ELECTRONIC TRANSPORT PHENOMENA IN CARBON-NANOTUBE AND DNA-BASED DEVICES

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ABSTRACT:

In recent years, the issue of charge transfer in (bio)-molecular based devices has become an overwhelming challenge, given its implications in novel nanoscale science, and impact in nano(bio)technologies. Carbon nanotubes are the ideal systems to push forward the frontier of science and applications. Indeed, their unique geometrical features have been conclusive to investigate challenging problems of quantum physics, from quantum interference phenomena to low-dimensional physics. Here we will emphasize on some specific and fundamental characteristics of electronic transport in carbon nanotubes (both in their single or multiwalled configuration) [1] that do not find any counterparts in conventional mesoscopic physics. New predictions will be made on Aharonov-Bohm phenomena occuring in nanotube-based field effect transistor devices, and the role of chemical doping on intrinsic transport and interface effects will be discussed. This last concern is of importance when addressing the sensing capability of molecular-based devices. We will outline recent progress in developing order N real space computational approach of quantum transport in the framework of Kubo-Greenwood or Landauer-Büttiker, able to tackle with the complexity of the devices without disregarding ab-initio related issues.

In a second part, the issue of charge transfer in DNA-based devices will be addressed. Charge transport in DNA biomolecules is a longstanding problem that is highly controversial. Many experiments have directly probed the electrical current as a function of the applied potential across DNA molecules. However, to date, results range from completely insulating to semiconducting and even superconducting behaviours. Setting a meaningful theoretical approach to the intrinsic DNA electrical transport properties is therefore a great challenge.

Any current measured through a DNA molecule results from the carrier injection onto the stack of bases, combined with the intrinsic conduction along the DNA sequence. At low voltage, the main contribution to the resistance comes from the metal-DNA junction potential mismatch (barrier), whereas for high enough voltage, new conduction channels are provided by the molecular states. The I(V) characteristics are thus somehow inferred from the energy difference between the metallic work function and the lowest ionization energy levels of the DNA (in case of hole transport). Charge transfer in DNA is expected to be mainly conveyed by intrastrand π–π coupling through sequential incoherent hopping or coherent tunneling (superexchange) The latter mechanism might be expected to dominate the conduction in the very low temperature regime.

We will present a theoretical study on coherent charge tunnelling in DNA molecules connected in between metallic contacts. An effective tight-binding hamiltonian of the DNA is constructed from ab-initio parameters. The role played by the DNA-metal interface in determining the overall transport and I(V) characteristics will be quantitatively addressed. In this way, we will pinpoint the limits for large turn-on currents, resulting from the resonance between the DNA molecular levels and the bias-modulated Fermi levels of contacts.

References

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