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On the Electronic and Geometric Structures of Armchair GeC Nanotubes: A Hybrid Density Functional Study[1] SOMILKUMAR RATHI, ASOK RAY, The University of Texas at 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 three different types of armchair germanium carbide nanotubes from (3, 3) to (11, 11). Full geometry and spin optimizations with unrestricted symmetry have been performed. A detailed comparison of the structures and stabilities of the three types of nanotubes will be presented. The 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. Radial buckling of tube along with bond length variations is also studied. All armchair GeC nanotubes investigated so far are semiconducting in nature. Applications in the field of nano-optoelectronic devices, molecular electronics and band gap engineering are envisioned for GeC nanotubes.

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Somilkumar Rathi
The University of Texas at Arlington

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