Effects of Quantum Interference: Analysis of the Influence of Electrode Geometry on Conjugated Polymers

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In previous investigations of electronic transport and effects of quantum interference, it was possible to observe the following effects: Blockade of Coulomb, Kondo effect **[1]**, different directions of excitation along the individual molecule **[2]** and the geometry type of the electrodes **[3]**. Normally the understanding of the properties of electrical conductivity in individual rectifying molecules, we subjected the device to the action of an external electric field **[4]**. However, due to the natural characteristics of these devices when subjected to low voltages, they present destructive quantum interference effects while at high voltages, constructive interference occurs. Our model devices are considered 1D or linear structures and have even numbers of carbon atoms containing single **(σ)** and double **(σ-π)** type bonds, starting with six (6) having up to twenty (20) atoms in their individual molecule, and for this work we will present polymer chains containing: 6, 10 and 20 ***C***. These devices will be subjected to two conditions: the first, at low voltages, ranging from 0 to 0.1 Volt and then to high voltages, from 0 to 1 Volt. We study effects of destructive quantum interference produced due to the geometry of the electrodes with gold electrodes **(Au)** connected at the ends of the individual molecules and we will use electrodes in the form of: ***(i)*** pyramid; ***(ii)*** plan. Our results show what conditions are observed and we can reduce the effects under low voltages. We use conjugated organic polymers that are not pure state, have low conductivity, but when doped, treated with oxidizing or reducing agents [5-6] or connected to gold electrodes (Au) and subjected to an external electric field; they have a behavior of the metallic type, i.e. with high conductivity. Our results show consonance with experimental works [7].

References

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Nossos resultados mostram em que condições são observadas e com podemos reduzir esses efeitos sob baixas tensões. Nós utilizamos polímeros orgânicos conjugados que no estado puro, têm baixa condutividade, mas quando dopados, tratados com agentes oxidantes ou redutores [5-6] ou conectados a eletrodos de ouro (Au) e submetidos a um campo elétrico externo, eles têm um comportamento do tipo metálico, isto é, com alta condutividade. Nossos resultados mostram consonacia com trabalhos experimentais [7].