

Curvature-induced effects in semiconducting alkaline-earth metal silicide nanotubes

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Abstract: By means of ab-initio techniques we have investigated changes in the structure and electronic properties of alkaline-earth metal silicide (Ca_2Si , Mg_2Si and MgCaSi) nanotubes caused by the curvature-induced effects. It is revealed that the curvature-induced effects can: 1) stabilize Mg_2Si nanotubes in a phase, which is metastable for the parent 2D Mg_2Si ; 2) lead to an energy gain as a result of 2D to nanotube

structural transformation in the case of ternary MgCaSi nanotubes; 3) modify the band dispersion and band gaps for nanotubes with the diameters less than 30 Å. In addition, Mg₂Si and MgCaSi nanotubes are found to be direct band-gap (0.5–1.2 eV) materials with appreciable oscillator strength of the first direct transitions.

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