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A Theoretical Study on Silicon and III-V Compound Nanotubes

Engin DURGUN, Salim ÇIRACI
Department of Physics, Bilkent University, Bilkent
Ankara 06800, TURKEY

Abstract: In this paper we present a theoretical study on single-wall silicon and III-V compound nanotubes. First principles plane wave calculations within density functional theory are used to predict energetics and electronic structures of armchair and zigzag nanotubes. The stability of tubular structures is further investigated at finite temperature by ab initio molecular dynamics calculations. Our results indicate that (n,0) zigzag and (n,n) armchair single-wall Si nanotubes are stable for n >= 6. Mechanically, the Si nanotubes are radially soft, however they are strong against axial deformations. Electronic analysis showed that zigzag nanotubes are metallic for n <=11, but they show semiconducting behavior for larger radii. On the other hand, all armchair nanotubes are metallic. (8,0) single wall nanotube has been chosen as prototypes for AlP, GaN, and GaAs compounds and we found that they are semiconducting and stable at room temperature.

Key Words: silicon, nanotube, first principles calculations.

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