1995 E Coalton rd 89-102, Boulder, CO 80027

801-358-1741 • r.alma.messerly@gmail.com

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.