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On the Electronic Structures of Ge Based Nanotubes.[1] SOMILKUMAR RATHI, ASOK RAY, The University of Texas at Arlington — In the context of elucidating the properties of Ge-based nanotubes, we provide here a systematic *ab initio* study of the electronic and geometric structures of three different types of armchair silicon germanium nanotubes from (3, 3) to (11, 11) and compare them with the corresponding properties of Ge and GeC nanotubes. The finite cluster approach with dangling bonds terminated with hydrogen has been used. The theoretical formalism used is hybrid density functional theory incorporating HF exchange with DFT exchange-correlation functional. Full geometry and spin optimizations with unrestricted symmetry have been performed. A detailed comparison of the structures and stabilities of the nanotubes with dependence of the electronic band gaps on the respective tube diameters, energy density of states, dipole moments as well as Mulliken charge distributions have been investigated for all the tubes. Radial buckling of the tubes along with bond length variations is also studied and implications for band gap engineering will be discussed.

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Somilkumar Rathi
The University of Texas at Arlington

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