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CARBON NANOSTRUCTURES: OPTICAL PROPERTIES FROM TDDFT STUDIES AND COMPLEX MAGNETIC BEHAVIOUR OF SUBSTITUTIONAL TRANSITION METAL IMPURITIES

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We report a theoretical study of substituinal Ni, Co and Fe impurities in graphene. Only Co impurity is magnetic with a moment of ~1μ_B. Ni substitutional impurities, whose presence in carbon nanotubes has been recently proposed by Ushiro *et al.*[1] from the analysis of extended x-ray absorption fine structure (EXAFS) and x-ray absorption near edge structure (XANES) data, show zero magnetic moment. However, the situation is different, and far more complex, for the Ni substitution in carbon nanotubes. Although the main features of the electronic structure of the Ni defect do not depart strongly from those of the substitutional dopant in graphene, some of the fine details are different leading to the appearance of a magnetic moment. In particular, the positions of some of the defect bands close to the Fermi level show a dependency on the curvature of the tube and the dopant concentration. This gives rise to a complex behavior of the magnetic moment of the Ni defect as a function of these parameters. The magnitude of the magnetic moment shows a complex, non-monotonic behavior as a function of the tube diameter and the impurity concentration (see the Figure below). Non-zero magnetic moments only occur for metallic tubes whereas for semiconducting tubes the magnetic moment remain always zero, like in the case of graphene. This may provide a route to unambiguously identify metallic carbon nanotubes.

In the second part of the talk we briefly present an ab initio study of the optical absorption and dielectric properties of small-diameter carbon nanotubes and other carbon nanostructures using time dependent density functional theory (TDDFT) is presented. The calculations have been performed using the SIESTA program [2]. This code performs standard pseudopotential density functional calculations using a linear combination of atomic orbitals as a flexible basis set. It has been specially optimized for the treatment of very large systems. I have recently participated in the implementation of TDDFT in this program [3]. The scheme used to calculate the optical response in this implementation follows closely the method proposed byYabana and Bertsch [4]. The idea is to apply an external perturbation to the system at time equal zero. The system is then allowed to evolve by solving the time dependent Kohn-Sham equations. The self-consistent Hamiltonian is computed at each time step and time evolution operator recalculated from it. From the computed time evolution of the density it is possible to obtain information about the dielectric response of the system. Besides the study of the optical properties of cabon nanotubes the method has been recently applied to the study of the electronic stopping in insulators [5].

The work on substitutionally doped carbon nanotubes has been performed in collaboration with E. J. G. Santos, A. Ayuela, S. B. Fagan, J. Mendes Filho , D. L. Azevedo and A. G. Souza Filho

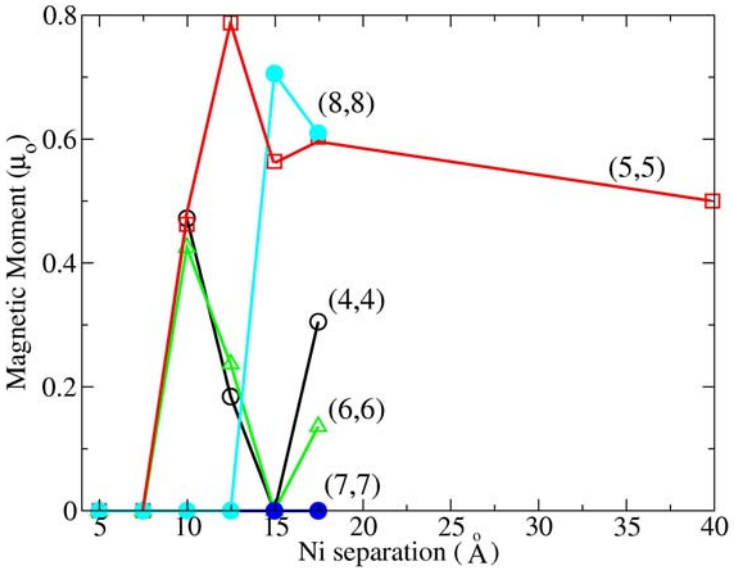

Figure. Magnetic moment associated to a nanotube with a Ni substitutional impurity as a function of the Ni-Ni separation (i.e., size of the supercell used in the calculations) for different metallic armchair tubes.

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