Electronic Transport using first-principles method in Carbon Nanotube [5,5] coupled boron and nitrogen nanowire

R. S. Pereira[1]; L.P. Cunha[1]; D. F. S. Ferreira[2]; J. F. P. Leal[3] ; J. Del Nero[4]

[1] *Graduação em Ciências Naturais - Física , Universidade do Estado Pará, Castanhal, PA, Brasil.*

[2] *Programa de Pós-graduação em Engenharia Elétrica, Universidade Federal do Pará, Belém, PA, Brasil.*

[3] *Departamento de Ciências Naturais, Universidade do Estado do Pará, Castanhal, PA, Brasil.*

[4] *Faculdade de Física, Universidade Federal do Pará, Campus Belém, Belém, PA, Brasil.*

ABSTRACT

In the creation of a molecular rectification diode by Aviram and Ratner in 1974, the miniaturization of circuits components as concerns of electronic transport of molecular junctions opened many new possibilities for the study of quantum interference phenomena and electronic behavior in atomic scale from the novel nanodevices development for application industrial [1]. In this work, it was realized a theoretical study about the electronics proprieties of wires junctions composed by atoms of boron and nitrogen with electrodes of a metallic carbon nanotube. However though, through of analyses of current-voltage, differential conductance, transmittance and the frontier molecular orbital, obtained through non-equilibrium green function with combined density functional method (NEGF-DFT) with formalism pertaining to Landauer-Buttiker [2,3] in the implementation of the SIESTA/TRANSIESTA package [4], it was observed negative differential resistance (NDR)[5], with an initial peak in values followed by a deterioration around 0.08V compared to the development of other studies [6,7]. This property occurs by aligning the system's Fermi level with the Frontier molecular orbital (FMO) [8]. This effect suggests applications in nano circuit compounds, as well as promising applications in photocatalysis, due to their resistance to chemical and physical modifications in the environment [9]. Therefore, this shows us good results for use in molecule engineering and plate component manufacturing.

REFERENCES

[1] AVIRAM, M. A.; RATNER, M. A. Molecular Rectifiers. Journal of Physical Chemistry, **144** (48), 20299-20319 (1974).

[2] DATTA, S. Exclusion principle and Landauer-Büttiker formalism. Physical Review, **136**, 864-871 (1964).

[3] BRANDBYGE, M.; "Density-funcional method for nanequilibrium electron transport". Physical Review B, **65**, 165401 (2002).

[4] SOLER, J. M. et al. The SIESTA method for ab initio order-Nmaterials simulation. Journal Physics Condense Matther, **14**, 2745-2779 (2002).

[5] KLETSOV, A.; DAHNOVSKY, Y. Ab initio electron propagator calculations in molecular transport junctions: Predictions of negative differential resistence. The Journal of Chemical Physics, **127**, 144716 (2007).

[6] WENJIANG, L.; XIAOQING, D.; SHAOHONG, C. Transport properties for carbon chain sandwiched between heteroatom-doped carbon nanotubes with different doping sites. AIP Advances, **6**, 075103 (2016).

[7] YIPENG, A. et al. The magnetism and spin-dependent electronic transport properties of boron nitride atomic chains. The Journal of Chemical Physics, **145**, 044301 (2016).

[8] WÓJIK, P. et al. Self-consistent Wigner distribution function study of gate-voltage controlled triple-barrier resonant tunneling diode. Semicondutor Science and Technology, **24** (9), 1-13 (2009).

[9] MILLER, T. S. et al. Carbon nitrides: synthesis and characterization of a new class of functional materials. Physical Chemistry Chemistry Physics, **19**, 15613 (2017).