SPECTROSCOPIC AND ELECTRONIC TRANSPORT MODELING IN ALKYNE JUNCTIONS WITH CARBON NANOTUBES

J. F. P. Leal[1]; J. C. Reis-Silva[2]; D. F. S. Ferreira[2]; J. Del Nero[3,4]

[1] Department of Natural Sciences, University of the Stare of Pará, Castanhal, PA, Brasil.
[2] Graduate Program in Electrical Engineering, Federal University of Pará, Belém, PA, Brasil.
[3] Department of Physics, Federal University of Pará, PA, Brasil.
[4] Department of Physics and Quantum Theory Project, University of Florida, Gainesville, USA
E-mail: jfpleal@uepa.br / jfpleal@ufpa.br

ABSTRACT

The investigation of the properties of electronic transport in molecule-electrode junctions based on the diode rectifier proposed by Molecular by Aviram and Ratner [1] has been extensively studied [2]. For this, it becomes crucial to understand the nature of these joints when the donor and acceptor groups are replaced by metal or semiconductor electrodes to investigate the dependence of the molecular bridge with the electronic properties of the bonds [3]. In this process, the molecule-electrode coupling depends on many parameters, such as the type of chemical bond between the two, the molecular conformation and the height of the tunneling barrier [4,5]. Thus, the properties of current-voltage, Differential conductance -voltage, transmittance - energy / voltage, device states density - energy, frontier molecular orbits, transition voltage spectroscopy and Millikan-Lauritsen plots were studied. Alkyne chain with metal carbon nanotube electrodes [6]. For that, the Density Functional Theory was combined with the Non-Equilibrium Green Function using SIESTA and TranSIESTA codes [7,8]. The results indicate the presence of a common diode characteristic [9]. In addition, the analysis of frontier molecular orbits reveals an organic semiconductor [10]. Finally, this electronic nanodevice presents a promising behavior and brought other contributions to new research in the area of nanoelectronics.

REFERENCES

[1] AVIRAM, A; RATNER, M. A., Molecular rectifiers, Chem. Phys. Lett. **29**, 277 - 283 (1974).
[2] MCCREERY, R. L., Molecular Electronic Junctions, Chem. Mater. **16**, 4477 - 4496 (2004).
[3] SAITNER, M. et al., Impact of Functional Groups onto the Electronic Structure of Metal Electrodes in Molecular Junctions, J. Phys. Chem. C **166**, 21810 - 21815 (2012).
[4] KUSHMERICK, J. G. et al., Metal-molecule contacts, Ann. N.Y. Acad. Sci. **1006**, 277 - 290 (2003).
[5] NAKAYAMA, H.; KIMURA, S., Oligo(phenyleneethynylene) as a molecular lead for STM measurement of single molecule conductance of a helical peptide, Chem. Phys. Lett. **508**, 281 - 284 (2011).
[6] SILVA JÚNIOR, C. A. B. et al., Electronic transport, transition-voltage spectroscopy, and the Fano effect in single molecule junctions composed of a biphenyl molecule attached to metallic and semiconducting carbon nanotube electrodes, Phys. Chem. Chem. Phys. **16**, 19602 - 19607 (2014).
[7] BRANDBYGE, M. et al., Density-functional method for nonequilibrium electron transport, Phys. Rev. B **65**, 165401(1) - 165401(17) (2002).
[8] STOKBRO, K. et al., TranSIESTA: a spice for molecular electronics, Ann. N. Y. Acad. Sci. **1006**, 212 – 226 (2003).
[9] OORSCHOT, P.F. Van; PUSTJENS, J.W., The Resistor Guide: the complete guide to the world of resistors, 2 ed. The resistorguide, 2013.
[10] SATTLER, Klaus D., Carbon nanomaterials sourcebook, London: CRC Press, 2016, 17p.