Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Simulation of non-ionic surfactant micelle formation across a range of temperature and pressure GREGORY CUSTER, University of Maryland, PAYEL DAS, IBM Thomas J. Watson Research Center, SILVINA MATYSIAK, University of Maryland — Non-ionic surfactants can, at certain concentrations and thermodynamic conditions, aggregate into micelles due to their amphiphilic nature. Our work looks at the formation and behavior of micelles at extremes of temperature and pressure. Due to the large system size and simulation time required to study micelle formation, we have developed a coarse-grained (CG) model of our system. This CG model represents each heavy atom with a single CG bead. We use the multibody Stillinger-Weber potential, which adds a three-body angular penalty to a two-body potential, to emulate hydrogen bonds in the system. We simulate the linear surfactant $C_{12}E_5$, which has a nonpolar domain of 12 carbons and a polar domain of 5 ethers. Our CG model has been parameterized to match structural properties from all-atom simulations of single and dimer surfactant systems. Simulations were performed using a concentration above the experimental critical micelle concentration at 300K and 1atm. We observe an expected region of stable micelle formation at intermediate temperature, with a breakdown at high and low temperature, as well as at high pressure. The driving forces behind the destabilization of micelles and the mechanism of micelle formation at different thermodynamic conditions will be discussed.

Gregory Custer
University of Maryland

Date submitted: 06 Nov 2015 Electronic form version 1.4