ELECTRONIC TRANSPORT ENGINEERING DEPENDENT ON THE BRIDGE SIZE

ALEIXO, Vicente F. P.[1]; **SILVA Jr, Carlos. A. B.**[1]; **DEL NERO, Jordan**[2,3]

[1]Faculdade de Física, Universidade Federal do Pará (UFPA), Ananindeua, PA, Brasil
[2]Faculdade de Física, Universidade Federal do Pará (UFPA), Belém, PA, Brasil
[3]Department of Physics and Quantum Theory Project, University of Florida (UF), Gainesville, FL, USA
E-mail: ferrer@ufpa.br; cabsjr@ufpa.br; jordan@ufpa.br

ABSTRACT

One of the goals for the expansion of knowledge in molecular electronics is the project focused on design of nanoscale circuits based in molecules under the action of an external electric potential where they present nonlinear behavior as Field Effect Transistor in current-voltage feature. The idea of proposing molecular components is based on understanding of charge transport mechanisms in systems containing electronic donors and acceptors groups. We investigated, by means of Density Functional Theory/Non-Equilibrium Green´s Function calculations, the electronic transport properties of molecular junctions in π conjugation systems composed by cyclic carotenoids because the polyenic chains (with five, seven, nine and eleven) are closed at two ends with benzene ring coupled to a thiol group (-SH) via methylene (CH2) junction to connect the molecule in the gold electrode. We found of the IxV curve that the Fowler-Nordheim and Millikan-Lauritsen plots exhibits one minimum voltage, V_{min} that occur whenever the tail of a resonant transmission peak enters in the bias window. We verified that V_{min} not depends of the carotenoids length. So, ours results exhibit that the best model to describe the electronic transport properties of this molecular system is the coherent molecular model given by the Landauer–Büttiker formula that takes into account the electronic energy levels of the molecule when coupled at the leads when it is coupled to the leads having different chemical potential generating a current.

Keywords: Cyclic carotenoids; Fowler-Nordheim; Millikan-Lauritsen.

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