

Augmented cylindrical wave and Green's function theory for electronic structure of pure, embedded, and doped nanotubes

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We develop a new quantum-mechanical method for calculating the electronic structure of the single-wall, double-wall, and embedded nanotubes both perfect and having impurities [1-5]. This is the linear augmented cylindrical wave (LACW) method. The main argument for using cylindrical waves is to account for the cylindrical geometry of the nanotubes in an explicit form that offers the obvious advantages. The approximations are made in the sense of muffin-tin potentials and local-density-functional theory only. In this model, the electronic spectrum of the single-wall nanotubes (SWNTs) is governed by movement of electrons in the interatomic space of cylindrical layer and by scattering of electrons on the atomic spheres. With account of rotational and helical symmetries of SWNTs, we developed a symmetry-adapted version of the method. In this case, the theory becomes applicable to any SWNT independent of the number of atoms in the translational unit cell [1]. The method is implemented as program package and applied to determine the total band structures and densities of states of the chiral and achiral, semiconducting and metallic both pure and transition metal intercalated single-wall carbon tubules. The electronic structure of double-wall carbon nanotubes consisting of two concentric graphene cylinders is calculated [2]. In this approach, the electronic spectrum of the double-wall carbon nanotubes is governed by the free movement of electron in the interatomic space of two cylindrical layers, by electron scattering on the muffin-tin spheres, and by electron tunneling between the layers. The electronic structure of SWNTs embedded in a crystal matrix is investigated too [3]. A delocalization of the nanotube electrons into the matrix region results in the strong band-structure perturbation. In the case of armchair nanotubes, the delocalization is responsible for the high-energy shift of the states and growth of the electron density of states at the Fermi level. For the semiconducting nanotubes, it causes the decay of the minimum energy gap and formation of metallic state. Based on a Green's function technique, the first-principles numerical method for calculation of the electronic structure of the point impurities in the SWNTs is elaborated [4]. The host SWNTs electron Green's function is calculated using the LACW theory. The Green's function of the impurities is calculated in the terms of matrix Dyson equation. It is shown that substitutional doping of bundles and composite materials, containing a mixture of semiconducting and metallic SWNTs, by either nitrogen or boron atoms substantially alters their electromagnetic characteristics in the terahertz and the far-infrared regimes [5].

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