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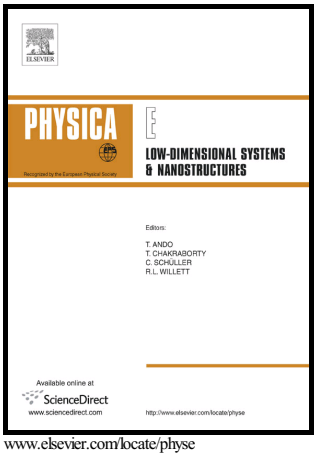

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First-principle study of nanotubes within the tetragonal, hexagonal and dodecagonal cycles structures

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Abstract

A systematic study has been done on the structural and electronic properties of carbon, boron nitride and aluminum nitride nanotubes with structure consisting of periodically distributed tetragonal (T $\equiv$ A_2X_2), hexagonal (H $\equiv$ A_3X_3) and dodecagonal (D $\equiv$ A_6X_6) (AX = C_2, BN, AlN) cycles. The method has been performed using first-principles calculations based on density functional theory (DFT). The optimized lattice parameters, density of states (DOS) curves and band structure of THD-NTs are obtained for (3, 0) and (0, 2) types. Our calculation results indicate that carbon nanotubes of these types (THD-CNTs) behave as a metallic, but the boron nitride nanotubes (THD-BNNTs) (with a band gap of around 4 eV) as well as aluminum nitride nanotubes (THD-AlNNTs) (with a band gap of around 2.6 eV) behave as an semiconductor. The inequality in number of atoms in different directions is affected on structures and diameters of nanotubes and their walls curvature.

Keywords: Nanotubes; Structural properties; Electronic properties; First principles calculations; Density functional theory

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