

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Silicon and III-V compound nanotubes: Structural and electronic properties ENGIN DURGUN, SEFAATTIN TONGAY, SALIM CIRACI, Bilkent University — Unusual physical properties of single-wall carbon nanotubes have started a search for similar tubular structures of other elements. We present a theoretical analysis of single-wall nanotubes of silicon and group-III-V compounds. Starting from precursor graphenelike structures we investigated the stability, energetics, and electronic structure of zigzag and armchair tubes using the first-principles pseudopotential plane wave method and finite temperature ab initio molecular dynamics calculations. We showed that $(n,0)$ zigzag and (n,n) armchair nanotubes of silicon having $n \geq 6$ are stable but those with $n < 6$ can be stabilized by internal or external adsorption of transition metal elements. Some of these tubes have a magnetic ground state leading to spintronic properties. We also examined the stability of nanotubes under radial and axial deformation. Owing to the weakness of radial restoring force, stable Si nanotubes are radially soft. Undeformed zigzag nanotubes are found to be metallic for $6 \leq n \leq 11$ due to the curvature effect; but a gap starts to open for $n \geq 12$. Furthermore, we identified stable tubular structures formed by the stacking of Si polygons. We found AlP, GaAs, and GaN $(8,0)$ single-wall nanotubes stable and semiconducting. Our results are compared with those of single-wall carbon nanotubes.[1] [1] E. Durgun, S. Tongay, and S. Ciraci Phys. Rev. B 72, 075420 (2005)

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Date submitted: 30 Nov 2005

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