RICHARD MESSERLY

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EDUCATION

Ph.D. Chemical Engineering, Brigham Young University, Provo, UT Apr. 2017
- Dissertation: How a Systematic Approach to Uncertainty Quantification Renders Molecular Simulation a Quantitative Tool in Predicting the Critical Constants for Large *n*-Alkanes
- Expertise: Force Field Development, Computational Chemistry, Configuration Reweighting, Uncertainty Quantification in Molecular Simulation, Thermodynamic Data Analysis
- Elective Courses: Quantum Chemistry, Statistical Mechanics, Nonlinear Statistical Analysis, Polymer Science and Engineering, Advanced Organic Chemistry, Classical Mechanics, Instrumental Analysis Lecture/Lab GPA: 4.0/4.0

B.S. Chemical Engineering, Brigham Young University, Provo, UT Dec. 2012
- Elective Courses: Molecular Modeling, Introduction to Partial Differential Equations
- Excelled in: Thermodynamics, Physical Chemistry, Reaction Engineering, Separations, Process Control, Statistics
- Minors: Spanish, French Overall GPA: 3.78/4.0

EXPERIENCE

Computational Scientist, Oak Ridge National Laboratory, Oak Ridge, TN Oct. 2024 – Present
- Served as artificial intelligence liaison for users of Frontier, the fastest supercomputer in the world

Staff Scientist, Los Alamos National Laboratory, Los Alamos, NM June 2021 – Oct. 2024
- Earned highly competitive Early Career Research Laboratory Directed Research & Development
- Developed machine learning interatomic potentials for diverse chemical and materials systems
- Mentored postdoc and five summer students with projects related to machine learning

Postdoctoral Researcher, Los Alamos National Laboratory, Los Alamos, NM Nov. 2019- June 2021
- Published literature review on aging and lifetime prediction of high explosives
- Predicted dissociative recombination rates based on excited-state *ab initio* molecular dynamics

Postdoc Research Scientist, National Renewable Energy Laboratory, Golden, CO Feb. 2019- Nov. 2019
- Employed accelerated molecular dynamics techniques to study low-temperature combustion pathways
- Estimated combustion reaction rates with transition state theory and machine learning
- Collaborated with researchers at Massachusetts Institute of Technology, Pennsylvania State University

NRC Postdoc Associate, National Institute of Standards and Technology, Boulder, CO Feb. 2017- 2019
- Received 91/100 scoring from National Research Council (NRC) selection committee
- Implemented alchemical free energy methods to accelerate Bayesian inference of force field parameters
- Collaborated with researchers at the NIST Gaithersburg, University of Colorado, University of Akron, Wayne State University, and the Open Force Field Initiative
- Mentored summer student while competing in the 10th Industrial Fluid Properties Simulation Challenge

Research Assistant, Design Institute for Physical Properties, Provo, UT Jan. 2012-Feb. 2014
- Evaluated literature experimental data and property prediction models for two biofuels
- Presented research updates for thirty minutes at biannual meetings with sponsors
- Mentored two undergraduate students performing experimental work and data analysis

Teaching Assistant, BYU Chemical Engineering, Provo, UT

- Courses: Chemical Process Principles, Dr. Thomas H. Fletcher — Jan.-Apr. 2012
  Plant Design & Synthesis, Dr. W. Vincent Wilding — Jan.-Apr. 2013/2014
  Molecular Modeling, Dr. Thomas A. Knotts IV — Jan.-Apr. 2015
- Conducted exam reviews, tutored students, and graded homework assignments

PUBLICATIONS

Allen, A. E. A.; Lubbers, N.; Matin, S.; Smith, J.; **Messerly, R.**; Tretiak, S.; Barros, K. Learning together: Towards foundation models for machine learning interatomic potentials with meta-learning. *npj Computational Materials*. 10, 154, 2024.

Zhang, S.; Makos M. Z.; Jadrich, R. B.; Kraka, E.; Barros, K.; Nebgen, B. T.; Tretiak, S.; Isayev, O.; Lubbers, N.; **Messerly, R. A**.; Smith, J. S. Exploring the frontiers of condensed-phase chemistry with a general reactive machine learning potential. *Nature Chemistry*. 16, 727-734, 2024.

Stippell, E.; Alzate-Vargas, L.; Subedi, K. N.; Tutchton, R. M.; Cooper, M. W. D.; Tretiak, S.; Gibson, T.; **Messerly, R. A.** Building a DFT+U Machine Learning Interatomic Potential for Uranium Dioxide. *Artificial Intelligence Chemistry.* 2 (1), 2024.

Fedik, N.; Nebgen, B.; Lubbers, N.; Barros, K.; Kulichenko, M.; Li, Y. W.; Zubatyuk, R.; **Messerly, R.**; Isayev, O.; Tretiak, S. Synergy of semiempirical models and machine learning in computational chemistry. *The Journal of Chemical Physics.* 159 (11), 2023.

Freixas, V. M.; Malone, W.; Li, X.; Song, H.; Negrin-Yuvero, H.; Pérez-Castillo, R.; White, A.; Gibson, T. R.; Makhov, D. V.; Shalashilin, D. V.; Zhang, Y.; Fedik, N.; Kulichenko, M.; **Messerly, R.**; Mohanam, L. N.; Sharifzadeh, S.; Bastida, A.; Mukamel, S.; Fernandez-Alberti, S.; Tretiak, S. NEXMD v2.0 software package for nonadiabatic excited state molecular dynamics simulations. *Journal of Chemical Theory and Computation.* 19 (16), 5356-5368, 2023.

Kulichenko, M.; Barros, K.; Lubbers, N.; Li, Y. W.; **Messerly, R.**; Tretiak, S.; Smith, J. S.; Nebgen, B. Uncertainty-driven dynamics for active learning of interatomic potentials. *Nature Computational Science.* 3 (3), 230-239, 2023.

Fedik, N.; Zubatyuk, R.; Kulichenko, M.; Lubbers, N.; Smith, J. S.; Nebgen, B.; **Messerly, R.**; Li, Y. W.; Boldyrev, A. I.; Barros, K.; Isayev, O.; Tretiak, S. Extending machine learning beyond interatomic potentials for predicting molecular properties. *Nature Reviews Chemistry.* 6 (9), 653-672, 2022.

Messerly, R. A.; Yoon, T. J.; Jadrich, R. B.; Currier, R. P.; Maerzke, K. A. Elucidating the temperature and density dependence of silver chloride hydration numbers in high-temperature water vapor: A first-principles molecular simulation study. *Chemical Geology*. 594, 120766, 2022.

Messerly, R. A.; Gifford, B. J.; Holland, T. M. Kinetic isotope effects for dissociative recombination of tritiated ketenyl ion (3HCCO+): A surface-hopping ab initio molecular dynamics study. *Computational and Theoretical Chemistry*. 1210, 113634, 2022.

Madin, O. C.; Boothroy, S.; **Messerly, R. A**.; Fass, J.; Chodera, J. D.; Shirts, M. R. Bayesian-inference-drive model parameterization and model selection for 2CLJQ fluid models. *Journal of Chemical Information and Modeling.* 62 (4), 874-889, 2022.

Sifain, A. E.; Lystrom, L.; **Messerly, R. A.**; Smith, J. S.; Nebgen, B.; Barros, K.; Tretiak, S.; Lubbers, N.; Gifford, B. J. Predicting phosphorescence energies and inferring wavefunction localization with machine learning. *Chemical Science*, 12 (30), 10207-10217, 2021.

Messerly, R. A.; Luecke, J. H.; St. John, P.; Etz, B. D.; Kim, Y.; Zigler, B.; McCormick, R.; Kim, S. Understanding how chemical structure affects ignition-delay-time ϕ-sensitivity. *Combustion & Flame,* 225, 377-387, 2021.

Messerly, R. A.; Rahimi, M.; St. John, P.; Luecke, J.; Park, J.; Huq, N. A.; Foust, T. D.; Lu, T.; Zigler, B.; McCormick, R.; Kim, S. Towards quantitative prediction of ignition-delay-time sensitivity on the fuel-to-air equivalence-ratio. *Combustion & Flame,* 214, 103-115, 2020.

Messerly, R. A.; Gokul, N; Schultz, A. J.; Kofke, D. A.; Harvey, A. H. Molecular calculation of the critical parameters of classical helium. *Journal of Chemical & Engineering Data,* 65, 3, 1028-1037, 2020.

Etz, B. D.; Fioroni G. M.; **Messerly, R. A.;** Rahimi, M. J.; St. John, P. C.; Robichaud, D. J.; Christensen E. D.; Beekley, B. P.; McEnally, C. S.; Pfefferle, L. D.; Xuan, Y.; Vyas, S.; Paton, R. S.; McCormick, R. L.; Kim, S. Elucidating the chemical pathways responsible for the sooting tendency of 1 and 2-phenylethanol. *Proceedings of the Combustion Institute,* 38, 1327-1334, 2020.

Kwon, H.; Etz, B. D.; Montgomery, M. J.; **Messerly, R. A.**; Shabnam, S.; Vyas, S.; van Duin, A. C.; McEnally, C. S.; Pfefferle, L. D.; Kim, S.; Xuan, Y.. Reactive molecular dynamics simulations and quantum chemistry calculations to investigate soot-relevant reaction pathways for hexylamine isomers. *Journal of Physical Chemistry A,* 124(21), 4290–4304, 2020.

Kim, Y.; Etz, B. D.; Fioroni, G. M.; Hays, C. K.; St. John, P.; **Messerly, R. A.;** Vyas, S.; Beekley, B. P.; Guo, F.; McEnally, C. S.; Pfefferle, L. D.; McCormick, R. L.; Kim, S. Investigation of structural effects of aromatic compounds on sooting tendency with mechanistic insight into ethylphenol isomers. *Proceedings of the Combustion Institute,* 38, 1143-1151, 2020.

Messerly, R. A.; Soroush Barhaghi, M.; Potoff, J. J.; Shirts, M. R. Histogram-free reweighting with grand canonical Monte Carlo: Post-simulation optimization of non-bonded potentials for phase equilibria. *Journal of Chemical & Engineering Data*, 64, 9, 3701-3717, 2019.

Messerly, R. A.; Anderson, M. C.; Razavi, S. M.; Elliott, J. R. Mie 16-6 force field predicts viscosity with faster-than-exponential pressure dependence for 2,2,4-trimethylhexane. *Fluid Phase Equilibria*, 495, 76-85, 2019.

Messerly, R. A.; Anderson, M. C.; Razavi, S. M.; Elliott, J. R. Improvements and limitations of Mie λ-6 potential for prediction of saturated and compressed liquid viscosity. *Fluid Phase Equilibria*, 483, 101-115, 2019.

Bell, I. H.; **Messerly, R. A.**; Thol, M.; Costigliola, L; Dyre, J. Modified residual entropy scaling of the transport properties of the Lennard-Jones fluid. *Journal of Physical Chemistry B,* 123(29), 6345-6363, 2019.

Razavi, S. M.; **Messerly, R. A.**; Elliott, J. R. Coexistence calculation using the isothermal-isochoric integration method. *Fluid Phase Equilibria,* 501, 2019.

Maginn, E. J.; **Messerly, R. A.**; Carlson, D. J.; Roe, D. R.; Elliott, J. R. Best Practices for Computing Transport Properties 1. Self-Diffusivity and Viscosity from Equilibrium Molecular Dynamics. *Living Journal of Computational Molecular Science*, 1(1), 2019.

Messerly, R. A.; Shirts, M. R.; Kazakov, A. F. Uncertainty quantification confirms unreliable extrapolation toward high pressures for united-atom Mie λ-6 force field. *The Journal of Chemical Physics,* 149(11), 114109, 2018.

Messerly, R. A.; Razavi, S. M.; Shirts, M. R. Configuration-sampling-based surrogate models for rapid parameterization of non-bonded interactions. *Journal of Chemical Theory and Computation*, 14 (6), 3144-3162, 2018.

Messerly, R. A.; Knotts IV, T. A.; Wilding, W. V. Uncertainty quantification and propagation of errors of the Lennard-Jones 12-6 parameters for *n*-alkanes. *The Journal of Chemical Physics,* 146, 194110(1-16), 2017.

Messerly, R. A.; Knotts IV, T. A.; Giles, N. F.; Wilding, W. V. Developing an internally consistent set of theoretically based prediction models for the critical constants and normal boiling points of large *n*-alkanes. *Fluid Phase Equilibria*, 449, 104-116, 2017.

Messerly, R. A. First principles prediction of the copolymerization process of 1,3-butadiene and vinyl chloride. *Journal of Theoretical & Computational Science*, 3:142, 1-4, 2016.

Messerly, R. A.; Knotts IV, T. A.; Rowley, R. L.; Wilding, W. V. Improved estimates of the critical point constants for large *n*-alkanes using Gibbs ensemble Monte Carlo simulations. *Journal of Chemical & Engineering Data*, 61(10), 3640-3649, 2016.

Messerly, R. A.; Knotts IV, T. A.; Rowley, R. L.; Wilding, W. V. An improved approach for predicting the critical constants of large molecules with Gibbs ensemble Monte Carlo simulation. *Fluid Phase Equilibria*, 425, 432-442, 2016.

Hogge, J. W.; **Messerly, R. A.**; Giles, N. F.; Knotts IV, T. A.; Rowley, R. L.; Wilding, W. V. Improving thermodynamic consistency among vapor pressure, heat of vaporization, and liquid and ideal gas isobaric heat capacities through multi-property optimization. *Fluid Phase Equilibria*, 418, 37-43, 2016.

Messerly, R. A.; Rowley, R. L.; Knotts IV, T. A.; Wilding, W. V. An improved statistical analysis for predicting the critical temperature and critical density with Gibbs ensemble Monte Carlo simulation. *The Journal of Chemical Physics*, 143(10), 104101(1-8), 2015.

Bell, J. C.; **Messerly, R. A.**; Gee, R.; Harrison, A.; Rowley, R. L.; Wilding, W. V. Ternary liquid-liquid equilibrium of biodiesel compounds for systems consisting of a methyl ester + glycerin + water. *Journal of Chemical & Engineering Data*, 58(4), 1001-1004, 2013.

PRESENTATIONS (ORAL)

Beyond United-Atom Lennard-Jones: Reliable Prediction of High Pressure Viscosities, *American Institute of Chemical Engineers Annual Meeting,* Pittsburgh, Pennsylvania, 2018.

Are Modern Force Fields Sufficiently Reliable for Developing Fundamental Equations of State from Hybrid Data Sets? *American Institute of Chemical Engineers Annual Meeting,* Pittsburgh, Pennsylvania, 2018.

Bayesian Inference Demonstrates Inadequacies of Mie λ-6 Repulsive Barrier at High Pressures, *American Institute of Chemical Engineers Annual Meeting,* Pittsburgh, Pennsylvania, 2018.

Uncertainty Quantification of Non-bonded Potentials for Prediction of Thermophysical Properties with Molecular Simulation, *20th Symposium on Thermophysical Properties,* Boulder Colorado, 2018.

Accelerating Force Field Parameterization to Improve the Quantitative Predictability of Thermophysical Properties, *American Institute of Chemical Engineers Annual Meeting,* Minneapolis, Minnesota, 2017.

Pushing the Frontier of Data-Driven Force Field Development, *Thermodynamics Research Center Consortium,* Boulder, Colorado, 2017.

A Novel Force Field Development Algorithm to Improve the Quantitative Predictability of Thermophysical Properties with Molecular Simulation, *European Symposium on Applied Thermodynamics 2017,* Bucharest, Romania, 2017.

How Uncertainty Quantification Renders Molecular Simulation a Quantitative Tool for Thermophysical Property Evaluation, *American Institute of Chemical Engineers Annual Meeting,* San Francisco CA, 2016.

Uncertainty Quantification of Intermolecular Parameters with a Transferable Potential Model for *n*-Alkanes, *American Institute of Chemical Engineers Annual Meeting,* San Francisco CA, 2016.

A Statistical Analysis of the Propagation of Error Associated with the Intermolecular Potential Model When Simulating Large Compounds, *American Institute of Chemical Engineers Annual Meeting,* Salt Lake City Utah, 2015.

A Statistical Approach to Reducing Finite-Size Effects from Gibbs Ensemble Monte Carlo Simulations for Predicting the Critical Point, *American Institute of Chemical Engineers Annual Meeting,* Salt Lake City Utah, 2015.

Group Contribution Model for Predicting Critical Volume with the Flory-Huggins Theory Asymptotic Behavior, *19th Symposium on Thermophysical Properties,* Boulder Colorado, 2015.

PRESENTATIONS (POSTER)

Uncertainty Quantification and Propagation Associated with a Transferable Intermolecular Potential Model for *n*-Alkanes, *International Conference on Properties and Phase Equilibria for Product and Process Design,* Porto Portugal, 2016.

Molecular Simulations of the Critical Point for Molecules that Decompose Experimentally, *American Institute of Chemical Engineers Annual Meeting,* Atlanta Georgia, 2014.

SKILLS/AWARDS

- **Programming languages:**
  - Python – advanced
  - MATLAB – advanced
  - Bash/Shell – intermediate
  - C++ – intermediate
  - Fortran 90 – intermediate
  - Visual Basic for Applications (VBA) – basic
  - R Project for Statistical Computing – basic
  - Structured Query Language (SQL) – basic
- **Simulation packages:**
  - Gromacs – advanced
  - Gaussian – advanced
  - Monte Carlo for Complex Chemical Systems (MCCCS) Towhee – advanced
  - Cassandra Monte Carlo – advanced
  - Atomic Simulation Environment (ASE) - intermediate

- CP2K – intermediate
- GPU Optimized Monte Carlo (GOMC) – intermediate
- MOLPRO – intermediate
- Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) – basic
- Amsterdam Density Functional (ADF) – basic

- **Additional software:**
  - Tensorflow, Scikit learn, PyTorch – advanced
  - LaTeX – advanced
  - Microsoft Office – advanced
  - Mathcad – advanced
  - Git – intermediate
- **Spoken languages:**
  - **Spanish** – advanced reading, writing, and speaking
  - **Portuguese** – advanced reading, writing, and speaking
  - **French** – intermediate reading, writing, and speaking
- **Dean's List Student** – achieved a 4.0 semester GPA as undergraduate Apr. 2009 & Jun. 2010
- **Eagle Scout Award** – erected a flag pole in front of a religious center Sept. 11th, 2002
- **3rd Place Award** – 10th Industrial Fluid Properties Simulation Challenge

VOLUNTEER WORK

Youth Basketball Coach, City of Rio Rancho, New Mexico 2022-2023
- Coached two teams of 9-10-year-olds simultaneously with multiple practices per week

Church Representative, The Church of Jesus Christ of Latter-day Saint, Guatemala Nov. 2006-2008
- Led a regional group of 12 representatives

Boy Scout Leader, Boy Scouts of America 1999-2006
- Inspired younger scouts to achieve their Eagle while organizing campouts and teaching activities

AREAS OF EXPERTISE

- **Computational chemistry (*ab initio* and density functional theory)**
- **Machine learning interatomic potentials (neural networks trained to quantum mechanics data)**
- **Dataset generation with active learning**
- **Free energy calculations with multistate reweighting**
- **Molecular dynamics and Monte Carlo simulations**
- **Classical force field development**
- **Vapor-liquid phase equilibria with Gibbs Ensemble and grand canonical Monte Carlo**
- **Prediction of thermodynamic and transport properties with classical molecular simulation**
- **Data analysis (non-linear statistics, Bayesian inference, machine learning)**

RESEARCH INTERESTS

- **Machine learning to improve electronic structure and computational chemistry methods**
- **Advanced sampling techniques, e.g., uncertainty-driven dynamics, meta dynamics**
- **Physics-informed machine learning to improve interpretability and transferability**

REFERENCES AVAILABLE UPON REQUEST