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.

   This was my first publication during my postdoctoral associateship at the National Institute of Standards and Technology (NIST). Furthermore, this publication marked the first time that my co-authors were collaborators outside of my own institution. Furthermore, Michael R. Shirts is an extremely well-published young professor and S. Mostafa Razavi is a graduate student for J. Richard Elliott, an established expert in the field. Thus, this was a landmark publication that helped to proliferate my name throughout the molecular simulation community. With respect to the actual content, this publication compared Michael Shirt's existing method (MBAR) with a novel approach I developed (PCFR). The comparison demonstrated that these two methods are complementary and should be implemented together. Furthermore, I demonstrated how to merge these two methods with an approach developed by J. Richard Elliott (ITIC). **Personal contribution: 75%.**

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.

   This publication was the culmination of my dissertation and led directly to my postdoctoral position with the Thermodynamics Research Center (TRC) at NIST. The main topic is uncertainty quantification (UQ) of thermophysical properties with molecular simulation, which is a strong interest at NIST. After presenting this research, the TRC group leader strongly encouraged me to apply for a National Research Council (NRC) postdoctoral position in his group, which was a pivotal step in developing my academic profile. Furthermore, this publication played a key role in joining the Open Force Field initiative, since this group utilizes Bayesian UQ methods as part of force field development. As a participant in this initiative, I have created strong connections and learned firsthand from a diverse set of experts in the field of molecular simulation. **Personal contribution: 90%.**

3. **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)

This study was motivated by the "hybrid data set" work performed previously by Vrabec. The results from this study were influential in my application to the Humboldt Research Fellowship. Specifically, this publication provided convincing evidence that the state-of-the-art Mie λ-6 force field is overly-repulsive at high pressures and, therefore, should not be used with the hybrid data set approach. Naturally, this conclusion sparked several ideas for how to improve force fields at high pressures. After discussing this issue with several colleagues, we proposed the more flexible and physically realistic extended Lennard-Jones (ex-LJ) non-bonded potential. The use of ex-LJ for hybrid data sets is the premise of my current proposal. **Personal contribution: 90%.**