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SEMINAIRE

Lundi 6 Novembre 2006 à 14h00

Bâtiment 466, salle 111 - CEA Saclay, 91191, Gif sur Yvette

Electronic structure and transport of disordered carbon nanotubes at the mesoscopic scale. Application to the presence of doping atoms in substitution/addition and physisorbed organic molecules

S. Latil

Laboratoire de Physique du Solide, Facultés Universitaires Notre-Dame de la Paix Namur,Belgium

Invité par M.C. Desjonquères

Abstract:

In view of incorporating carbon nanotubes (CNTs) as building blocks for nanoelectronics, a tuning of their electronic properties by chemical doping has been proposed early on. Structures doped by boron or nitrogen substitutions, or potassium addition have been produced, and their transport properties have been fully characterized [1]. However a deeper understanding of the scattering that is induced by these defects is still missing.

In a very different domain of study, the effect of physisorption of small ring hydrocarbon molecules (benzene e.g.), adsorbed onto the CNTs has been investigated experimentally, through thermopower measurements [2]. It appears that, in spite of a negligible charge transfer between CNT and molecular system, the aromatic character affects significantly the electronic transport in the underlying CNT. It is possible to give a microscopic explanation of this scattering? and, besides, to predict how a given non-covalent functionnalization will affect (or not) the transport in nanotubes?

Our theoretical study is then devoted to electronic transport in carbon nanotubes, in presence of doping atoms (substitutions or in addition), and grafted pi-conjugated molecular systems. Since our motivations are clearly related to experimental data, our work aims to simulate the transport in CNT-based structures, as realistic as possible.

So, on the one hand, we address large devices with a mesoscopic approach, in order to randomize the scattering centers location, to take random multiple interference effects into account and then to follow the evolution of the generic transport properties (conduction regime, conductance, etc.)

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versus the density of dopants/molecules. On the other hand, a good description of the electronic structure in the vicinity of a defect (dopant or molecule) is crucial, otherwise the resulting scattering will be ill-estimated.

We have then developed an hybrid approach, based on the combination of ab initio (density functionnal theory - DFT) and tight-binding (TB) techniques. First, the local study of a defect is carried out help to DFT calculations (structural optimization, formation energy, localized states, etc.). Seconds, the electronic properties at the mesoscopic scale are treated with a TB model, whose parameters are adjusted on the previous ab initio results. At last, the transport properties are calculated with both Kubo and Landauer formulae (that will be shortly described during the presentation).

In the case of boron/nitrogen substitutions, the regime is found to be highly sensitive upon the energy and the density of dopants, whereas the transport in CNTs doped by potassium addition is found to be less affected [3]. In the case of molecular systems grafted on the surface of the CNT, we have established that the value of the molecular HOMO-LUMO gap drives directly the scattering rate at the Fermi level [4].

This presentation will be followed by a short description of my CV, and an overview of my research prospective

[1] V. Krstic et al., Phys. Rev. B 67, 041401 (2003), Radosavlevic et al., Appl. Phys. Lett. 84, 3693 (2004).
[2] G.U. Sumanasekera et al., Phys. Rev. Lett. 89, 166801 (2004).
[3] S. Latil et al., Phys. Rev. Lett. 92, 256805 (2004), 95, 126802 (2005), C. Adessi et al., Phys. Rev. B 73, 125414 (2006).
[4] S. Latil et al., Nanolett. 5, 2216 (2005).