Abstract Submitted
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A Hybrid Density Functional Study of Si Nanotubes[1] SOMILKUMAR RATHI, ASOK RAY, Physics Department, University of Texas, Arlington — First principles calculations have been used to study the electronic and geometric structures of zigzag and chiral silicon nanotubes. 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 (HF) exchange with density functional theory (DFT) 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 represented by core potentials and the remaining electrons as valence states. 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 been investigated. We will also compare our results with previously published data on Si armchair nanotubes published by our group* and with other results published in the literature. *P. Pradhan and A. K. Ray, J. Comp. Th. Nanosci. **3**, 128 (2006).

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