RICHARD MESSERLY

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EDUCATION

Ph.D. Chemical Engineering, Brigham Young University, Provo, UT 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, Uncertainties 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

B.S. Chemical Engineering, Brigham Young University, Provo, UT 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

WORK EXPERIENCE

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
- Presented research updates for thirty minutes at annual meetings with consortium members
- Collaborated with researchers at the National Institute of Standards and Technology, University of Colorado, University of Akron, Wayne State University, and the Open Force Field Initiative
- Mentored undergraduate student during three-month project for the 10th Industrial Fluid Properties Simulation Challenge

Research Assistant, Design Institute for Physical Properties, Provo, UT Jan. 2012-Feb. 2014
- Performed experimental work that involved: preparation, execution, cleaning, and processing data
- 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, held office hours, and graded homework assignments

VOLUNTEER WORK

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

SKILLS/AWARDS

- **Programming languages:**
  - Python – advanced
  - MATLAB – advanced
  - Bash/Shell – intermediate
  - C++ – basic
  - Visual Basic for Applications (VBA) – basic
  - R Project for Statistical Computing – basic
  - Structured Query Language (SQL) – basic
- **Molecular simulation packages:**
  - Gromacs – advanced
  - Monte Carlo for Complex Chemical Systems (MCCCS) Towhee – advanced
  - Cassandra – intermediate
  - Gaussian – intermediate
  - GPU Optimized Monte Carlo (GOMC) – intermediate
  - Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) – basic
- **Additional software:**
  - LaTeX – advanced
  - Microsoft Office – advanced
  - Mathcad – advanced
  - Git – intermediate
- **Spoken languages:**
  - **Spanish** – advanced reading, writing, and speaking
  - **French** – intermediate reading, writing, and speaking
  - **Portuguese** – basic 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

PUBLICATIONS

Uncertainty quantification confirms unreliable extrapolation toward high pressures for united-atom Mie λ-6 force field. *The Journal of Chemical Physics.* Pending publication.

Best Practices for Computing Transport Properties 1. Self-Diffusivity and Viscosity from Equilibrium Molecular Dynamics v1. *Living Journal of Computational Molecular Science.* Pending publication.

Configuration-sampling-based surrogate models for rapid parameterization of non-bonded interactions. *Journal of Chemical Theory and Computation*, 14 (6), pp. 3144-3162, 2018.

Uncertainty quantification and propagation of errors of the Lennard-Jones 12-6 parameters for *n*-alkanes, *The Journal of Chemical Physics,* 146, pp. 194110(1-16), 2017.

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.

Improved estimates of the critical point constants for large *n*-alkanes using Gibbs ensemble Monte Carlo simulations, *Journal of Chemical & Engineering Data,* 61(10), pp. 3640-3649, 2016.

An improved approach for predicting the critical constants of large molecules with Gibbs ensemble Monte Carlo simulation, *Fluid Phase Equilibria,* 425, pp. 432-442, 2016.

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

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), pp. 104101(1-8), 2015.

PRESENTATIONS

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.

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.

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.

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