Ab initio study of substitutionally Ni-doped single wall carbon nanotubes: structural and electronic properties

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We report the structural and electronic properties of substitutionally Ni-doped in armchair and zigzag single-wall carbon nanotube (SWNT) [1] by using spin-polarized total-energy ab initio calculations. We find two stable geometries for these systems with Ni atom in an outward or inward local distortion relative to the tube surface (Figure 1). These structures agree with the previous experimental results by Ushiro et al. using extended x-ray absorption fine structure (EXAFS) and x-ray absorption near edge structure (XANES) techniques [2]. The outward configurations are always more stable that the inward ones. We explore the change on the electronic properties after Ni doping SWNT's. A strong dependence between the Ni concentration and the electronic features have been observed. Varying the Ni concentration the, initially metallic, (5,5) SWNT can become either semiconducting, with an energy gap of 0.33 eV for the outward geometry (Figure 1) and 0.14 eV for the inward one, without magnetic behaviour, or remain metallic, but with a total magnetization mean of 0.61 (μ). For the (8,0) SWNT a reduction of the gap is observed from 0.80 eV to 0.39 eV for the outward geometry and 0.37 eV for the inward one. We study in detail the changes in the electronic band structure after the doping. Due to the symmetry reduction most of the expected degeneracies for the tubes are removed. Several bands with strong Ni 3d character appear near the Fermi level. The character and symmetry of these d-bands and its dependence on the bonding configuration and curvature are also studied (Figure 1) [3].

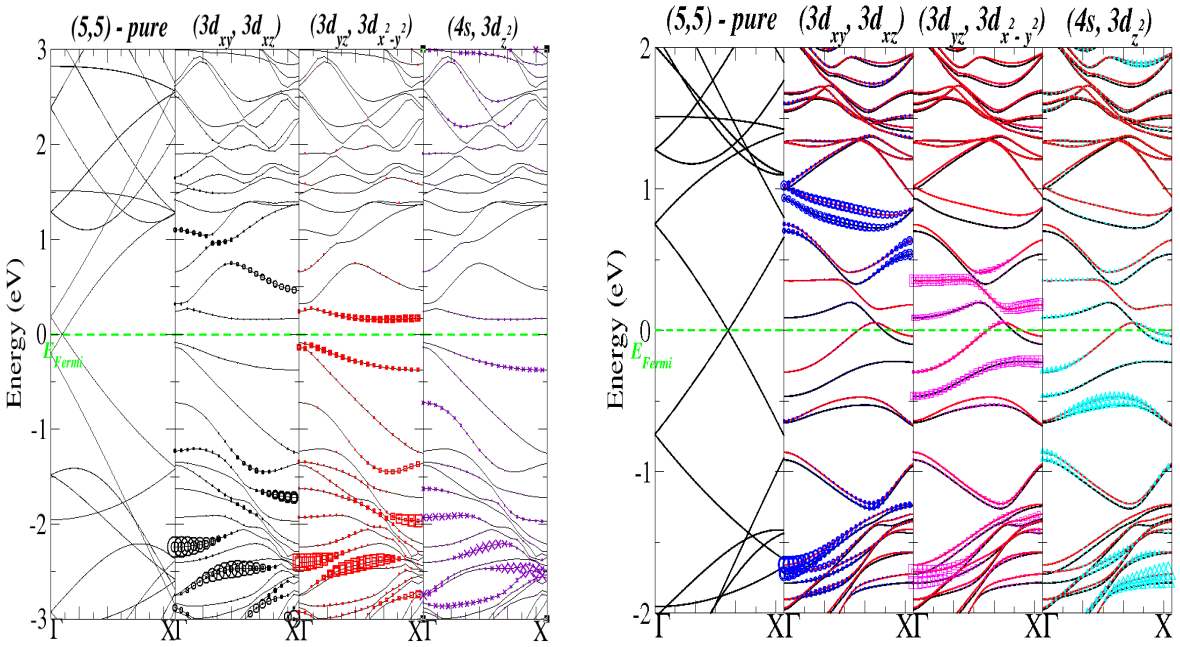

Figure 1. The representation of the electronic band structures for the Ni-doped (5,5) in the outward configuration for a Ni concentration of 1.69 % (right panel) and 1.27 % (left panel). The bands mainly associated with the Ni orbitals has been highlighted using solid symbols. The Ni-orbitals are grouped following the remaining symmetries after the Ni dopping. The strong spin split is one of the principal features of the right panel, where the states around the E_{Fermi} have a major contribution from the d-levels. The states in approximatelly -1.70 eV have also a large hibridization with the sp-carbon states, but the contribution of the $3d_{xy}$, $3d_{xz}$, $3d_{yz}$, $3d_{x2-y2}$ orbitals near to the Γ point is important to stress.

References:

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