Brennon Shanks

Curriculum Vitae

Department of Chemical Engineering
University of Utah

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Education

2019 – Doctor of Philosophy in Chemical Engineering, University of Utah, Salt Lake City, UT. Neutron scattering analysis, statistical and quantum statistical mechanics, materials science, molecular simulation, thermodynamics, Bayesian statistics and machine learning

2015 – 2019 Bachelor of Engineering in Chemical and Biomolecular Engineering and Mathematics, *Ohio State University*, Columbus, OH.

Protein complex synthesis and chemical processing, chemical informatics, computational quantum chemistry, electronic transitions in strongly correlated systems

Publications

Journal Articles

2022 **B. L. Shanks, J. J. Potoff, and M. P. Hoepfner**, *Transferable Force Fields from Experimental Scattering Data with Machine Learning Assisted Structure Refinement*, J. Phys. Chem. Lett, 13, 49, 11512–11520.

Industry

Honda, Columbus, OH

Jan, 2019 – May, *Process Engineering Intern*.

2019 Proposed a heat exchanger network to improve thermal efficiency in body paint process.

The Procter & Gamble Company, Cincinnati, OH

May, 2017 – Aug, *Process Engineering Intern*.

2017 Development of dye mixing model that recovers an estimated net loss of $\sim 1.3 million/year.

May, 2016 – Aug, *Strategic Innovation and Technology Intern*.

2016 Molecule development and intellectual property filing strategy in China and Brazil.

Research

University of Utah, Salt Lake City UT

Aug, 2019 - Neutron scattering analysis with molecular simulation and machine learning.

Application of statistical and quantum statistical mechanics to determine interatomic forces from microstructure of condensed matter.

Advisor: **Dr. Michael Hoepfner**, Associate Professor, Department of Chemical Engineering, University of Utah (Personal Web-page)

Ohio State University, Columbus OH

Oct, 2017 - May, Theoretical quantum chemistry of strongly correlated systems.

2018 Developed software designed to calculate properties of charged excited states in metals.

Advisor: **Dr. Alexander Sokolov**, Assistant Professor, Department of Chemistry and Biochemistry (Personal Web-page)

- Oct, 2015 June, Apohemoglobin processing and reconstitution of cancer therapeutics.
 - 2017 Developed an improved method to separate heme from hemoglobin and initiated project aimed to determine the most likely drug candidates for apohemoglobin cancer therapeutic reconstitution as a treatment for leukemia.
 - Advisor: **Dr. Andre Palmer**, Professor, Department of Chemical and Biomolecular Engineering (Personal Web-page)

Conference Presentations

- Mar, 2022 Recent Advances in Machine Learning Accelerated Molecular Dynamics,

 CECAM (Centre Européen de Calcul Atomique et Moléculaire), Trieste, IT.

 Poster: Bayesian optimized force fields enabled by a radial distribution function surrogate model
- Jan, 2022 Combining Multi-scale Simulation and Scattering for Structural Analysis of Complex Systems, CECAM (Centre Européen de Calcul Atomique et Moléculaire), Lausanne, CH.

 Contributed Talk: Transferable force fields with structure-optimized potential refinement
- Oct, 2021 *US Total Scattering School*, Oak Ridge National Laboratory, TN.

 Poster: Transferable force fields with structure-optimized potential refinement
- Jan, 2021 Utah Biomedical Engineering Conference, Salt Lake City, UT.
 Contributed Talk: Characterizing self-assembly in biological liquids with machine learning
- Jan, 2021 Combining Multi-scale Simulation and Scattering for Structural Analysis of Complex Systems, CECAM (Centre Européen de Calcul Atomique et Moléculaire), Lausanne, CH.

 Poster: Neutron scattering predicts emergent thermodynamic behavior in noble gas liquids

Fellowships & Awards

- 2023 *University Teaching Award* at the University of Utah.
- 2022 **Researcher** at the Energy Frontier Research Center for Multi-scale Fluid-Solid Interactions in Architected and Natural Materials (MUSE), University of Utah.
- 2019 Graduate Research Fellow at the University of Utah.
 - 2016 Undergraduate Research Scholar at the Department of Chemical, Ohio State University.

Academic Achievements & Recognition

Feb, 2021 1st Place Presentation at the *Graduate Engineering Symposium*, University of Utah.

Teaching Experience

University of Utah

- Fall, 2023 CHEN 5960 | Introduction to Molecular Simulations, Lecturer, bshanks.netlify.app.
- Fall, 2022 CHEN 6853 | Advanced Thermodynamics, Guest Lecturer.
- 2021 2023 CHEN 7973 | Undergraduate Research Mentor.
 - Fall, 2021 CHEN 7703 | Uncertainty Quantification, Validation, and Machine Learning, GTA.
 - Fall, 2020 CHEN 6853 | Advanced Thermodynamics, GTA.

Ohio State University

- Spring, 2019 CBE 2523 | Separation Processes, UTA.
 - Fall, 2018 CBE 2420 | Transport Phenomena I, UTA.