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Structural Properties and Stability of Double Walled Armchair Silicon Nanotubes[1] HAOLIANG CHEN, ASOK RAY, Physics Department, University of Texas at Arlington, Arlington, Texas 76019 — A systematic study of armchair double-walled Si nanotubes (DWNT) (n,n)@(m,m) ($3 \leq n \leq 6$; $7 \leq m \leq 12$) using the finite cluster approximation is presented. The geometries of the tubes have been spin optimized with an all electron 3-21G* basis set and the B3LYP functional. The study indicates that the stabilities of the double-walled Si nanotubes are of the same order as those of single-walled Si nanotubes suggesting the possibilities of experimental synthesis of both single-walled and double-walled Si nanotubes. The binding energy per atom or the cohesive energy of the double-walled nanotubes depends not only on the number of atoms but also on the coupling of the constituent single-walled nanotubes. Some nanotubes with small interlayer separations do not hold the coaxial cylindrical structure after optimization. The NTS (n, n)@(n+3, n+3) are found to have large formation energies and binding energies per atom. For example, (3,3)@(6,6), (4,4)@(7,7), (5,5)@(8,8), and (6,6)@(9,9) all have large binding energies per atom, around 3.7eV/atom. All double-walled Si nanotubes are found to be semiconductors. However, the band gap, in general, is observed to decrease from single walled nanotubes to double walled nanotubes.

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