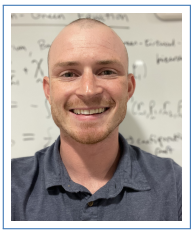
Brennon L. Shanks

Curriculum Vitae

Department of Chemical Engineering
University of Utah
513-256-4541
brennon.shanks@chemeng.utah.edu
bshanks.netlify.app/
Github *Linkedin*



Professional Summary

- Ph.D. chemical engineer specializing in statistical mechanics, quantum theory, and probabilistic machine learning. My research develops Bayesian methods for interpreting experimental data and constructing uncertainty-aware molecular models.
- First author on multiple publications in top-tier journals (JCP, JCTC, JPCL) and lead developer of novel Bayesian algorithms for molecular simulations. Experienced mentor of graduate researchers in computational modeling and statistical inference.
- Dedicated educator with teaching experience in molecular simulation, thermodynamics, and machine learning. Committed to interdisciplinary collaboration, scientific communication, and inclusive research environments.

Education

2019 – 2024 **Doctor of Philosophy in Chemical Engineering**, *University of Utah*, SLC, UT.
Bayesian statistics and probabilistic machine learning algorithm development with applications to neutron scattering, statistical and quantum statistical mechanics, and molecular simulation.

2015 – 2019 **Bachelors in Chemical and Biomolecular Engineering**, *Ohio State*, 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, CZ, **Dr. Pavel Jungwirth**, *Professor* (*link*).
- Developing biomolecular force fields with Bayesian uncertainty quantification.
- Combining statistical mechanics with machine learning to model complex biomolecular interactions.
- Collaborating with international experts in theory and simulation.

2019 – 2024 **Liquid Structure Analysis with Machine Learning and Molecular Simulation**, *University of Utah*, Salt Lake City, UT, **Dr. Michael Hoepfner**, *Associate Professor* (*link*).
- Developed probabilistic machine learning algorithms for analyzing neutron scattering data.
- Integrated Gaussian Process models with iterative Boltzmann inversion to infer pair potentials.
- Mentored graduate researchers and published as first author in JCP, JPCL, and JCTC.

2017 – 2018 **Electronic Structure in Strongly Correlated Systems**, *Ohio State University*, Columbus, OH, **Dr. Alexander Sokolov**, *Assistant Professor* (*link*).
- Studied excited states and charge transfer in open-shell molecular systems.
- Applied multireference quantum chemistry methods to characterize electronic transitions.

2015 – 2017 **Apohemoglobin Reconstitution for Cancer Therapeutics**, *Ohio State University*, Columbus, OH, **Dr. Andre Palmer**, *Professor, Associate Dean* (*link*).
- Developed an improved separation method for heme from hemoglobin.
- Initiated reconstitution screening strategy for leukemia-targeting apohemoglobin therapies.

Publications

June, 2025 M. Cervenka, **B.L. Shanks**, P.E. Mason, P. Jungwirth, *Cation-π Interactions in Biomolecular Contexts by Neutron Scattering and Molecular Dynamics: Case Study of the Tetramethylammonium Cation*, J. Phys. Chem. B, (*link*).

April, 2025 **B.L. Shanks*,** H.W. Sullivan, P.J. Jungwirth, M.P. Hoepfner, *Experimental Evidence of Quantum Drude Oscillator Behavior in Liquids Revealed with Machine Learning Assisted Iterative Boltzmann Inversion*, J. Chem. Phys., (*link*).
*Corresponding Author

December, 2024 **B.L. Shanks,** H.W. Sullivan, M.P. Hoepfner, *Bayesian Analysis Reveals the Key to Extracting Pair Potentials from Neutron Scattering Data*, J. Phys. Chem. Lett., (*link*).

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

March, 2024 **B.L. Shanks,** H.W. Sullivan, A.R. Shazed, M.P. Hoepfner, *Accelerated Bayesian Inference for Molecular Simulations using Local Gaussian Process Surrogate Models*, J. Chem. Theory Comput., (*link*).

September, 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., (*link*).

December, 2022 **B.L. Shanks,** J.J. Potoff, M.P. Hoepfner, *Transferable Force Fields from Experimental Scattering Data with Machine Learning Assisted Structure Refinement*, J. Phys. Chem. Lett., (*link*).

Submitted / In Preparation

Submitted, 2025 Shujie Fan, Philip E. Mason, Victor Cruces Chamorro, **B.L. Shanks**, Hector Martinez-Seara, Pavel Jungwirth, *Charge Scaling Force Field for Biologically Relevant Ions Utilizing a Global Optimization Method*, chemRxiv, (*link*).

Submitted, 2025 H.W. Sullivan, **B.L. Shanks***, M. Cervenka, M.P. Hoepfner, *Inference of Radial Distribution Functions with Non-Stationary Gaussian Processes*, arXiv, (*link*).
*Corresponding Author

In Preparation, 2025 A.R. Vishwakarma, **B.L. Shanks**, R.S. Pierre, J. Li, *Experimental Characterization and Hyperelastic Constitutive Modeling of Ecoflex Silicone Elastomers*.

In Preparation, 2025 V. Kostal, **B.L. Shanks**, Hector Martinez-Seara, Pavel Jungwirth, *Bayesian inference of force field charge distributions for biomolecular simulations guided by ab initio molecular dynamics*.

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*.

Peer Reviewing

2025 - **Journal of Chemical Physics**, *Reviewed 2 Articles*.

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

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

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

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

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

Awards

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

February, 2021 **1st Place Presentation**, *University of Utah Graduate Engineering Symposium*, SLC, UT.
Selected among 30 graduate students for outstanding presentation of scientific research.

Conference Presentations

Invited Talks

June, 2025 **Embracing Uncertainty in Computational Chemistry the Bayesian Way**, *Masaryk University*, Brno, CZ, Invited by Dr. Robert Vacha.

March, 2025 **Bayesian Approaches to Force Field Optimization and Surrogate Modeling**, *Q-Scaling Workshop, IOCB*, Prague, CZ.

March, 2024 **Bayesian Methods in Computational Chemistry with Applications to Neutron Diffraction**, *Johns Hopkins University*, Baltimore, MD, Invited by Dr. Paulette Clancy.

February, 2024 **Bayesian Methods in Computational Chemistry**, *Institute of Organic Chemistry and Biochemistry (IOCB)*, Prague, CZ, Invited by Dr. Pavel Jungwirth.

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

September, 2023 **Bayesian Methods in Neutron Diffraction Analysis**, *University of Utah*, Salt Lake City, UT, Invited by Dr. Valeria Molinero.

Contributed Talks

November, 2025 **Combining Quantum Theory and Scattering Experiments in Machine Learning Potentials**, *AIChE Annual Meeting*, Boston, MA, ML for Soft and Hard Materials.

November, 2025 **Bridging Neutron Scattering and Quantum Polarization for Aqueous Ions**, *AIChE Annual Meeting*, Boston, MA, Molecular Simulation Methods II.

November, 2025 **Radial Distribution Function Uncertainty Quantification with Non-Stationary Gaussian Processes**, *AIChE Annual Meeting*, Boston, MA, ML for Soft and Hard Materials.

August, 2025 **Toward a Bayesian Framework for Liquid State Theory**, *Gordon Research Seminar: Chemistry and Physics of Liquids*, Holderness, NH.

January, 2024 **Challenges in Reconstructing Classical Force Fields from Scattering Data**, *EFRC Workshop*, Salt Lake City, UT, Department of Energy.

November, 2023 **Structure Optimized Potential Refinement for Molecular Simulation**, *AIChE Annual Meeting*, Orlando, FL, Session: Molecular Simulation Methods.

November, 2023 **Learning Atomic Forces from Fluid Structure Measurements**, *AIChE Annual Meeting*, Orlando, FL, Session: ML for Soft and Hard Materials.

September, 2023 **State-Dependent Atomic Forces in Fluid Ensembles**, *EFRC Principal Investigators Meeting – Lightning Talk*, Virtual, DOE.

August, 2023 **ML for Interatomic Forces from Experimental Structure**, *ACS Fall Meeting (COMP Session)*, San Francisco, CA, Chair: ML in Chemistry.

January, 2022 **Transferable Force Fields with Structure-Optimized Potential Refinement**, *CECAM Workshop*, Lausanne, CH, Centre Européen de Calcul Atomique et Moléculaire.

October, 2021 **Structure Optimized Force Fields for Fluids**, *US Total Scattering School*, Oak Ridge National Laboratory, TN.

February, 2021 **Machine Learning for Neutron Diffraction Analysis**, *Graduate Research Symposium*, Salt Lake City, UT, University of Utah.

January, 2021 **Self-Assembly in Biological Liquids via Machine Learning**, *Utah Biomedical Engineering Conference*, Salt Lake City, UT.

Poster Presentations

November, 2025 **Quantum + Scattering Data for Machine Learning Potentials**, *AIChE Annual Meeting*, Boston, MA.

August, 2025 **Toward a Bayesian Framework for Liquid State Theory**, *Gordon Research Conference: Chemistry and Physics of Liquids*, Holderness, NH.

July, 2024 **Exploring State-Dependence of Classical Pair Potentials**, *Foundations of Molecular Modeling and Simulation*, Salt Lake City, UT.

September, 2023 **Translating Atomistic Modeling to the Continuum Scale**, *EFRC Principal Investigators Meeting*, Virtual.

August, 2023 **Structure Optimized Potential Refinement from Scattering Data**, *ACS Fall Meeting – COMP Division*, San Francisco, CA.

August, 2023 **ML Prediction of Force Fields from Scattering Measurements**, *Gordon Research Conference: Chemistry and Physics of Liquids*, Holderness, NH.

March, 2022 **Bayesian Optimized Force Fields with RDF Surrogates**, *CECAM Workshop on ML-Accelerated MD*, Trieste, IT.

January, 2021 **Neutron Scattering Predicts Emergent Thermodynamics**, *CECAM*, Lausanne, CH.

Positions of Responsibility

Internal

April, 2023 **Chair**, *Retention, Promotion, and Tenure Decisions Student Committee*, University of Utah.

April, 2021 **Member**, *Retention, Promotion, and Tenure Decisions Student 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.

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.