The Workshop on Renewable Energy Sources and Nanotechnology – WREN 2019

Modeling of Electronic Transport from Quantum Dot and Molecular Bridge variation in Au nanodevices

J. C. Reis-Silva[1,2]; M. Moura-Moreira[1,2]; J. Del Nero[3,4]

[1] Graduate Program in Electrical Engineering, Federal University of Pará, Belém, PA, Brazil.

[2] Department of Natural Sciences, State University of Pará, Castanhal, PA, Brazil.

[3] Department of Physics, Federal University of Pará, PA, Brazil.

[4] Department of Physics and Quantum Theory Project, University of Florida, Gainesville, USA.

ABSTRACT

One of the great challenges of today is the effective manipulation of electronics at the nanoscale. This idea was initiated by Aviram and Ratner in 1974 in the creation of a unimolecular rectifier diode [1]. Since then, important investigations have been emphasized in theoretical modeling of electronic transport, in order to study the dependence relationship of the structure of the molecular bridge with the electronic properties of the connections made with the electrodes, and in this way to build an electronic device functional. Thus, the research work carried out a theoretical study of the electron properties in single-molecule Au junctions, subjected to variations of molecular and quantum dots [2], through analysis of the characteristic curves of Current-Voltage, Differential Condutance-Voltage, Transmittance - Energy and Voltage, Density of the Device States as a function of Energy and Autochannels of Conduction. For that, the Density Functional Theory was combined with the Green Function of Non-Equilibrium via free Siesta and Transiesta software packages [3-6]. The results indicate the presence of many interlacings of regions of electronic transport probabilities, mainly generating changes with those that have quantum dots. Finally, these electronic devices of Au presented several indications for other researches with other types of materials involved in the same central ideas of change of geometry with moleculares bridges and quantum dots for the control of loads and generation of new phenomena [7].

REFERENCES

[1] AVIRAM, M. A.; RATNER, M. A. Molecular Rectifiers. Journal of physical chemistry, **114** (48), 20299–20319 (1974).

[2] WEN, F.; ZHANG, Y.; GOTTHEIM, S.; KING, N. S.; ZHANG, Y.; NORDLANDER, P.; HALAS, N. J. Charge transfer plasmons: optical frequency conductances and tunable infrared resonances. ACS Nano, 9 (6), 6428-6435, 2015.

[3] HOHENBERG, P.; KOHN. Inhomogeneous electron gas. Physics Review, **136**, 864-871 (1964).

[4] DATTA, S.; TIAN, W.; HONG, S.; REIFENBERGER, R.; HENDERSON, J. I.; KUBIAK, C. P. Current–voltage characteristics of self-assembled monolayers by scanning tunneling microscopy. Physics Review Letters, **79**, 2530-2533 (1997).

[5] SOLER, J. M.; ARTACHO, E.; GALE, J. D.; GARCÍA, A.; JUNQUERA, J.; ORDEJÓN, P.; SÁNCHEZ-PORTAL, D. The SIESTA method for ab initio order-N-materials simulation. Journal Physics Condense Matter, **14**, 2745-2779 (2002).

[6] BRANDBYGE, M. Density-functional method for nonequilibrium electron transport. Physical Review B, **65**, 165401 (2002).

[7] FUECHSLE, M.; MIWA, J. A.; MAHAPATRA, S.; RYU, H.; LEE, S.; WARSCHKOW, O.; SIMMONS, M. Y. A single-atom transistor. Nature Nanotechnology, 7(4), 242-246 (2012).