# Refereed Journal Articles

8. Richard A. Messerly, Michael R. Shirts, and Andrei F. Kazakov. "United-atom, Mie $\lambda$-6 force fields for normal and branched alkanes perform poorly at high pressures when parameterized using vapor-liquid equilibria properties." *The Journal of Physical Chemistry B.* Pending publication.

7. Richard A. Messerly, S. Mostafa Razavi, and Michael R. Shirts. "Configuration-sampling-based surrogate models for rapid parameterization of non-bonded interactions." *Journal of Chemical Theory and Computation.* Pending publication.

6. Richard A. Messerly, Thomas A. Knotts IV, and W. Vincent Wilding. "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.

5. Richard A. Messerly, Thomas A. Knotts IV, Neil F. Giles, and W. Vincent Wilding. "Developing an internally consistent set of theoretically based prediction models for the critical constants and normal boiling point of large $n$-alkanes." *Fluid Phase Equilibria.* 449, 104-116, 2017.

4. Richard A. Messerly, Thomas A. Knotts IV, Richard L. Rowley, and W. Vincent Wilding. "Improved estimates of the critical point constants for large $n$-alkanes using Gibbs ensemble Monte Carlo simulations." *Journal of Chemical & Engineering Data.* 2016.

3. Richard A. Messerly, Thomas A. Knotts IV, Richard L. Rowley, and W. Vincent Wilding. "An improved approach for predicting the critical constants of large molecules with Gibbs ensemble Monte Carlo simulation." *Fluid Phase Equilibria.* 425, 432-442. 2016.

2. Richard A. Messerly. "First Principles Prediction of the Copolymerization Process of 1,3-Butadiene and Vinyl Chloride." *Journal of Theoretical & Computational Science.* 3:142. 2016.

1. Richard A. Messerly, Richard L. Rowley, Thomas A. Knotts IV, and W. Vincent Wilding. "An improved statistical analysis for predicting the critical temperature and critical density with Gibbs ensemble Monte Carlo simulation." *Journal of Chemical Physics.* 143, 104101, 1-8. 2015.

# Presentations

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

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

8. Richard A Messerly. "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.

7. Richard A Messerly. "How Uncertainty Quantification Renders Molecular Simulation a Quantitative Tool for Thermophysical Property Evaluation." *American Institute of Chemical Engineers Annual Meeting.* San Francisco, California. 2016.

6. Richard A Messerly. "Uncertainty Quantification of Intermolecular Parameters with a Transferable Potential Model for *n*-Alkanes." *American Institute of Chemical Engineers Annual Meeting.* San Francisco, California. 2016.

5. Richard A Messerly. "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.

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

3. Richard A Messerly. "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.

2. Richard A Messerly. "Group Contribution Model for Predicting Critical Volume with the Flory-Huggins Theory Asymptotic Behavior." *19$^{th}$ Symposium on Thermophysical Properties.* Boulder, Colorado. 2015.

1. Richard A Messerly. "Molecular Simulations of the Critical Point for Molecules That Decompose Experimentally." *American Institute of Chemical Engineers Annual Meeting.* Atlanta, Georgia. 2014.