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An Ab Initio Study of Molecular Hydrogen Interaction with SiC Nanotube – A Precursor to Hydrogen Storage[1] SOUPTIK MUKHERJEE, ASOK RAY, Department of Physics, University of Texas at Arlington, Arlington, Texas 76019 — First principles calculations have been performed to study the adsorption of molecular hydrogen (H2) on three types of armchair (9,9) silicon carbide nanotubes. The distances of H2 from the outer walls of the nanotubes have been optimized using the B3LYP and PW91 functionals. For the PW91 functional, the carbon top site for type 1, the second hollow site for type 2 and the C-C bridge site for type 3 nanotubes are the most preferred adsorption sites. For the B3LYP functional, the C-Si normal bridge site for type 1, and the C-C bridge site for type 2 and type 3 nanotubes are the most preferred sites. The adsorption energies using the PW91 functional are found to be always higher than those using the B3LYP functional; however, the adsorption distances using the B3LYP functional are greater than the corresponding distances using the PW91 functional. Current studies indicate that silicon carbide nanotubes can possibly be used as a proper media for hydrogen storage at ambient conditions.

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