Sessions: Nanotechnology.
Preferred presentation Type: Poster.

Electronic transport in carbon hybrid systems coupled to linear Fe and Fe / Au electrodes

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Abstract: The use of unique molecules to compose electronic devices has been growing in recent years [1], due to the limits set in the miniaturization of electronic devices [1-3]. In the field of miniaturization the molecular nanowires have good characteristics as applied in components of the bridge type in circuits in nanofabrication [3]. From a perspective of analysis of the behavior of hybrid systems with organic and inorganic coupling for the formation of molecular wires, the Carbyne (Polyyne and Cumulene) alottrope with a variation in the amount of carbon [4-6] in the chain coupled to Fe and Fe/Au nanowires electrodes [7], ranging from 7 to 10 carbons atoms, constituting a molecular yarn possible variation. Using the Density Functional Theory (DFT) method [8], with the implementation of the Non-Equilibrium Green Function (NEGF) implemented in SIESTA [9] code, possible to obtain the structures in their state of minimum energy and to obtain characteristics regarding the electronic structure. The analyzes allowed to characterize current curves, border molecular orbitals, transmission probability, differential conductance curves and the density of states for transport. Finally, the results verified the effects on the chain variation, allowed to assimilate a characterization of increase in the current due to the addition of carbons to devices with Fe electrodes with similar characteristics of crossing of currents under the same voltage, as well as for the second proposal with Fe/Au electrodes that allowed to visualize the alternation in the density of states in regions of negative and positive energy for carbons in odd and even respectively. Also observed are NDR effects for some devices via addition of the Au atoms.
Keywords: Electronic Transport; Hybrid Nanowires ; Carbyne;

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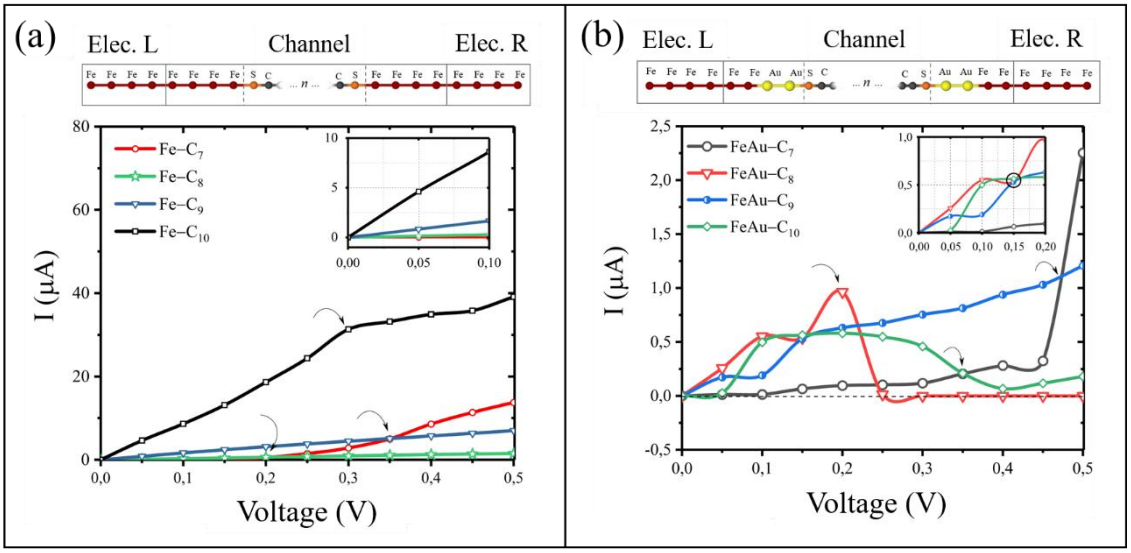

Fig.1. Coupled nanowires with carbon variation of 7 to 10 atoms. In (a) nanowire based solely on the bonding of Fe atoms with carbons and on (b) Fe-nanowire with Au interface attached to the carbon atoms.