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A Hybrid Density Functional Study Of Pure Ge And GeC Nanotubes: Zigzag Configuration[1] SOMILKUMAR J. RATHI, Colorado School of Mines, ASOK K. RAY, Department of Physics, The University of Texas, Arlington — Ab initio calculations within the framework of hybrid density functional theory and finite cluster approximation have been performed for the electronic and geometric structures of pure zigzag Ge and three different types of zigzag germanium carbide nanotubes from (3, 3) to (11, 11). Full geometry and spin optimizations with unrestricted symmetry have been performed. A detailed stability investigation of the topologically similar nanotubes with dependence of the electronic band gaps on the respective tube diameters, energy density of states, and dipole moments have been carried out for all the tubes. Using Mulliken charge analysis charge density distribution along the tube lengths is calculated. In depth structural analysis of the structure and molecular orbitals are also reported. From our results it is clear that type I zigzag nanotubes are the most stable structures. For pure Ge, type II, and type III GeC nanotubes the chemical bonding have mixed ionic-covalent character, while for type I GeC tubes are ionic in nature. A wide spectrum of band gap values is also obtained for these nanotubes. This present study also opens up the possibilities for numerous applications of hybrid Ge based nanotubes.

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Somilkumar Rathi
Colorado School of Mines

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