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Electronic Transport in Molecular Junction by Tunneling Composed by heteroatom and SWCNTs Electrodes.

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Abstract:
Currently, molecular electronics, which is a subfield of nanotechnology, has in recent decades achieved great progress. One of the first proposals of electronic device based on molecules was attributed to Aviram and Ratner 1974 [1] who studied a device that presented the behavior of a diode of molecular rectification. In the area of nanotechnology, the nanostructures most known and used, including molecular electronics, are the carbon allotropes, which result from the different possibilities of electronic states that the carbon atom takes on in the formation of chemical bonds [2]. Among the most studied carbon allotropes are Single-Walled Carbon Nanotubes (SWCNTs), which are cylindrical structures obtained from the winding of one graphene sheet and have sp^2 hybridization [3]. Such structures present a great diversity of applications due to their electronic properties. Several works in electronic transport have shown satisfactory and promising results when using metallic CNTs in place of inorganic metal electrodes [4-5]. This work proposes to carry out a theoretical investigation through molecular junction by tunneling formed by a single atom in the central region and SWCNTs as electrodes. The electronic transport properties were obtained through the Density Functional Theory methodology combined with the Non-Equilibrium Green Function formalism [6] as implemented in the SIESTA/TRANSIESTA packages [7-8]. The results obtained for transport calculations such as voltage-current curve, differential conductance curve, transmittance and voltage channels show that the central atom contributes significantly to the electronic conduction process even without being effectively connected with the electrodes.

Keywords: Electronic Transport, SWCNT, heteroatom, Molecular Junction by Tunneling.

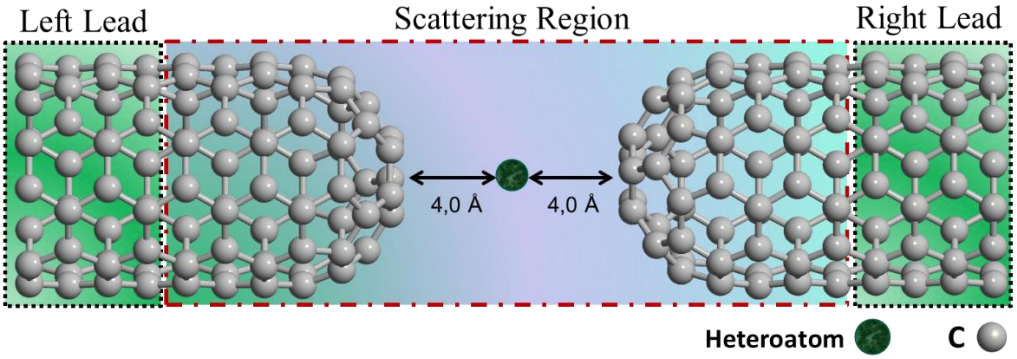

Figure 1: Schematic representation of the studied system formed by a heteroatom in the center (without effective bonding) and SWCNTs electrodes.

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