Wang-Landau Simulations for Self-assembling Systems

Katie Maerzkev[S], Lili Gai, Peter Cummings and Clare McCabe[C]
Vanderbilt University, Department of Chemical and Biomolecular Engineering, Nashville, TN, U.S.A.
c.mccabe@vanderbilt.edu

Understanding the relative free energies of various conformations of macromolecules and the phase transitions in self-assembled systems is an extremely important area of study; however, limited progress has been made to date since the calculation of free energy remains a significant challenge for molecular simulation. A recent breakthrough in this area is the Wang-Landau method, which allows for the direct calculation of the density of states, and thus the free energy. However, Wang-Landau simulations for continuous molecular systems present several challenges regarding efficient implementation and sampling techniques that must be overcome to utilize the method broadly. One promising approach is a hybrid Wang-Landau/transition matrix technique, wherein the Wang-Landau method quickly achieves broad sampling of phase space and the transition-matrix method accelerates convergence. We will report our results for the self-assembly of a simple off-lattice model using a hybrid Wang-Landau/transition matrix method.