General session VIII

Atomistic simulations of defect containing tubular nanostructures

S. Bellucci, Yu. Zhukovskii, J. Kazerovskis, S. Piskunov, P. Dyachkov
INFN-Laboratori Naziionali di Frascati, Italy

Contemporary quantum-chemical simulations are becoming more and more capable to predict physical, chemical, and even mechanical properties of many interesting materials. However, very little has been reported on computer simulations of defective nanostructures, mainly because the lack of periodicity makes their study both very time-consuming computationally and costly. We demonstrate the advantage of first principles methods, which can exploit periodic rototranslation symmetry for efficient calculations on defect-containing nanotubes. Using density functional theory (DFT) realized either within the LCAO method or the formalism of linear augmented cylindrical waves, we calculate the equilibrium geometry and energetics of a Ni filament inside carbon nanotubes (CNTs), and single atom substitutions inside the wall of boron nitride nanotubes (BNNTs). As for CNTs, we consider monoatomic chains of nickel atoms encapsulated into CNTs of (n,0) and (n,n) chiralities with varied n indices. Our calculations show that CNTs with Ni filament exhibit metallic behavior, even if the pristine nanotube is semiconducting. Thus, we predict that the encapsulation of a Ni filament inside CNTs is a way for the reliable realization of stable conductive quasi-one-dimensional hybrid nanostructures. In BNNTs with (5,5) and (9,0) chiralities we consider P, As, Sb substitutions for the host N atom while In, Ga and Al substitute the host boron. The band gap of the BNNTs is virtually closed, due to the effect imposed by Sb, while the introduction of the In, Ga or Al atom in the BNNT results in a minor increase of its band gap. The obtained results can help to understand better the optical and photoelectron spectroscopy experiments, and the measured electrical properties of the doped BNNTs.

NOTES

Reflectance properties of nanocarbons: nanodiamond (ND), sp2/sp3 composites, onion-like carbon and multiwalled carbon nanotubes

V.Kuznetsov[1, 2], S. Moseenkov[1,2], T. Larina[1], A. Ishchenko[1], S. Bokova[3], E. Obraztsova[3], A. Romanenko[2,4], O. Anikeeva[2,4], E. Tkachev[4], P.Lambin[5]
[1]Boreskov Institute of Catalysis SB RAS, Russia

Carbon nanomaterials are the promising candidates for potential broadband limiting applications and design of extremely low reflectance coatings, particularly in the infrared, visible and UV spectral regions. The reflectance properties of nanocarbons are important for the design of absorbing paints, low reflectance coatings, sensors etc. We have performed the comparative study of diffuse reflectance of nanodiamond (ND), sp2/sp3 composites, onion-like carbon (OLC) and multiwalled carbon nanotubes (MWNTs) in infrared, visible and UV regions. The diffuse reflectance spectra of these materials are analyzed taking into account the size and defectiveness of graphene sheets which are the main building blocks of sp2-carbon based nanocarbons. We have controlled defectiveness of all nanocarbons with the uniform set of physical methods, namely HR TEM, Raman spectroscopy, temperature dependence conductivity and magnetoresistance measurements. The diffuse reflectance of carbon nanomaterials depends mainly on the electronic configuration, defect concentration, size of graphene-like ordered fragments and agglomerates of nanoparticles along with their morphology.

NOTES