Ab initio Quantum Transport in Carbon Nanostructures

Jean-Christophe Charlier

Université Catholique de Louvain
Unité de Physico-Chimie et de Physique des Matériaux (PCPM),
Place Croix du Sud 1, B-1348 Louvain-la-Neuve, Belgium
Email: Jean-Christophe.Charlier@uclouvain.be

Their unusual electronic and structural properties promote carbon nanostructures as promising candidates for a wide range of nanoscience and nanotechnology applications. Not only can carbon nanotubes be metallic, but they are mechanically very stable and strong, and their carrier mobility is equivalent to that of good metals, suggesting that they would make ideal interconnects in nanosized devices. Further, the intrinsic semiconducting character of other tubes and graphene nanoribbons, as controlled by their topology, allows us to build logic devices at the nanometer scale, as already demonstrated in many laboratories.

The tremendous importance of the transport properties of nanotubes [1], both from a fundamental and technological point of view, justifies wealth of work and theories developed to deal with 1D systems involving a confined electron gas. The purpose of the present talk consists in defining the electronic and quantum transport properties of both nanotubes and nanoribbons in relation with their atomic structures. Since quantum effects are prominent in carbon nanostructure physics, the electronic quantum transport has been investigated using both the Landauer-Buttiker and the Kubo-Greenwood formalisms, allowing to extract generic properties such as quantum conductance, conduction mechanisms, mean-free-paths... Within both frameworks, the well-known ballistic properties of armchair metallic nanotubes have been reproduced.

However, like in most materials, the presence of defects in carbon nanotube and graphene has been demonstrated experimentally. These defects may take different forms : vacancy, bi-vacancy, “Stone-Wales” defect, 5/7 pair, atom in substitution, … and are known to modify the electronic properties of the host graphene material [2]. It is crucial to understand the properties of these defects in order to conquer their detrimental effects, but also because controlled defect introduction may be used to tune carbon-nanostructure properties in a desired direction. Consequently, the modifications induced by those defects in the electronic properties of the carbon hexagonal network have been investigated using *first-principles* calculations. Computed constant-current STM images of these defects have been calculated within a *tight-binding* approach in order to facilitate the interpretation of STM images of defected carbon nanostructures. As these defects should also play a key role in the chemical reactivity of carbon nanotubes, the study of the modulation of the conductance due to specific molecules adsorbed at the defected nanotube surface will also be presented [3].

In contrast to carbon nanotubes, graphene nanoribbons (GNRs) exhibit a high degree of edge chemical reactivity, which, for instance, prevents the existence of truly metallic nanostructures. Additionally, the discrepancy between the theoretical electronic confinement gap and the experimentally measured transport gap has been attributed to localized states induced by edge disorder. To date, most of the transport studies of edge disordered GNRs have assumed simplified defect topologies, although recent ab initio calculations have proposed and edge chemistry, with evidence of the stability of certain types of geometries such as the Stone-Wales reconstruction. Several experimental studies have also reported the characterization of individual edge defects either by means of Raman, scanning tunneling or transmission electronic microscopy. Consequently, it is presently mandatory to investigate and illustrate the impact of realistic edge defect topology on the electronic transport properties of long and disordered GNRs [4].

In addition, the ground state of zigzag graphene nanoribbons (zGNRs) with hydrogen passivated zigzag edges presents finite magnetic moments on each edge with negligible change in atomic structure, thus suggesting these carbon nanostructures to be attractive for spintronics. Indeed, zGNRs are predicted to exhibit a magnetic insulating ground state with ferromagnetic ordering at each zigzag edge and antiparallel spin orientation between the two edges. However, ideal zigzag GNRs are not efficient spin injectors due to the symmetry between the edges with opposite magnetization. In order to obtain net spin injection, this symmetry must be broken. Incorporating defects (such as vacancies or adatoms) in the GNR or imperfections at the edge which usually cannot be avoided experimentally, break the symmetry between the edges and could thus influence the spin conductance of the GNR. Finally, the introduction of magnetic point defects in zGNRs favors a specific spin configuration of the edges [5]. Consequently, magnetic point defects are also expected to play a key role on the transport properties of graphene nanoribbons.

References :

[1] *Electronic and transport properties of nanotubes,*
J.-C. Charlier, X. Blase, and S. Roche, Reviews of Modern Physics 79, 677-732 (2007)

[2] *Scanning tunneling microscopy fingerprints of point defects in graphene : a theoretical prediction,*
H. Amara, S. Latil, V. Meunier, Ph. Lambin, and J.-C. Charlier, Physical Review B 76, 115423 (2007)

[3] *Defective carbon nanotubes for single molecule sensing,*
Z. Zanolli and J.-C. Charlier, submitted for publication (2009).

[4] *Electron-Hole transport asymmetry and conduction gaps in edge-defected graphene nanoribbons,*
S.M.-M. Dubois, J.-C. Charlier, A. Lopez-Bezanilla, A. Cresti, F. Triozon, and S. Roche,
submitted for publication (2009).

[5] *Spin-transport in defective graphene nanoribbons,*
S.M.-M. Dubois, G.-M. Rignanese, and J.-C. Charlier, submitted for publication (2009).