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ELECTRONIC TRANSPORT IN BIPHENYL MOLECULE JUNCTIONS WITH CARBYNE ELECTRODES

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ABSTRACT

Nanoscience has developed in the last decades. Theoretical studies on electronic transport modeling in organic semiconductor materials have provided important progress in nanotechnology [1]. Among these molecular electronic materials we highlight those formed by carbons composed of pi-conjugated molecules, the biphenyls, which are smaller structures comprising two adjacent benzenes and they are the ideal model compounds for investigating properties of electronic transport [2]. The device studied in this work is formed by a biphenyl molecule coupled to carbyne electrodes [1,3], according to the schematic representation of Figure 1. Carbyne is a monodimensional material consisting of a single filament formed by simple bonded carbon atoms and alternating triple bonds [3]. The electronic transport was calculated using the SIESTA/ TRANSIESTA [4] computational package, through the combination of DFT (Density Functional Theory) and NEGF (Non-Equilibrium Greens Function) [5], which has been efficient in describing the electronic properties in molecular devices. The results show the behavior of the system when a polarization voltage is applied, the symmetry of the I-V curve and the differential conductance.

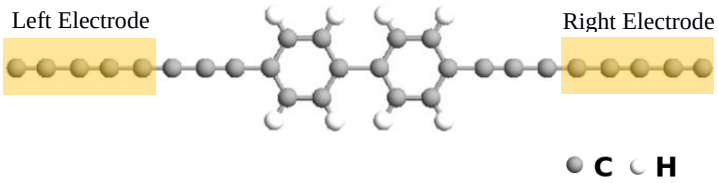

Figure 1- Schematic representation of the studied system.

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