: 10.1093/mnras/stu1918.  
  
D. J. Muñoz, K. Kratter, M. Vogelsberger, L. Hernquistand V. Springel, “Stellar orbit evolution in close circumstellar disc encounters”, *Monthly Notices of the Royal Astronomical Society*, vol. 446, no. 2. Oxford University Press (OUP), pp. 2010–2029, Nov. 22, 2014. doi: 10.1093/mnras/stu2220.  
  
D. J. Muñoz, V. Springel, R. Marcus, M. Vogelsbergerand L. Hernquist, “Multidimensional, compressible viscous flow on a moving Voronoi mesh”, *Monthly Notices of the Royal Astronomical Society*, vol. 428, no. 1. Oxford University Press (OUP), pp. 254–279, Oct. 26, 2012. doi: 10.1093/mnras/sts015.  
  
B. Murray, “A2T and A2V Aβ peptides exhibit different aggregation kinetics, primary nucleation, morphology, structure, and LTP inhibition”, *Proteins: Structure, Function, and Bioinformatics*, vol. 84, no. 4. Wiley, pp. 488–500, Feb. 23, 2016. doi: 10.1002/prot.24995.  
  
A. Nair, “Combining self-supervised learning and imitation for vision-based rope manipulation”, *2017 IEEE International Conference on Robotics and Automation (ICRA)*. IEEE, May 2017. doi: 10.1109/icra.2017.7989247.  
  
A. K. Nair, A. Gautieri, S.-W. Changand M. J. Buehler, “Molecular mechanics of mineralized collagen fibrils in bone”, *Nature Communications*, vol. 4, no. 1. Springer Science and Business Media LLC, Apr. 16, 2013. doi: 10.1038/ncomms2720.  
  
N. Nakamura, “Automated specimen search in cryo-TEM observation with DIFF-defocus imaging”, *Journal of Electron Microscopy*, vol. 59, no. 4. Oxford University Press (OUP), pp. 299–310, Mar. 30, 2010. doi: 10.1093/jmicro/dfq009.  
  
A. Nakayama, G. Arai, S. Yamazakiand T. Taketsugu, “Solvent effects on the ultrafast nonradiative deactivation mechanisms of thymine in aqueous solution: Excited-state QM/MM molecular dynamics simulations”, *The Journal of Chemical Physics*, vol. 139, no. 21. AIP Publishing, p. 214304, Dec. 07, 2013. doi: 10.1063/1.4833563.  
  
S. K. Mohan Nalluri, “Discrete Dimers of Redox-Active and Fluorescent Perylene Diimide-Based Rigid Isosceles Triangles in the Solid State”, *Journal of the American Chemical Society*, vol. 141, no. 3. American Chemical Society (ACS), pp. 1290–1303, Dec. 11, 2018. doi: 10.1021/jacs.8b11201.  
  
D. J. Needleman, “Ion specific effects in bundling and depolymerization of taxol-stabilized microtubules”, *Faraday Discussions*, vol. 166. Royal Society of Chemistry (RSC), p. 31, 2013. doi: 10.1039/c3fd00063j.  
  
L. M. Negrón, Y. Meléndez-Contésand J. M. Rivera, “Patchy Supramolecules as Versatile Tools To Probe Hydrophobicity in Nanoglobular Systems”, *Journal of the American Chemical Society*, vol. 135, no. 10. American Chemical Society (ACS), pp. 3815–3817, Feb. 27, 2013. doi: 10.1021/ja401373h.  
  
A. Neisius, “Improving the lens design and performance of a contemporary electromagnetic shock wave lithotripter”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 13. Proceedings of the National Academy of Sciences, Mar. 17, 2014. doi: 10.1073/pnas.1319203111.  
  
N.-. phuong D. Nguyen, S. Mirarab, K. Kumarand T. Warnow, “Ultra-large alignments using phylogeny-aware profiles”, *Genome Biology*, vol. 16, no. 1. Springer Science and Business Media LLC, Jun. 16, 2015. doi: 10.1186/s13059-015-0688-z.  
  
N.-. phuong . Nguyen, S. Mirarab, B. Liu, M. Popand T. Warnow, “TIPP: taxonomic identification and phylogenetic profiling”, *Bioinformatics*, vol. 30, no. 24. Oxford University Press (OUP), pp. 3548–3555, Oct. 29, 2014. doi: 10.1093/bioinformatics/btu721.  
  
N. Nguyen, S. Miraraband T. Warnow, “MRL and SuperFine+MRL: new supertree methods”, *Algorithms for Molecular Biology*, vol. 7, no. 1. Springer Science and Business Media LLC, Jan. 26, 2012. doi: 10.1186/1748-7188-7-3.  
  
N.-P. Nguyen, T. Warnow, M. Popand B. White, “A perspective on 16S rRNA operational taxonomic unit clustering using sequence similarity”, *npj Biofilms and Microbiomes*, vol. 2, no. 1. Springer Science and Business Media LLC, Apr. 20, 2016. doi: 10.1038/npjbiofilms.2016.4.  
  
N.-P. Nguyen, T. Warnow, M. Popand B. White, “A perspective on 16S rRNA operational taxonomic unit clustering using sequence similarity”, *npj Biofilms and Microbiomes*, vol. 2, no. 1. Springer Science and Business Media LLC, Apr. 20, 2016. doi: 10.1038/npjbiofilms.2016.4.  
  
T. H. Nguyen and D. D. L. Minh, “Intermediate Thermodynamic States Contribute Equally to Free Energy Convergence: A Demonstration with Replica Exchange”, *Journal of Chemical Theory and Computation*, vol. 12, no. 5. American Chemical Society (ACS), pp. 2154–2161, Apr. 21, 2016. doi: 10.1021/acs.jctc.6b00060.  
  
A. E. Noble, N. M. Temme, W. F. Faganand T. H. Keitt, “A sampling theory for asymmetric communities”, *Journal of Theoretical Biology*, vol. 273, no. 1. Elsevier BV, pp. 1–14, Mar. 2011. doi: 10.1016/j.jtbi.2010.12.021.  
  
S. Nouranian, S. R. Gwaltney, M. I. Baskes, M. A. Tschoppand M. F. Horstemeyer, “Simulations of tensile bond rupture in single alkane molecules using reactive interatomic potentials”, *Chemical Physics Letters*, vol. 635. Elsevier BV, pp. 278–284, Aug. 2015. doi: 10.1016/j.cplett.2015.06.071.  
  
S. Nouranian, M. A. Tschopp, S. R. Gwaltney, M. I. Baskesand M. F. Horstemeyer, “An interatomic potential for saturated hydrocarbons based on the modified embedded-atom method”, *Phys. Chem. Chem. Phys.*, vol. 16, no. 13. Royal Society of Chemistry (RSC), pp. 6233–6249, 2014. doi: 10.1039/c4cp00027g.  
  
A. Nova, S. Keten, N. M. Pugno, A. Redaelliand M. J. Buehler, “Molecular and Nanostructural Mechanisms of Deformation, Strength and Toughness of Spider Silk Fibrils”, *Nano Letters*, vol. 10, no. 7. American Chemical Society (ACS), pp. 2626–2634, Jun. 02, 2010. doi: 10.1021/nl101341w.  
  
B. Novakovic and G. Klimeck, “Atomistic quantum transport approach to time-resolved device simulations”, *2015 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)*. IEEE, Sep. 2015. doi: 10.1109/sispad.2015.7292245.  
  
C. M. Oaida, Y. Xue, M. G. Flanner, S. M. Skiles, F. De Salesand T. H. Painter, “Improving snow albedo processes in WRF/SSiB regional climate model to assess impact of dust and black carbon in snow on surface energy balance and hydrology over western U.S.”, *Journal of Geophysical Research: Atmospheres*, vol. 120, no. 8. American Geophysical Union (AGU), pp. 3228–3248, Apr. 27, 2015. doi: 10.1002/2014jd022444.  
  
J. S. Oh, “Evidence for Anionic Excess Electrons in a Quasi-Two-Dimensional Ca2N Electride by Angle-Resolved Photoemission Spectroscopy”, *Journal of the American Chemical Society*, vol. 138, no. 8. American Chemical Society (ACS), pp. 2496–2499, Feb. 17, 2016. doi: 10.1021/jacs.5b12668.  
  
M. A. Ojeda-Lopez, “Transformation of taxol-stabilized microtubules into inverted tubulin tubules triggered by a tubulin conformation switch”, *Nature Materials*, vol. 13, no. 2. Springer Science and Business Media LLC, pp. 195–203, Jan. 19, 2014. doi: 10.1038/nmat3858.  
  
C. Y. Ok, “Prevalence and Clinical Implications of Epstein–Barr Virus Infection in *De Novo* Diffuse Large B-Cell Lymphoma in Western Countries”, *Clinical Cancer Research*, vol. 20, no. 9. American Association for Cancer Research (AACR), pp. 2338–2349, Apr. 30, 2014. doi: 10.1158/1078-0432.ccr-13-3157.  
  
G. S. Oliveira, “Molecular modeling of enzyme attachment on AFM probes”, *Journal of Molecular Graphics and Modelling*, vol. 45. Elsevier BV, pp. 128–136, Sep. 2013. doi: 10.1016/j.jmgm.2013.08.007.  
  
E. Onuk, “Effects of Catalytic Action and Ligand Binding on Conformational Ensembles of Adenylate Kinase”, *Biochemistry*, vol. 56, no. 34. American Chemical Society (ACS), pp. 4559–4567, Aug. 16, 2017. doi: 10.1021/acs.biochem.7b00351.  
  
Y. W. Oo, “Essential Role of Calmodulin in RyR Inhibition by Dantrolene”, *Molecular Pharmacology*, vol. 88, no. 1. American Society for Pharmacology & Experimental Therapeutics (ASPET), pp. 57–63, Apr. 28, 2015. doi: 10.1124/mol.115.097691.  
  
M. A. Opazo, S. P. Ong, P. Vargas, C. A. Rossand J. M. Florez, “Oxygen-vacancy tuning of magnetism in perovskite”, *Physical Review Materials*, vol. 3, no. 1. American Physical Society (APS), Jan. 10, 2019. doi: 10.1103/physrevmaterials.3.014404.  
  
C. N. M. Ouma, M. Z. Mapelu, N. W. Makau, G. O. Amoloand R. Maezono, “Quantum Monte Carlo study of pressure-inducedphase transition in GaAs”, *Physical Review B*, vol. 86, no. 10. American Physical Society (APS), Sep. 28, 2012. doi: 10.1103/physrevb.86.104115.  
  
C. N. M. Ouma and W. E. Meyer, “Ab initio study of metastability of Eu3+ defect complexes in GaN”, *Physica B: Condensed Matter*, vol. 439. Elsevier BV, pp. 141–143, Apr. 2014. doi: 10.1016/j.physb.2013.11.004.  
  
M. Owkes and O. Desjardins, “A discontinuous Galerkin conservative level set scheme for interface capturing in multiphase flows”, *Journal of Computational Physics*, vol. 249. Elsevier BV, pp. 275–302, Sep. 2013. doi: 10.1016/j.jcp.2013.04.036.  
  
M. Owkes and O. Desjardins, “A computational framework for conservative, three-dimensional, unsplit, geometric transport with application to the volume-of-fluid (VOF) method”, *Journal of Computational Physics*, vol. 270. Elsevier BV, pp. 587–612, Aug. 2014. doi: 10.1016/j.jcp.2014.04.022.  
  
P. Padmanabhan, M. Chavis, C. K. Oberand F. A. Escobedo, “Phase behaviour of PMMA-b-PHEMA with solvents methanol and THF: modelling and comparison to the experiment”, *Soft Matter*, vol. 10, no. 33. Royal Society of Chemistry (RSC), pp. 6172–6181, 2014. doi: 10.1039/c4sm00856a.  
  
F. Palacios, “Stanford University Unstructured (SU2): Analysis and Design Technology for Turbulent Flows”, *52nd Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 10, 2014. doi: 10.2514/6.2014-0243.  
  
G. Pandav, V. Pryamitsyn, J. Erringtonand V. Ganesan, “Multibody Interactions, Phase Behavior, and Clustering in Nanoparticle–Polyelectrolyte Mixtures”, *The Journal of Physical Chemistry B*, vol. 119, no. 45. American Chemical Society (ACS), pp. 14536–14550, Oct. 30, 2015. doi: 10.1021/acs.jpcb.5b07905.  
  
G. Pandav, V. Pryamitsynand V. Ganesan, “Interactions and Aggregation of Charged Nanoparticles in Uncharged Polymer Solutions”, *Langmuir*, vol. 31, no. 45. American Chemical Society (ACS), pp. 12328–12338, Nov. 04, 2015. doi: 10.1021/acs.langmuir.5b02885.  
  
F. Pan, C. Rolandand C. Sagui, “Ion distributions around left- and right-handed DNA and RNA duplexes: a comparative study”, *Nucleic Acids Research*, vol. 42, no. 22. Oxford University Press (OUP), pp. 13981–13996, Nov. 26, 2014. doi: 10.1093/nar/gku1107.  
  
L. Pan and S. G. Aller, “Allosteric Role of Substrate Occupancy Toward the Alignment of P-glycoprotein Nucleotide Binding Domains”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, Oct. 02, 2018. doi: 10.1038/s41598-018-32815-2.  
  
L. Pan and J. P. Segrest, “Computational studies of plasma lipoprotein lipids”, *Biochimica et Biophysica Acta (BBA) - Biomembranes*, vol. 1858, no. 10. Elsevier BV, pp. 2401–2420, Oct. 2016. doi: 10.1016/j.bbamem.2016.03.010.  
  
T. Pan, Y. Luand S. Lloyd, “Quantum-Chemistry Study of Asphalt Oxidative Aging: An XPS-Aided Analysis”, *Industrial & Engineering Chemistry Research*, vol. 51, no. 23. American Chemical Society (ACS), pp. 7957–7966, May 24, 2012. doi: 10.1021/ie3007215.  
  
S. S. Park and J. Gervay-Hague, “Synthesis of Partially *O-*Acetylated *N*-Acetylneuraminic Acid Using Regioselective Silyl Exchange Technology”, *Organic Letters*, vol. 16, no. 19. American Chemical Society (ACS), pp. 5044–5047, Sep. 23, 2014. doi: 10.1021/ol502389g.  
  
P. E. Pascuzzi, “In Vivo Mapping of *Arabidopsis* Scaffold/Matrix Attachment Regions Reveals Link to Nucleosome-Disfavoring Poly(dA:dT) Tracts”, *The Plant Cell*, vol. 26, no. 1. Oxford University Press (OUP), pp. 102–120, Jan. 2014. doi: 10.1105/tpc.113.121194.  
  
S. S. Patel, M. Min, K. C. Ugaand T. Lee, “A spectral-element discontinuous Galerkin lattice Boltzmann method for simulating natural convection heat transfer in a horizontal concentric annulus”, *Computers & Fluids*, vol. 95. Elsevier BV, pp. 197–209, May 2014. doi: 10.1016/j.compfluid.2014.02.021.  
  
B. Paxton, L. Bildsten, A. Dotter, F. Herwig, P. Lesaffreand F. Timmes, “MODULES FOR EXPERIMENTS IN STELLAR ASTROPHYSICS (MESA)”, *The Astrophysical Journal Supplement Series*, vol. 192, no. 1. American Astronomical Society, p. 3, Dec. 15, 2010. doi: 10.1088/0067-0049/192/1/3.  
  
B. Paxton, “MODULES FOR EXPERIMENTS IN STELLAR ASTROPHYSICS (MESA): PLANETS, OSCILLATIONS, ROTATION, AND MASSIVE STARS”, *The Astrophysical Journal Supplement Series*, vol. 208, no. 1. American Astronomical Society, p. 4, Aug. 28, 2013. doi: 10.1088/0067-0049/208/1/4.  
  
G. Paytakov, T. Dinadayalaneand J. Leszczynski, “Toward Selection of Efficient Density Functionals for van der Waals Molecular Complexes: Comparative Study of C–H···π and N–H···π Interactions”, *The Journal of Physical Chemistry A*, vol. 119, no. 7. American Chemical Society (ACS), pp. 1190–1200, Feb. 06, 2015. doi: 10.1021/jp511450u.  
  
F. Peng, Y. Yao, H. Liuand Y. Ma, “Crystalline LiN5 Predicted from First-Principles as a Possible High-Energy Material”, *The Journal of Physical Chemistry Letters*, vol. 6, no. 12. American Chemical Society (ACS), pp. 2363–2366, Jun. 09, 2015. doi: 10.1021/acs.jpclett.5b00995.  
  
P.-C. Peng, M. A. Hassan Sameeand S. Sinha, “Incorporating Chromatin Accessibility Data into Sequence-to-Expression Modeling”, *Biophysical Journal*, vol. 108, no. 5. Elsevier BV, pp. 1257–1267, Mar. 2015. doi: 10.1016/j.bpj.2014.12.037.  
  
Y. Peng, “A Metastable Contact and Structural Disorder in the Estrogen Receptor Transactivation Domain”, *Structure*, vol. 27, no. 2. Elsevier BV, pp. 229–240.e4, Feb. 2019. doi: 10.1016/j.str.2018.10.026.  
  
Y. Peng, “A Metastable Contact and Structural Disorder in the Estrogen Receptor Transactivation Domain”, *Structure*, vol. 27, no. 2. Elsevier BV, pp. 229–240.e4, Feb. 2019. doi: 10.1016/j.str.2018.10.026.  
  
E. Perepelitsky and B. Sriram Shastry, “Extremely correlated Fermi liquids in the limit of infinite dimensions”, *Annals of Physics*, vol. 338. Elsevier BV, pp. 283–301, Nov. 2013. doi: 10.1016/j.aop.2013.09.010.  
  
E. Perepelitsky and B. Sriram Shastry, “Diagrammatic series for extremely correlated Fermi liquids”, *Annals of Physics*, vol. 357. Elsevier BV, pp. 1–39, Jun. 2015. doi: 10.1016/j.aop.2015.03.010.  
  
J. Pérez-Mayoral, A. L. Pacheco-Torres, L. Morales, H. Acosta-Rodríguez, J. L. Mattaand J. Dutil, “Genetic polymorphisms in *RAD23B* and *XPC* modulate DNA repair capacity and breast cancer risk in Puerto Rican women”, *Molecular Carcinogenesis*, vol. 52, no. S1. Wiley, pp. 127–138, Jun. 18, 2013. doi: 10.1002/mc.22056.  
  
B. Phillabaum, E. W. Carlsonand K. A. Dahmen, “Spatial complexity due to bulk electronic nematicity in a superconducting underdoped cuprate”, *Nature Communications*, vol. 3, no. 1. Springer Science and Business Media LLC, Jun. 26, 2012. doi: 10.1038/ncomms1920.  
  
T. Phillips, R. DeLeonand I. Senocak, “Dynamic rating of overhead transmission lines over complex terrain using a large-eddy simulation paradigm”, *Renewable Energy*, vol. 108. Elsevier BV, pp. 380–389, Aug. 2017. doi: 10.1016/j.renene.2017.02.072.  
  
G. D. Pintilie, J. Zhang, T. D. Goddard, W. Chiuand D. C. Gossard, “Quantitative analysis of cryo-EM density map segmentation by watershed and scale-space filtering, and fitting of structures by alignment to regions”, *Journal of Structural Biology*, vol. 170, no. 3. Elsevier BV, pp. 427–438, Jun. 2010. doi: 10.1016/j.jsb.2010.03.007.  
  
M. Plecnik and J. M. McCarthy, “Dimensional Synthesis of Six-Bar Linkage as a Constrained RPR Chain”, *New Trends in Mechanism and Machine Science*. Springer Netherlands, pp. 273–280, Aug. 10, 2012. doi: 10.1007/978-94-007-4902-3\_29.  
  
M. M. Plecnik and J. Michael McCarthy, “Numerical Synthesis of Six-Bar Linkages for Mechanical Computation”, *Journal of Mechanisms and Robotics*, vol. 6, no. 3. ASME International, Jun. 17, 2014. doi: 10.1115/1.4027443.  
  
M. Plecnik, J. M. McCarthyand C. W. Wampler, “Kinematic Synthesis of a Watt I Six-Bar Linkage for Body Guidance”, *Advances in Robot Kinematics*. Springer International Publishing, pp. 317–325, 2014. doi: 10.1007/978-3-319-06698-1\_33.  
  
B. H. Pogostin, A. Malmendal, C. H. Londerganand K. S. Åkerfeldt, “pKa Determination of a Histidine Residue in a Short Peptide Using Raman Spectroscopy”, *Molecules*, vol. 24, no. 3. MDPI AG, p. 405, Jan. 23, 2019. doi: 10.3390/molecules24030405.  
  
P. Pongkitiwanichakul, K. D. Makwanaand D. Ruffolo, “Driving reconnection in sheared magnetic configurations with forced fluctuations”, *Physics of Plasmas*, vol. 25, no. 2. AIP Publishing, p. 022114, Feb. 2018. doi: 10.1063/1.5014026.  
  
I. Ponomarev, A. C. T. van Duinand P. Kroll, “Reactive Force Field for Simulations of the Pyrolysis of Polysiloxanes into Silicon Oxycarbide Ceramics”, *The Journal of Physical Chemistry C*, vol. 123, no. 27. American Chemical Society (ACS), pp. 16804–16812, Jun. 10, 2019. doi: 10.1021/acs.jpcc.9b03810.  
  
M. Popowski, “Bright/Arid3A Acts as a Barrier to Somatic Cell Reprogramming through Direct Regulation of Oct4, Sox2, and Nanog”, *Stem Cell Reports*, vol. 2, no. 1. Elsevier BV, pp. 26–35, Jan. 2014. doi: 10.1016/j.stemcr.2013.12.002.  
  
M. L. Powers, A. G. McDermott, N. C. Shanerand S. H. D. Haddock, “Expression and characterization of the calcium-activated photoprotein from the ctenophore Bathocyroe fosteri: Insights into light-sensitive photoproteins”, *Biochemical and Biophysical Research Communications*, vol. 431, no. 2. Elsevier BV, pp. 360–366, Feb. 2013. doi: 10.1016/j.bbrc.2012.12.026.  
  
S. K. Prasad, “A vision for GPU-accelerated parallel computation on geo-spatial datasets”, *SIGSPATIAL Special*, vol. 6, no. 3. Association for Computing Machinery (ACM), pp. 19–26, Apr. 22, 2015. doi: 10.1145/2766196.2766200.  
  
S. K. Prasad, S. Shekhar, M. McDermott, X. Zhou, M. Evansand S. Puri, “GPGPU-accelerated interesting interval discovery and other computations on GeoSpatial datasets”, *Proceedings of the 2nd ACM SIGSPATIAL International Workshop on Analytics for Big Geospatial Data*. ACM, Nov. 04, 2013. doi: 10.1145/2534921.2535837.  
  
V. Pryamitsyn and V. Ganesan, “Interplay between Depletion and Electrostatic Interactions in Polyelectrolyte–Nanoparticle Systems”, *Macromolecules*, vol. 47, no. 17. American Chemical Society (ACS), pp. 6095–6112, Aug. 19, 2014. doi: 10.1021/ma501014u.  
  
V. Pryamitsyn and V. Ganesan, “Pair interactions in polyelectrolyte-nanoparticle systems: Influence of dielectric inhomogeneities and the partial dissociation of polymers and nanoparticles”, *The Journal of Chemical Physics*, vol. 143, no. 16. AIP Publishing, p. 164904, Oct. 28, 2015. doi: 10.1063/1.4934242.  
  
V. Prytkova, M. Heyden, D. Tobiasand J. A. Freites, “Introducing Molecular Flexibility in Efficient Simulations of Many-Protein Systems”, *Biophysical Journal*, vol. 108, no. 2. Elsevier BV, p. 470a, Jan. 2015. doi: 10.1016/j.bpj.2014.11.2567.  
  
N. M. Pugno, S. W. Cranfordand M. J. Buehler, “Synergetic Material and Structure Optimization Yields Robust Spider Web Anchorages”, *Small*, vol. 9, no. 16. Wiley, pp. 2747–2756, Apr. 15, 2013. doi: 10.1002/smll.201201343.  
  
S. Qin, D. D. L. Minh, J. A. McCammonand H.-X. Zhou, “Method to Predict Crowding Effects by Postprocessing Molecular Dynamics Trajectories: Application to the Flap Dynamics of HIV-1 Protease”, *The Journal of Physical Chemistry Letters*, vol. 1, no. 1. American Chemical Society (ACS), pp. 107–110, Nov. 09, 2009. doi: 10.1021/jz900023w.  
  
Y. Qin, “Rationally Designed 3D Fe and N Codoped Graphene with Superior Electrocatalytic Activity toward Oxygen Reduction”, *Small*, vol. 12, no. 19. Wiley, pp. 2549–2553, Mar. 23, 2016. doi: 10.1002/smll.201600282.  
  
Z. Qin and M. J. Buehler, “Structure and dynamics of human vimentin intermediate filament dimer and tetramer in explicit and implicit solvent models”, *Journal of Molecular Modeling*, vol. 17, no. 1. Springer Science and Business Media LLC, pp. 37–48, Apr. 01, 2010. doi: 10.1007/s00894-010-0696-6.  
  
Z. Qin and M. J. Buehler, “Flaw Tolerance of Nuclear Intermediate Filament Lamina under Extreme Mechanical Deformation”, *ACS Nano*, vol. 5, no. 4. American Chemical Society (ACS), pp. 3034–3042, Mar. 25, 2011. doi: 10.1021/nn200107u.  
  
Z. Qin and M. J. Buehler, “Impact tolerance in mussel thread networks by heterogeneous material distribution”, *Nature Communications*, vol. 4, no. 1. Springer Science and Business Media LLC, Jul. 23, 2013. doi: 10.1038/ncomms3187.  
  
Z. Qin and M. J. Buehler, “Molecular mechanics of mussel adhesion proteins”, *Journal of the Mechanics and Physics of Solids*, vol. 62. Elsevier BV, pp. 19–30, Jan. 2014. doi: 10.1016/j.jmps.2013.08.015.  
  
Z. Qin, L. Dimas, D. Adler, G. Bratzeland M. J. Buehler, “Biological materials by design”, *Journal of Physics: Condensed Matter*, vol. 26, no. 7. IOP Publishing, p. 073101, Jan. 22, 2014. doi: 10.1088/0953-8984/26/7/073101.  
  
Z. Qin, A. Gautieri, A. K. Nair, H. Inbarand M. J. Buehler, “Thickness of Hydroxyapatite Nanocrystal Controls Mechanical Properties of the Collagen–Hydroxyapatite Interface”, *Langmuir*, vol. 28, no. 4. American Chemical Society (ACS), pp. 1982–1992, Jan. 18, 2012. doi: 10.1021/la204052a.  
  
Z. Qin, A. Kalinowski, K. N. Dahland M. J. Buehler, “Structure and stability of the lamin A tail domain and HGPS mutant”, *Journal of Structural Biology*, vol. 175, no. 3. Elsevier BV, pp. 425–433, Sep. 2011. doi: 10.1016/j.jsb.2011.05.015.  
  
Z. Qin, N. M. Pugnoand M. J. Buehler, “Mechanics of fragmentation of crocodile skin and other thin films”, *Scientific Reports*, vol. 4, no. 1. Springer Science and Business Media LLC, May 27, 2014. doi: 10.1038/srep04966.  
  
Z. Qin, M. Taylor, M. Hwang, K. Bertoldiand M. J. Buehler, “Effect of Wrinkles on the Surface Area of Graphene: Toward the Design of Nanoelectronics”, *Nano Letters*, vol. 14, no. 11. American Chemical Society (ACS), pp. 6520–6525, Oct. 24, 2014. doi: 10.1021/nl503097u.  
  
Z. Qin, “Quantitative Comparison of Photothermal Heat Generation between Gold Nanospheres and Nanorods”, *Scientific Reports*, vol. 6, no. 1. Springer Science and Business Media LLC, Jul. 21, 2016. doi: 10.1038/srep29836.  
  
H. Qiu, A. Sarathy, J.-P. Leburtonand K. Schulten, “Intrinsic Stepwise Translocation of Stretched ssDNA in Graphene Nanopores”, *Nano Letters*, vol. 15, no. 12. American Chemical Society (ACS), pp. 8322–8330, Nov. 25, 2015. doi: 10.1021/acs.nanolett.5b03963.  
  
H. Qiu, A. Sarathy, J.-P. Leburtonand K. Schulten, “Stepwise Transport of Stretched ssDNA Through Graphene Nanopores”, *Biophysical Journal*, vol. 110, no. 3. Elsevier BV, p. 508a, Feb. 2016. doi: 10.1016/j.bpj.2015.11.2716.  
  
H. Qiu, A. Sarathy, K. Schultenand J.-P. Leburton, “Detection and mapping of DNA methylation with 2D material nanopores”, *npj 2D Materials and Applications*, vol. 1, no. 1. Springer Science and Business Media LLC, Apr. 11, 2017. doi: 10.1038/s41699-017-0005-7.  
  
N. Ramakrishnan, P. B. Sunil Kumarand R. Radhakrishnan, “Mesoscale computational studies of membrane bilayer remodeling by curvature-inducing proteins”, *Physics Reports*, vol. 543, no. 1. Elsevier BV, pp. 1–60, Oct. 2014. doi: 10.1016/j.physrep.2014.05.001.  
  
P. S. Ramos, “Genetic analyses of interferon pathway-related genes reveal multiple new loci associated with systemic lupus erythematosus”, *Arthritis & Rheumatism*, vol. 63, no. 7. Wiley, pp. 2049–2057, Jun. 29, 2011. doi: 10.1002/art.30356.  
  
A. Rasmussen, “Comparison of the American-European Consensus Group Sjögren’s syndrome classification criteria to newly proposed American College of Rheumatology criteria in a large, carefully characterised sicca cohort”, *Annals of the Rheumatic Diseases*, vol. 73, no. 1. BMJ, pp. 31–38, Aug. 22, 2013. doi: 10.1136/annrheumdis-2013-203845.  
  
C. Rasmussen, J. D. Pelletier, P. A. Troch, T. L. Swetnamand J. Chorover, “Quantifying Topographic and Vegetation Effects on the Transfer of Energy and Mass to the Critical Zone”, *Vadose Zone Journal*, vol. 14, no. 11. Wiley, pp. 1–16, Feb. 23, 2015. doi: 10.2136/vzj2014.07.0102.  
  
W. B. Redwine, R. Hernández-López, S. Zou, J. Huang, S. L. Reck-Petersonand A. E. Leschziner, “Structural Basis for Microtubule Binding and Release by Dynein”, *Science*, vol. 337, no. 6101. American Association for the Advancement of Science (AAAS), pp. 1532–1536, Sep. 21, 2012. doi: 10.1126/science.1224151.  
  
P. M. Reed, N. W. Chaney, J. D. Herman, M. P. Ferringerand E. F. Wood, “Internationally coordinated multi-mission planning is now critical to sustain the space-based rainfall observations needed for managing floods globally”, *Environmental Research Letters*, vol. 10, no. 2. IOP Publishing, p. 024010, Feb. 01, 2015. doi: 10.1088/1748-9326/10/2/024010.  
  
P. M. Reed, N. W. Chaney, J. D. Herman, M. P. Ferringerand E. F. Wood, “Internationally coordinated multi-mission planning is now critical to sustain the space-based rainfall observations needed for managing floods globally”, *Environmental Research Letters*, vol. 10, no. 2. IOP Publishing, p. 024010, Feb. 01, 2015. doi: 10.1088/1748-9326/10/2/024010.  
  
P. M. Reed, N. W. Chaney, J. D. Herman, M. P. Ferringerand E. F. Wood, “Internationally coordinated multi-mission planning is now critical to sustain the space-based rainfall observations needed for managing floods globally”, *Environmental Research Letters*, vol. 10, no. 2. IOP Publishing, p. 024010, Feb. 01, 2015. doi: 10.1088/1748-9326/10/2/024010.  
  
S. L. Reichow, “Allosteric mechanism of water-channel gating by Ca2+–calmodulin”, *Nature Structural & Molecular Biology*, vol. 20, no. 9. Springer Science and Business Media LLC, pp. 1085–1092, Jul. 28, 2013. doi: 10.1038/nsmb.2630.  
  
H. Ren, “Selective Hydrodeoxygenation of Biomass-Derived Oxygenates to Unsaturated Hydrocarbons using Molybdenum Carbide Catalysts”, *ChemSusChem*, vol. 6, no. 5. Wiley, pp. 798–801, Apr. 04, 2013. doi: 10.1002/cssc.201200991.  
  
T. Respondek, R. N. Garner, M. K. Herroon, I. Podgorski, C. Turroand J. J. Kodanko, “Light Activation of a Cysteine Protease Inhibitor: Caging of a Peptidomimetic Nitrile with RuII(bpy)2”, *Journal of the American Chemical Society*, vol. 133, no. 43. American Chemical Society (ACS), pp. 17164–17167, Oct. 12, 2011. doi: 10.1021/ja208084s.  
  
T. Respondek, “Inhibition of Cathepsin Activity in a Cell-Based Assay by a Light-Activated Ruthenium Compound”, *ChemMedChem*, vol. 9, no. 6. Wiley, pp. 1306–1315, Apr. 11, 2014. doi: 10.1002/cmdc.201400081.  
  
J. Řezáč, Y. Huang, P. Hobzaand G. J. O. Beran, “Benchmark Calculations of Three-Body Intermolecular Interactions and the Performance of Low-Cost Electronic Structure Methods”, *Journal of Chemical Theory and Computation*, vol. 11, no. 7. American Chemical Society (ACS), pp. 3065–3079, Jun. 17, 2015. doi: 10.1021/acs.jctc.5b00281.  
  
M. K. Ridley, M. L. Macheskyand J. D. Kubicki, “Experimental Study of Strontium Adsorption on Anatase Nanoparticles as a Function of Size with a Density Functional Theory and CD Model Interpretation”, *Langmuir*, vol. 31, no. 2. American Chemical Society (ACS), pp. 703–713, Jan. 06, 2015. doi: 10.1021/la503932e.  
  
C. L. Rodriguez, S. Chatterjeeand F. A. Rasio, “Binary black hole mergers from globular clusters: Masses, merger rates, and the impact of stellar evolution”, *Physical Review D*, vol. 93, no. 8. American Physical Society (APS), Apr. 15, 2016. doi: 10.1103/physrevd.93.084029.  
  
C. L. Rodriguez, C.-J. Haster, S. Chatterjee, V. Kalogeraand F. A. Rasio, “DYNAMICAL FORMATION OF THE GW150914 BINARY BLACK HOLE”, *The Astrophysical Journal*, vol. 824, no. 1. American Astronomical Society, p. L8, Jun. 06, 2016. doi: 10.3847/2041-8205/824/1/l8.  
  
C. L. Rodriguez, M. Morscher, B. Pattabiraman, S. Chatterjee, C.-J. Hasterand F. A. Rasio, “Binary Black Hole Mergers from Globular Clusters: Implications for Advanced LIGO”, *Physical Review Letters*, vol. 115, no. 5. American Physical Society (APS), Jul. 30, 2015. doi: 10.1103/physrevlett.115.051101.  
  
C. L. Rodriguez, M. Morscher, L. Wang, S. Chatterjee, F. A. Rasioand R. Spurzem, “Million-body star cluster simulations: comparisons between Monte Carlo and direct*N*-body”, *Monthly Notices of the Royal Astronomical Society*, vol. 463, no. 2. Oxford University Press (OUP), pp. 2109–2118, Aug. 24, 2016. doi: 10.1093/mnras/stw2121.  
  
C. L. Rodriguez, M. Zevin, C. Pankow, V. Kalogeraand F. A. Rasio, “ILLUMINATING BLACK HOLE BINARY FORMATION CHANNELS WITH SPINS IN ADVANCED LIGO”, *The Astrophysical Journal*, vol. 832, no. 1. American Astronomical Society, p. L2, Nov. 11, 2016. doi: 10.3847/2041-8205/832/1/l2.  
  
L. M. Rodriguez-R, J. C. Castro, N. C. Kyrpides, J. R. Cole, J. M. Tiedjeand K. T. Konstantinidis, “How Much Do rRNA Gene Surveys Underestimate Extant Bacterial Diversity?”, *Applied and Environmental Microbiology*, vol. 84, no. 6. American Society for Microbiology, Mar. 15, 2018. doi: 10.1128/aem.00014-18.  
  
L. M. Rodriguez-R, “The Microbial Genomes Atlas (MiGA) webserver: taxonomic and gene diversity analysis of Archaea and Bacteria at the whole genome level”, *Nucleic Acids Research*, vol. 46, no. W1. Oxford University Press (OUP), pp. W282–W288, Jun. 14, 2018. doi: 10.1093/nar/gky467.  
  
S. P. Roy, P. G. Arias, V. R. Lecoustre, D. C. Haworth, H. G. Imand A. Trouvé, “Development of High Fidelity Soot Aerosol Dynamics Models using Method of Moments with Interpolative Closure”, *Aerosol Science and Technology*, vol. 48, no. 4. Informa UK Limited, pp. 379–391, Jan. 28, 2014. doi: 10.1080/02786826.2013.878017.  
  
S. Roy, P. Schopfand A. Warshel, “Origin of the Non-Arrhenius Behavior of the Rates of Enzymatic Reactions”, *The Journal of Physical Chemistry B*, vol. 121, no. 27. American Chemical Society (ACS), pp. 6520–6526, Jul. 05, 2017. doi: 10.1021/acs.jpcb.7b03698.  
  
V. A. Roytman, R. W. Karugu, Y. Hong, J. S. Hirschiand M. J. Vetticatt, “13 C Kinetic Isotope Effects as a Quantitative Probe To Distinguish between Enol and Enamine Mechanisms in Aminocatalysis”, *Chemistry - A European Journal*, vol. 24, no. 32. Wiley, pp. 8098–8102, May 14, 2018. doi: 10.1002/chem.201801748.  
  
T. Rumbell, J. Barnden, S. Denhamand T. Wennekers, “Emotions in autonomous agents: comparative analysis of mechanisms and functions”, *Autonomous Agents and Multi-Agent Systems*, vol. 25, no. 1. Springer Science and Business Media LLC, pp. 1–45, Feb. 13, 2011. doi: 10.1007/s10458-011-9166-5.  
  
T. Rumbell, S. L. Denhamand T. Wennekers, “A Spiking Self-Organizing Map Combining STDP, Oscillations, and Continuous Learning”, *IEEE Transactions on Neural Networks and Learning Systems*, vol. 25, no. 5. Institute of Electrical and Electronics Engineers (IEEE), pp. 894–907, May 2014. doi: 10.1109/tnnls.2013.2283140.  
  
S. Saha, T. C. Dinadayalane, J. S. Murray, D. Leszczynskaand J. Leszczynski, “Surface Reactivity for Chlorination on Chlorinated (5,5) Armchair SWCNT: A Computational Approach”, *The Journal of Physical Chemistry C*, vol. 116, no. 42. American Chemical Society (ACS), pp. 22399–22410, Oct. 11, 2012. doi: 10.1021/jp307090t.  
  
M. Salciccioli, W. Yu, M. A. Barteau, J. G. Chenand D. G. Vlachos, “Differentiation of O–H and C–H Bond Scission Mechanisms of Ethylene Glycol on Pt and Ni/Pt Using Theory and Isotopic Labeling Experiments”, *Journal of the American Chemical Society*, vol. 133, no. 20. American Chemical Society (ACS), pp. 7996–8004, Apr. 28, 2011. doi: 10.1021/ja201801t.  
  
M. A. H. Samee, B. G. Bruneauand K. S. Pollard, “A De Novo Shape Motif Discovery Algorithm Reveals Preferences of Transcription Factors for DNA Shape Beyond Sequence Motifs”, *Cell Systems*, vol. 8, no. 1. Elsevier BV, pp. 27–42.e6, Jan. 2019. doi: 10.1016/j.cels.2018.12.001.  
  
M. A. H. Samee, “A Systematic Ensemble Approach to Thermodynamic Modeling of Gene Expression from Sequence Data”, *Cell Systems*, vol. 1, no. 6. Elsevier BV, pp. 396–407, Dec. 2015. doi: 10.1016/j.cels.2015.12.002.  
  
M. A. H. Samee, “Quantitative Measurement and Thermodynamic Modeling of Fused Enhancers Support a Two-Tiered Mechanism for Interpreting Regulatory DNA”, *Cell Reports*, vol. 21, no. 1. Elsevier BV, pp. 236–245, Oct. 2017. doi: 10.1016/j.celrep.2017.09.033.  
  
M. A. H. Samee and S. Sinha, “Evaluating thermodynamic models of enhancer activity on cellular resolution gene expression data”, *Methods*, vol. 62, no. 1. Elsevier BV, pp. 79–90, Jul. 2013. doi: 10.1016/j.ymeth.2013.03.005.  
  
M. A. H. Samee and S. Sinha, “Quantitative Modeling of a Gene’s Expression from Its Intergenic Sequence”, *PLoS Computational Biology*, vol. 10, no. 3. Public Library of Science (PLoS), p. e1003467, Mar. 06, 2014. doi: 10.1371/journal.pcbi.1003467.  
  
J. G. Sanders, “Baleen whales host a unique gut microbiome with similarities to both carnivores and herbivores”, *Nature Communications*, vol. 6, no. 1. Springer Science and Business Media LLC, Sep. 22, 2015. doi: 10.1038/ncomms9285.  
  
B. J. Sanderson, L. Wang, P. Tiffin, Z. Wuand M. S. Olson, “Sex‐biased gene expression in flowers, but not leaves, reveals secondary sexual dimorphism in *Populus balsamifera*”, *New Phytologist*, vol. 221, no. 1. Wiley, pp. 527–539, Sep. 04, 2018. doi: 10.1111/nph.15421.  
  
A. Sarathy, H. Qiu, K. Schultenand J.-P. Leburton, “Single-Site Resolution Detection of Methylation in DNA with Graphene Nanopores”, *Biophysical Journal*, vol. 110, no. 3. Elsevier BV, p. 654a, Feb. 2016. doi: 10.1016/j.bpj.2015.11.3501.  
  
S. M. Sarhangi, M. M. Waskasi, S. M. Hashemianzadeh, D. R. Martinand D. V. Matyushov, “Half Reactions with Multiple Redox States Do Not Follow the Standard Theory: A Computational Study of Electrochemistry of C60”, *The Journal of Physical Chemistry C*, vol. 122, no. 30. American Chemical Society (ACS), pp. 17080–17087, Jul. 07, 2018. doi: 10.1021/acs.jpcc.8b04764.  
  
S. M. Sarhangi, M. M. Waskasi, S. M. Hashemianzadehand D. V. Matyushov, “Interfacial structural crossover and hydration thermodynamics of charged C60in water”, *Physical Chemistry Chemical Physics*, vol. 20, no. 42. Royal Society of Chemistry (RSC), pp. 27069–27081, 2018. doi: 10.1039/c8cp05422c.  
  
S. M. Sarhangi, M. M. Waskasi, S. M. Hashemianzadehand D. V. Matyushov, “Effective Dielectric Constant of Water at the Interface with Charged C60Fullerenes”, *The Journal of Physical Chemistry B*, vol. 123, no. 14. American Chemical Society (ACS), pp. 3135–3143, Mar. 19, 2019. doi: 10.1021/acs.jpcb.9b00901.  
  
J. Sastri, “Restriction of HIV-1 by Rhesus TRIM5α Is Governed by Alpha Helices in the Linker2 Region”, *Journal of Virology*, vol. 88, no. 16. American Society for Microbiology, pp. 8911–8923, Aug. 15, 2014. doi: 10.1128/jvi.01134-14.  
  
R. D. Schaeffer, Y. Liao, H. Chengand N. V. Grishin, “ECOD: new developments in the evolutionary classification of domains”, *Nucleic Acids Research*, vol. 45, no. D1. Oxford University Press (OUP), pp. D296–D302, Nov. 29, 2016. doi: 10.1093/nar/gkw1137.  
  
C. J. Schneider, M. Bezaireand I. Soltesz, “Toward a full-scale computational model of the rat dentate gyrus”, *Frontiers in Neural Circuits*, vol. 6. Frontiers Media SA, 2012. doi: 10.3389/fncir.2012.00083.  
  
C. J. Schneider, H. Cuntzand I. Soltesz, “Linking Macroscopic with Microscopic Neuroanatomy Using Synthetic Neuronal Populations”, *PLoS Computational Biology*, vol. 10, no. 10. Public Library of Science (PLoS), p. e1003921, Oct. 23, 2014. doi: 10.1371/journal.pcbi.1003921.  
  
T. W. Schneider, M. T. Hren, M. Z. Ertemand A. M. Angeles-Boza, “[RuII(tpy)(bpy)Cl]+-Catalyzed reduction of carbon dioxide. Mechanistic insights by carbon-13 kinetic isotope effects”, *Chemical Communications*, vol. 54, no. 61. Royal Society of Chemistry (RSC), pp. 8518–8521, 2018. doi: 10.1039/c8cc03009j.  
  
M. T. Sears, “NtERF32: a non-NIC2 locus AP2/ERF transcription factor required in jasmonate-inducible nicotine biosynthesis in tobacco”, *Plant Molecular Biology*, vol. 84, no. 1–2. Springer Science and Business Media LLC, pp. 49–66, Aug. 11, 2013. doi: 10.1007/s11103-013-0116-2.  
  
P. Selvaraj, “A computational study of ethylene–air sooting flames: Effects of large polycyclic aromatic hydrocarbons”, *Combustion and Flame*, vol. 163. Elsevier BV, pp. 427–436, Jan. 2016. doi: 10.1016/j.combustflame.2015.10.017.  
  
I. Senocak, M. Sandusky, R. DeLeon, D. Wade, K. Felzienand M. Budnikova, “An Immersed Boundary Geometric Preprocessor for Arbitrarily Complex Terrain and Geometry”, *Journal of Atmospheric and Oceanic Technology*, vol. 32, no. 11. American Meteorological Society, pp. 2075–2087, Nov. 2015. doi: 10.1175/jtech-d-14-00023.1.  
  
V. Sethuraman, V. Pryamitsynand V. Ganesan, “Influence of molecular weight and degree of segregation on local segmental dynamics of ordered block copolymers”, *Journal of Polymer Science Part B: Polymer Physics*, vol. 54, no. 9. Wiley, pp. 859–864, Jan. 15, 2016. doi: 10.1002/polb.23985.  
  
S. Seyedi, D. R. Martinand D. V. Matyushov, “Screening of Coulomb interactions in liquid dielectrics”, *Journal of Physics: Condensed Matter*, vol. 31, no. 32. IOP Publishing, p. 325101, May 28, 2019. doi: 10.1088/1361-648x/ab1e6f.  
  
S. Seyedi and D. V. Matyushov, “Ergodicity breaking of iron displacement in heme proteins”, *Soft Matter*, vol. 13, no. 44. Royal Society of Chemistry (RSC), pp. 8188–8201, 2017. doi: 10.1039/c7sm01561e.  
  
S. S. Seyedi and D. V. Matyushov, “Protein Dielectrophoresis in Solution”, *The Journal of Physical Chemistry B*, vol. 122, no. 39. American Chemical Society (ACS), pp. 9119–9127, Sep. 11, 2018. doi: 10.1021/acs.jpcb.8b06864.  
  
S. Seyedi and D. V. Matyushov, “Dipolar susceptibility of protein hydration shells”, *Chemical Physics Letters*, vol. 713. Elsevier BV, pp. 210–214, Dec. 2018. doi: 10.1016/j.cplett.2018.10.045.  
  
M. A. Sgambellone, A. David, R. N. Garner, K. R. Dunbarand C. Turro, “Cellular Toxicity Induced by the Photorelease of a Caged Bioactive Molecule: Design of a Potential Dual-Action Ru(II) Complex”, *Journal of the American Chemical Society*, vol. 135, no. 30. American Chemical Society (ACS), pp. 11274–11282, Jul. 19, 2013. doi: 10.1021/ja4045604.  
  
D. Shannahoff-Khalsa and S. Golshan, “Nasal cycle dominance and hallucinations in an adult schizophrenic female”, *Psychiatry Research*, vol. 226, no. 1. Elsevier BV, pp. 289–294, Mar. 2015. doi: 10.1016/j.psychres.2014.12.065.  
  
A. Sharma, “A model Scientific Computing course for freshman students at liberal arts Colleges”, *The Journal of Computational Science Education*, vol. 8, no. 2. The Shodor Education Foundation, Inc., pp. 2–9, Jul. 2017. doi: 10.22369/issn.2153-4136/8/2/1.  
  
B. S. Shastry, “Theory of extreme correlations using canonical Fermions and path integrals”, *Annals of Physics*, vol. 343. Elsevier BV, pp. 164–199, Apr. 2014. doi: 10.1016/j.aop.2014.02.005.  
  
B. S. Shastry and E. Perepelitsky, “Low-energy physics of themodel inusing extremely correlated Fermi liquid theory: Cutoff second-order equations”, *Physical Review B*, vol. 94, no. 4. American Physical Society (APS), Jul. 28, 2016. doi: 10.1103/physrevb.94.045138.  
  
B. S. Shastry, E. Perepelitskyand A. C. Hewson, “Extremely correlated Fermi liquid study of theAnderson impurity model”, *Physical Review B*, vol. 88, no. 20. American Physical Society (APS), Nov. 12, 2013. doi: 10.1103/physrevb.88.205108.  
  
M. W. Shen, “Predictable and precise template-free CRISPR editing of pathogenic variants”, *Nature*, vol. 563, no. 7733. Springer Science and Business Media LLC, pp. 646–651, Nov. 2018. doi: 10.1038/s41586-018-0686-x.  
  
P. J. Shepard, “Consanguinity and rare mutations outside of MCCC genes underlie nonspecific phenotypes of MCCD”, *Genetics in Medicine*, vol. 17, no. 8. Elsevier BV, pp. 660–667, Aug. 2015. doi: 10.1038/gim.2014.157.  
  
R. Shidpour, M. Vossoughi, A. R. Simchiand M. Micklich, “Extended Quantum Yield: A Dimensionless Factor Including Characteristics of Light Source, Photocatalyst Surface, and Reaction Kinetics in Photocatalytic Systems”, *Industrial & Engineering Chemistry Research*, vol. 53, no. 30. American Chemical Society (ACS), pp. 11973–11978, Jul. 16, 2014. doi: 10.1021/ie5021987.  
  
Q. Shi, Y. Huangand C. Jing, “Synthesis, characterization and application of lanthanum-impregnated activated alumina for F removal”, *Journal of Materials Chemistry A*, vol. 1, no. 41. Royal Society of Chemistry (RSC), p. 12797, 2013. doi: 10.1039/c3ta12548c.  
  
Q. Shi, L. Yan, T. Chanand C. Jing, “Arsenic Adsorption on Lanthanum-Impregnated Activated Alumina: Spectroscopic and DFT Study”, *ACS Applied Materials & Interfaces*, vol. 7, no. 48. American Chemical Society (ACS), pp. 26735–26741, Nov. 23, 2015. doi: 10.1021/acsami.5b08730.  
  
A. G. Shtukenberg, “The Third Ambient Aspirin Polymorph”, *Crystal Growth & Design*, vol. 17, no. 6. American Chemical Society (ACS), pp. 3562–3566, May 24, 2017. doi: 10.1021/acs.cgd.7b00673.  
  
A. G. Shtukenberg, “Powder diffraction and crystal structure prediction identify four new coumarin polymorphs”, *Chemical Science*, vol. 8, no. 7. Royal Society of Chemistry (RSC), pp. 4926–4940, 2017. doi: 10.1039/c7sc00168a.  
  
P. Silvestrov, T. A. Müller, K. N. Clark, R. P. Hausingerand G. A. Cisneros, “Homology modeling, molecular dynamics, and site-directed mutagenesis study of AlkB human homolog 1 (ALKBH1)”, *Journal of Molecular Graphics and Modelling*, vol. 54. Elsevier BV, pp. 123–130, Nov. 2014. doi: 10.1016/j.jmgm.2014.10.013.  
  
M. J. Skocik and L. N. Long, “On the Capabilities and Computational Costs of Neuron Models”, *IEEE Transactions on Neural Networks and Learning Systems*, vol. 25, no. 8. Institute of Electrical and Electronics Engineers (IEEE), pp. 1474–1483, Aug. 2014. doi: 10.1109/tnnls.2013.2294016.  
  
D. R. Slochower, Y.-H. Wang, R. W. Tourdot, R. Radhakrishnanand P. A. Janmey, “Counterion-mediated pattern formation in membranes containing anionic lipids”, *Advances in Colloid and Interface Science*, vol. 208. Elsevier BV, pp. 177–188, Jun. 2014. doi: 10.1016/j.cis.2014.01.016.  
  
E. N. Smith, “Genetic and epigenetic profiling of CLL disease progression reveals limited somatic evolution and suggests a relationship to memory-cell development”, *Blood Cancer Journal*, vol. 5, no. 4. Springer Science and Business Media LLC, pp. e303–e303, Apr. 10, 2015. doi: 10.1038/bcj.2015.14.  
  
E. N. Smith, K. Jepsen, A. D. Arias, P. J. Shepard, C. D. Chambersand K. A. Frazer, “Genetic ancestry of participants in the National Children’s Study”, *Genome Biology*, vol. 15, no. 2. Springer Science and Business Media LLC, p. R22, 2014. doi: 10.1186/gb-2014-15-2-r22.  
  
E. N. Smith, “Biased estimates of clonal evolution and subclonal heterogeneity can arise from PCR duplicates in deep sequencing experiments”, *Genome Biology*, vol. 15, no. 7. Springer Science and Business Media LLC, Aug. 2014. doi: 10.1186/s13059-014-0420-4.  
  
M. Solaimani, R. Gopalan, L. Khan, P. T. Brandtand B. Thuraisingham, “Spark-Based Political Event Coding”, *2016 IEEE Second International Conference on Big Data Computing Service and Applications (BigDataService)*. IEEE, Mar. 2016. doi: 10.1109/bigdataservice.2016.30.  
  
M. Solar and M. J. Buehler, “Comparative analysis of nanomechanics of protein filaments under lateral loading”, *Nanoscale*, vol. 4, no. 4. Royal Society of Chemistry (RSC), pp. 1177–1183, 2012. doi: 10.1039/c1nr11260k.  
  
M. Solar and M. J. Buehler, “Tensile deformation and failure of amyloid and amyloid-like protein fibrils”, *Nanotechnology*, vol. 25, no. 10. IOP Publishing, p. 105703, Feb. 14, 2014. doi: 10.1088/0957-4484/25/10/105703.  
  
M. Solar, Z. Qinand M. J. Buehler, “Molecular mechanics and performance of crosslinked amorphous polymer adhesives”, *Journal of Materials Research*, vol. 29, no. 9. Springer Science and Business Media LLC, pp. 1077–1085, May 13, 2014. doi: 10.1557/jmr.2014.82.  
  
J. Song, Y. Zhong, H. Luo, Y. Dingand R. Du, “Hydrodynamics of larval fish quick turning: A computational study”, *Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science*, vol. 232, no. 14. SAGE Publications, pp. 2515–2523, Dec. 01, 2017. doi: 10.1177/0954406217743271.  
  
P. Soto Garcia, “A Nanobiosensor Based on 4-Hydroxyphenylpyruvate Dioxygenase Enzyme for Mesotrione Detection”, *IEEE Sensors Journal*, vol. 15, no. 4. Institute of Electrical and Electronics Engineers (IEEE), pp. 2106–2113, Apr. 2015. doi: 10.1109/jsen.2014.2371773.  
  
E. B. Sözer, Z. A. Levineand P. T. Vernier, “Quantitative Limits on Small Molecule Transport via the Electropermeome — Measuring and Modeling Single Nanosecond Perturbations”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, Mar. 03, 2017. doi: 10.1038/s41598-017-00092-0.  
  
J. S. Spilker, “SUB-KILOPARSEC IMAGING OF COOL MOLECULAR GAS IN TWO STRONGLY LENSED DUSTY, STAR-FORMING GALAXIES”, *The Astrophysical Journal*, vol. 811, no. 2. American Astronomical Society, p. 124, Sep. 28, 2015. doi: 10.1088/0004-637x/811/2/124.  
  
J. S. Spilker, “THE REST-FRAME SUBMILLIMETER SPECTRUM OF HIGH-REDSHIFT, DUSTY, STAR-FORMING GALAXIES”, *The Astrophysical Journal*, vol. 785, no. 2. American Astronomical Society, p. 149, Apr. 04, 2014. doi: 10.1088/0004-637x/785/2/149.  
  
J. S. Spilker, “ALMA IMAGING AND GRAVITATIONAL LENS MODELS OF SOUTH POLE TELESCOPE—SELECTED DUSTY, STAR-FORMING GALAXIES AT HIGH REDSHIFTS”, *The Astrophysical Journal*, vol. 826, no. 2. American Astronomical Society, p. 112, Jul. 26, 2016. doi: 10.3847/0004-637x/826/2/112.  
  
L. Spiridon and D. D. L. Minh, “Hamiltonian Monte Carlo with Constrained Molecular Dynamics as Gibbs Sampling”, *Journal of Chemical Theory and Computation*, vol. 13, no. 10. American Chemical Society (ACS), pp. 4649–4659, Sep. 27, 2017. doi: 10.1021/acs.jctc.7b00570.  
  
E. M. Sproviero, “Opsin Effect on the Electronic Structure of the Retinylidene Chromophore in Rhodopsin”, *Journal of Chemical Theory and Computation*, vol. 11, no. 3. American Chemical Society (ACS), pp. 1206–1219, Feb. 27, 2015. doi: 10.1021/ct500612n.  
  
K. Srinivasan, F. Currimand S. Ram, “Predicting High-Cost Patients at Point of Admission Using Network Science”, *IEEE Journal of Biomedical and Health Informatics*, vol. 22, no. 6. Institute of Electrical and Electronics Engineers (IEEE), pp. 1970–1977, Nov. 2018. doi: 10.1109/jbhi.2017.2783049.  
  
K. Srinivasan and W. R. Young, “Zonostrophic Instability”, *Journal of the Atmospheric Sciences*, vol. 69, no. 5. American Meteorological Society, pp. 1633–1656, May 01, 2012. doi: 10.1175/jas-d-11-0200.1.  
  
K. Srinivasan and W. R. Young, “Reynolds Stress and Eddy Diffusivity of β-Plane Shear Flows”, *Journal of the Atmospheric Sciences*, vol. 71, no. 6. American Meteorological Society, pp. 2169–2185, May 30, 2014. doi: 10.1175/jas-d-13-0246.1.  
  
S. Srivastava, W. Wang, G. Manyam, C. Ordonezand V. Baladandayuthapani, “Integrating multi-platform genomic data using hierarchical Bayesian relevance vector machines”, *EURASIP Journal on Bioinformatics and Systems Biology*, vol. 2013, no. 1. Springer Science and Business Media LLC, Jun. 28, 2013. doi: 10.1186/1687-4153-2013-9.  
  
M. Staton, “Preliminary Genomic Characterization of Ten Hardwood Tree Species from Multiplexed Low Coverage Whole Genome Sequencing”, *PLOS ONE*, vol. 10, no. 12. Public Library of Science (PLoS), p. e0145031, Dec. 23, 2015. doi: 10.1371/journal.pone.0145031.  
  
M. Staton, “Substantial genome synteny preservation among woody angiosperm species: comparative genomics of Chinese chestnut (Castanea mollissima) and plant reference genomes”, *BMC Genomics*, vol. 16, no. 1. Springer Science and Business Media LLC, Oct. 05, 2015. doi: 10.1186/s12864-015-1942-1.  
  
A. Stern, “The Evolutionary Pathway to Virulence of an RNA Virus”, *Cell*, vol. 169, no. 1. Elsevier BV, pp. 35–46.e19, Mar. 2017. doi: 10.1016/j.cell.2017.03.013.  
  
S. A. Stoian, G. Xue, E. L. Bominaar, L. Que Jr.and E. Münck, “Spectroscopic and Theoretical Investigation of a Complex with an [O═FeIV–O–FeIV═O] Core Related to Methane Monooxygenase Intermediate **Q**”, *Journal of the American Chemical Society*, vol. 136, no. 4. American Chemical Society (ACS), pp. 1545–1558, Jan. 14, 2014. doi: 10.1021/ja411376u.  
  
M. L. Strandet, “THE REDSHIFT DISTRIBUTION OF DUSTY STAR-FORMING GALAXIES FROM THE SPT SURVEY”, *The Astrophysical Journal*, vol. 822, no. 2. American Astronomical Society, p. 80, May 10, 2016. doi: 10.3847/0004-637x/822/2/80.  
  
C. Su, X. Yang, S. Gao, Y. Tang, C. Zhaoand L. Li, “Identification and characterization of a subset of microRNAs in wheat ( Triticum aestivum L.)”, *Genomics*, vol. 103, no. 4. Elsevier BV, pp. 298–307, Apr. 2014. doi: 10.1016/j.ygeno.2014.03.002.  
  
J. Su, “Targeting the Biophysical Properties of the Myeloma Initiating Cell Niches: A Pharmaceutical Synergism Analysis Using Multi-Scale Agent-Based Modeling”, *PLoS ONE*, vol. 9, no. 1. Public Library of Science (PLoS), p. e85059, Jan. 27, 2014. doi: 10.1371/journal.pone.0085059.  
  
Y. Suleimenov, A. Ay, M. A. H. Samee, J. M. Dresch, S. Sinhaand D. N. Arnosti, “Global parameter estimation for thermodynamic models of transcriptional regulation”, *Methods*, vol. 62, no. 1. Elsevier BV, pp. 99–108, Jul. 2013. doi: 10.1016/j.ymeth.2013.05.012.  
  
B. Sun, D. Vaughan, S. Tikunova, T. P. Creamer, J. P. Davisand P. M. Kekenes-Huskey, “Calmodulin–Calcineurin Interaction beyond the Calmodulin-Binding Region Contributes to Calcineurin Activation”, *Biochemistry*, vol. 58, no. 39. American Chemical Society (ACS), pp. 4070–4085, Sep. 04, 2019. doi: 10.1021/acs.biochem.9b00626.  
  
J. Sun, “Structural and mechanistic insights into Mcm2–7 double-hexamer assembly and function”, *Genes & Development*, vol. 28, no. 20. Cold Spring Harbor Laboratory, pp. 2291–2303, Oct. 15, 2014. doi: 10.1101/gad.242313.114.  
  
W. Sun, “The thermodynamic scale of inorganic crystalline metastability”, *Science Advances*, vol. 2, no. 11. American Association for the Advancement of Science (AAAS), Nov. 04, 2016. doi: 10.1126/sciadv.1600225.  
  
W. Sun and Z. Wei, “Multiple Testing for Pattern Identification, With Applications to Microarray Time-Course Experiments”, *Journal of the American Statistical Association*, vol. 106, no. 493. Informa UK Limited, pp. 73–88, Mar. 2011. doi: 10.1198/jasa.2011.ap09587.  
  
W. Sun and Z. Wei, “Hierarchical recognition of sparse patterns in large-scale simultaneous inference”, *Biometrika*, vol. 102, no. 2. Oxford University Press (OUP), pp. 267–280, May 08, 2015. doi: 10.1093/biomet/asv012.  
  
Y. Sun, W. Zhang, Y. Chen, Q. Ma, J. Weiand Q. Liu, “Identifying anti-cancer drug response related genes using an integrative analysis of transcriptomic and genomic variations with cell line-based drug perturbations”, *Oncotarget*, vol. 7, no. 8. Impact Journals, LLC, pp. 9404–9419, Jan. 25, 2016. doi: 10.18632/oncotarget.7012.  
  
P. Swamy, M. M. Raghuwanshiand A. Gholghate, “An Improved Approach for k-Means Using Parallel Processing”, *2015 International Conference on Computing Communication Control and Automation*. IEEE, Feb. 2015. doi: 10.1109/iccubea.2015.75.  
  
A. T. Swesi, “Textured NiSe2 Film: Bifunctional Electrocatalyst for Full Water Splitting at Remarkably Low Overpotential with High Energy Efficiency”, *Scientific Reports*, vol. 7, no. 1. Springer Science and Business Media LLC, May 25, 2017. doi: 10.1038/s41598-017-02285-z.  
  
M. R. Talipov, Q. K. Timerghazin, R. L. Safiullinand S. L. Khursan, “No Longer a Complex, Not Yet a Molecule: A Challenging Case of Nitrosyl *O*-Hydroxide, HOON”, *The Journal of Physical Chemistry A*, vol. 117, no. 3. American Chemical Society (ACS), pp. 679–685, Jan. 14, 2013. doi: 10.1021/jp3110858.  
  
W. Tang, L. Zhangand G. Henkelman, “Catalytic Activity of Pd/Cu Random Alloy Nanoparticles for Oxygen Reduction”, *The Journal of Physical Chemistry Letters*, vol. 2, no. 11. American Chemical Society (ACS), pp. 1328–1331, May 19, 2011. doi: 10.1021/jz2004717.  
  
A. Tarakanova and M. J. Buehler, “The role of capture spiral silk properties in the diversification of orb webs”, *Journal of The Royal Society Interface*, vol. 9, no. 77. The Royal Society, pp. 3240–3248, Aug. 15, 2012. doi: 10.1098/rsif.2012.0473.  
  
A. Tarakanova and M. J. Buehler, “Molecular modeling of protein materials: case study of elastin”, *Modelling and Simulation in Materials Science and Engineering*, vol. 21, no. 6. IOP Publishing, p. 063001, Jul. 12, 2013. doi: 10.1088/0965-0393/21/6/063001.  
  
A. Tarakanova, W. Huang, Z. Qin, D. L. Kaplanand M. J. Buehler, “Modeling and Experiment Reveal Structure and Nanomechanics across the Inverse Temperature Transition in *B. mori* Silk-Elastin-like Protein Polymers”, *ACS Biomaterials Science & Engineering*, vol. 3, no. 11. American Chemical Society (ACS), pp. 2889–2899, Apr. 18, 2017. doi: 10.1021/acsbiomaterials.6b00688.  
  
A. Tchekhovskoy, “Launching of Active Galactic Nuclei Jets”, *The Formation and Disruption of Black Hole Jets*. Springer International Publishing, pp. 45–82, Oct. 08, 2014. doi: 10.1007/978-3-319-10356-3\_3.  
  
J. C. Thibault and I. Senocak, “Accelerating incompressible flow computations with a Pthreads-CUDA implementation on small-footprint multi-GPU platforms”, *The Journal of Supercomputing*, vol. 59, no. 2. Springer Science and Business Media LLC, pp. 693–719, Aug. 17, 2010. doi: 10.1007/s11227-010-0468-1.  
  
Y. Tian, F. A. Jaberiand D. Livescu, “Density Effects on the Flow Structure in Multi-fluid Shock-turbulence Interaction”, *2018 AIAA Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 07, 2018. doi: 10.2514/6.2018-0374.  
  
K. J. Tinto and R. E. Bell, “Progressive unpinning of Thwaites Glacier from newly identified offshore ridge: Constraints from aerogravity”, *Geophysical Research Letters*, vol. 38, no. 20. American Geophysical Union (AGU), p. n/a–n/a, Oct. 2011. doi: 10.1029/2011gl049026.  
  
B. C. Tlach, A. L. Tomlinson, K. D. Morgan, C. R. Collins, M. D. Zennerand M. Jeffries-EL, “Effect of Extended Conjugation on the Optoelectronic Properties of Benzo[1,2-d:4,5-d′]bisoxazole Polymers”, *Australian Journal of Chemistry*, vol. 67, no. 5. CSIRO Publishing, p. 711, 2014. doi: 10.1071/ch13528.  
  
B. C. Tlach, “Influence of Conjugation Axis on the Optical and Electronic Properties of Aryl-Substituted Benzobisoxazoles”, *The Journal of Organic Chemistry*, vol. 78, no. 13. American Chemical Society (ACS), pp. 6570–6581, Jun. 25, 2013. doi: 10.1021/jo4007927.  
  
O. Tokareva, M. Jacobsen, M. Buehler, J. Wongand D. L. Kaplan, “Structure–function–property–design interplay in biopolymers: Spider silk”, *Acta Biomaterialia*, vol. 10, no. 4. Elsevier BV, pp. 1612–1626, Apr. 2014. doi: 10.1016/j.actbio.2013.08.020.  
  
Ç. Tokgöz and S. Dardona, “Physics-based RF/microwave characterization of wave interactions within electrical connectors with partial insertion faults”, *Radio Science*, vol. 51, no. 9. American Geophysical Union (AGU), pp. 1489–1502, Sep. 2016. doi: 10.1002/2016rs006101.  
  
Ç. Tokgöz and S. Dardona, “Interrogation of electrical connector faults using miniaturized UWB sources”, *Radio Science*, vol. 52, no. 1. American Geophysical Union (AGU), pp. 94–104, Jan. 2017. doi: 10.1002/2016rs006153.  
  
Ç. Tokgöz, S. Dardona, N. C. Soldnerand K. R. Wheeler, “Modeling and characterization of partially inserted electrical connector faults”, *Journal of Applied Physics*, vol. 119, no. 10. AIP Publishing, p. 104501, Mar. 14, 2016. doi: 10.1063/1.4943178.  
  
H. Torabifard, L. Reed, M. T. Berry, J. E. Hein, E. Menkeand G. A. Cisneros, “Computational and experimental characterization of a pyrrolidinium-based ionic liquid for electrolyte applications”, *The Journal of Chemical Physics*, vol. 147, no. 16. AIP Publishing, p. 161731, Oct. 28, 2017. doi: 10.1063/1.5004680.  
  
H. Torabifard, O. N. Starovoytov, P. Renand G. A. Cisneros, “Development of an AMOEBA water model using GEM distributed multipoles”, *Theoretical Chemistry Accounts*, vol. 134, no. 8. Springer Science and Business Media LLC, Aug. 2015. doi: 10.1007/s00214-015-1702-y.  
  
G. Tóth, “Adaptive numerical algorithms in space weather modeling”, *Journal of Computational Physics*, vol. 231, no. 3. Elsevier BV, pp. 870–903, Feb. 2012. doi: 10.1016/j.jcp.2011.02.006.  
  
R. W. Tourdot, R. P. Bradley, N. Ramakrishnanand R. Radhakrishnan, “Multiscale computational models in physical systems biology of intracellular trafficking”, *IET Systems Biology*, vol. 8, no. 5. Institution of Engineering and Technology (IET), pp. 198–213, Oct. 2014. doi: 10.1049/iet-syb.2013.0057.  
  
A. Travesset, “Binary nanoparticle superlattices of soft-particle systems”, *Proceedings of the National Academy of Sciences*, vol. 112, no. 31. Proceedings of the National Academy of Sciences, pp. 9563–9567, Jul. 20, 2015. doi: 10.1073/pnas.1504677112.  
  
A. Travesset, “Topological structure prediction in binary nanoparticle superlattices”, *Soft Matter*, vol. 13, no. 1. Royal Society of Chemistry (RSC), pp. 147–157, 2017. doi: 10.1039/c6sm00713a.  
  
N. M. Tubman, J. Lee, T. Y. Takeshita, M. Head-Gordonand K. B. Whaley, “A deterministic alternative to the full configuration interaction quantum Monte Carlo method”, *The Journal of Chemical Physics*, vol. 145, no. 4. AIP Publishing, p. 044112, Jul. 28, 2016. doi: 10.1063/1.4955109.  
  
R. K. R. Tumkur, R. Calderer, A. Masud, A. J. Pearlstein, L. A. Bergmanand A. F. Vakakis, “Computational study of vortex-induced vibration of a sprung rigid circular cylinder with a strongly nonlinear internal attachment”, *Journal of Fluids and Structures*, vol. 40. Elsevier BV, pp. 214–232, Jul. 2013. doi: 10.1016/j.jfluidstructs.2013.03.008.  
  
M. A. Turabekova, T. C. Dinadayalane, D. Leszczynskaand J. Leszczynski, “Comprehensive Study on the Dissociative Chemisorption of NH3 on the Sidewalls of Stone–Wales Defective Armchair (5,5) Single-Walled Carbon Nanotubes”, *The Journal of Physical Chemistry C*, vol. 116, no. 10. American Chemical Society (ACS), pp. 6012–6021, Mar. 02, 2012. doi: 10.1021/jp2098685.  
  
S. Turgman-Cohen, J. C. Araque, E. M. V. Hoekand F. A. Escobedo, “Molecular Dynamics of Equilibrium and Pressure-Driven Transport Properties of Water through LTA-Type Zeolites”, *Langmuir*, vol. 29, no. 40. American Chemical Society (ACS), pp. 12389–12399, Sep. 26, 2013. doi: 10.1021/la402895h.  
  
K. C. Uga, M. Min, T. Leeand P. F. Fischer, “Spectral-element discontinuous Galerkin lattice Boltzmann simulation of flow past two cylinders in tandem with an exponential time integrator”, *Computers & Mathematics with Applications*, vol. 65, no. 2. Elsevier BV, pp. 239–251, Jan. 2013. doi: 10.1016/j.camwa.2011.12.059.  
  
C. Umphrey, R. DeLeonand I. Senocak, “Direct Numerical Simulation of Turbulent Katabatic Slope Flows with an Immersed-Boundary Method”, *Boundary-Layer Meteorology*, vol. 164, no. 3. Springer Science and Business Media LLC, pp. 367–382, Apr. 28, 2017. doi: 10.1007/s10546-017-0252-3.  
  
U. Unnikrishnan, J. C. Oefeleinand V. Yang, “Direct Numerical Simulation of a Turbulent Reacting Liquid-Oxygen/Methane Mixing Layer at Supercritical Pressure”, *2018 Joint Propulsion Conference*. American Institute of Aeronautics and Astronautics, Jul. 08, 2018. doi: 10.2514/6.2018-4564.  
  
R. Kirmse, Z. Qin, C. M. Weinert, A. Hoenger, M. J. Buehlerand L. Kreplak, “Plasticity of Intermediate Filament Subunits”, *PLoS ONE*, vol. 5, no. 8. Public Library of Science (PLoS), p. e12115, Aug. 12, 2010. doi: 10.1371/journal.pone.0012115.  
  
D. F. van Helden, D. R. Laver, J. Holdsworthand M. S. Imtiaz, “Generation and propagation of gastric slow waves”, *Clinical and Experimental Pharmacology and Physiology*, vol. 37, no. 4. Wiley, pp. 516–524, Apr. 2010. doi: 10.1111/j.1440-1681.2009.05331.x.  
  
D. F. van Helden, P. A. Thomas, P. J. Dosen, M. S. Imtiaz, D. R. Laverand G. K. Isbister, “Pharmacological Approaches That Slow Lymphatic Flow As a Snakebite First Aid”, *PLoS Neglected Tropical Diseases*, vol. 8, no. 2. Public Library of Science (PLoS), p. e2722, Feb. 27, 2014. doi: 10.1371/journal.pntd.0002722.  
  
E. Vázquez-Montelongo, J. Vázquez-Cervantesand G. Cisneros, “Polarizable ab initio QM/MM Study of the Reaction Mechanism of N-tert-Butyloxycarbonylation of Aniline in [EMIm][BF4]”, *Molecules*, vol. 23, no. 11. MDPI AG, p. 2830, Oct. 31, 2018. doi: 10.3390/molecules23112830.  
  
J.-B. Fan, “Correction: Highly Parallel Genome-Wide Expression Analysis of Single Mammalian Cells”, *PLoS ONE*, vol. 7, no. 2. Public Library of Science (PLoS), Feb. 21, 2012. doi: 10.1371/annotation/3f0ddf41-2e7a-4b56-93c2-2731f2890b19.  
  
J.-B. Fan, “Highly Parallel Genome-Wide Expression Analysis of Single Mammalian Cells”, *PLoS ONE*, vol. 7, no. 2. Public Library of Science (PLoS), p. e30794, Feb. 08, 2012. doi: 10.1371/journal.pone.0030794.  
  
A. Velasquez and S. K. Jha, “Parallel computing using memristive crossbar networks: Nullifying the processor-memory bottleneck”, *2014 9th International Design and Test Symposium (IDT)*. IEEE, Dec. 2014. doi: 10.1109/idt.2014.7038603.  
  
I. Venkatesh, V. Mehra, Z. Wang, B. Califfand M. G. Blackmore, “DevelopmentalChromatinRestriction ofPro‐GrowthGeneNetworksActs as anEpigeneticBarrier toAxonRegeneration inCorticalNeurons”, *Developmental Neurobiology*, vol. 78, no. 10. Wiley, pp. 960–977, Jun. 14, 2018. doi: 10.1002/dneu.22605.  
  
M. J. Vetticatt, A. A. Desaiand W. D. Wulff, “How the Binding of Substrates to a Chiral Polyborate Counterion Governs Diastereoselection in an Aziridination Reaction: H-Bonds in Equipoise”, *Journal of the American Chemical Society*, vol. 132, no. 38. American Chemical Society (ACS), pp. 13104–13107, Sep. 29, 2010. doi: 10.1021/ja103863j.  
  
P.-Y. von der Weid, S. Lee, M. S. Imtiaz, D. C. Zawiejaand M. J. Davis, “Electrophysiological Properties of Rat Mesenteric Lymphatic Vessels and their Regulation by Stretch”, *Lymphatic Research and Biology*, vol. 12, no. 2. Mary Ann Liebert Inc, pp. 66–75, Jun. 2014. doi: 10.1089/lrb.2013.0045.  
  
P.-Y. von der Weid, “Mechanisms of VIP-induced inhibition of the lymphatic vessel pump”, *The Journal of Physiology*, vol. 590, no. 11. Wiley, pp. 2677–2691, May 31, 2012. doi: 10.1113/jphysiol.2012.230599.  
  
Q. N. Vo, C. A. Hawkins, L. X. Dang, M. Nilssonand H. D. Nguyen, “Computational Study of Molecular Structure and Self-Association of Tri-*n*-butyl Phosphates in*n*-Dodecane”, *The Journal of Physical Chemistry B*, vol. 119, no. 4. American Chemical Society (ACS), pp. 1588–1597, Jan. 17, 2015. doi: 10.1021/jp510365c.  
  
G. L. Wagner and W. R. Young, “Available potential vorticity and wave-averaged quasi-geostrophic flow”, *Journal of Fluid Mechanics*, vol. 785. Cambridge University Press (CUP), pp. 401–424, Nov. 23, 2015. doi: 10.1017/jfm.2015.626.  
  
J. A. Wallace and J. K. Shen, “Charge-leveling and proper treatment of long-range electrostatics in all-atom molecular dynamics at constant pH”, *The Journal of Chemical Physics*, vol. 137, no. 18. AIP Publishing, p. 184105, Nov. 14, 2012. doi: 10.1063/1.4766352.  
  
K. Walweel, “Differences in the regulation of RyR2 from human, sheep, and rat by Ca2+ and Mg2+ in the cytoplasm and in the lumen of the sarcoplasmic reticulum”, *Journal of General Physiology*, vol. 144, no. 3. Rockefeller University Press, pp. 263–271, Aug. 25, 2014. doi: 10.1085/jgp.201311157.  
  
K. Walweel, “Ryanodine receptor modification and regulation by intracellular Ca2+ and Mg2+ in healthy and failing human hearts”, *Journal of Molecular and Cellular Cardiology*, vol. 104. Elsevier BV, pp. 53–62, Mar. 2017. doi: 10.1016/j.yjmcc.2017.01.016.  
  
B. Wang, J. Sun, E. N. Hahnand X. Wang, “Shear Localization and its Related Microstructure Mechanism in a Fine-Grain-Sized Near-Beta Ti Alloy”, *Journal of Materials Engineering and Performance*, vol. 24, no. 1. Springer Science and Business Media LLC, pp. 477–483, Oct. 25, 2014. doi: 10.1007/s11665-014-1285-0.  
  
B.-T. Wang, P. Zhang, H.-Y. Liu, W.-D. Liand P. Zhang, “First-principles calculations of phase transition, elastic modulus, and superconductivity under pressure for zirconium”, *Journal of Applied Physics*, vol. 109, no. 6. AIP Publishing, p. 063514, Mar. 15, 2011. doi: 10.1063/1.3556753.  
  
C. Wang, G. L. Rosnerand R. B. S. Roden, “A Bayesian design for phase I cancer therapeutic vaccine trials”, *Statistics in Medicine*, vol. 38, no. 7. Wiley, pp. 1170–1189, Oct. 25, 2018. doi: 10.1002/sim.8021.  
  
D. Wang and D. Liu, “MusiteDeep: A deep-learning framework for protein post-translational modification site prediction”, *2017 IEEE International Conference on Bioinformatics and Biomedicine (BIBM)*. IEEE, Nov. 2017. doi: 10.1109/bibm.2017.8218046.  
  
D. Wang, “MusiteDeep: a deep-learning framework for general and kinase-specific phosphorylation site prediction”, *Bioinformatics*, vol. 33, no. 24. Oxford University Press (OUP), pp. 3909–3916, Aug. 03, 2017. doi: 10.1093/bioinformatics/btx496.  
  
H. Wang, M. I. Eremets, I. Troyan, H. Liu, Y. Maand L. Vereecken, “Nitrogen Backbone Oligomers”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, Aug. 19, 2015. doi: 10.1038/srep13239.  
  
H. Wang, Q. Li, H. Wang, H. Liu, T. Cuiand Y. Ma, “Design of Superhard Ternary Compounds under High Pressure: SiC2N4 and Si2CN4”, *The Journal of Physical Chemistry C*, vol. 114, no. 18. American Chemical Society (ACS), pp. 8609–8613, Apr. 06, 2010. doi: 10.1021/jp100990b.  
  
J. Wang, Z. Lyu, S. Hossain, G. Stacey, D. Xuand T. Joshi, “SoyTSN: A web-based prediction tool for soybean tissue specific network within SoyKB”, *2017 IEEE International Conference on Bioinformatics and Biomedicine (BIBM)*. IEEE, Nov. 2017. doi: 10.1109/bibm.2017.8218045.  
  
L. Wang, T. M. Beissinger, A. Lorant, C. Ross-Ibarra, J. Ross-Ibarraand M. B. Hufford, “The interplay of demography and selection during maize domestication and expansion”, *Genome Biology*, vol. 18, no. 1. Springer Science and Business Media LLC, Nov. 13, 2017. doi: 10.1186/s13059-017-1346-4.  
  
L. Wang, “The Leukemogenicity of AML1-ETO Is Dependent on Site-Specific Lysine Acetylation”, *Science*, vol. 333, no. 6043. American Association for the Advancement of Science (AAAS), pp. 765–769, Aug. 05, 2011. doi: 10.1126/science.1201662.  
  
L. Wang and L. D. Stein, “Localizing triplet periodicity in DNA and cDNA sequences”, *BMC Bioinformatics*, vol. 11, no. 1. Springer Science and Business Media LLC, Nov. 08, 2010. doi: 10.1186/1471-2105-11-550.  
  
L. Wang and L. D. Stein, “Modeling the evolution dynamics of exon-intron structure with a general random fragmentation process”, *BMC Evolutionary Biology*, vol. 13, no. 1. Springer Science and Business Media LLC, p. 57, 2013. doi: 10.1186/1471-2148-13-57.  
  
Q. Wang, “Proline-Rich Chaperones Are Compared Computationally and Experimentally for Their Abilities to Facilitate Recombinant Butyrylcholinesterase Tetramerization in CHO Cells”, *Biotechnology Journal*, vol. 13, no. 3. Wiley, p. 1700479, Nov. 17, 2017. doi: 10.1002/biot.201700479.  
  
Q. Wang and M. S. Cheung, “A Physics-Based Approach of Coarse-Graining the Cytoplasm of Escherichia coli (CGCYTO)”, *Biophysical Journal*, vol. 102, no. 10. Elsevier BV, pp. 2353–2361, May 2012. doi: 10.1016/j.bpj.2012.04.010.  
  
Q. Wang, M. R. Diehl, B. Jana, M. S. Cheung, A. B. Kolomeiskyand J. N. Onuchic, “Molecular origin of the weak susceptibility of kinesin velocity to loads and its relation to the collective behavior of kinesins”, *Proceedings of the National Academy of Sciences*, vol. 114, no. 41. Proceedings of the National Academy of Sciences, Sep. 27, 2017. doi: 10.1073/pnas.1710328114.  
  
Q. Wang, “Direct Band Gap Silicon Allotropes”, *Journal of the American Chemical Society*, vol. 136, no. 28. American Chemical Society (ACS), pp. 9826–9829, Jul. 03, 2014. doi: 10.1021/ja5035792.  
  
T. Wang, C. Niand A. Janotti, “Band alignment and -type doping of ”, *Physical Review B*, vol. 95, no. 20. American Physical Society (APS), May 31, 2017. doi: 10.1103/physrevb.95.205205.  
  
W. Wang, V. Baladandayuthapani, J. S. Morris, B. M. Broom, G. Manyamand K.-A. Do, “iBAG: integrative Bayesian analysis of high-dimensional multiplatform genomics data”, *Bioinformatics*, vol. 29, no. 2. Oxford University Press (OUP), pp. 149–159, Nov. 09, 2012. doi: 10.1093/bioinformatics/bts655.  
  
W. Y. Wang, “Solid-Solution Hardening in Mg-Gd-TM (TM = Ag, Zn, and Zr) Alloys: An Integrated Density Functional Theory and Electron Work Function Study”, *JOM*, vol. 67, no. 10. Springer Science and Business Media LLC, pp. 2433–2441, Aug. 04, 2015. doi: 10.1007/s11837-015-1555-9.  
  
X. Wang, H. Huo, U. Unnikrishnanand V. Yang, “A systematic approach to high-fidelity modeling and efficient simulation of supercritical fluid mixing and combustion”, *Combustion and Flame*, vol. 195. Elsevier BV, pp. 203–215, Sep. 2018. doi: 10.1016/j.combustflame.2018.04.030.  
  
Y. Wang, C. H. Chen, D. Hu, M. B. Ulmschneiderand J. P. Ulmschneider, “Spontaneous formation of structurally diverse membrane channel architectures from a single antimicrobial peptide”, *Nature Communications*, vol. 7, no. 1. Springer Science and Business Media LLC, Nov. 22, 2016. doi: 10.1038/ncomms13535.  
  
Y. Wang, “Crystal structures, stability, electronic and elastic properties of 4d and 5d transition metal monoborides: First-principles calculations”, *Journal of Alloys and Compounds*, vol. 538. Elsevier BV, pp. 115–124, Oct. 2012. doi: 10.1016/j.jallcom.2012.05.114.  
  
Y. Wang, H. Liu, J. Lv, L. Zhu, H. Wangand Y. Ma, “High pressure partially ionic phase of water ice”, *Nature Communications*, vol. 2, no. 1. Springer Science and Business Media LLC, Nov. 29, 2011. doi: 10.1038/ncomms1566.  
  
Y. Wang, “An effective structure prediction method for layered materials based on 2D particle swarm optimization algorithm”, *The Journal of Chemical Physics*, vol. 137, no. 22. AIP Publishing, p. 224108, Dec. 14, 2012. doi: 10.1063/1.4769731.  
  
Z. Wang, “KLF6 and STAT3 co-occupy regulatory DNA and functionally synergize to promote axon growth in CNS neurons”, *Scientific Reports*, vol. 8, no. 1. Springer Science and Business Media LLC, Aug. 22, 2018. doi: 10.1038/s41598-018-31101-5.  
  
Z. Wang, “Metallization and superconductivity of BeH2 under high pressure”, *The Journal of Chemical Physics*, vol. 140, no. 12. AIP Publishing, p. 124707, Mar. 28, 2014. doi: 10.1063/1.4869145.  
  
G. Li, Q. Ma, B. Liu, Z. Chang, C. Zhouand Z. Wang, “An Insight into Species from Same Descendent Aspect and the Application into Clostridia”, *Current Bioinformatics*, vol. 12, no. 2. Bentham Science Publishers Ltd., pp. 140–146, Mar. 03, 2017. doi: 10.2174/1574893611666160616130126.  
  
K. E. Wardle and T. Lee, “Finite element lattice Boltzmann simulations of free surface flow in a concentric cylinder”, *Computers & Mathematics with Applications*, vol. 65, no. 2. Elsevier BV, pp. 230–238, Jan. 2013. doi: 10.1016/j.camwa.2011.09.020.  
  
M. M. Waskasi, D. R. Martinand D. V. Matyushov, “Wetting of the Protein Active Site Leads to Non-Marcusian Reaction Kinetics”, *The Journal of Physical Chemistry B*, vol. 122, no. 46. American Chemical Society (ACS), pp. 10490–10495, Oct. 26, 2018. doi: 10.1021/acs.jpcb.8b10376.  
  
A. J. Waters, “Comprehensive analysis of imprinted genes in maize reveals allelic variation for imprinting and limited conservation with other species”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 48. Proceedings of the National Academy of Sciences, pp. 19639–19644, Nov. 11, 2013. doi: 10.1073/pnas.1309182110.  
  
A. J. Waters, “Parent-of-Origin Effects on Gene Expression and DNA Methylation in the Maize Endosperm”, *The Plant Cell*, vol. 23, no. 12. Oxford University Press (OUP), pp. 4221–4233, Dec. 01, 2011. doi: 10.1105/tpc.111.092668.  
  
J. L. Wegrzyn, “Uniform standards for genome databases in forest and fruit trees”, *Tree Genetics & Genomes*, vol. 8, no. 3. Springer Science and Business Media LLC, pp. 549–557, Mar. 27, 2012. doi: 10.1007/s11295-012-0494-7.  
  
A. Weiß, “ALMA REDSHIFTS OF MILLIMETER-SELECTED GALAXIES FROM THE SPT SURVEY: THE REDSHIFT DISTRIBUTION OF DUSTY STAR-FORMING GALAXIES”, *The Astrophysical Journal*, vol. 767, no. 1. American Astronomical Society, p. 88, Mar. 28, 2013. doi: 10.1088/0004-637x/767/1/88.  
  
X. Wei, J. Chen, Q. Xie, S. Zhang, L. Geand X. Qiao, “Distinct Photolytic Mechanisms and Products for Different Dissociation Species of Ciprofloxacin”, *Environmental Science & Technology*, vol. 47, no. 9. American Chemical Society (ACS), pp. 4284–4290, Apr. 16, 2013. doi: 10.1021/es400425b.  
  
Z. Wei, “Large Sample Size, Wide Variant Spectrum, and Advanced Machine-Learning Technique Boost Risk Prediction for Inflammatory Bowel Disease”, *The American Journal of Human Genetics*, vol. 92, no. 6. Elsevier BV, pp. 1008–1012, Jun. 2013. doi: 10.1016/j.ajhg.2013.05.002.  
  
Z. Wei, W. Wang, P. Hu, G. J. Lyonand H. Hakonarson, “SNVer: a statistical tool for variant calling in analysis of pooled or individual next-generation sequencing data”, *Nucleic Acids Research*, vol. 39, no. 19. Oxford University Press (OUP), pp. e132–e132, Aug. 03, 2011. doi: 10.1093/nar/gkr599.  
  
N. Welikala, “Probing star formation in the dense environments of z ∼ 1 lensing haloes aligned with dusty star-forming galaxies detected with the South Pole Telescope”, *Monthly Notices of the Royal Astronomical Society*, vol. 455, no. 2. Oxford University Press (OUP), pp. 1629–1646, Nov. 17, 2015. doi: 10.1093/mnras/stv2302.  
  
P. T. West, “Genomic Distribution of H3K9me2 and DNA Methylation in a Maize Genome”, *PLoS ONE*, vol. 9, no. 8. Public Library of Science (PLoS), p. e105267, Aug. 14, 2014. doi: 10.1371/journal.pone.0105267.  
  
A. Wetzel, J. Bakaland M. Dittrich, “A Virtual File System for On-Demand Processing of Multidimensional Datasets”, *Proceedings of the XSEDE16 Conference on Diversity, Big Data, and Science at Scale*. ACM, Jul. 17, 2016. doi: 10.1145/2949550.2949656.  
  
Z. J. Whitfield, “The Diversity, Structure, and Function of Heritable Adaptive Immunity Sequences in the Aedes aegypti Genome”, *Current Biology*, vol. 27, no. 22. Elsevier BV, pp. 3511–3519.e7, Nov. 2017. doi: 10.1016/j.cub.2017.09.067.  
  
N. J. Wickett, “Phylotranscriptomic analysis of the origin and early diversification of land plants”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 45. Proceedings of the National Academy of Sciences, Oct. 29, 2014. doi: 10.1073/pnas.1323926111.  
  
N. J. Wickett, “Phylotranscriptomic analysis of the origin and early diversification of land plants”, *Proceedings of the National Academy of Sciences*, vol. 111, no. 45. Proceedings of the National Academy of Sciences, Oct. 29, 2014. doi: 10.1073/pnas.1323926111.  
  
C. Willis, M. Lambert, K. McHenryand C. Kirkpatrick, “Container-based Analysis Environments for Low-Barrier Access to Research Data”, *Proceedings of the Practice and Experience in Advanced Research Computing 2017 on Sustainability, Success and Impact*. ACM, Jul. 09, 2017. doi: 10.1145/3093338.3104164.  
  
C. Willis, D. LeBauer, M. Lambertand M. Burnette, “Terra-Ref Analysis Workbench: Container-Based Environments For Low-Barrier Access To Research Data”, *Zenodo*, May 2017, doi: 10.5281/ZENODO.580057.  
  
G. Wlazłowski, J. W. Holt, S. Moroz, A. Bulgacand K. J. Roche, “Auxiliary-Field Quantum Monte Carlo Simulations of Neutron Matter in Chiral Effective Field Theory”, *Physical Review Letters*, vol. 113, no. 18. American Physical Society (APS), Oct. 30, 2014. doi: 10.1103/physrevlett.113.182503.  
  
M. J. Wolovick, R. E. Bell, T. T. Creytsand N. Frearson, “Identification and control of subglacial water networks under Dome A, Antarctica”, *Journal of Geophysical Research: Earth Surface*, vol. 118, no. 1. American Geophysical Union (AGU), pp. 140–154, Mar. 2013. doi: 10.1029/2012jf002555.  
  
M. J. Wolovick, T. T. Creyts, W. R. Buckand R. E. Bell, “Traveling slippery patches produce thickness‐scale folds in ice sheets”, *Geophysical Research Letters*, vol. 41, no. 24. American Geophysical Union (AGU), pp. 8895–8901, Dec. 16, 2014. doi: 10.1002/2014gl062248.  
  
D. P. Woods, M. A. McKeown, Y. Dong, J. C. Prestonand R. M. Amasino, “Evolution of *VRN2/Ghd7-*Like Genes in Vernalization-Mediated Repression of Grass Flowering”, *Plant Physiology*, vol. 170, no. 4. Oxford University Press (OUP), pp. 2124–2135, Feb. 04, 2016. doi: 10.1104/pp.15.01279.  
  
J. Wu, F. Hagelberg, T. C. Dinadayalane, D. Leszczynskaand J. Leszczynski, “Do Stone–Wales Defects Alter the Magnetic and Transport Properties of Single-Walled Carbon Nanotubes?”, *The Journal of Physical Chemistry C*, vol. 115, no. 45. American Chemical Society (ACS), pp. 22232–22241, Oct. 21, 2011. doi: 10.1021/jp207510n.  
  
J. Wu, “WDL-RF: predicting bioactivities of ligand molecules acting with G protein-coupled receptors by combining weighted deep learning and random forest”, *Bioinformatics*, vol. 34, no. 13. Oxford University Press (OUP), pp. 2271–2282, Feb. 08, 2018. doi: 10.1093/bioinformatics/bty070.  
  
L. Wu, “Unraveling Stable Vanadium Tetraboride and Triboride by First-Principles Computations”, *The Journal of Physical Chemistry C*, vol. 119, no. 37. American Chemical Society (ACS), pp. 21649–21657, Sep. 03, 2015. doi: 10.1021/acs.jpcc.5b06721.  
  
X. Wu, P. Moin, R. J. Adrianand J. R. Baltzer, “Osborne Reynolds pipe flow: Direct simulation from laminar through gradual transition to fully developed turbulence”, *Proceedings of the National Academy of Sciences*, vol. 112, no. 26. Proceedings of the National Academy of Sciences, pp. 7920–7924, Jun. 15, 2015. doi: 10.1073/pnas.1509451112.  
  
P. Xiao, J. Duncan, L. Zhangand G. Henkelman, “Ridge-based bias potentials to accelerate molecular dynamics”, *The Journal of Chemical Physics*, vol. 143, no. 24. AIP Publishing, p. 244104, Dec. 28, 2015. doi: 10.1063/1.4937393.  
  
Y. Xiao, “Poliovirus intrahost evolution is required to overcome tissue-specific innate immune responses”, *Nature Communications*, vol. 8, no. 1. Springer Science and Business Media LLC, Aug. 29, 2017. doi: 10.1038/s41467-017-00354-5.  
  
Y. Xiao, “RNA Recombination Enhances Adaptability and Is Required for Virus Spread and Virulence”, *Cell Host & Microbe*, vol. 19, no. 4. Elsevier BV, pp. 493–503, Apr. 2016. doi: 10.1016/j.chom.2016.03.009.  
  
Y. Xiao, “RNA Recombination Enhances Adaptability and Is Required for Virus Spread and Virulence”, *Cell Host & Microbe*, vol. 22, no. 3. Elsevier BV, p. 420, Sep. 2017. doi: 10.1016/j.chom.2017.08.006.  
  
B. Xie, T. H. Nguyenand D. D. L. Minh, “Absolute Binding Free Energies between T4 Lysozyme and 141 Small Molecules: Calculations Based on Multiple Rigid Receptor Configurations”, *Journal of Chemical Theory and Computation*, vol. 13, no. 6. American Chemical Society (ACS), pp. 2930–2944, May 01, 2017. doi: 10.1021/acs.jctc.6b01183.  
  
L. Xiong, Q. Deng, G. J. Tucker, D. L. McDowelland Y. Chen, “Coarse-grained atomistic simulations of dislocations in Al, Ni and Cu crystals”, *International Journal of Plasticity*, vol. 38. Elsevier BV, pp. 86–101, Nov. 2012. doi: 10.1016/j.ijplas.2012.05.002.  
  
L. Xiong, D. L. McDowelland Y. Chen, “Nucleation and growth of dislocation loops in Cu, Al and Si by a concurrent atomistic-continuum method”, *Scripta Materialia*, vol. 67, no. 7–8. Elsevier BV, pp. 633–636, Oct. 2012. doi: 10.1016/j.scriptamat.2012.07.026.  
  
L. Xiong, D. L. McDowelland Y. Chen, “Sub-THz Phonon drag on dislocations by coarse-grained atomistic simulations”, *International Journal of Plasticity*, vol. 55. Elsevier BV, pp. 268–278, Apr. 2014. doi: 10.1016/j.ijplas.2013.11.004.  
  
L. Xiong, G. Tucker, D. L. McDowelland Y. Chen, “Coarse-grained atomistic simulation of dislocations”, *Journal of the Mechanics and Physics of Solids*, vol. 59, no. 2. Elsevier BV, pp. 160–177, Feb. 2011. doi: 10.1016/j.jmps.2010.11.005.  
  
L. Xiong, S. Xu, D. L. McDowelland Y. Chen, “Concurrent atomistic–continuum simulations of dislocation–void interactions in fcc crystals”, *International Journal of Plasticity*, vol. 65. Elsevier BV, pp. 33–42, Feb. 2015. doi: 10.1016/j.ijplas.2014.08.002.  
  
C. Xu, “Accelerating plant DNA barcode reference library construction using herbarium specimens: improved experimental techniques”, *Molecular Ecology Resources*, vol. 15, no. 6. Wiley, pp. 1366–1374, Apr. 28, 2015. doi: 10.1111/1755-0998.12413.  
  
J. Xue, “Task-D: A Task Based Programming Framework for Distributed System”, *2015 IEEE 17th International Conference on High Performance Computing and Communications, 2015 IEEE 7th International Symposium on Cyberspace Safety and Security, and 2015 IEEE 12th International Conference on Embedded Software and Systems*. IEEE, Aug. 2015. doi: 10.1109/hpcc-css-icess.2015.299.  
  
K. Xu, L. Jinand M. Xiong, “Functional regression method for whole genome eQTL epistasis analysis with sequencing data”, *BMC Genomics*, vol. 18, no. 1. Springer Science and Business Media LLC, May 18, 2017. doi: 10.1186/s12864-017-3777-4.  
  
Z. Y. Xu-Monette, “MDM2 phenotypic and genotypic profiling, respective to TP53 genetic status, in diffuse large B-cell lymphoma patients treated with rituximab-CHOP immunochemotherapy: a report from the International DLBCL Rituximab-CHOP Consortium Program”, *Blood*, vol. 122, no. 15. American Society of Hematology, pp. 2630–2640, Oct. 10, 2013. doi: 10.1182/blood-2012-12-473702.  
  
Z. Xu, “A novel device for air removal from vascular access line: a bench study”, *Journal of Clinical Monitoring and Computing*, vol. 32, no. 6. Springer Science and Business Media LLC, pp. 1041–1047, Feb. 17, 2018. doi: 10.1007/s10877-018-0114-7.  
  
J. Yalim, J. M. Lopezand B. D. Welfert, “Vertically forced stably stratified cavity flow: instabilities of the basic state”, *Journal of Fluid Mechanics*, vol. 851. Cambridge University Press (CUP), Jul. 31, 2018. doi: 10.1017/jfm.2018.571.  
  
D. F. Yancey, S. T. Chill, L. Zhang, A. I. Frenkel, G. Henkelmanand R. M. Crooks, “A theoretical and experimental examination of systematic ligand-induced disorder in Au dendrimer-encapsulated nanoparticles”, *Chemical Science*, vol. 4, no. 7. Royal Society of Chemistry (RSC), p. 2912, 2013. doi: 10.1039/c3sc50614b.  
  
D. F. Yancey, L. Zhang, R. M. Crooksand G. Henkelman, “Au@Pt dendrimer encapsulated nanoparticles as model electrocatalysts for comparison of experiment and theory”, *Chemical Science*, vol. 3, no. 4. Royal Society of Chemistry (RSC), p. 1033, 2012. doi: 10.1039/c2sc00971d.  
  
B. Yang, R. Kalyanam, C. Willis, M. Lambertand C. Kirkpatrick, “CHEESE”, *Proceedings of the 20th Annual SIG Conference on Information Technology Education*. ACM, Sep. 26, 2019. doi: 10.1145/3349266.3351393.  
  
H. Yang, “Orientation-Dependent Interfacial Mobility Governs the Anisotropic Swelling in Lithiated Silicon Nanowires”, *Nano Letters*, vol. 12, no. 4. American Chemical Society (ACS), pp. 1953–1958, Mar. 28, 2012. doi: 10.1021/nl204437t.  
  
J. Yang, C. T. Hu, X. Zhu, Q. Zhu, M. D. Wardand B. Kahr, “DDT Polymorphism and the Lethality of Crystal Forms”, *Angewandte Chemie*, vol. 129, no. 34. Wiley, pp. 10299–10303, Jun. 13, 2017. doi: 10.1002/ange.201703028.  
  
S. Yang and Y. Chen, “Concurrent atomistic and continuum simulation of bi-crystal strontium titanate with tilt grain boundary”, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 471, no. 2175. The Royal Society, p. 20140758, Mar. 2015. doi: 10.1098/rspa.2014.0758.  
  
S. Yang, L. Xiong, Q. Dengand Y. Chen, “Concurrent atomistic and continuum simulation of strontium titanate”, *Acta Materialia*, vol. 61, no. 1. Elsevier BV, pp. 89–102, Jan. 2013. doi: 10.1016/j.actamat.2012.09.032.  
  
W. Yang, “Protective role of Arapaima gigas fish scales: Structure and mechanical behavior”, *Acta Biomaterialia*, vol. 10, no. 8. Elsevier BV, pp. 3599–3614, Aug. 2014. doi: 10.1016/j.actbio.2014.04.009.  
  
Y. Yang, E. Faraggi, H. Zhaoand Y. Zhou, “Improving protein fold recognition and template-based modeling by employing probabilistic-based matching between predicted one-dimensional structural properties of query and corresponding native properties of templates”, *Bioinformatics*, vol. 27, no. 15. Oxford University Press (OUP), pp. 2076–2082, Jun. 11, 2011. doi: 10.1093/bioinformatics/btr350.  
  
Z. Yang, “Comparative Transcriptome Analyses Reveal Core Parasitism Genes and Suggest Gene Duplication and Repurposing as Sources of Structural Novelty”, *Molecular Biology and Evolution*, vol. 32, no. 3. Oxford University Press (OUP), pp. 767–790, Dec. 21, 2014. doi: 10.1093/molbev/msu343.  
  
R. Yan, J. Liand C. Ren, “Intermittent laser-plasma interactions and hot electron generation in shock ignition”, *Physics of Plasmas*, vol. 21, no. 6. AIP Publishing, p. 062705, Jun. 2014. doi: 10.1063/1.4882682.  
  
R. Yan, “Generating energetic electrons through staged acceleration in the two-plasmon-decay instability in inertial confinement fusion”, *Physical Review Letters*, vol. 108, no. 17. American Physical Society (APS), Apr. 24, 2012. doi: 10.1103/physrevlett.108.175002.  
  
J. Yao, “Serine Protease Activation Essential for Endothelial–Mesenchymal Transition in Vascular Calcification”, *Circulation Research*, vol. 117, no. 9. Ovid Technologies (Wolters Kluwer Health), pp. 758–769, Oct. 09, 2015. doi: 10.1161/circresaha.115.306751.  
  
Y. Yao, “Reducing Jagged 1 and 2 levels prevents cerebral arteriovenous malformations in matrix Gla protein deficiency”, *Proceedings of the National Academy of Sciences*, vol. 110, no. 47. Proceedings of the National Academy of Sciences, pp. 19071–19076, Nov. 04, 2013. doi: 10.1073/pnas.1310905110.  
  
A. Yaseen and Y. Li, “Accelerating knowledge-based energy evaluation in protein structure modeling with Graphics Processing Units”, *Journal of Parallel and Distributed Computing*, vol. 72, no. 2. Elsevier BV, pp. 297–307, Feb. 2012. doi: 10.1016/j.jpdc.2011.10.005.  
  
A. Yaseen and Y. Li, “Context-Based Features Enhance Protein Secondary Structure Prediction Accuracy”, *Journal of Chemical Information and Modeling*, vol. 54, no. 3. American Chemical Society (ACS), pp. 992–1002, Mar. 12, 2014. doi: 10.1021/ci400647u.  
  
K. Yin, Y. Wang, H. Liu, F. Pengand L. Zhang, “N2H: a novel polymeric hydronitrogen as a high energy density material”, *Journal of Materials Chemistry A*, vol. 3, no. 8. Royal Society of Chemistry (RSC), pp. 4188–4194, 2015. doi: 10.1039/c4ta06555g.  
  
H. Yoon, V. Kolevand A. Warshel, “Validating the Water Flooding Approach by Comparing It to Grand Canonical Monte Carlo Simulations”, *The Journal of Physical Chemistry B*, vol. 121, no. 40. American Chemical Society (ACS), pp. 9358–9365, Oct. 02, 2017. doi: 10.1021/acs.jpcb.7b07726.  
  
H. Yoon and A. Warshel, “Simulating the fidelity and the three Mg mechanism of pol η and clarifying the validity of transition state theory in enzyme catalysis”, *Proteins: Structure, Function, and Bioinformatics*, vol. 85, no. 8. Wiley, pp. 1446–1453, May 04, 2017. doi: 10.1002/prot.25305.  
  
K. Yoon, “Measuring the thermal conductivity of residue-free suspended graphene bridge using null point scanning thermal microscopy”, *Carbon*, vol. 76. Elsevier BV, pp. 77–83, Sep. 2014. doi: 10.1016/j.carbon.2014.04.051.  
  
S. E. Yost, “Identification of high-confidence somatic mutations in whole genome sequence of formalin-fixed breast cancer specimens”, *Nucleic Acids Research*, vol. 40, no. 14. Oxford University Press (OUP), pp. e107–e107, Apr. 06, 2012. doi: 10.1093/nar/gks299.  
  
Z. You, “Plastic anisotropy and associated deformation mechanisms in nanotwinned metals”, *Acta Materialia*, vol. 61, no. 1. Elsevier BV, pp. 217–227, Jan. 2013. doi: 10.1016/j.actamat.2012.09.052.  
  
L. Yuan, “GAAP: Genome-organization-framework-Assisted Assembly Pipeline for prokaryotic genomes”, *BMC Genomics*, vol. 18, no. S1. Springer Science and Business Media LLC, Jan. 2017. doi: 10.1186/s12864-016-3267-0.  
  
H.-F. Yu, C.-J. Hsieh, H. Yun, S. V. N. Vishwanathanand I. S. Dhillon, “A Scalable Asynchronous Distributed Algorithm for Topic Modeling”, *Proceedings of the 24th International Conference on World Wide Web*. International World Wide Web Conferences Steering Committee, May 18, 2015. doi: 10.1145/2736277.2741682.  
  
H.-F. Yu, C.-J. Hsieh, S. Siand I. S. Dhillon, “Parallel matrix factorization for recommender systems”, *Knowledge and Information Systems*, vol. 41, no. 3. Springer Science and Business Media LLC, pp. 793–819, Sep. 01, 2013. doi: 10.1007/s10115-013-0682-2.  
  
H. Yu and Xin Li, “Intelligent corner synthesis via cycle-consistent generative adversarial networks for efficient validation of autonomous driving systems”, *2018 23rd Asia and South Pacific Design Automation Conference (ASP-DAC)*. IEEE, Jan. 2018. doi: 10.1109/aspdac.2018.8297275.  
  
W. Yu, M. A. Barteauand J. G. Chen, “Glycolaldehyde as a Probe Molecule for Biomass Derivatives: Reaction of C—OH and C═O Functional Groups on Monolayer Ni Surfaces”, *Journal of the American Chemical Society*, vol. 133, no. 50. American Chemical Society (ACS), pp. 20528–20535, Nov. 30, 2011. doi: 10.1021/ja208786f.  
  
W. Yu, Z. J. Mellinger, M. A. Barteauand J. G. Chen, “Comparison of Reaction Pathways of Ethylene Glycol, Acetaldehyde, and Acetic Acid on Tungsten Carbide and Ni-Modified Tungsten Carbide Surfaces”, *The Journal of Physical Chemistry C*, vol. 116, no. 9. American Chemical Society (ACS), pp. 5720–5729, Feb. 28, 2012. doi: 10.1021/jp210756f.  
  
W. Yu, M. D. Porosoffand J. G. Chen, “Review of Pt-Based Bimetallic Catalysis: From Model Surfaces to Supported Catalysts”, *Chemical Reviews*, vol. 112, no. 11. American Chemical Society (ACS), pp. 5780–5817, Aug. 24, 2012. doi: 10.1021/cr300096b.  
  
W. Yu, M. Salciccioli, K. Xiong, M. A. Barteau, D. G. Vlachosand J. G. Chen, “Theoretical and Experimental Studies of C–C versus C–O Bond Scission of Ethylene Glycol Reaction Pathways via Metal-Modified Molybdenum Carbides”, *ACS Catalysis*, vol. 4, no. 5. American Chemical Society (ACS), pp. 1409–1418, Apr. 08, 2014. doi: 10.1021/cs500124n.  
  
W. Yu, K. Xiong, N. Ji, M. D. Porosoffand J. G. Chen, “Theoretical and experimental studies of the adsorption geometry and reaction pathways of furfural over FeNi bimetallic model surfaces and supported catalysts”, *Journal of Catalysis*, vol. 317. Elsevier BV, pp. 253–262, Aug. 2014. doi: 10.1016/j.jcat.2014.06.025.  
  
W.-Y. Yu, L. Zhang, G. M. Mullen, E. J. Evans, G. Henkelmanand C. B. Mullins, “Effect of annealing in oxygen on alloy structures of Pd–Au bimetallic model catalysts”, *Physical Chemistry Chemical Physics*, vol. 17, no. 32. Royal Society of Chemistry (RSC), pp. 20588–20596, 2015. doi: 10.1039/c5cp03515e.  
  
W.-Y. Yu, L. Zhang, G. M. Mullen, G. Henkelmanand C. B. Mullins, “Oxygen Activation and Reaction on Pd–Au Bimetallic Surfaces”, *The Journal of Physical Chemistry C*, vol. 119, no. 21. American Chemical Society (ACS), pp. 11754–11762, May 07, 2015. doi: 10.1021/acs.jpcc.5b02970.  
  
E. A. Yuzbashyan, B. S. Shastryand J. A. Scaramazza, “Rotationally invariant ensembles of integrable matrices”, *Physical Review E*, vol. 93, no. 5. American Physical Society (APS), May 09, 2016. doi: 10.1103/physreve.93.052114.  
  
M. Zamaninasab, E. Clausen-Brown, T. Savolainenand A. Tchekhovskoy, “Dynamically important magnetic fields near accreting supermassive black holes”, *Nature*, vol. 510, no. 7503. Springer Science and Business Media LLC, pp. 126–128, Jun. 2014. doi: 10.1038/nature13399.  
  
M. Zaratiegui, “CENP-B preserves genome integrity at replication forks paused by retrotransposon LTR”, *Nature*, vol. 469, no. 7328. Springer Science and Business Media LLC, pp. 112–115, Dec. 12, 2010. doi: 10.1038/nature09608.  
  
N. Zarifi, H. Liuand J. S. Tse, “Structures of the metallic and superconducting high pressure phases of solid CS2”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, May 18, 2015. doi: 10.1038/srep10458.  
  
C. Zdanski, “Quantitative assessment of the upper airway in infants and children with subglottic stenosis”, *The Laryngoscope*, vol. 126, no. 5. Wiley, pp. 1225–1231, Jul. 30, 2015. doi: 10.1002/lary.25482.  
  
M. Zerbetto, “Analysis of 15N–1H NMR Relaxation in Proteins by a Combined Experimental and Molecular Dynamics Simulation Approach: Picosecond–Nanosecond Dynamics of the Rho GTPase Binding Domain of Plexin-B1 in the Dimeric State Indicates Allosteric Pathways”, *The Journal of Physical Chemistry B*, vol. 117, no. 1. American Chemical Society (ACS), pp. 174–184, Dec. 28, 2012. doi: 10.1021/jp310142f.  
  
H.-M. Zhang, “Polarized and persistent Ca2+ plumes define loci for formation of wall ingrowth papillae in transfer cells”, *Journal of Experimental Botany*, vol. 66, no. 5. Oxford University Press (OUP), pp. 1179–1190, Dec. 10, 2014. doi: 10.1093/jxb/eru460.  
  
H. Zhang, G. Liu, M. P. Timko, J. Li, W. Wangand H. Ma, “Solanaceae Plant Malformation in Chongqing City, China, Reveals a Pollution Threat to the Yangtze River”, *Environmental Science & Technology*, vol. 48, no. 20. American Chemical Society (ACS), pp. 11787–11793, Oct. 09, 2014. doi: 10.1021/es501502y.  
  
H. Zhang, Y. Maand Z. Chen, “Quantum spin hall insulators in strain-modified arsenene”, *Nanoscale*, vol. 7, no. 45. Royal Society of Chemistry (RSC), pp. 19152–19159, 2015. doi: 10.1039/c5nr05006e.  
  
J. Zhang, “Mechanism of folding chamber closure in a group II chaperonin”, *Nature*, vol. 463, no. 7279. Springer Science and Business Media LLC, pp. 379–383, Jan. 2010. doi: 10.1038/nature08701.  
  
J. Zhang, “Cryo-EM Structure of a Group II Chaperonin in the Prehydrolysis ATP-Bound State Leading to Lid Closure”, *Structure*, vol. 19, no. 5. Elsevier BV, pp. 633–639, May 2011. doi: 10.1016/j.str.2011.03.005.  
  
J. Zhang, P. Minaryand M. Levitt, “Multiscale natural moves refine macromolecules using single-particle electron microscopy projection images”, *Proceedings of the National Academy of Sciences*, vol. 109, no. 25. Proceedings of the National Academy of Sciences, pp. 9845–9850, Jun. 04, 2012. doi: 10.1073/pnas.1205945109.  
  
J. Zhang and Z. Wei, “An empirical Bayes change-point model for identifying 3′ and 5′ alternative splicing by next-generation RNA sequencing”, *Bioinformatics*, vol. 32, no. 12. Oxford University Press (OUP), pp. 1823–1831, Feb. 11, 2016. doi: 10.1093/bioinformatics/btw060.  
  
L. Zhang, R. M. Anderson, R. M. Crooksand G. Henkelman, “Correlating Structure and Function of Metal Nanoparticles for Catalysis”, *Surface Science*, vol. 640. Elsevier BV, pp. 65–72, Oct. 2015. doi: 10.1016/j.susc.2015.03.018.  
  
L. Zhang, “Bayesian hierarchical structured variable selection methods with application to molecular inversion probe studies in breast cancer”, *Journal of the Royal Statistical Society: Series C (Applied Statistics)*, vol. 63, no. 4. Oxford University Press (OUP), pp. 595–620, Mar. 10, 2014. doi: 10.1111/rssc.12053.  
  
L. Zhang, S. Bouguet-Bonnetand M. Buck, “Combining NMR and Molecular Dynamics Studies for Insights into the Allostery of Small GTPase–Protein Interactions”, *Methods in Molecular Biology*. Springer New York, pp. 235–259, Sep. 18, 2011. doi: 10.1007/978-1-61779-334-9\_13.  
  
L. Zhang, S. T. Chilland G. Henkelman, “Distributed replica dynamics”, *The Journal of Chemical Physics*, vol. 143, no. 17. AIP Publishing, p. 174112, Nov. 07, 2015. doi: 10.1063/1.4934987.  
  
L. Zhang and G. Henkelman, “Tuning the Oxygen Reduction Activity of Pd Shell Nanoparticles with Random Alloy Cores”, *The Journal of Physical Chemistry C*, vol. 116, no. 39. American Chemical Society (ACS), pp. 20860–20865, Sep. 24, 2012. doi: 10.1021/jp305367z.  
  
L. Zhang and G. Henkelman, “Computational Design of Alloy-Core@Shell Metal Nanoparticle Catalysts”, *ACS Catalysis*, vol. 5, no. 2. American Chemical Society (ACS), pp. 655–660, Dec. 24, 2014. doi: 10.1021/cs501176b.  
  
L. Zhang, R. Iyyamperumal, D. F. Yancey, R. M. Crooksand G. Henkelman, “Design of Pt-Shell Nanoparticles with Alloy Cores for the Oxygen Reduction Reaction”, *ACS Nano*, vol. 7, no. 10. American Chemical Society (ACS), pp. 9168–9172, Sep. 23, 2013. doi: 10.1021/nn403788a.  
  
L. Zhang, H. Y. Kimand G. Henkelman, “CO Oxidation at the Au–Cu Interface of Bimetallic Nanoclusters Supported on CeO2(111)”, *The Journal of Physical Chemistry Letters*, vol. 4, no. 17. American Chemical Society (ACS), pp. 2943–2947, Aug. 19, 2013. doi: 10.1021/jz401524d.  
  
L. Zhang, A. Polyanskyand M. Buck, “Modeling Transmembrane Domain Dimers/Trimers of Plexin Receptors: Implications for Mechanisms of Signal Transmission across the Membrane”, *PLOS ONE*, vol. 10, no. 4. Public Library of Science (PLoS), p. e0121513, Apr. 02, 2015. doi: 10.1371/journal.pone.0121513.  
  
M. Zhang, “Two-dimensional boron–nitrogen–carbon monolayers with tunable direct band gaps”, *Nanoscale*, vol. 7, no. 28. Royal Society of Chemistry (RSC), pp. 12023–12029, 2015. doi: 10.1039/c5nr03344f.  
  
M. Zhang, H. Liu, Y. Du, X. Zhang, Y. Wangand Q. Li, “Orthorhombic C32: a novel superhard sp3 carbon allotrope”, *Physical Chemistry Chemical Physics*, vol. 15, no. 33. Royal Society of Chemistry (RSC), p. 14120, 2013. doi: 10.1039/c3cp51746b.  
  
M. Zhang, M. Lu, Y. Du, L. Gao, C. Luand H. Liu, “Hardness of FeB4: Density functional theory investigation”, *The Journal of Chemical Physics*, vol. 140, no. 17. AIP Publishing, p. 174505, May 07, 2014. doi: 10.1063/1.4871627.  
  
M.-Q. Zhang, X. Xuand S.-J. Luo, “The genetics of brown coat color and white spotting in domestic yaks (*Bos grunniens*)”, *Animal Genetics*, vol. 45, no. 5. Wiley, pp. 652–659, Jul. 03, 2014. doi: 10.1111/age.12191.  
  
M. Zhang, H. Yan, Q. Weiand H. Liu, “A new high-pressure polymeric nitrogen phase in potassium azide”, *RSC Advances*, vol. 5, no. 16. Royal Society of Chemistry (RSC), pp. 11825–11830, 2015. doi: 10.1039/c4ra15699d.  
  
Q. Zhang, “Cryo-EM Structure of a Molluscan Hemocyanin Suggests Its Allosteric Mechanism”, *Structure*, vol. 21, no. 4. Elsevier BV, pp. 604–613, Apr. 2013. doi: 10.1016/j.str.2013.02.018.  
  
X. Zhang, “Pressure-induced zigzag phosphorus chain and superconductivity in boron monophosphide”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, Mar. 04, 2015. doi: 10.1038/srep08761.  
  
Y. Zhang, K. Abiraman, H. Li, D. M. Pierce, A. V. Tzingounisand G. Lykotrafitis, “Modeling of the axon membrane skeleton structure and implications for its mechanical properties”, *PLOS Computational Biology*, vol. 13, no. 2. Public Library of Science (PLoS), p. e1005407, Feb. 27, 2017. doi: 10.1371/journal.pcbi.1005407.  
  
Y. Zhang, J. Xie, J. Yang, A. Fennell, C. Zhangand Q. Ma, “QUBIC: a bioconductor package for qualitative biclustering analysis of gene co-expression data”, *Bioinformatics*. Oxford University Press (OUP), p. btw635, Oct. 06, 2016. doi: 10.1093/bioinformatics/btw635.  
  
Y. Zhang, C. Zhouand H. Luo, “Effect of mass ratio on thrust production of an elastic panel pitching or heaving near resonance”, *Journal of Fluids and Structures*, vol. 74. Elsevier BV, pp. 385–400, Oct. 2017. doi: 10.1016/j.jfluidstructs.2017.07.003.  
  
Z. Zhang, H. Liuand M. Zhang, “Superhard sp 3 carbon allotrope: Ab initio calculations”, *EPL (Europhysics Letters)*, vol. 108, no. 4. IOP Publishing, p. 46006, Nov. 01, 2014. doi: 10.1209/0295-5075/108/46006.  
  
Z. Zhang, Y. Xue, G. MacDonald, P. M. Coxand G. J. Collatz, “Investigation of North American vegetation variability under recent climate: A study using the SSiB4/TRIFFID biophysical/dynamic vegetation model”, *Journal of Geophysical Research: Atmospheres*, vol. 120, no. 4. American Geophysical Union (AGU), pp. 1300–1321, Feb. 23, 2015. doi: 10.1002/2014jd021963.  
  
C. Zheng and D. L. James, “Rigid-body fracture sound with precomputed soundbanks”, *ACM Transactions on Graphics*, vol. 29, no. 4. Association for Computing Machinery (ACM), pp. 1–13, Jul. 26, 2010. doi: 10.1145/1778765.1778806.  
  
C. Zheng and D. L. James, “Toward high-quality modal contact sound”, *ACM Transactions on Graphics*, vol. 30, no. 4. Association for Computing Machinery (ACM), pp. 1–12, Jul. 2011. doi: 10.1145/2010324.1964933.  
  
L. Zheng, T. Lee, Z. Guoand D. Rumschitzki, “Shrinkage of bubbles and drops in the lattice Boltzmann equation method for nonideal gases”, *Physical Review E*, vol. 89, no. 3. American Physical Society (APS), Mar. 05, 2014. doi: 10.1103/physreve.89.033302.  
  
X. Zheng, H. Babaee, S. Dong, C. Chryssostomidisand G. E. Karniadakis, “A phase-field method for 3D simulation of two-phase heat transfer”, *International Journal of Heat and Mass Transfer*, vol. 82. Elsevier BV, pp. 282–298, Mar. 2015. doi: 10.1016/j.ijheatmasstransfer.2014.11.052.  
  
J. Zhong and E. A. Kellogg, “Duplication and expression of*CYC2*‐like genes in the origin and maintenance of corolla zygomorphy in Lamiales”, *New Phytologist*, vol. 205, no. 2. Wiley, pp. 852–868, Oct. 20, 2014. doi: 10.1111/nph.13104.  
  
J. Zhong, “Greenhouse gas emission from the total process of swine manure composting and land application of compost”, *Atmospheric Environment*, vol. 81. Elsevier BV, pp. 348–355, Dec. 2013. doi: 10.1016/j.atmosenv.2013.08.048.  
  
X. Zhong, Y. Wang, F. Peng, H. Liu, H. Wangand Y. Ma, “Pressure stabilization of long-missing bare C6 hexagonal rings in binary sesquicarbides”, *Chem. Sci.*, vol. 5, no. 10. Royal Society of Chemistry (RSC), pp. 3936–3940, 2014. doi: 10.1039/c4sc01383b.  
  
D. Zhou, “Experimental selection of hypoxia-tolerant *Drosophila melanogaster*”, *Proceedings of the National Academy of Sciences*, vol. 108, no. 6. Proceedings of the National Academy of Sciences, pp. 2349–2354, Jan. 24, 2011. doi: 10.1073/pnas.1010643108.  
  
L. Zhu, H. Liu, C. J. Pickard, G. Zouand Y. Ma, “Reactions of xenon with iron and nickel are predicted in the Earth’s inner core”, *Nature Chemistry*, vol. 6, no. 7. Springer Science and Business Media LLC, pp. 644–648, Apr. 20, 2014. doi: 10.1038/nchem.1925.  
  
Q. Zhu, A. R. Oganov, A. O. Lyakhovand X. Yu, “Generalized evolutionary metadynamics for sampling the energy landscapes and its applications”, *Physical Review B*, vol. 92, no. 2. American Physical Society (APS), Jul. 13, 2015. doi: 10.1103/physrevb.92.024106.  
  
Q. Zhu, A. R. Oganovand Q. Zeng, “Formation of Stoichiometric CsFn Compounds”, *Scientific Reports*, vol. 5, no. 1. Springer Science and Business Media LLC, Jan. 22, 2015. doi: 10.1038/srep07875.  
  
Q. Zhu, “Resorcinol Crystallization from the Melt: A New Ambient Phase and New “Riddles””, *Journal of the American Chemical Society*, vol. 138, no. 14. American Chemical Society (ACS), pp. 4881–4889, Apr. 05, 2016. doi: 10.1021/jacs.6b01120.  
  
T. Zhu, R. Kumar, E. V. Titovand D. A. Levin, “Analysis of Fractal-Like Spore Aggregates in Direct Simulation Monte Carlo”, *Journal of Thermophysics and Heat Transfer*, vol. 26, no. 3. American Institute of Aeronautics and Astronautics (AIAA), pp. 417–429, Jul. 2012. doi: 10.2514/1.t3824.  
  
T. Zhu, Z. Liand D. A. Levin, “Modeling of NO Radiation from Unsteady and Steady Shocks Using DSMC”, *44th AIAA Thermophysics Conference*. American Institute of Aeronautics and Astronautics, Jun. 22, 2013. doi: 10.2514/6.2013-2786.  
  
T. Zhu, Z. Li, N. S. Parsonsand D. A. Levin, “High Fidelity Modeling of Energy Transfer and Chemical Reactions in Shock Waves”, *7th AIAA Theoretical Fluid Mechanics Conference*. American Institute of Aeronautics and Astronautics, Jun. 13, 2014. doi: 10.2514/6.2014-3207.  
  
T. Zhu, Z. Li, N. S. Parsonsand D. A. Levin, “Simulation of Radiation Generated by Chemical Reactions in Weakly Ionized Shock Waves using DSMC”, *52nd Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 10, 2014. doi: 10.2514/6.2014-1212.  
  
T. Zhu, Z. Li, N. S. Parsonsand D. A. Levin, “State Specific Modeling of Energy Transfer in N2-N2 Under High Temperature Condition”, *53rd AIAA Aerospace Sciences Meeting*. American Institute of Aeronautics and Astronautics, Jan. 03, 2015. doi: 10.2514/6.2015-0477.  
  
T. Zhu, Z. Li, N. S. Parsons, D. A. Levinand M. Panesi, “State Specific Modeling of Energy Transfer under Shock Conditions in Nitrogen using High Fidelity Models”, *45th AIAA Thermophysics Conference*. American Institute of Aeronautics and Astronautics, Jun. 18, 2015. doi: 10.2514/6.2015-2510.  
  
Z. Zhu, Z.-Y. Wengand T.-L. Ho, “Spin and charge modulations in a single-hole-doped Hubbard ladder: Verification with optical lattice experiments”, *Physical Review A*, vol. 93, no. 3. American Physical Society (APS), Mar. 07, 2016. doi: 10.1103/physreva.93.033614.  
  
R. Žitko, D. Hansen, E. Perepelitsky, J. Mravlje, A. Georgesand B. S. Shastry, “Extremely correlated Fermi liquid theory meets dynamical mean-field theory: Analytical insights into the doping-driven Mott transition”, *Physical Review B*, vol. 88, no. 23. American Physical Society (APS), Dec. 30, 2013. doi: 10.1103/physrevb.88.235132.  
  
Q. Zou, D. Mrozek, Q. Maand Y. Xu, “Scalable Data Mining Algorithms in Computational Biology and Biomedicine”, *BioMed Research International*, vol. 2017. Hindawi Limited, pp. 1–3, 2017. doi: 10.1155/2017/5652041.  
  
X. Zuo, “Potentiation of Colon Cancer Susceptibility in Mice by Colonic Epithelial PPAR-δ/β Overexpression”, *JNCI: Journal of the National Cancer Institute*, vol. 106, no. 4. Oxford University Press (OUP), Mar. 28, 2014. doi: 10.1093/jnci/dju052.