Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Molecular Dynamics Simulations of DNA-Functionalized Carbon Nanotube Chemical Sensors ROBERT JOHNSON, MICHAEL KLEIN, ALAN JOHNSON, University of Pennsylvania — We have conducted all-atom classical molecular dynamics simulations onDNA-functionalized carbon nanotube chemical sensors, including the presence of water. Our simulations verify that single stranded DNA (ssDNA) binds to a single-wall carbon nanotube (swCN) via a pi-pi stacking interaction. Preliminary simulations of a partially hydrated system also suggest that the ssDNA conformation about a swCN exhibits nanoscale pockets that can result in additional binding sites for analytes. Molecular dynamics simulations have also been performed to determine binding orientations of analytes adsorbed to the swCN-ssDNA system. To determine possible chemical gating effects of analytes on the swCN, we numerically calculate changes in the electric potential at the surface of the swCN due to the introduction of ssDNA and analytes. Results of further simulations of a fully hydrated system will also be presented

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Date submitted: 10 Jan 2006 Electronic form version 1.4