Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Surfactants at Single-Walled Carbon Nanotube-Water Interface: Physics of Surfactants, Counter-Ions, and Hydration Shell[1] KETAN S. KHARE, MSED, NIST, Gaithersburg, MD 20899 and Physics, Georgetown Univ., DC 20057, FREDERICK R. PHELAN JR., MSED, NIST, Gaithersburg, MD 20899
— Specialized applications of single-walled carbon nanotubes (SWCNTs) require an efficient and reliable method to sort these materials into monodisperse fractions with respect to their defining metrics (chirality, length, etc.) while retaining their physical and chemical integrity. A popular method to achieve this goal is to use surfactants that individually disperse SWCNTs in water and then to separate the resulting colloidal mixture into fractions that are enriched in monodisperse SWCNTs. Recently, experiments at NIST have shown that subtle point mutations of chemical groups in bile salt surfactants have a large impact on the hydrodynamic properties of SWCNT-surfactant complexes during ultracentrifugation. These results provide strong motivation for understanding the rich physics underlying the assembly of surfactants around SWCNTs, the structure and dynamics of counter ions around the resulting complex, and propagation of these effects into the first hydration shell. Here, all-atom molecular dynamics simulations are used to investigate the thermodynamics of SWCNT-bile salt surfactant complexes in water with an emphasis on the buoyant characteristics of the SWCNT-surfactant complexes. Simulation results will be presented along with a comparison with experimental data.

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Date submitted: 04 Nov 2015 Electronic form version 1.4