ELECTRONIC TRANSPORT IN SINGLE-MOLECULE JUNCTIONS

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Present trends in the miniaturization of electronic devices suggest that ultimately single molecules may be used as electronically active elements in a variety of applications. Recent advances in the manipulation of single molecules now permit to contact an individual molecule between two electrodes and measure its electronic transport properties. In contrast to single-electron transistors based on metallic islands, molecular devices have a more complicated, but in principle tunable, electronic structure. In addition to generic principles of nanoscale physics, such as Coulomb blockade, the chemistry and geometry of the molecular junction emerge as the fundamental tunable characteristics of molecular junctions.

In my talk, I will present our recent efforts to describe theoretically the electronic transport through single-molecule junctions. Our work is based on the combination of ab initio quantum chemistry calculations and Green functions techniques [1]. Such an approach allows us to elucidate the relation between the electronic structure of individual molecules and the electrical conduction of the circuits in which they are embedded. This fact will be illustrated in my talk with the discussion of the following important topics motivated by recent experiments:

1. *Conductance of aluminium break-junction in the presence of oxygen molecules and other absorbates* [2]. In collaboration with the experimental group of Marcelo Goffman (CEA, Saclay), we show how the use of superconducting electrodes can be very valuable to understand the nature of the conduction through simple molecules such as oxygen or hydrogen.
2. *Role of the conjugation in biphenyl single-molecule junctions* [3]. In relation to the recent experiments of Venkataraman *et al.* [4], we show how one can tune the conductance of biphenyl molecules by introducing suitable side-groups which control the degree of conjugation of the π-electron system.
3. *Length dependence of the conductance of oligophenylenes* [5]. In this case, in relation to recent experiments [6], we study how the length of different

oligophenylene molecules determines basic transport properties such as the low-bias conductance and the thermopower.

4. *Huge photoconductances in organic single-molecule contacts* [7]. It is essential to not only understand the conduction through single molecules, but also to find ways to control it using external stimuli. We have recently studied the transport through organic single-molecule contacts in the presence of an electromagnetic radiation and found that it is possible to enhance their low-bias conductance by several orders of magnitude by applying radiation of the appropriate wavelength.

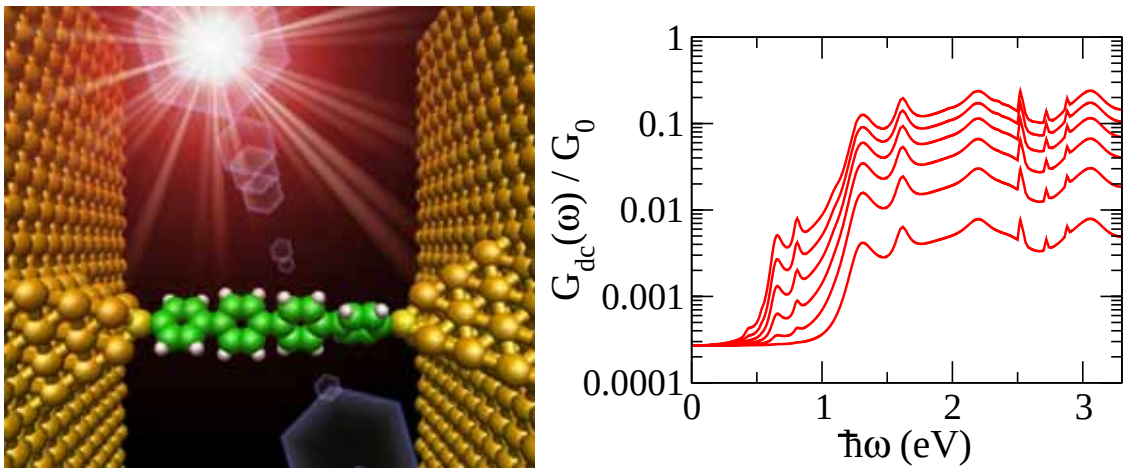

Figure: (Left) Schematic representation of a single-molecule junction subjected to an external electromagnetic radiation. (Right) Photoconductance vs. radiation frequency of an oligophenylene junction for different radiation powers exhibiting a huge enhancement in the infrared and visible range of the electromagnetic spectrum.

References

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