

# Bradley S. Harris

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## Research Interests

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

## Education

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**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

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**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

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[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.jpcc.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.jpcc.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*. Pacificchem 2021, Honolulu HI, December 2021
- [4] **Harris, B. S.** et al. *Molecular modeling of lipid bilayer and multilayer formation from dynamically confined environments*. Pacificchem 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	Fall 2017
<b>Head Teaching Assistant</b> , University of California, Davis	
CHE 104, Forensic Analytical Chemistry	Fall 2018

<b>Teaching Assistant</b> , 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

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### Ph.D Student

Yasmene W. Elhady, Physics, University of Washington	Spring 2023-present
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### Undergraduate Students

Bo Chen, Chemical Engineering, University of California, Davis	January 2018 - July 2019
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## Skills

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**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, NWChem, ORCA, Modeller, Rosetta, OpenLB, ESPResSo, MDAnalysis