Electron Transport Modeling of triparafenylene with polarons defect coupled in carbon nanotubes

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ABSTRACT

In 1974, Aviran and Ratner have purposed the first molecular rectifier [1]. They have idealized a single-molecule device as consequence of the miniaturization in circuits components and studied their electrical conductance. It would makes economy of power and open new ways to develop new sources of energy. After then, the manipulation of electronics properties of matter follows in the direction of the atomic and molecular properties of each compound. This new front of studies comes from theoretical and experimental efforts around the world. In this work, we have performed theoretical studies about electronic properties in nanojunctions of tribenzene under bipolaron structural defect [2] coupled to metallic carbon nanotubes. The current-voltage, differential conductance, transmission and frontier molecular orbitals were analyzed. These results were obtained using the NEGF-DFT methodology in the Landauer-Buttiker formalism [3-5], as implemented in SIESTA/TRANSIESTA package [6,7]. The results shows Negative Differential Resistance and resonances, like a Esaki diode [8] and in comparison with reference [9], the fact of inserting more rings in the middle of rings with defects bipolaron, there is a gradual decrease of the current, thus suggesting the synthesis of possible nanoelectronic components that need a smaller current, using the same one idea of unimolecular bridge in systems with carbon nanotubes. The final behavior is one organic-metallic device, in agreement with the frontier orbitals [10]. Finally, these results have good properties for new materials in molecular engineering and new projects in the direction to miniaturization of integrated circuits.

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