Quantum Transport in Carbon Nanotubes

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Their unusual electronic and structural physical properties promote carbon nanotubes as promising candidates for a wide range of nanoscience and nanotechnology applications. Not only can 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, 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 is to define the electronic and transport properties of nanotubes in relation with their atomic structures. Since quantum effects are prominent in nanotube 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, defects, doping and chemical functionalisation can alter this ideal situation. For example, even a small amount of boron or nitrogen dopants can drastically modify the electronic transport properties of the tube, which is certainly a key effect for future nanoelectronics [2]. The chemical sensitivity of the electronic transport in carbon nanotubes under the physisorption of molecular species [3] or covalent functionalisation is also an important issue as for example in sensing applications.

Like in most materials, the presence of defects in carbon nanotube 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 carbon nanotubes [4]. 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 nanotube 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. At last, 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 be presented.

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] *Mesoscopic transport in chemically doped carbon nanotubes*, S. Latil, S. Roche, D. Mayou, and J.-C. Charlier, Physical Review Letters 92, 256805 (2004)
[3] *Electronic transport in carbon nanotubes with random coverage of physisorbed molecules*, S. Latil, S. Roche, and J.-C. Charlier, Nano Letters 5, 2216-2219 (2005)
[4] *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)