Bradley S. Harris

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Research Interests

Multiscale molecular modeling, computational chemistry and physics at the intersection of biology, material science and data science.

Education

University of California, Davis, Davis, CA, USA — Sep. 2016 – Mar. 2022
Ph.D in Chemical Engineering

University of Kansas, Lawrence, KS, USA — Aug. 2012 – May. 2016
B.S. in Chemical Engineering

Experience

Pacific Northwest National Lab, Richland, WA, USA — Sep. 2022 – present
Postdoctoral Scholar
Mentor: Marcel Baer

University of California, Davis, Davis, CA, USA — Jan. 2017 – Mar. 2022
Graduate Student Researcher
Mentors: Roland Faller, Gang-yu Liu

University of Kansas, Lawrence, KS, USA — Jan. 2014 – Jul. 2016
Undergraduate Student Researcher
Mentor: Stevin Gehrke

Lawrence Free State High School, Lawrence, KS, USA — May. 2015 – Jun. 2016
Assistant Speech and Debate Coach

Refereed Manuscripts

[15] Chakma, P., **Harris, B. S.**, Shi, C., Hao, B., Whitaker, K., Baer, M. D., Chen, C.-L., (2025) Multi-stimuli Responsive Nanomaterials Assembled from Spiropyran-containing Peptoids. Nanoscale, https://doi.org/10.1039/D5NR03491D

[14] Chakma, P., Chen, Y., **Harris, B. S.**, Elhady, Y. W., Zheng, R., Bowden, M. E., Shutthanandan, V. Bard, A., Trinh, T. K. H., Zheng, X., Mundy, C. J., Baer, M. D., & Chen, C.-L. (2025). Assembled peptoid crystalline nanomaterials as carbonic anhydrase mimics for promoted hydration and sequestration of CO_2. Nature Communications, 16, 7348. https://doi.org/10.1038/s41467-025-62366-w

[13] Elhady, Y. W., **Harris, B. S.**, Mundy, C. J., & Baer, M. D. (2025). Steps-sol a peptoid force field parameterization to include solvent effects. The Journal of Physical Chemistry B, 129(23),5901-5912. https://doi.org/10.1021/acs.jpcb.5c02834

[12] Li, Y., **Harris, B. S.**, Li, Z., Shi, C., Abdullah, J., Majumder, S., Berhanu, S., Vorobieva, A. A, Myers, S. K., Hettige, J., Baer, M. D., De Yoreo, J., Baker, D., & Noy, A. (2025) Water, solute, and ion transport in de novo designed membrane protein channels. ACS Nano, 19(2), 2185-2195. https://doi.org/10.1021/acsnano.4c11317

[11] Zhang, S., Zhou, W., **Harris, B. S.**, Zheng, R., Monahan, M., Mu, P., Yang, W., Chen, J., Noy, A., Baer, M., Chen, C.-L., & De Yoreo, J. (2024). Hierarchical assembly of peptoids on mos2. Materials Today Physics, 101406. https://doi.org/https://doi.org/10.1016/j.mtphys.2024.101406

[10] Yadav Schmid, S., Ma, X., Hammons, J. A., Mergelsberg, S. T., **Harris, B. S.**, Ferron, T., Yang, W., Zhou, W., Zheng, R., Zhang, S., Legg, B. A., Van Buuren, A., Baer, M. D., Chen, C.-L., Tao, J., & De Yoreo, J. J. (2024). Influence of peptoid sequence on the mechanisms and kinetics of 2d assembly [PMID: 38215492]. ACS Nano, 18(4), 3497–3508. https://doi.org/10.1021/acsnano.3c10810

[9] **Harris, B. S.**, Bejagam, K. K., & Baer, M. D. (2023). Development of a systematic and extensible force field for peptoids (steps) [PMID: 37462325]. The Journal of Physical Chemistry B, 127(29), 6573–6584. https://doi.org/10.1021/acs.jpcb.3c01424

[8] Karnes, J. J., Weisgraber, T. H., Cook, C. C., Wang, D. N., Crowhurst, J. C., Fox, C. A., **Harris, B. S.**, Oakdale, J. S., Faller, R., & Shusteff, M. (2023). Isolating chemical reaction mechanism as a variable with reactive coarse-grained molecular dynamics: Step-growth versus chain-growth polymerization. Macromolecules, 56(6), 2225–2233. https://doi.org/10.1021/acs.macromol.2c02069

[7] Rollins, Z., **Harris, B. S.**, George, S. & Faller, R. (2023). A molecular dynamics investigation of n-glycosylation effects on t-cell receptor kinetics [PMID: 35763488]. Journal of Biomolecular Structure and Dynamics, 41(12), 5614–5623. https://doi.org/10.1080/07391102.2022.2091660

[6] **Harris, B. S.**, Liu, G.-y., & Faller, R. (2023). Genevapa: A generic evaporation package for modeling evaporation in molecular dynamics simulations. Computer Physics Communications, 282, 108539. https://doi.org/https://doi.org/10.1016/j.cpc.2022.108539

[5] **Harris, B. S.**, Huang, Y., Karsai, A., Su, W.-C., Sambre, P. D., Parikh, A. N., Liu, G.-y., & Faller, R. (2022). Impact of surface polarity on lipid assembly under spatial confinement [PMID: 35671406]. Langmuir, 38(24), 7545–7557. https://doi.org/10.1021/acs.langmuir.2c00636

[4] Minami, S. A., Jung, S., Huang, Y., **Harris, B. S.**, Kenaston, M. W., Faller, R., Nandi, S., McDonald, K. A., & Shah, P. S. (2022). Production of novel sars-cov-2 spike truncations in chinese hamster ovary cells leads to high expression and binding to antibodies. Biotechnology Journal, 17(9), 2100678. https://doi.org/https://doi.org/10.1002/biot.202100678

[3] **Harris, B. S.**∗, Huang, Y.∗, Minami, S. A., Jung, S., Shah, P. S., Nandi, S., McDonald, K. A., & Faller, R. (2022). Sars-cov-2 spike binding to ace2 is stronger and longer ranged due to glycan interaction. Biophysical Journal, 121(1), 79–90. https://doi.org/10.1016/j.bpj.2021.12.002, (∗ Co 1st Authors)

[2] Bernardi, A., Huang, Y., **Harris, B. S.**, Xiong, Y., Nandi, S., McDonald, K. A., & Faller, R. (2020). Development and simulation of fully glycosylated molecular models of ace2-fc fusion proteins and their interaction with the sars-cov-2 spike protein binding domain. PLOS ONE, 15(8), 1–12. https://doi.org/10.1371/journal.pone.0237295

[1] Zhang, J., Yu, H., **Harris, B. S.**, Zheng, Y., Celik, U., Na, L., Faller, R., Chen, X., Haudenschild, D. R., & Liu, G.-y. (2020). New means to control molecular assembly. The Journal of Physical Chemistry C, 124(11), 6405–6412. https://doi.org/10.1021/acs.jpcc.9b11377

Submitted Manuscripts

[1] Owen, M., Chaudhary, S., Ismet, S., **Harris, B. S.**, Celik, U., Jasper, Y., Faller, R., Haudenschild, D,. & Liu, G-y., (n.d) New insight into drug release profiles of flavopiridol loaded poly(lactic-co-glycolic acid) microparticles [Submitted].

Conferences and Workshops

[5] Owen M. & **Harris, B. S.**, et al. *Structural changes of flavopiridol encapsulated PLGA microparticles in correlation with drug release profile.* Pacifichem 2021, Honolulu HI, December 2021

[4] **Harris, B. S.** et al. *Molecular modeling of lipid bilayer and multilayer formation from dynamically confined environments.* Pacifichem 2021, Honolulu HI, December 2021

[3] **Harris, B. S.**, & Faller R. *Extending reactive molecular dynamics simulations of acrylate polymers through specific reactive coarse-graining for applications in volumetric additive manufacturing,* LLNL VAM workshop 2021, Livermore CA, August 10-11 2021

[2] **Harris, B. S.**, et al. *A new means to control the assembly of carbohydrate materials.* Oral Presentation at MIP/CCI workshop, Davis CA. October 15, 2019

[1] **Harris, B. S.**, et al. *Molecular dynamics simulation of tetrasaccharide assemblies in the context of 3D nanoprinting.* LLNL Data Science Institute Workshop, Livermore CA. August 7-8, 2018

Teaching Experience

Guest Lecturer, University of California, Davis
ECH 252, Statistical Thermodynamics   Fall 2020, Fall 2021

Graduate Assistance in Areas Of National Need, American River College, Sacramento, CA
General Chemistry Lab design   Spring 2017

Head Teaching Assistant, University of California, Davis
CHE 104, Forensic Analytical Chemistry   Fall 2018

Teaching Assistant, University of California, Davis
CHE 104, Forensic Analytical Chemistry   Fall 2017, Fall 2021

CHE 145, Good Quality Practices,   Winter 2018

CHE 107B, Physical Chemistry for the Life Sciences   Spring 2018

CHE 8A, Organic Chemistry,   Spring 2018

CHE 107A, Physical Chemistry for the Life Sciences   Summer Session I 2018

CHE 110B, Physical Chemistry: Properties of Atoms & Molecules,   Summer Session II 2018

CHE 2B, General Chemistry   Spring 2019

ECH 152B, Chemical Engineering Thermodynamics   Winter 2020

Mentoring

Ph.D Student
Yasmene W. Elhady, Physics, University of Washington   Spring 2023-present

Undegraduate Students
Bo Chen, Chemical Engineering, University of California, Davis   January 2018 - July 2019

Skills

Technologies: Molecular Dynamics, Density Functional Theory, Computational Fluid Dynamics, Python (Pandas, Jupyter, Scipy), Bash, TCL, C++, VBA, MATLAB, Excel, Linux, HPC, Git, SciKitLearn

Software: GROMACS, LAMMPS, AMBER, OpenMM, NWCHEM, ORCA, Modeller, Rosetta, OpenLB, ESPResSo, MDAnalysis