Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

A Molecular Dynamics Study of Single-Walled Carbon Nanotubes (SWCNTs) Dispersed in Bile Salt Surfactants FREDERICK PHELAN JR., NIST - National Institute of Standards and Technology, HUAI SUN, Shanghai Jiao Tong University — Single-walled carbon nanotubes (SWNCTs) are materials with structural, electronic and optical properties that make them attractive for a myriad of advanced technology applications. A practical barrier to their use is that SWCNT synthesis techniques produce heterogeneous mixtures of varying lengths and chirality, whereas applications generally require tubes with narrow size distributions and individual type. Most separation techniques currently in use to obtain monodisperse tube fractions rely on dispersion of these materials in aqueous solution using surfactants. The dispersion process results in a mixture of colloidal structures in which individual tubes are dispersed and contained 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, is key to understanding and improving separations processes. In this study, we use molecular dynamics (MD) simulations to study the structure and properties of SWCNT-surfactant colloidal complexes. We tested a number of methods and protocols in order to build an accurate model for simulating SWCNT systems for a variety of bile salt surfactants as well as anionic co-surfactants, components that are widely used and important in experimental separation studies at NIST. The custom force field parameters used here will be stored in WebFF, a Web-hosted smart force-field repository for polymeric and organic materials being developed at NIST for the Materials Genome Initiative.

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Date submitted: 15 Nov 2013 Electronic form version 1.4