# Brennon L. Shanks

# Curriculum Vitae

Department of Chemical Engineering
University of Utah

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⑥ Github in Linkedin

# Professional Summary Statement

- Engineering Ph.D. candidate with a strong expertise in statistical mechanics, quantum mechanics, molecular simulations, neutron scattering, and machine learning. My in-depth knowledge and experience in these fields have resulted in publications and presentations at international conferences, specifically focused on neutron scattering analysis, machine learning, and uncertainty quantification.
- Versatile and innovative researcher with a wide range of experiences in academic and industry settings. My background encompasses fundamental scientific research, process engineering and design, intellectual property strategy, marketing, and manufacturing. This diverse skill set enables me to approach problems from multiple perspectives and deliver comprehensive solutions that bridge the gap between theory and practical applications.
- Thoughtful and driven team member who prioritizes building strong professional relationships. I strive to foster an interdisciplinary, inclusive, and productive work environment where collaboration and open communication thrive. By promoting a positive and supportive atmosphere, I aim to bring out the best in myself and my colleagues, leading to enhanced teamwork and successful outcomes.

## Education

- 2019 2024 **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 Bachelors 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.

## Research Experience

- 2019 2024 Neutron scattering analysis with molecular simulation and machine learning, *University* of Utah, Salt Lake City, UT, Dr. Michael Hoepfner, Associate Professor (link).

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

  2017 2018 Theoretical quantum chemistry of strongly correlated systems, *Ohio State University*,

Columbus, OH, **Dr. Alexander Sokolov**, Assistant Professor (link).

- Quantum mechanical properties of charged excited states in strongly correlated electronic systems.
- 2015 2017 **Apohemoglobin processing and reconstitution for novel cancer therapies**, *Ohio State University*, Columbus, OH, **Dr. Andre Palmer**, *Professor* (*link*).

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.

# Industry Experience

2019 Process Engineer, Honda Motor Company, Ltd.

Heat exchanger network design to improve thermal efficiency and recovery for a body paint process.

- 2017 **Process Engineer**, *The Procter & Gamble Company*.

  Development of dye mixing model that recovers an estimated net loss of  $\sim$  \$ 1.3 million/year.
- 2016 **Strategic Innovation and Technology Engineer**, *The Procter & Gamble Company*. Molecule development and intellectual property filing strategy in China and Brazil.

## **Publications**

- Sept, 2023 M.M. Seeley, N.R. Vaughn, **B.L. Shanks**, R.E. Martin, M.König, G.A. Asner, *Classifying a highly polymorphic tree species across landscapes using airborne imaging spectroscopy*, Remote Sens., 13, 49, 11512–11520 (*link*).
- Dec, 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 (*link*).

## Conference Presentations

### Invited Talks

- Oct, 2023 Kirchner Group Seminar (Invited by Barbara Kirchner), University of Bonn, Bonn, DE. The Role of Uncertainty Quantification in Force Field Optimization to Complex Experimental Data
- Sept, 2023 **Theoretical Chemistry Seminar (Invited by Valeria Molinero)**, *University of Utah*, Salt Lake City, UT.

  Learning Interatomic Forces from Experimental Measurements of Fluid Structure

#### Contributed Talks

- Nov, 2023 Recent Advances in Molecular Simulation Methods , *AIChE*, Orlando, FL. Force Field Development for Molecular Simulations with Structure Optimized Potential Refinement
- Nov, 2023 Machine Learning for Soft and Hard Materials, AIChE, Orlando, FL. Learning Interatomic Forces from Experimental Measurements of Fluid Structure
- Sept, 2023 **EFRC Principal Investigators Meeting Lightning Talk**, *Department of Energy*, Virtual. Experimentally Informed State-Dependent Atomic Forces in Real Fluid Ensembles
- Aug, 2023 Machine Learning in Chemistry (Chair), American Chemical Society, San Francisco, CA.

  Machine learning accelerated methods to predict interatomic forces from experimental structure measurements
- Jan, 2022 Combining Multi-scale Simulation and Scattering for Structural Analysis of Complex Systems, Centre Européen de Calcul Atomique et Moléculaire, Lausanne, CH.

  Transferable force fields with structure-optimized potential refinement
- Oct, 2021 **US Total Scattering School**, Oak Ridge National Laboratory, TN. Transferable force fields with structure-optimized potential refinement
- Feb, 2021 **Graduate Research Symposium**, Salt Lake City, UT. Machine learning for neutron diffraction analysis
- Jan, 2021 Utah Biomedical Engineering Conference, Salt Lake City, UT. Characterizing self-assembly in biological liquids with machine learning Poster Sessions
- Sept, 2023 **EFRC Principal Investigators Meeting**, *Department of Energy*, Online, Virtual. Improvement of Atomistic Modeling for Confined Fluid Properties: Translating from the Statistical to Continuum Scale
- Aug, 2023 **Computers in Chemistry (COMP)**, American Chemical Society, San Francisco, CA.

  Constructing transferable force fields from neutron scattering measurements with structure optimized potential refinement

- Aug, 2023 **Chemistry and Physics of Liquids**, *Gordon Research Conferences*, Holderness, NH.

  Advancing Interatomic Force Prediction with Machine Learning: Accelerated Methods for Extracting Force Fields from Experimental Scattering Measurements
- Mar, 2022 Recent Advances in Machine Learning Accelerated Molecular Dynamics, Centre Européen de Calcul Atomique et Moléculaire, Trieste, IT.

  Bayesian optimized force fields enabled by a radial distribution function surrogate model
- Jan, 2021 Combining Multi-scale Simulation and Scattering for Structural Analysis of Complex Systems, Centre Européen de Calcul Atomique et Moléculaire, Lausanne, CH.

  Neutron scattering predicts emergent thermodynamic behavior in noble gas liquids

## Fellowships & Awards

## **Fellowships**

- Jan, 2023 University Teaching Assistantship Award at the University of Utah.
- Aug, 2019 Graduate Research Fellow at the University of Utah.

#### **Grant Proposals**

Sept, 2016 Undergraduate Research Scholar Grant at the Ohio State University.

#### **Awards**

- Jun, 2023 **Research Leader Award** at the *Energy Frontier Research Center for Multi-scale Fluid-Solid Interactions in Architected and Natural Materials*, University of Utah.
- Feb. 2021 1st Place Presentation at the Graduate Engineering Symposium, University of Utah.

## Positions of Responsibility

#### Internal

- April, 2023 Chair, Retention, Promotion, and Tenure Decisions Committee, University of Utah.
- April, 2021 Member, Retention, Promotion, and Tenure Decisions Committee, University of Utah.
- 2019 2023 Vice President, Graduate Student Advisory Committee, University of Utah.

#### External

2023 – 2024 **Early Career Network Representative**, *Basic Energy Sciences*, United States Department of Energy.

## Teaching Experience

### Courses

- Fall, 2023 CHEN 5960 | Introduction to Molecular Simulation, University of Utah, (link).

  Mentorship
- 2023 2024 CHEN 7973 | Research Mentor, University of Utah, William Kelly.
- 2021 2024 CHEN 7973 | Research Mentor, University of Utah, Harry W. Sullivan.

## Teaching Assistantship

- Fall, 2022 CHEN 6853 | Advanced Thermodynamics, University of Utah, Guest Lecturer.
- Fall, 2021 CHEN 6853 | Advanced Thermodynamics, University of Utah, Guest Lecturer.
- Fall, 2021 CHEN 7703 | Uncertainty Quantification and Machine Learning, University of Utah.
- Fall, 2020 CHEN 6853 | Advanced Thermodynamics, University of Utah.
- Spring, 2019 C&BE 2523 | Separation Processes, Ohio State University.
  - Fall, 2018 **C&BE 2420** | **Transport Phenomena I**, *Ohio State University*.