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Tuning Desirable Properties in Molecular Electronics

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Abstract

Molecular electronics has attracted attention due application in nanoscale electronic devices. Feynman was the first scientist to propose that a molecular machine could be built, in which atoms would work the same role as the bricks of a regular size structure, composing a nanometer appliance. These nanostructures can present features which are sometimes similar to well-known devices as Zener diodes, resonant tunnel diode, field-effect transistors, thyristors, capacitors, electrochromic devices and so on. However, it offers a viable alternative to overcome difficulties associated with the continuing shrinking of electronic devices in the silicon-based technology. In this presentation we discuss recent finds in the field, focusing on one- and two-dimensional organic systems working as usual and non-usual devices and addressing important effects related with electronic transport, such as push-pull molecules, Coulomb blockage, negative differential resistance, strong and weak coupling, quantum interference, topological insulator behavior, edge passivation, coherent and incoherent transport, tunnelling regime, semiconductor-metal transition ,switches, and a few applications will be addressed. Also, as example, we have investigated by means of nonequilibrium Green's functions method coupled to Density Functional Theory, the electronic transport properties of molecular heterojunctions attached to metallic organic electrodes. We are going to show how tuning electronic properties as current and conductance and how they are strongly correlated to Fowler-Nordheim and Millikan-Lauritsen signatures for several systems.

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