Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Adsorption of SDS surfactant inside and around carbon nanotubes with DPD simulation MINH VO, The University of Oklahoma, DIMITRIOS PAPAVASSILIOU, National Science Foundation — The inner diameter of a carbon nanotube (CNT) is generally from 1 to 20 nm, while its inner space could be filled by certain compounds. In our study, Dissipative Particle Dynamics (DPD) simulations were utilized to investigate the ability of sodium dodecyl sulfate (SDS) to adsorb inside a single-walled CNT. First of all, the DPD interaction parameters for SDS surfactants were validated by determining the CMC of surfactants from DPD calculation. The SDS micelle shape and size in water were also calculated. Water-CNT interactions were obtained from a prior study [1]. When the SDS aqueous system reached equilibrium, an open-ended, hydrophobic CNT (a hollow cylinder in the simulation) was inserted into the solution. The diameter of the CNT varied from 1 to 5 nm. All simulations were run up to $2x10^6$ time steps at room temperature. For the system of water and CNT, the radial and axial density profiles of water were computed and compared with published Molecular Dynamics results. In the presence of SDS, the distribution of water and SDS inside the CNT was found to be comparable to that in bulk solution after the system reached equilibrium. In addition, the diffusivity and residence time of water and SDS inside CNTs of different were calculated. This study would give insights into the dynamics and morphology of surfactants in nanoconfined structures. References [1] Vo, M.; Papavassiliou, D. V., Molecular Simulation, 2015, DOI:10.1080/08927022.2015.1089989

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Date submitted: 06 Nov 2015 Electronic form version 1.4