

Abstract Submitted
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Four Types of Single-Walled SiGe Nanotubes: Existence and Stability¹ PRABATH WANAGURU, ASOK K. RAY, The University of Texas at Arlington — Four types of SiGe armchair nanotubes from (3, 3) to (12, 12) have been studied using the cluster approximation and the dangling bonds saturated by H atoms. The tubes have been spin- and geometry optimized using the hybrid functional B3LYP, the all electron 6-31G**//3-21G* basis set and the GAUSSIAN 03/09 suite of software. Cohesive energies, band gaps, bond lengths, hybridization of Ge and Si atoms, among others will be presented in details. In general, cohesive energy of type I tubes decrease and saturate around 3.389eV and that of, type IV tubes increase and saturate around 3.411eV. The cohesive energy of both type II and type III tubes indicates oscillatory behavior eventually reaching saturation as the tube diameter increases. Band gaps, in general for all four types decrease as the tube diameter increases. The band gap of type I tubes saturate at around 1.0eV and type IV tubes indicate the lowest saturation gap of about 0.3eV. While most types I-III tubes show sp² or a mixture of sp² and sp³ bonding, some type IV tubes show predominantly p bonding. Results of types I-III will be compared with previous results using the cluster approximation and the B3LYP/LANL2DZ level of theory.²

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²S. Rathi and A. K. Ray, Chem. Phys. Lett. 466, 79 (2008).

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