Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Molecular Simulation of Reverse Micelles[1] JANAMEJAYA CHOWDHARY, BRANKA LADANYI, Department of Chemistry, Colorado State University — Reverse micelles (RM) are surfactant assemblies containing a nano-sized water pool dissolved in a hydrophobic solvent. Understanding their properties is crucial for insight into the effect of confinement on aqueous structure, dynamics as well as physical processes associated with solutes in confinement. We perform molecular dynamics simulations for the RM formed by the surfactant Aerosol-OT (AOT) in isooctane (2,2,4-trimethyl pentane) in order to study the effect of reverse micelle size on the aqueous phase. The structure of the RM is quantified in terms of the radial and pair density distributions. Dynamics are studied in terms of the mean squared displacements and various orientational time correlation functions in different parts of the RM so as to understand the effect of proximity to the interface on aqueous dynamics. Shape fluctuations of the RM are also analyzed.

[1]NSF

Janamejaya Chowdhary
Colorado State University

Date submitted: 21 Nov 2008 Electronic form version 1.4