Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Curvature and nanoscale forces in controlling self-assembly of carbon nanotube-amphiphile complexes JUKKA MAATTA, Department of Chemistry, Aalto University, Helsinki, Finland, PAUL VAN TASSEL, Department of Chemical and Environmental Engineering, Yale University, New Haven, CT, USA., MARIA SAMMALKORPI, Department of Chemistry, Aalto University, Helsinki, Finland — In aqueous solution, carbon nanotubes (CNTs) bundle strongly via hydrophobicity induced aggregation, yet the extraordinary properties are best realized when CNTs are dispersed as individual tubes. As a result, pure and well isolated individual CNTs are typically desired and extensive effort has been devoted to achieving good aqueous dispersion of CNTs through covalent or non-covalent functionalization. Here, we examine by molecular simulations the non-covalent solubilization of CNTs with a special focus on curvature effects. We employ molecular dynamics simulations and theoretical models to systematically study the amphiphile interactions at the CNT surface. We report that micelle-forming amphiphiles form hemimicellar structures whereas bilayer-forming lipids form tubular coatings. We characterize the energetics of the underlying physical components - the electrostatic, hydration, and geometric effects on CNT dispersion to examine the efficiency of the various CNT solubilization strategies. The observed differences in amphiphile absorption provide a microscopic understanding on the curvature-dependence in amphiphile-coated CNTs solubility in the aqueous phase and will facilitate the bottom-up design of soft nanoscale materials for nanotechnology.

Jukka Maatta
Aalto Univ

Date submitted: 15 Nov 2013 Electronic form version 1.4