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**An *Ab Initio* Study of Atomic Hydrogen and Oxygen Adsorptions on Armchair Si Nanotubes**[1] 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 and geometric 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. Atomic hydrogen and oxygen adsorptions on a (6, 6) tube have been studied by optimizing the distances of the adatoms from both inside and outside the tube. The on-top external site is the most preferred site for hydrogen with an adsorption energy of 5.97eV and an optimized distance of 1.50 A. For oxygen, the external bridge site is the most preferred site with an adsorption energy of 11.36eV, the optimized distance being 1.66A.

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