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A Hybrid Density Functional Study of Armchair SiC Nanotubes[1]

KAZI ALAM, ASOK RAY, Department of Physics, University of Texas at Arlington, TX-76019 — As a continuation of our previous work on SiC nanoclusters, we report here first principles calculations on the electronic and geometric structures of armchair silicon carbide nanotubes from (3,3) to (9,9). The finite cluster approach with dangling bonds terminated with hydrogen has been used. The theoretical formalism used is hybrid density functional theory incorporating Hartree-Fock exchange with density functional theory exchange-correlation. In particular, we have used the B3LYP hybrid functional and the Los Alamos pseudopotential LANL2DZ as implemented in the Gaussian 03 suite of programs. For silicon, the 1s, 2s, and 2p electrons have been treated as core states and the remaining electrons as valence states. For carbon and hydrogen, all electron basis sets have been used. A detailed comparison of the structures and stabilities of the nanotubes has been performed and the dependence of the electronic band gaps on the respective tube diameters has also been investigated. Results will be compared with other published data in the literature.

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