

Abstract Submitted  
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**Coarse Grained Modelling of Nanotube Stabilization by PEO Adsorption and Grafting** JUSTIN HOOPER, DMITRY BEDROV, GRANT SMITH, University of Utah — Coarse grained, implicit solvent models have been developed to represent the interaction between two infinite (periodic) single-walled carbon nanotubes and poly(ethylene oxide) in an aqueous environment. The polymer is modelled at a monomeric level of granularity, while the nanotubes are represented as cylindrical effective fields anchored to infinite, periodic lines. This coarse-grained model has been utilized to determine the potential of mean force between two nanotubes with either freely adsorbing or grafted polymer association models. The similarities and differences in relative stabilization of the nanotubes due to the polymer presence and association method is discussed.

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