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Electronic structure of carbon-boron nitride nanotubes RAÚL SANGINÉS-MENDOZA, EDGAR MARTINEZ, Universidad Autónoma de Nuevo León — Structures of carbon and boron nitride nanotubes (CNTs, BNNTs) are quite similar, conversely, electronic properties are radically different from each other. Carbon nanotubes, whose electronic properties can be either metallic or semiconducting depending on their chiral structure, boron nitride nanotubes are always semiconductors with bandgaps over 4 eV. We have looked to hybrid systems, to predict a new kind of nanostructures with novel electronic properties. In this way, we explore the electronic properties of C-BN nanotubes. In particular, we studied the electronic structure of armchair C-BN nanotubes. The calculations were performed using the pseudopotential LCAO method with a Generalized Gradient Approximation for the exchange-correlation energy functional. The band structure of most of these systems have semiconductor character with an indirect gap smaller than its analogous BNNTs. In addition, the most prominent feature of these systems is the existence of flat bands both at the valence band top and at the conduction band minimum. Such flat bands results in sharp and narrow peaks on the total density of states. The behavior of these flat bands mainly indicates that electrons are largely localized. Thus, a detailed analysis on the electronic band structure shows that hybridization between those orbitals on the interfaces is responsible to exhibit localization effects on the hybrid systems.This research was supported by Conacyt under Grant No. 133022.

Edgar Martinez-Guerra
Universidad Autónoma de Nuevo León

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