Abstract Submitted
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Can Silicon Carbide Nanotubes Be Effective Storage Medium for Hydrogen Storage[1] SOUPTIK MUKHERJEE, ASOK RAY, UTA — A systematic study of molecular hydrogen adsorption on three different atomic configurations of armchair SICNTs has been performed. In the first stage of our study, first principles calculations using both density functional theory (DFT) and hybrid density functional theory (HDFT) as well as the finite cluster approximation have been performed to study the adsorption of molecular hydrogen on three types of armchair (9, 9) silicon carbide nanotubes. The distances of molecular hydrogen from the outer wall of the nanotubes have been optimized manually using the B3LYP and PW91 functionals and results have been compared in detail with published literature results. In the second part of our study, hydrogen molecule has been adsorbed from both inside as well as from the outer wall of nanotubes ranging from (3, 3) to (6, 6) for all three types. A detailed comparison of the binding energies, equilibrium positions and Mulliken charges has been performed for all three types of nanotubes and for all possible sites in those nanotubes. In the third phase, co-adsorption of two hydrogen molecules has been carried out. Possibilities of hydrogen storage have been explored in detail.

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