Abstract Submitted
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Atomic Hydrogen and Oxygen Adsorptions in Single-Walled Zigzag Silicon Nanotubes[1] HAOLIANG CHEN, ASOK RAY, University of Texas at Arlington — *Ab initio* calculations have been performed to study the electronic and geometric structure properties of zigzag Si nanotubes. 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 zigzag silicon nanotube (12, 0) studied has a binding energy per atom of 3.584eV. Atomic hydrogen and oxygen adsorption on (9, 0) and (10, 0) nanotubes have been studied by optimizing the distances of the adatoms from both inside and outside the tube. The adatom can be placed initially in four adsorption sites- parallel bridge, zigzag bridge, hollow, and on-top site. The on-top site is the most preferred site for hydrogen atom adsorbed on (9, 0) with an adsorption energy of 3.0eV and an optimized distance of 1.49Å. For oxygen adsorption on (9, 0), the most preferred site is the zigzag bridge site with an adsorption energy of 5.987eV. For atomic hydrogen adsorption on (10, 0), the most preferred site is also the on-top site with an adsorption energy of 2.974eV and an optimized distance of 1.49 Å. For adsorption of atomic oxygen on (10, 0), the most preferred site is parallel bridge site with an adsorption energy of 6.275eV.

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