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Properties of Electronic Transport on Molecular Devices

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Abstract – Molecular electronics has recently attracted a lot of attention due to promising application in nanoscale electronic devices. In this presentation we highlight recent results in this field, focusing on single organic molecules working as devices and addressing important effects related with electronic transport, such as push-pull molecules, s or p bridges, Coulomb blockage, negative differential resistance, molecular radicals, temperature dependence, environment sensibility, strong and weak coupling, quantum interference, coherent and incoherent transport, tunneling regime, switches, and a few applications will be addressed.

Feynman was probably the first scientist to imagine that a molecular machine could be built, in which atoms would play the same role as the bricks of a regular size structure, composing a sub-μm device. In 1974, Aviram and Ratner were the first to suggest an organic molecular system showing current rectification, composed by a donor and an acceptor group attached by a carbon bridge with single bonds. Since them, several works have been done and many review articles related to molecular electronics as well nanoelectronics have been written, by Petty, Ellenborgen et al., Merkle, Love et al., LeClair, Heath et al., Read, Nitzan et al. and Pati et al.. Book reviews covering issues related to molecular electronics have also been written [1 and reference therein].

The first thing to deal with a possible molecular device is the molecular structure of the bridge. This includes defining several aspects of the system: sigma or pi bridges between a push-pull system, different bridge length and of course how these choices affect the electronic transport. Theory plays a major role in helping designing and guiding the synthesis of these organic molecules. Therefore, it is often crucial to study theoretically the electronic transport in these structures [2,3,4,5 and references therein].

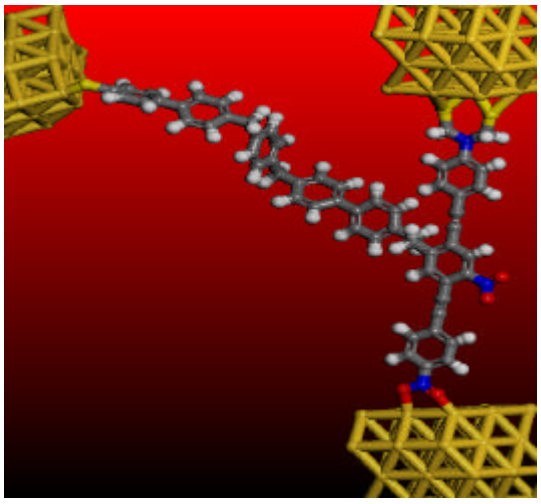

Figure 1: Pictogram of the Controlled Molecular Rectifier utilized in this work. The diagonal-left terminal is the Gate terminal ($\mathbf{T_{Gate}}$). *Top* and *Bottom* terminal are $\mathbf{T_1}$ and $\mathbf{T_2}$ terminals, respectively. Note that the structure is composed by heterogeneous electrons-type, i.e., conjugated rings attached with saturated Carbons in the gate molecule (sp^3 and sp^2 electrons participating of conduction process) and conjugated rings attached with triple bonds Carbons (sp bond) in the main molecule.

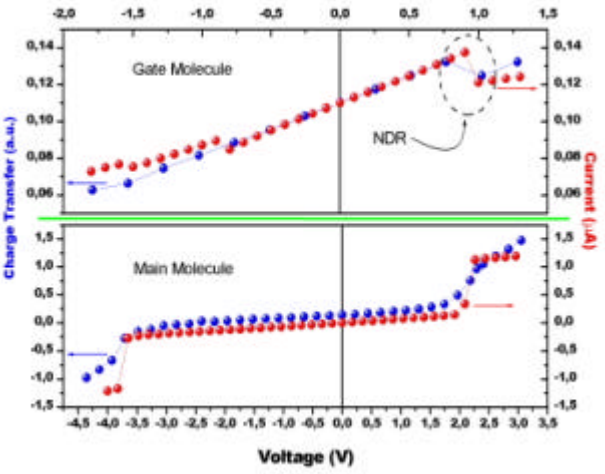

Figure 2: Charge accumulated and current versus bias voltage for a resonant tunnel junction within (*top*) a capacitive model and (*bottom*) asymmetric tunneling barriers. (*top*) Around *V=1 volt* we observe a negative differential resistance (NDR) effect. This NDR in the *I-V* curve is related to the Coulomb blockade in the molecule, which suppresses the current for some particular bias voltage range and (*bottom*) an asymmetric rectification behavior between the $\mathbf{T_1}$-$\mathbf{T_2}$ terminals.

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