Brennon L. Shanks

Curriculum Vitae

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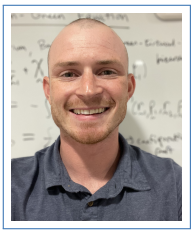

Professional Summary Statement

- Engineering Ph.D. with expertise in statistical mechanics, quantum mechanics, molecular simulation, neutron scattering, and probabilistc machine learning. My in-depth experience in these fields have resulted in publications in top tier journals.
- Versatile and innovative researcher with a wide range of experiences in academic and industry settings. My background encompasses fundamental scientific research, process engineering, 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 strongly believe in interdisciplinary, inclusive, and productive work environments with a culture for collaboration and open communication. 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*, SLC, 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

2024 – Present **Uncertainty aware force field design for ion-controlled biomolecular processes**, *Czech Academy of Sciences*, Prague, CZEC, **Dr. Pavel Jungwirth**, *Group Leader* (*link*).
Designing uncertainty-aware biomolecular force fields at the interface of theoretical statistical mechanics and probabilistic machine learning.

2019 – 2024 **Liquid structure analysis with molecular simulation and probabilistic machine learning**, *University of Utah*, SLC, UT, **Dr. Michael Hoepfner**, *Associate Professor* (*link*).
Application of statistical and quantum statistical mechanics to determine interatomic forces from neutron diffraction experiments.

2017 – 2018 **Electron structure in 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**, *Associate Dean, 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 ~$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

In Review **B.L. Shanks,** H.W. Sullivan, and M.P. Hoepfner, *Bayesian Analysis Reveals the Key to Extracting Pair Potentials from Neutron Scattering Data*, arXiv, (*link*).

August, 2024 **B.L. Shanks**, *Uncertainty Aware Liquid State Modeling from Experimental Scattering Measurements*, arXiv, (*link*).

Mar, 2024 **B.L. Shanks,** H.W. Sullivan, A. R. Shazed and M.P. Hoepfner, *Accelerated Bayesian Inference for Molecular Simulations using Local Gaussian Process Surrogate Models**, J. Chem. Theory Comput., (*link*).
*Published as part of Journal of Chemical Theory and Computation virtual special issue "*Machine Learning and Statistical Mechanics: Shared Synergies for Next Generation of Chemical Theory and Computation*".

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*).
*Computational lead on Gaussian process classification.

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*).

Peer Reviewing

2024 - **Nature Communications**, *Reviewed 1 Article.*

Conference Presentations

Invited Talks

Mar, 2024 **Seminar (Invited by Dr. Paulette Clancy)**, *Johns Hopkins*, Baltimore, MD.
Bayesian methods in computational chemistry with applications to neutron diffraction

Feb, 2024 **Seminar (Invited by Dr. Pavel Jungwirth)**, *IOCB*, Prague, CZEC.
Bayesian methods in computational chemistry

Oct, 2023 **Seminar (Invited by Dr. Barbara Kirchner)**, *University of Bonn*, Bonn, DE.
Probabilistic Machine Learning for Statistical Mechanical Inverse Problems

Sept, 2023 **Seminar (Invited by Dr. Valeria Molinero)**, *Univ. of Utah*, SLC, UT.
Bayesian methods in neutron diffraction analysis

Contributed Talks

Jan, 2024 **Multi-scale Fluid-Solid Interactions in Architected and Natural Materials EFRC**, *DOE*, SLC, UT.
Current Challenges in Reconstructing Classical Force Fields from Neutron Scattering Data

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**, *DOE*, 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**, SLC, UT.
Machine learning for neutron diffraction analysis

Jan, 2021 **Utah Biomedical Engineering Conference**, SLC, UT.
Characterizing self-assembly in biological liquids with machine learning

Poster Sessions

July, 2024 **Foundations of Molecular Modeling and Simulation**, *Department of Energy*, SLC, UT.
Exploring the State-Dependence of Classical Pair Potentials with Neutron Scattering

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

Funded Fellowships and Proposals

April, 2024 **Postdoctoral Fellowship**, *Institute of Organic Chemistry and Biochemistry (IOCB) at the Czech Academy of Sciences*, Prague, CZEC.
Uncertainty Aware Force Field Design for Ion-Controlled Biological Processes

Jan, 2023 **Teaching Fellowship**, *University of Utah Department of Chemical Engineering*, SLC, UT.
Designed upper level undergraduate course on Molecular Simulations for Engineers

Aug, 2019 **Graduate Research Fellowship**, *University of Utah Chemical Engineering*, SLC, UT.

Sept, 2016 **Undergraduate Research Scholarship**, *Ohio State University*, Columbus, OH.
Apohemoglobin reconstitution for experimental leukemia drug delivery

Awards

Jun, 2023 **Research Leader Award**, *Energy Frontier Research Center for Multi-scale Fluid-Solid Interactions in Architected and Natural Materials*, SLC, University of Utah.

Feb, 2021 **1st Place Presentation**, *University of Utah Graduate Engineering Symposium*, SLC, UT.

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

August 2024 **Scientific Communication and Storytelling Webinar Leader**, *Basic Energy Sciences*, US Department of Energy.

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

Teaching Experience

Courses

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

Mentorship

2021 – 2024 **CHEN 7973** | **Research Mentor**, *University of Utah*, Harry W. Sullivan, PhD Student. University of Minnesota - Twin Cities

Guest Lectures

Fall, 2022 **CHEN 6853** | **Advanced Thermodynamics**, *University of Utah*, Statistical Correlation Functions and Kirkwood-Buff Theory.

Fall, 2021 **CHEN 6853** | **Advanced Thermodynamics**, *University of Utah*, Statistical Correlation Functions and Kirkwood-Buff Theory.

Teaching Assistantship

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*.