INVESTIGATION OF ELECTRONIC TRANSPORT IN AZOBENZENE DEVICES WITH CARBON NANOTUBE ELECTRODES

José Weliton de Oliveira Araújo(1), Alexandre de Souza Oliveira(1), Jordan Del Nero(2).

(1) Pós-graduação em Engenharia Elétrica, Universidade Federal do Pará.
(2) Departamento de Física, Universidade Federal do Pará.

Electronic devices based on individual molecules are considered one of the newest technologies to semiconductor electronics [1-2]. In this work we used devices from azobenzene connected to carbon nanotubes electrodes when subjected to an external electrical voltage are replaced by a metallic or semiconducting-type behavior, depending on the geometry of the electrodes [2-3]. We will consider devices consisting of azobenzene molecules in the Cis and Trans configurations, with transverse and longitudinal geometry electrodes. In these devices will apply low voltages, ranging from 0 to 0.1 Volt and then to high voltages of 0 to 1 Volt. We intend to establish in detail the extended Hückel method combined with the Non-Equilibrium Green Function (FGNE) using the State Density measurements in the region around the Fermi level, that is, in the region between the largest occupied orbital HOMO) and the lowest unoccupied orbital (LUMO). Recalling that after the application of an external voltage, the electric current will be given by the Landauer-Büttiker formula [4]. Previous studies have shown that we must take into account the effects of influence due to the geometry of the electrodes [2], as well as the molecular junctions [3]. Thus, we will analyze current and conductance curves to classify these devices.

References

[1] Nitzan, A. and Ratner, M. A. Science 300, 1384 (2003).
[2] Current-voltage characteristics through a single light-sensitive molecule. C. Zhang, Y. He, H.-P. Cheng, Y. Xue, M.A. Ratner, X.-G. Zhang and P. Krstic, Phys. Rev. B 73, 125445 (2006).
[3] Electronic and transport properties of azobenzene monolayer junctions as molecular switches. Y. Wang and H.-P. Cheng, Phys. Rev. B 86, 035444 (2012).
[4] Landauer, R. IBM J. Res. Dev. 1, 223 (1957);