TRANSITION VOLTAGE SPECTROSCOPY IN JUNCTIONS DERIVATIVES FROM BIPHENYL AND CARBON NANOTUBES ELECTRODES

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ABSTRACT

We investigate, by means of Extended Hückel Theory (EHT) coupled NonEqulibrium Green's Functions (NEGF), Transition Voltage Spectroscopy (TVS) in molecular junctions composed of molecules derived from biphenyl attached to metallic carbon nanotubes electrodes. Experimental works have been made with molecules derived from biphenyl coupled to inorganic electrodes. EHT has some advantage to realize the calculations, as: ***(i)*** the lower computational cost, ***(ii)*** capture the electronic and atomic properties of large molecules, i.e., greater than 200 atoms (which is our case), ***(iii)*** it has recently been applied very well the molecular transport coupled with NEGF. We find the current by Landauer-Buttiker formule and Fowler-Nordheim (FN) and Lauritssen-Millikan (LM) Plots, i. e, $\ln[I/V^2]$ and $\ln[I]$ versus V^{-1} show a good performance of electronic transport properties in the application in electronic device. So, the three structures exhibit: ***(1)*** **ZZ9_B2_ZZ9**: three negative differential resistances (NDRs) at V= 1.6V (I = 3.42nA), V= 2V (I = 2.42nA) and V= 2.6V (I = 523.36nA) shown Tunnel or Easaki Diode behavior. At V= 3V, I_{max} = 1,132.37nA. One resonance at V= 1.2V (I = 0.72nA) shown Transistor behavior. The inflection point at V_{min} = 2V ($V^{-1} = 0.5V^{-1}$) in $\ln(I/V^2) = 2.27$ and $\ln(I) = 0.88$ that match with the second point of NDR. ***(2)*** **ZZ9_B2EE_ZZ9**: one NDR at V= 0.6V (I = -5.22nA) with Tunnel or Easaki Diode behavior and one resonance at V= 0.8V (I = 0.012nA). At 3V, I_{max} = 37.68nA. The V_{min} = 0.8V ($V^{-1} = 1.25V^{-1}$) in $\ln(I/V^2) = -4.81$ and $\ln(I) = -4.37$ that match with the resonance. ***(3)*** **ZZ9_B2EA_ZZ9**: three NDRs at 1.6V, 2V and 3V with 246.98nA, 288.43nA and 162.61nA, respectively. I_{max} = 479.25nA at 2.4V. The V_{min} = 1.6V ($V^{-1} = 0.625V^{-1}$) in $\ln(I/V^2) = 6.45$ and $\ln(I) = 5.51$ that match with the first NDR.

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