Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Probing the Structure of DNA-Carbon Nanotube Hybrids with Molecular Dynamics Simulations[1] ROBERT R. JOHNSON, ALAN T. JOHNSON, MICHAEL L. KLEIN, University of Pennsylvania — DNA-carbon nanotube hybrids (DNA-NT) consist of a single-walled carbon nanotube (SWNT) wrapped with a self-assembled monolayer of single-stranded DNA (ssDNA). Recent experiments involving DNA-NT have shown that this material holds a wide range of technologically useful properties. However, a detailed understanding of its microscopic structure and interactions is lacking. To assist the interpretation of contemporary experiments, we have performed atomistic molecular dynamics (MD) simulations using empirical force fields. MD reveals the nature of the interactions and structural arrangements involved in DNA-NT. We find that the hybrid material spontaneously self-assembles via the attractive $\pi - \pi$ stacking interaction between ssDNA nucleobases and SWNT sidewall. Under ambient conditions, ssDNA adopts various wrapping conformations about SWNT including right- and left- handed helices as well as disordered, kinked structures. These conformations are energetically distinct with the compact right-handed helix the most favorable.

[1]Research supported by NSF Grant No. DMR05-20020 and by the JSTO DTRA and the Army Research Office Grant No. 911NF-06-1-0462.

Robert R. Johnson
University of Pennsylvania

Date submitted: 20 Nov 2006 Electronic form version 1.4