

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Calculation of the free energy of binding of DNA bases on a single-wall carbon nanotube¹ ROBERT JOHNSON, A.T. CHARLIE JOHNSON, MICHAEL KLEIN, University of Pennsylvania — Biological molecules can be combined with inorganic nanostructures to form multifunctional hybrid materials with unique properties that will drive advances in nanoelectronics, environmental safety, medicine and homeland security. One such material of contemporary interest is the DNA-carbon nanotube hybrid (DNA-CN), which consists of a single-wall carbon nanotube (SWCN) coated with a self-assembled monolayer of single-stranded DNA (ssDNA). Computation and experiment indicate that DNA-CN self-assembles with DNA bases binding to SWCN sidewall. However, the nature, strength and solvation effects of base-SWCN binding have not been studied in detail. To address these issues and expand our understanding of DNA-CN, we have computed the binding free energy of individual DNA bases with SWCN using alchemical free energy methods. Such calculations provide detailed information about the importance of electrostatic, van der Waals and hydrophobic interactions in base-SWCN binding.

¹This work was supported by JSTO, DTRA and the Army Research Office Grant # W911NF-06-1-0462.

Robert Johnson
University of Pennsylvania

Date submitted: 29 Nov 2008

Electronic form version 1.4