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Title. Electronic Transport Between Metallic Nanoparticles.

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Abstract:
Since the idea proposed by Aviram and Ratner [1] in 1974 on unimolecular rectifier diode, many important investigations have been highlighted in theoretical modeling of electronic transport, in order to study the dependence relation of the structure of molecular junctions with the electronic properties of the connections made with the electrodes, and in this way build a functional electronic device [2]. Thus, in this work was performed a theoretical study of the electronic properties in three different configurations of molecular junctions by tunneling formed by gold (Au) electrodes and quantum dots as central region and without effective bonding with the electrodes [3]. From the obtained results were analyzed the characteristic curves of Current-Voltage, Differential Conductance-Voltage, Transmittance - Energy and Voltage, Density of the States of the Device as a function of Energy, Molecular Orbitals and Eigenchannels. The electronic transport calculations were performed using Density Functional Theory (DFT) combined with Non Equilibrium Green's Functions (DFT-NEGF) [4] methodology as implemented in the SIESTA/TranSIESTA packages [5-6]. The results indicate the presence of many interlacing of regions of probabilities of electronic transport with certain differences in the increase of the width of the systems. Finally, these electronic devices of Au presented several indications for other researches with other types of materials involved in the same central ideas of quantum dots for the control of loads and generation of new phenomena.
Keywords: Electronic transport; Au; Quantum dots

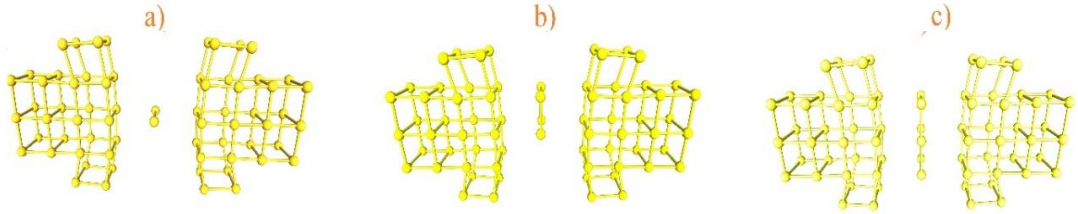

Figure 1. Schematic representation of the studied systems composed by Gold (Au) electrodes and quantum dots of Au as central region and without effective bonding with electrodes for a) two, b) four and c) six atoms in the central regions.

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