

## List of the selected key publications of Richard Messerly

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**, Michael R. Shirts, and Andrei F. Kazakov. “Uncertainty quantification confirms unreliable extrapolation toward high pressures for united-atom Mie -6 force field.” *The Journal of Chemical Physics*. (publisher’s acknowledgment of receipt enclosed)