W. Seth Horne

Associate Professor

Department of Chemistry

Publications

N.A. Tavenor, K.I. Silva, S. Saxena, W.S. Horne "Origins of structural flexibility in protein-based supramolecular polymers revealed by DEER spectroscopy." *J. Phys. Chem. B* **2014**, *118*, 9881-9889.

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Peng Liu

Chemistry

Publications

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Yang, Y.; Liu, P.: “Mechanism and Origins of Selectivities in the Copper-Catalyzed Dearomatization-Induced ortho C–H Cyanation of Vinylarenes,” ACS. Catal., 2015, 5, 2944–2951.

Lu, G.; Fang, C.; Xu, T.; Dong, G.; Liu, P.: “Computational Study of Rh-Catalyzed Carboacylation of Olefins: Ligand-Promoted Rhodacycle Isomerization Enables Regioselective C–C Bond Functionalization of Benzocyclobutenones,” submitted.

Kennedy, N.; Lu, G.; Liu, P.; Cohen, T.: “Reductive Lithiation in the Absence of Aromatic Electron Carriers. A Steric Effect Manifested on the Surface of Lithium Metal Leads to a Remarkable Difference in Selectivity Depending on Whether the Aromatic Electron Carrier is Present or Absent,” submitted.

Dave Waldeck

Chemistry

X. Yin, E. Wierzbinski, H. Lu, S. Bezer, A. R. de Leon, K. L. Davis, C. Achim, and D. H. Waldeck A Three-Step Kinetic Model for Electrochemical Charge Transfer in the Hopping Regime J. Phys. Chem. A  **118**(2014) 7579-7589

X. Yin, J. Kong, A. DeLeon, YL Li, Z. J. Ma, E. Wierzbinski, C. Achim, and D. H. Waldeck Luminescence Quenching by Photoinduced Charge Transfer between Metal Complexes in Peptide Nucleic Acids J. Phys Chem. B **118** (2014) 9037-9045.

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Greg Constantine

Department of Mathematics

Publications

 An alternative to Hadamard codes: one error for the price of existence, Annals of Combinatorics, in press 2015, DOI:10.1007/s00026-015-0274-9  
  
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Bohnen NI, Frey KA, Studenski S, Kotagal V, Koeppe RA, Constantine GM, Scott PJH, Albin RL, Muller MLTM. Extra-nigral pathologies are common in Parkinson disease with freezing of gait: an in vivo PET study. Movement Disorders, accepted.  
  
Impact of Chemically-Modified Tetracycline 3 on Intertwined Physiological, Biochemical, and Inflammatory Networks in Porcine Sepsis/ARDS, submitted to JAMA Surgery, with Sadowsky D et al

Patrick Moore

Microbio Genetics Science (Health Sciences)

Publications

[Restricted protein phosphatase 2A targeting by Merkel cell polyomavirus small T antigen.](http://www.ncbi.nlm.nih.gov/pubmed/25631078)

Kwun HJ, Shuda M, Camacho CJ, Gamper AM, Thant M, Chang Y, Moore PS.

J Virol. 2015 Apr;89(8):4191-200. doi: 10.1128/JVI.00157-15. Epub 2015 Jan 28.

PMID: 25631078

Paolo Zunino

MEMS

Workshop/Conference Participation

Advanced Numerical Method in the Mathematical Sciences, Texas A&M, May 2015 (Poster presentation)

Third Annual Midwest Women in Mathematics Symposium, Illinois, March 2015 (Oral presentation)

Advancing Research Through HPC, University of Pittsburgh, October 2014

17th US National Congress on Theoretical and Applied Mechanics, MI, June 2014 (Oral presentation)

Workshop on Aneurysm Research at the University of Pittsburgh, Pittsburgh, PA, July 2014

Workshop on Computational Geomechanics, Pittsburgh, PA, May 22, 2014 (Poster Presentation)

Publications

Rana Zakerzadeh. Martina Bukac, Paolo Zunino. “Computational Analysis of Energy Distribution of Coupled Blood Flow and Arterial Deformation”, (Submitted)

Bukac, M., Yotov, I., Zakerzadeh, R., and Zunino, P. “Partitioning strategies for the interaction of a fluid with a poroelastic material based on Nitsche's coupling approach”, Computer Methods in Applied Mechanics and Engineering, 2014. (In press), 4 citation

·Bukac, M., Yotov, I., Zakerzadeh, R., and Zunino P. “Effects of poroelasticity on fluid-structure interaction in arteries: a computational sensitivity study”, In Modeling the Heart and the Circulatory System, pp. 197-220. Springer International Publishing, 2015.(Published)

G.P. Galdi, M. Mohebbi, R. Zakerzadeh, P. Zunino, Fluid-structure interaction and biomedical applications, Book Chapter: "Hyperbolic-Parabolic Coupling in Partially Dissipative Systems," In Fluid-Structure Interaction and Biomedical Applications, pp. 197-256. Springer Basel, 2014. (Published)

Rana Zakerzadeh, Paolo Zunino, “Fluid-Structure Interaction in the Arteries with a Poroelastic Wall Model”, proceeding of 21st Iranian Conference in Biomedical Engineering (ICBME), Tehran, Iran, 26-28 November 2014. Page 35-39. IEEE, DOI: 10.1109/ICBME.2014.7043889. (Published)

Kyle Bibby

Civil and Environmental Engineering

Publications

Amit Vikram, Daniel Lipus, and Kyle Bibby. Produced Water Exposure Alters Bacterial Response to Biocides.Environmental Science and Technology. 2014, 48 (21), pp 13001–13009.

Elyse Stachler and Kyle Bibby. Metagenomic Evaluation of the Highly Abundant Human Gut Bacteriophage CrAssphage for Source Tracking of Human Fecal Pollution. Environmental Science and Technology Letters. 2014. 1(10) 405-409.

Arvind Murali-Mohan, Daniel Lipus, Kyle Bibby, Kelvin Gregory. The Functional Potential of Microbial Communities in Hydraulic Fracturing Source Water and Produced Water from Natural Gas Extraction Characterized by Metagenomic Sequencing. PLoS ONE. 2014. 9 (10), e107682.

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Benay Akyon, Elyse Stachler, Na Wei, and Kyle Bibby. Microbial Mats as a Biological Treatment Approach for Saline Wastewaters: The Case of Produced Water from Hydraulic Fracturing. Environmental Science & Technology 2015 49 (10), 6172-6180. DOI: 10.1021/es505142t

Lillian Chong

Chemistry

Publications

MC Zwier, JL Adelman, JW Kaus, AJ Pratt, KF Wong, NB Rego, E Suarez, S. Lettieri, DW wang, M Grabe, MD Zuckerman, and LT Chong. “WESTPA: An interoperable, highly scalable software package for weighted ensemble simulation and analysis” *J. Chem. Theory Comput.* 2015, 11, 800.

E Syarez, S Lettieri, MC Zwier, CA Stri;nger, SR Subramanian, LT Chong, and DM Zuckerman. “Simultaneous computation of dynamical and equilibrium information using a weighted ensemble of trajectories.” *J Chem Theory Comput*, 2014. 10, 2658

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Nathan Clark

Computational and Systems Biology

Publications

Priedigkeit NM, Wolfe NW, Clark NL. Evolutionary signatures amongst disease genes permit novel methods for gene prioritization and construction of informative gene networks. PLOS Genetics. 2015; 11(2): e1004967.

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John Keith

Chemical and Petroleum Engineering

Publications

Ping Li, Graeme Henkelman, John A. Keith, J. Karl Johnson “Elucidation of Aqueous Solvent Mediated Hydrogen Transfer Reactions by Ab Initio Molecular Dynamics and Nudged Elastic Band Studies of NaBH4 Hydrolysis” J. Phys. Chem. C, 2014. 118, 21385-21399. DOI: 10.1021/jp507872d.

Ken Jordan

Chemistry

Publications

V. K. Voora and K. D. Jordan, "Non-valence Correlation-bound Anion State of C6F6: Doorway to Low-energy Electron Capture", J. Phys. Chem. A., 118, 7201-7205 (2014).

O. Karalti, X. Su, W. A. Al-Saidi, and K. D. Jordan, "Correcting Density Functionals for Dispersion Interactions using Pseudopotentials, Chem. Phys. Lett., 591, 133-136 (2014).

D. C. Sorescu, S. Civiš, and K. D. Jordan, "Mechanism of Oxygen Exchange Between CO2 and TiO2(101) Anatase", J. Phys. Chem. C, 118, 1628-1639 (2014).

K. D. Jordan, V. K. Voora, and J. Simons, "Negative Electron Affinities - Fact or Fiction?" Theor. Chem. Accts., 133, 1445:1-15 (2014).

M. F. Falcetta, L. A. DiFalco, D. S. Ackerman, J. C. Barlow, and K. D. Jordan, "Assessment of Various Electronic Structure Methods for Characterizing Temporary Anion States: Application to the Ground State Anions of N2, C2H2, C2H4 and C6H6", J. Phys. Chem. A, 118, 7489-7497 (2014).

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S. Civiš, M. Ferus, M. Zukalová, A. Zukal, L. Kavan, K. D. Jordan, and D. C. Sorescu, "Oxygen Atom Exchange Between Gaseous CO2 and TiO2 Nanoparticles", J. Phys Chem. C, in press.

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John Brigham

Civil and Environmental Engineering

Publications

G.A. Banyay, M. Ahmadpoor, and J.C. Brigham (2014), “Proper Orthogonal Decomposition Based Reduced Order Modeling of the Very High Temperature Reactor Lower Plenum Hydrodynamics,” ASME 2014 4th Joint US-European Fluids Engineering Division Summer Meeting, Chicago, IL, August.

B. Notghi and J.C. Brigham (2014), “Robust Nondestructive Test Design Maximizing Material Characterization Capabilities for Solids and Structures Subject to Uncertainty,” Conference of the Engineering Mechanics Institute, Hamilton, ON, Canada, August.

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Christopher Ewing

Chemical & Petroleum Engineering

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CS Ewing, MJ Hartmann, KR Martin, A Musto, SJ Padinjarekutt, EM Weiss, G Veser, JJ McCarthy, JK Johnson, DS Lambrecht, “[Structural and Electronic Properties of Pt13 Nanoclusters on Amorphous Silica Supports](http://pubs.acs.org/doi/abs/10.1021/jp5105104)”*J. Phys. Chem. C* 119 (2015) 2503-2512.

Lambrecht, Daniel

Chemistry

K. A. Werling, M. Griffin, G. R. Hutchison, and D. S. Lambrecht, "Piezoelectric Hydrogen Bonding: Computational Screening for a Design Rationale", J. Phys. Chem. A, DOI 10.1021/jp412740j (Ken Jordan Festschrift)

Mpourmpakis, G

Chemical and Petroleum Engineering

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Andriotis A.N., Mpourmpakis G., Broderick S., Rajan K., Datta S., Sunkara M., and Menon M. J. Chem. Phys. 140, 094705 (2014)

Leu, Paul W.

Chemistry

T. Gao, Z. Li, P.-S. Huang, G. J. Shenoy, D. Parobek, S. Tan, J.-K. Lee, H. Liu, and P. W. Leu, “Hierarchical graphene/metal grid structures for stable, flexible transparent conductors,” ACS Nano, 2015. <http://pubs.acs.org/doi/abs/10.1021/acsnano.5b01243>  
  
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silicon thin film solar cells,” Nano Energy, 2015. <http://www.sciencedirect.com/science/article/pii/S221128551420108X>  
  
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in PbS/TiO2 heterojunction solar cells,” Solar Energy Materials & Solar Cells, vol. 128, pp. 386–93,  
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