Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

A First-Principles Study of SiGe Nanotubes[1] PRABATH WANAGURU, ASOK K. RAY, Department of Physics, University of Texas at Arlington, Arlington, TX 76019 — A systematic study of the electronic structures of three types of SiGe armchair nanotubes from (3, 3) to (11, 11) using periodic boundary conditions has been performed. Geometries of the tubes have been optimized using the hybrid functional B3LYP, the double-zeta LANL2DZ basis set and the GAUSSIAN 03/09 software. Variations of the cohesive energies, band gaps, bond lengths, and Mulliken charges, among others, with the tube diameters will be presented in detail. The cohesive energies of all tubes, in general, increase as the diameters increase and appear to saturate at about 2.98eV for (11, 11) tubes. However, band gaps indicate an oscillatory pattern, with type 2 tubes, in general, with smaller band gaps. Results will be compared with previous results for SiGe tubes using the cluster approximation.[2]

[1]This work is supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525).
[2]S. Rathi and A. K. Ray, Chem. Phys. Lett. 466, 79 (2008).

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Date submitted: 29 Nov 2010 Electronic form version 1.4