THEORETICAL STUDY OF ELECTRON TRANSPORT IN 6-HYDROXY-2-NAPHTHOIC SINGLE-MOLECULE USED ON THE SYNTHESIS OF LIQUID CRISTAL POLYMERS.

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ABSTRACT

Polymers are compounds that can be obtained artificially by polymerization. In general, they exhibits many common characteristics that are very interesting in each application in each kind of polymer. Some properties can change from insulator to semiconductor behavior. In this sense, one class with great interest is the Liquid Cristal Polymers (LCP) which are aromatic polymers with the especial capability to form regions with highly ordered structure while in liquid phase. This level of order, therefore, is lower than a solid crystal. These materials have high mechanical resistance at high temperatures, extreme chemical resistance, inherent flame retardancy and good weatherability [1]. This work presents a theoretical study of electron transport properties of 6-Hydroxy-2-naphthoic Acid (6,2-HNA), which is one of compounds used in the LCP synthesis [2]. The electron transport calculations were performed using the SIESTA/TRANSIESTA package [3,4] that uses the Non-Equilibrium Green's Functions Methodology with Density Functional Theory (NEGF-DFT) and the Landauer-Büttiker formalism [5]. Our results shows the behavior of the system when a bias voltage is applied using the I-V curve and the molecular energy levels.

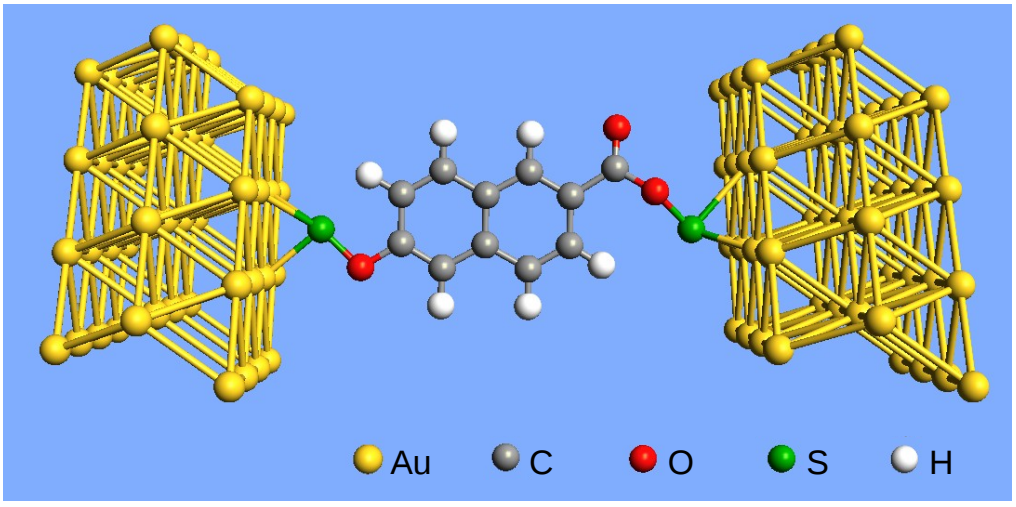

Figure 1: 6-hydroxy-2-naphthoic molecule coupled between two Au electrodes using sulfur as ligand.

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