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Molecular Dynamics Study of Surfactant Self-Assembly on Single-Walled Carbon Nanotubes (SWCNTs) FREDERICK PHELAN JR., NIST - Natl Inst of Stds & Tech — Single-walled carbon nanotubes (SWNCTs) are materials with structural, electronic and optical properties that make them attractive for a myriad of advanced technology applications. Increased adaptation of these materials requires advancement in separation techniques which enables them to be sorted with increased reliability into monodisperse fractions with respect to length and chirality. Most separation techniques currently in use rely on dispersion of tubes in aqueous solution using surfactants. This results in a colloidal mixture in which tubes are packed and individually dispersed in a surfactant shell. Understanding the structure and properties of the SWCNT-surfactant complex at the molecular level, and how this is affected by chirality, will help to improve separations processes. In this work, we study the structure and properties of SWCNT-surfactant colloidal complexes using all-atom molecular dynamics. Self-assembled structures are computed for a number of combinations SWCNT/surfactant, and also, co-surfactant mixtures for the bile salt surfactant sodium deoxycholate (DOC) and the anionic surfactant sodium dodecyl sulfate (SDS). From the radial distribution function we estimate the size of the SWCNT hydration layer, and use that information to compute the buoyant densities of unfilled tubes for a number of concentrations. Estimates of the change in hydrodynamic radius with increased surfactant packing and the binding energies of the individual surfactants are also obtained.

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