Abstract Submitted
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An Ab Initio Study on Silicon and Germanium Nanotubes PRACHI PRADHAN, ASOK K. RAY, The University of Texas at Arlington — First principles calculations using hybrid density functional theory have been performed to examine the electronic and geometric structure properties of single-walled silicon (SWSiNT) and germanium (SWGeNT) nanotubes. Finite clusters X_mH_n(X = Si or Ge) are used to model the nanotubes (*e.g.* the smallest SWSiNT is modeled as $Si_{60}H_{12}$). Hydrogen termination is done to simulate the effect of longer tubes as well as to take care of end effects. A pseudopotential basis set has been used for the silicon atoms[1] and complete geometry optimizations of the structures has been carried out using the Gaussian 03 suite of programs.[2] Computer simulations predict that the existence and stability of the nanotubes are highly dependent on the ratio of the sp^2 to sp^3 hybridization. Results will be presented on cohesive energies, HOMO-LUMO gaps, and other electronic structure properties and their dependence on the tube diameter. We will discuss the density of states (DOS) to explain the possible metallic or semi-conducting character of the tubes. Detailed comparisons with published data in the literature will also be presented. * Work supported, in part, by the Welch Foundation, Houston, Texas (Grant No. Y-1525). [1]P. J. Hay and W. R. Wadt, J. Chem. Phys. **82**, 270 (1985). [2]*Gaussian03*, Revision A.1, M. J. Frisch *et al.*, Gaussian Inc., Pittsburgh, PA , 2003.

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