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Role of Surfactant Molecular Structure on Self Assembly: Aqueous SDBS on Carbon Nanotubes[1] MANASWEE SUTTIPONG, Chulalongkorn University, JOHN R. THOMPSON, NAGA RAJESH TUMMALA, The University of Oklahoma, BOONYARACH KITIYANAN, Chulalongkorn University, ALBERTO STRIOLO, The University of Oklahoma — Stabilizing aqueous dispersions of carbon nanotubes mono-dispersed in diameter and chirality remains elusive. Surfactants have proven useful in deploying ultra-centrifugation techniques, but the molecular mechanism responsible for their effectiveness remains not fully understood. Based on a number of recent molecular simulation results, including those from our group, it appears that the morphology of the self-assembled surfactant aggregates on the carbon nanotubes strongly affects the effective potential of mean force between pairs of interacting carbon nanotubes. In this work we explore the effect of surfactant molecular structure on the properties of aqueous surfactant self-assembled aggregates. We employ equilibrium all-atom molecular dynamics simulations. We consider the surfactant SDBS (sodium dodecyl benzene sulfonate) with benzene ring located on the fifth or on the twelfth carbon atom in the tail, and the surfactant AOT [sodium bis(2-ethylhexyl) sulfosuccinate]. The simulations are conducted at room conditions for different surface coverages on (6,6), (12,12), and (20,20) single walled carbon nanotubes. These new results will help us identify the surfactant properties that allow us to manipulate nanotube-nanotube effective interactions.

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