# Electro / Optical Properties study of Molecule Propyl Red through Quantum Calculus for Application as Molecular Device.

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## RESUMO

Molecular systems are considered attractive options for the development of nanoscale electronic devices in a few years ago [1], [2]. For this reason, the analysis of characteristics of current-voltage (IxV) made it possible to glimpse structures varied with different behaviors [3].

This paper aims to analyze the electronic behavior of organic compound Propyl Red (4 - [4 - (dipropylamino) phenylazo] benzoic acid). The radical $NO_2$ is in position to, other than the usual target [4]. A compound commonly used as an indicator of Ph, a feature found in other molecules already studied [5]. The intention is to observe a considerable stability of the system, when subjected to application of an external electric field.

The methodology deals with properties that govern the electron transport through molecule, with emphasis on a model of transport which uses the formalism of Landauer-Büttiker. Although are made calculations based on Quantum Chemistry methods such as Hartree-Fock (HF), semi-empirical methods and Technique of Configuration Interaction (CI).

Below is shown the formula of Landauer-Büttiker for construction of curve IxV, which will shape the transport system of electronic equilibrium [6]:

$$I = \frac{2e}{h} \int d\varepsilon [\mu_L(\varepsilon) - \mu_R(\varepsilon)] T(\varepsilon)$$

(1)

Where $e$ is the electron charge in modulus ($e > 0$), $h$ is the Plank's constant, $\mu_{L/R}$ is the Fermi distribution function for the left (L) or the right (R) of the molecular junction, and $T(\varepsilon)$ is the transmission coefficient of system with multiple levels and coupled to

reservoirs located (in this specific system will be the group donor and acceptor), which is given by:

$$T(\varepsilon) = \sum_{l} \frac{\Gamma_0^L \Gamma_0^R}{(\varepsilon - E_l)^2 + \left(\dfrac{\Gamma_0^L + \Gamma_0^R}{2}\right)^2} \qquad (2)$$

In what $\Gamma_0^{L/R}$ is the electron tunneling rate between the left / right and the central region (molecule). The sum covers all localized levels. An additional assumption was made in the transmission expression above, i.e., the rates $\Gamma_0^L$ and $\Gamma_0^R$ are independent of energy. To complete the description, we need only specify how the bias voltage drop along the system. The simplest assumption is to obtain a drop below [7], [8].

$$E_l = E_l^0 - xeV_{LR} \qquad (3)$$

Where $E_l^0$ is the level $l$ without bias, $V_{LR}$ the voltage between donor and acceptor end x the voltage drop asymmetry of system. That latter is also responsible by purposes of correction seen in IxV curves.

The value of $E_l^0$ and x may change according to the arrangement of system. In particular, these adjustments were made for the molecule in isolated stages and connected to electrodes.

The resonance points that give rise to the steps on the curve IxV occur when $E_l = E_F^L$ or $E_l = E_F^R$, for positive or negative polarity, respectively. Already the magnitude of these steps is adjusted by the value of $\Gamma_0^{L/R}$. A possible slope on the curve can be associated with an overlap between conductor levels. This levels overlap is achieved making so many times that you want as the curve slope IxV.

The design and simulation optimization of compound electronic transport uses semi-empirical method PM3 (Parametric Method 3). In order is give a absorption spectrum by ZINDO / S-CI (Zerner-Intermediate Neglect of Differential overlap / Spectroscopy - Configuartion Interation) method.

After optimization, referring to the system fundamental state, applies an external electric field in x direction of the area where the molecule is. In order, the structure is optimized using the PM3 method. This procedure is repeated for field gradual values, as positive as negative, until occurs the nano-structure breaking. Every interaction, the charge to molecule attached redistributes along it self. All information, around of the charge successive redistribution, are stored and accounted for the two molecule halves to generate curves of charge accumulation x electric field, graph of HOMO-LUMO orbital of systems.

Moreover, they were determined the spectrum absorption in region between the visible and ultraviolet (UV-visible). The build these spectrum will be made optimizing structures are related to the field values that provide the saturation point on the curve **e** x **E**. Generally, these field values are responsible for a significant shift of the spectrum.

The molecule propyl red has undergone three different stages to observe their behavior as possible nano-device:

- Propyl Red (alone molecule M);

- HS – M – SH (+ tiol group);

- AlS – M – SAl (molecule + atom sulfur + Aluminum electrode).

The molecule has been studied in form alone and with the electrodes addition. The results are theoretical and were obtained through simulation and can serve as basis for experimental studies. This study allows the understanding of molecular structure charge transport of along the. From the results, it was possible to conclude that:

- The charge transport along the molecule is asymmetrical under bias direct and reverse;

- The transport is type resonant tunneling in the current x voltage indicative curve;

- The investigated molecular system show feature of molecular rectifier.

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