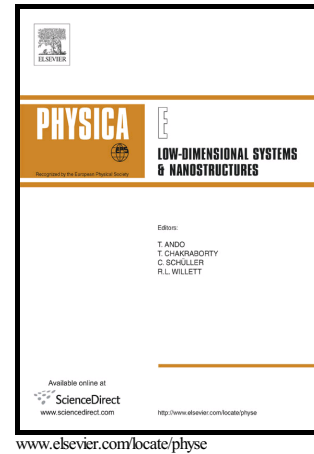


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# First-principle study of nanotubes within the tetragonal, hexagonal and dodecagonal cycles structures

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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 a 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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