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Co-adsorptions of Hydrogen and Oxygen Molecules in Armchair Silicon Nanotubes[1] HAOLIANG CHEN, ASOK RAY, University of Texas at Arlington — A systematic study of the interactions of hydrogen and oxygen molecules with armchair silicon nanotubes using the finite cluster approximation and the Gaussian09 suite of software is presented. Hydrogen and oxygen molecules have been adsorbed from both inside and outside of the nanotube. The admolecules were placed initially perpendicular to the tube axis in four different adsorption sites- normal bridge, zigzag bridge, hollow and on-top sites. After adsorption, the two hydrogen molecules maintained their original diatomic linear structure and the most preferred site is the on-top site, with the highest adsorption energy being 3.714eV. For adsorption of two oxygen molecules, complete dissociation, partial dissociation and non-dissociation were noted, with the highest adsorption energy being 7.659eV. We propose several precursor (or metastable) states, such as the Si-O-O-Si peroxide structure, which has a lower ground state energy than dissociative adsorption. For the co-adsorption of one hydrogen molecule with one oxygen molecule, the oxygen molecule dissociated into oxygen atoms and hydrogen molecule prefers to stay in on-top site, the highest adsorption energy being 5.563eV.

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