REDUCTION OF THE EFFECTS OF DESTRUCTIVE QUANTUM INTERFERENCE ON CONJUGATED POLYMERS

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The understanding of electronic transport in nano-devices has been of great relevance in recent years due to its numerous technological applications with low cost, high performance and for better understanding regarding the properties of electrical conductivity in individual molecules rectifiers under action Of an external electric field [1]. However because of the natural characteristics of these devices when submitted to low voltages show destructive quantum interference effects while at high voltages it's assumed that there is constructive quantum interference. Therefore, We'll find a way to reduce the effects of quantum interference under low voltages. Initially introducing a neutral doping in the device.

In this work conjugated organic polymers were used and in the pure state they presented low conductivity, but when doped, treated with oxidizing or reducing agents [2-3] or connected to gold electrodes (Au) and subjected to an external electric field. A behavior of the metallic type, that is, with high conductivity in consonance with experimental works [4]. We will consider devices composed of conjugated organic polymers in the pure state with chains containing single (σ) and double (σ-π) type bonds, alternating between the carbons and these only bound to hydrogen atoms, with gold electrodes (Au) in Form of pyramid connected at the ends of the individual molecules. Our model devices are considered 1D or linear structures and have unpaired numbers of carbon atoms starting with five (5) having up to nineteen (19) atoms in their individual molecule and for this work we will present polymer chains containing 5, 9 and 19 C, (Figure 1). These devices will be subjected to two conditions: the first at low voltages ranging from 0 to 0.1 Volt and then at high voltages from 0 to 1 Volt.

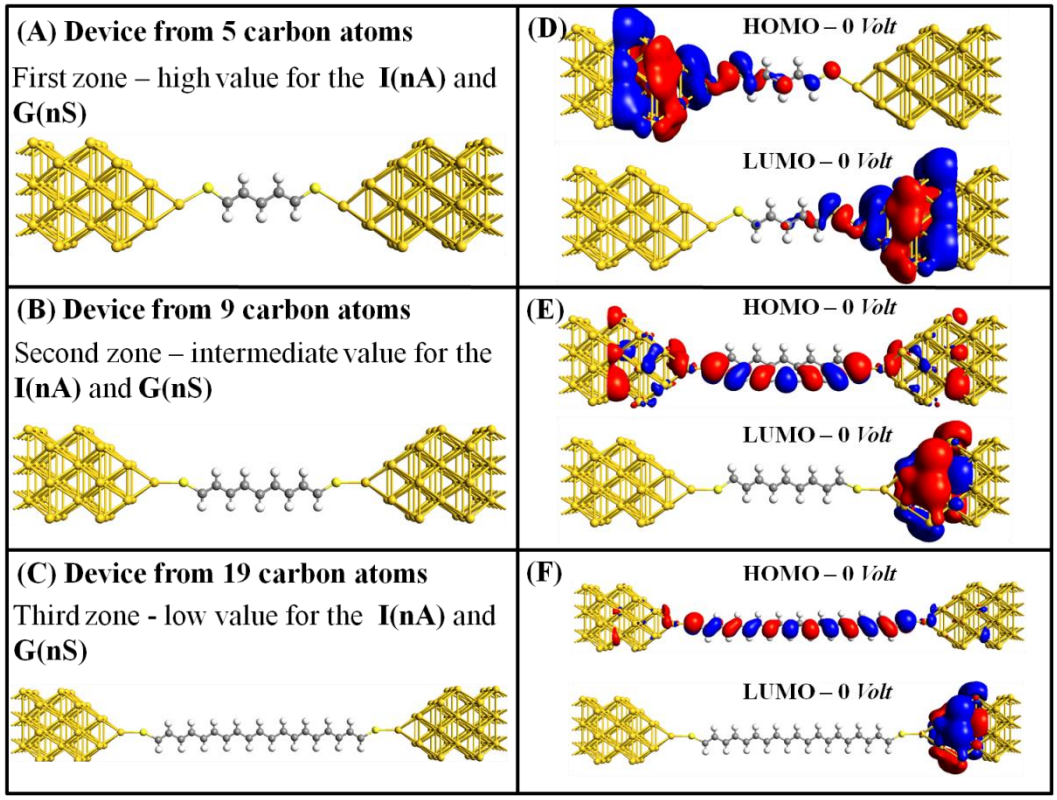

Figure 1: *Conjugated polymers geometric model for three operations zones: (A) first zone - containing 5 carbon atoms. (B) the second zone - intermediate with a polymer chain composed of 9 carbon atoms and (C) a third zone - presenting 19 carbon atoms in their structure. While in (D), (E) and (F) have the molecular orbital in the region of HOMO and LUMO under the null voltage of the devices respectively.*

Previous studies on tunneling in electronic transport and interference effects have shown that we should take into account the effects of molecular junctions, Kondo and Coulomb Block [5], as well as the influence due to electrode geometry [6] and finally, The different directions of excitation along the individual molecule [7]. For this work, we will only analyze the effects of destructive quantum interference produced due to anti-resonance in transmittance and mainly to show under what conditions are observed and how we can obtain the reduction of these effects under low voltages.

References

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