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Effects of Destructive Quantum Interference on Conjugated Polymers: analysis of electrode geometry

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Abstract

The study of electronic transport in nano-devices proved to be of great relevance in the understanding of the phenomena of quantum interference (QI). Molecular polyacetylene wires connected to gold electrodes with pyramid-shaped geometry, Figure 1(a), when submitted to low voltages, showed anti-resonance in the transmission responsible for producing destructive quantum interference (DQI) [1]. On the other hand, other parameters, such as molecular junctions, Kondo effects and Coulomb block [10] as well as the geometry of the electrodes [11] can influence the production of (IQD). In this work conjugated organic polymers were used, and in the pure state they present low conductivity but when doped, treated with oxidizing agents or reducers [7-8] or connected to gold electrodes (Au) and submitted to an external electric field, they start to have a metallic behavior [9]. We will consider devices constituted of organic polymers conjugated in the pure state with chains containing connections of the simple type (σ) and double type (σ - π), alternated between the carbon and these connected only to hydrogen atoms with gold electrodes (Au) with flat geometry, Figure 1(b), connected at the ends of the individual molecules. The model devices are considered almost 1D or linear structures and have odd amounts of carbon atoms, starting with five (5) having up to nineteen (19) atoms in its individual molecule, and for this work only the polymeric chain containing 5 C should be presented. This device will be submitted to two conditions: the first, in low voltage, varying from 0 to 0.1 Volt and then high voltage, from 0 to 1 Volt. Finally, we will compare the current-voltage (I-V) and conductance-voltage (G-V) curves of the same polymeric chain, but connected to pyramid-shaped electrodes, besides observing the effects of destructive quantum interference when subjected to low voltages.

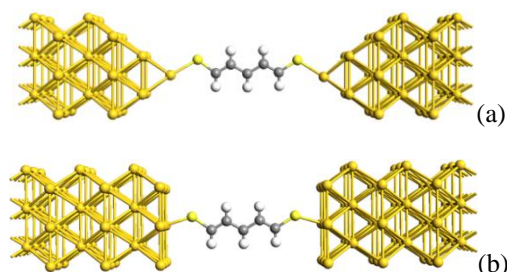


Figure 1: (a) Device containing a polymeric chain with 5 carbon atoms connected to pyramid-shaped electrodes. While in (b) with plane geometry.

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