

SDS Surfactants on Carbon Nanotubes: Aggregate Morphology

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Although carbon nanotubes have attracted enormous research interest, their practical application is still hindered, primarily, by the difficulty of separating them into samples monodispersed in diameter, chirality, and length. Recent advances show that ultracentrifugating carbon nanotube dispersions stabilized by surfactants is a promising route for achieving the desired separation. For further perfecting this procedure it is necessary to know how surfactants adsorb on nanotubes of different diameters, which determines the nanotube-surfactant aggregate effective density and the nanotube-nanotube potential of mean force. Because only limited experimental data are available to elucidate these phenomena, we report here an extensive all-atom molecular dynamics study on the morphology of sodium dodecyl sulfate (SDS) surfactant aggregates adsorbed on (6,6), (12,12), and (20,20) single walled carbon nanotubes at room conditions. Our calculations reveal that the nanotube diameter is the primary factor that determines the morphology of the aggregates because of a competition between the entropic and energetic advantage encountered by the surfactants when they wrap one nanotube, and the enthalpic penalty faced during this process due to bending of the surfactant molecule. The data are in qualitative agreement with the neutron scattering results reported by Yurekli et al. [J. Am. Chem. Soc. 126, 2004, 9902], and for the first time provide an atomic-level description helpful in designing better separation, as well as stabilization techniques for aqueous carbon nanotube dispersions.