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Electronic Transport Mechanism by Tunneling

M. Moura-Moreira[1], D. F. S. Ferreira[1], J. Del Nero[1,2]

[1] *Pós-Graduação em Engenharia Elétrica, UFPA, Belém, PA, Brazil.*
[2] *Faculdade de Física, UFPA, Belém, PA, Brazil.*

In the field of electronic structure, one of the first studies on molecular devices has been attributed to Aviram and Ratner 1974 [1] who conducted a study about diode of molecular rectification. Among the systems studied in electronic structure are the electronic devices from carbon allotropes that present several advantages [REF] in the nanotechnology area as, for example, the Single-Walled Carbon Nanotubes (SWCNTs), which are sp^2-hybridized cylindrical structures obtained from the winding of one graphene sheet [2-4] and Carbyne polyyne type wires, which are structures with *sp* hybridization formed por carbon linear chain [4-6]. In the present work, we have investigated the electronic transport mechanism through molecular junctions by tunneling in 1D and *quasi*-1D systems. The first is composed of a central atom as a scattering region and polyynes as electrodes. The second system has single-walled carbon nanotubes as electrodes and a central atom as scattering region. In both systems, there is not effective bond between the atom and the electrodes. The electronic transport properties were obtained through the Density Functional Theory methodology combined with the Non-Equilibrium Green Function formalism [7] as implemented in the SIESTA/TRANSIESTA packages [8-9]. From results obtained for transport calculations it will be possible to understand the dynamics of the transport mechanism that control the electronic conduction in the presence of the central atom and without.

Keywords: Electronic Transport, SWCNTs, polyyne, central atom, Transport mechanism

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