Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Adhesion of single functional groups to individual carbon nanotubes: electronic effects probed by *ab-initio* calculations[1] JEFFREY GROSSMAN, University of California, Berkeley, GIANCARLO CICERO, INFM, Torino Polytechnic, GIULIA GALLI, University of California, Davis — The interfacial interaction of simple functional groups (-NH_2, -CN, -CH_3 -$CHOCH_2$) with single wall carbon nanotubes (SWCNT) was investigated using *ab-initio* calculations. Binding energies and attachment forces were computed using Density Functional Theory (DFT) in the local density approximation, and Quantum Monte Carlo calculations were employed to test DFT accuracy in describing weak interactions for the controversial case of an oxygen molecule. We find that computed energies and forces are very sensitive to small variations of the electronic charge on the nanotube. In particular, the presence of a solvent (polar or non-polar), and thus of a small charge transfer from or to the tube, may alter the relative strength of adhesion forces for different functional groups, as compared to vacuum.

[1]This material is based upon work supported by the National Science Foundation under Grant No. EEC-0425914.

Jeffrey C. Grossman
University of California, Berkeley

Date submitted: 30 Nov 2005 Electronic form version 1.4