Complete list of publications of Richard Messerly

A Publications with peer review process

1. **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.* 14 (6), 3144-3162, 2018.

2. **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.

3. **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.* 61 (10), 3640-3649, 2016.

5. **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.

6. **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.

7. Joseph W. Hogge*, **Richard A. Messerly**, Neil Giles, Thomas Knotts, Richard Rowley, W. Vincent Wilding. "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.

8. **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.

9. Joseph C. Bell*, **Richard A. Messerly**, Ryan Gee, Aaron Harrison, Richard L. Rowley, and W. Vincent Wilding. "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.

B Submitted publications with peer review process

1. **Richard A. Messerly***, Michael R. Shirts, and Andrei F. Kazakov. "Uncertainty quantification confirms unreliable extrapolation toward high pressures for united-atom Mie λ-6 force field." *The Journal of Chemical Physics.* (publisher's acknowledgment of receipt enclosed)

2. Edward J. Maginn, **Richard A. Messerly***, Daniel J. Carlson, Daniel R. Roe, J. Richard Elliott. "Best Practices for Computing Transport Properties 1. Self-Diffusivity and Viscosity from Equilibrium Molecular Dynamics v1." *Living Journal of Computational Molecular Science.* (publisher's acknowledgment of receipt enclosed)

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The following above mentioned publications have evolved from my doctoral dissertation: A2, A3, A4, A5, A8

as of July 2018