Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Molecular dynamics study of shape transitions in aqueous micelle solutions[1] A. SANGWAI, R. SURESHKUMAR, Syracuse University, Syracuse, NY 13244, USA. — It is well known that surfactant molecules self-assemble in aqueous solutions to form various micellar structures such as spheres, rods or sheets. Although this phenomenon is widely studied experimentally, the molecular mechanisms of shape transitions are not well understood. Atomistic simulations of self-assembled micellar systems are computationally prohibitive to sample several hundred nanoseconds necessary to capture shape transitions. We demonstrate that MARTINI coarse-grained (CG) force field for CTAC is capable of accurately representing micellar assemblies by comparing the CG system to fully atomistic ones. Microsecond molecular dynamic simulations using MARTINI CG models in explicit water are used to predict sphere to rod transitions in micelles. Inter-micelle association free energies are estimated to distinguish between the chemical environments in which the micelle assumes a spherical versus rod-like shape. Presence of hydrophobic salt e.g. Sodium Salicylate, is shown to greatly promote the formation of rodlike structures. CG MARTINI molecular dynamics is benchmarked as a practical approach to study nano-scale micellar structures.

[1]NSF Grant 1049454

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Date submitted: 18 Nov 2010 Electronic form version 1.4