First principles calculation of the electronic structure and energy-loss near edge spectra of chiral carbon nanotubes

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Single-wall carbon nanotubes (CNTs) are obtained by rolling up a graphene sheet. They are model structures for investigating the effect of the curvature and the diameter in fullerene materials. Different possible orientations of the graphitic hexagons are possible in the tube wall (chirality, expressed by the chiral angle $\theta$), with very big unit cells in some case ($0^\circ < \theta < 30^\circ$ or chiral tubes). Diameter and chiral angle influence the electronic properties of these quasi 1D systems. A conventional approach for theoretical calculations is based on nearest neighbour tight binding by zone folding of the graphene $\pi$ bands [1]. This method describes quite well the modification of the $\pi$-$\pi^*$ bands due to the finite diameter and chiral angle of the tubes. Of course, it cannot describe the $\pi$-$\sigma$ hybridisation [2] expected for these systems (and resulting in $sp^{2+\delta}$ hybrids). Other techniques are based on Density Functional Theory (DFT) calculations [3], but few results are available for chiral tubes (due to the dimensions of the unit cells).

In this work, we present full potential DFT-LDA (Local Density Approximation) calculations on small nanotubes ($d < 1$ nm) with different chiral angles and diameters to determine the modifications induced in the electronic properties, with particular attention to the energy-loss near edge (ELNES) spectra (the first calculated for chiral tubes), and we compare them with spectra from zigzag ($\theta = 0^\circ$) and armchair ($\theta = 30^\circ$) tubes of similar diameters. The symmetry projected final density of states intrinsic in the ELNES spectrum permits to investigate the $\pi^*$ and $\sigma^*$ contributions to the spectra and evaluate the degree of hybridisation.

References