

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Molecular Hydrogen and Oxygen Interactions with Armchair Si Nanotubes¹ HAOLIANG CHEN, ASOK RAY, Physics Department, University of Texas at Arlington, Arlington, Texas 76019 — First principles calculations based on hybrid density functional theory have been used to study the electronic structure properties of armchair silicon nanotubes from (3, 3) to (12, 12). Full geometry and spin optimizations have been performed without any symmetry constraints with an all electron 3-21G* basis set and the B3LYP functional. The largest silicon nanotube studied has a cohesive energy of 3.47eV/atom. Molecular hydrogen and oxygen adsorptions on a (6, 6) tube have been studied by optimizing the distances of the admolecules from both inside and outside the tube. The molecule is originally placed perpendicular or parallel to the tube axis. The on-top external site is the most preferred site for the hydrogen molecule with adsorption energy of 3.71eV and an optimized distance of 3.31 Å when it is perpendicular to the tube axis. For oxygen, the molecule dissociates into two atoms with adsorption energy of 7.45eV, the optimized distances being 1.65/1.68Å. The buckling of the nanotubes increased significantly indicating structural deformation and an increase of sp³ structure. The band gap increases from 0.98eV of bare nanotube to 1.26eV after adsorption of hydrogen molecule. For oxygen molecule, the band gap slightly increases from 0.98eV to 1.01eV.

¹Work partially supported by the Welch Foundation. (Grant No. Y-1525)

Haoliang Chen
Physics Dept, University of Texas at Arlington, Arlington, Texas 76019

Date submitted: 26 Nov 2011

Electronic form version 1.4