MOLECULAR ELECTRONICS DEVICE COMPOSED BY CARBON NANOTUBES ELECTRODES COUPLED WITH BIPYRIDINE DERIVATIVES

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ABSTRACT

Experimental works have been made with molecules derived from bipyridine coupled to inorganic electrodes. We develop a computational research to investigate the electronic transport properties and Transition Voltage Spectroscopy (TVS) of molecular junctions based bipyridine derivative attached to Single-Walled Carbon Nanotube (SWCN) electrodes. The methodology used were the Extended Hückel Theory (EHT) coupled NonEqulibrium Green's Functions (NEGF) because it has lower computational cost, capture the electronic and atomic properties of large molecules, i.e., greater than 200 atoms (which is our case), and it has recently been applied very well the molecular transport as well as DFT/NEGF calculations. Thus, the calculations used in T = 300K are: (i) Hückel basis set for the C (Cerda.Carbon [graphite]) and H (Hoffmann.Hydrogen); (ii) mesh density cut-off (200 Rydberg); (iii) k-points (1x1x100) and (iv) vary the Fermi level (E_F) of the electrode left and fix the right to get a voltage between the terminals of the electrodes and generate a current given by Landauer-Buttiker formule. The calculations performed for transmittance, density of states, I-V Curve; and Fowler-Nordheim (FN) and Lauritssen-Millikan (LM) Plots show a good performance of electronic transport properties in the application in electronic device.

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