Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Encapsulation of floating carbon nanotubes in SiO_2 LEONIDAS TSETSERIS, SOKRATES PANTELIDES, Vanderbilt University — In many applications of carbon nanotubes (CNT), it is desirable to have them embedded in a dielectric such as SiO_2, without significantly impacting their electronic properties. Here we study the CNT-SiO_2 interface of an embedded CNT using first-principles calculations. Our results suggest that a carbon nanotube can be incorporated inside a SiO_2 matrix that nucleates around it through the formation of Si-O-C bridges. The large distortion associated with the formation of these bridges can be alleviated by hydrogenation of the composite. Introduction of hydrogen in the vicinity of the bridges leads to their elimination, whereby the nanotube loses its anchoring to the matrix and it floats. For CNTs of suitable diameter, the final floating structure has electronic properties very close to the structure in vacuum. Overall, our results provide atomic-scale information that is relevant to a broad range of applications using embedded or adsorbed nanotubes, for example, sensors, electronics, actuators, and CNT coatings. This work was supported in part by DOE Grant DEFG0203ER46096.

Leonidas Tsetseris
Vanderbilt University

Date submitted: 17 Nov 2006 Electronic form version 1.4