



# Evaluation of electronic and transport properties of a nano-scale device in the presence of electric field

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## ARTICLE INFO

### Article history:

Received 10 July 2010

Received in revised form

9 August 2010

Accepted 20 August 2010

Available online 26 August 2010

## ABSTRACT

The effect of external electric field (EF) in electronic properties of an organic semiconductor (OSE) molecule sandwiched between two ferromagnetic electrodes has been carried out. We adopt a modified Su–Schrieffer–Heeger (SSH) Hamiltonian for describing the isolated Pentathiophene molecule. The ground state of the molecule is obtained by Hellmann–Feynman theorem. Our calculation results show that by taking into account the presence of EF lattice distortion, electron density and HOMO–LUMO gap will be changed. Using Green’s function formalism we have also studied the effect of these changes on transport properties of molecule. Our results show that in the presence of EF current and TMR decrease, the negative differential resistance (NDR) occurs.

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## 1. Introduction

Spin dependent transport through organic semiconductors (OSEs) is quite interesting for most researchers specifically because of its application in electronic devices. As a result it has been studied both theoretically and experimentally [1–8]. Due to weakness of spin-orbit coupling and hyperfine interactions in an organic material, the spin relaxation length is large and spin-flip can be neglected during conduction process. As a result OSEs are good candidate for future spintronics devices. Negative differential resistance (NDR) has been experimentally observed in OSEs [1,2]. And tunneling magnetoresistance (TMR) also has been observed in a spin-valve structure with an OSE spacer [3]. There are some recommended mechanisms to explain NDR in OSEs [4,5]. Here we relate NDR to the presence of external electric field (EF) along molecule and we have also studied the effect of this phenomenon on transport properties and TMR in the sandwiched molecule. A strong electron–phonon interaction plays an important role in electronic and transport properties of OSEs. The Su–Schrieffer–Heeger (SSH) Hamiltonian contains this interaction and has been used in many different articles for describing OSEs [5–7]. Green’s function formalism has been used for calculation of transmission coefficient in different bias voltage. In this work ferromagnetic electrodes have been described in the wide-band approximation [8,9].

## 2. Model and method

The Hamiltonian of a molecule that is sandwiched between two electrodes can be written as

$$H = \begin{pmatrix} H_L & H_{L,M} & 0 \\ H_{L,M}^+ & H_{PTh} + H_{EF} & H_{R,M}^+ \\ 0 & H_{R,M} & H_R \end{pmatrix} \quad (1)$$

where  $H_{L/R,M}$  shows the coupling between molecule and electrodes.  $H_{PTh}$  shows the Hamiltonian of isolated polythiophene molecule. We have considered the *PTh* molecule as a quasi one dimensional chain with  $N$  rings, which can be described by using a modified SSH Hamiltonian as follows [6,10,11]:

$$H_{PTh} = \sum_{i=1}^{4N} \sum_{\sigma} \{ \varepsilon_0 C_{i,\sigma}^+ C_{i,\sigma} - t_{i,i+1} (C_{i+1,\sigma}^+ C_{i,\sigma} + C_{i,\sigma}^+ C_{i+1,\sigma}) \} \\ - \sum_{n=1}^N \sum_{\sigma} \{ \varepsilon' (C_{4n,\sigma}^+ C_{4n,\sigma} + C_{4n-3,\sigma}^+ C_{4n-3,\sigma}) \\ + t'(C_{4n,\sigma}^+ C_{4n-3,\sigma} + C_{4n-3,\sigma}^+ C_{4n,\sigma}) \} \quad (2)$$

where

$$t_{i,i+1} = t_0 - \left( t_1 \cos\left(\frac{i\pi}{2}\right) - \alpha(u_{i+1} - u_i) \right) \quad (3)$$

The index  $i$  runs over the orbitals of Carbon chain of the molecule. The operator  $C_i^+$  ( $C_i$ ) creates/annihilates a  $\pi$  electron with spin  $\sigma$  at the  $i$ -th site of PTh molecule.  $\varepsilon_0$  is the onsite energy of Carbon atoms and  $t_{i,i+1}$  denotes the hopping integral between two neighboring sites.  $t_0$  is the transfer integral in a undimerized

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molecule and  $t_1$  is confinement constant which guarantees the nondegenerate characteristics of the ground state [11]. The electron–phonon coupling constant is denoted by  $\alpha$ ,  $\varepsilon'$  and  $t'$  show the effect of Sulfur atom on Hamiltonian of molecule [6].  $u_i$  is the displacement of the  $i$ -th Carbon atom, which is evaluated with the help of Hellmann–Feynman theorem. The second term in Eq. (1) shows the contribution of EF (which is uniform along the molecule) in the Hamiltonian and can be written as [7]

$$H_{EF}(V_B) = -\sum_{i,\sigma} q_{i,\sigma} \left(\frac{V_B}{L}\right) \left[\frac{L}{2} - X(i)\right] C_{i,\sigma}^+ C_{i,\sigma} \quad (4)$$

where  $L$  and  $V_B$  are the molecule length and bias voltage, respectively.  $X(i)$  shows the position of  $i$ -th Carbon atoms and is determined from Fig. 1.

$q_{i,\sigma}$  shows the charge density on the  $i$ -th site with spin  $\sigma$  and is written as follows:

$$q_{i,\sigma,V_B} = |e| \sum_{\mu}^{\text{occ}} \Psi_{i,\mu,\sigma,V_B} \Psi_{i,\mu,\sigma,V_B} \quad (5)$$

where  $\Psi_{i,\mu,\sigma,V_B}$  is the wave function for an electron on the  $i$ -th site with eigenvalue  $\varepsilon_{\mu}$ , spin  $\sigma$  and applied voltage  $V_B$ . For simplicity we assume that the molecule is in the ground state and only the lowest levels of molecule are occupied. Relaxation of molecule in the presence of EF has been done with the help of Hellmann–Feynman theorem, which leads to the following equation [11,12]:

$$u_i = \frac{1}{2} \left[ u_{i-1} + u_{i+1} + \frac{2\alpha}{K} \sum_{\mu,\sigma}^{\text{occ}} (\Psi_{i+1,\mu,\sigma,V_B} \Psi_{i,\mu,\sigma,V_B} - \Psi_{i,\mu,\sigma,V_B} \Psi_{i-1,\mu,\sigma,V_B}) \right] \quad (6)$$

The electronic eigenstate and the eigenvalue can be solved from the Schrodinger equation of the electronic part of Hamiltonian as follows:

$$\begin{aligned} & \left( \varepsilon_0 - q_{i,\sigma} \left(\frac{V_B}{L}\right) \left[\frac{L}{2} - X(i)\right] \right) \Psi_{i,\mu,\sigma,V_B} - t_i (\Psi_{i-1,\mu,\sigma,V_B} + \Psi_{i+1,\mu,\sigma,V_B}) \\ & - (\varepsilon' \Psi_{i,\mu,\sigma,V_B} + t' \Psi_{i-3,\mu,\sigma,V_B}) \Delta\left(\frac{i}{4}, \text{int}\right) \\ & - (\varepsilon' \Psi_{i,\mu,\sigma,V_B} + t' \Psi_{i+3,\mu,\sigma,V_B}) \Delta\left(\frac{i-3}{4}, \text{int}\right) = \varepsilon_{\mu,\sigma,V_B} \Psi_{i,\mu,\sigma,V_B} \quad (7) \end{aligned}$$

where:  $\Delta(x, \text{int}) = \begin{cases} 1 & x \text{ is Integer} \\ 0 & \text{otherwise} \end{cases}$

Eqs. (6) and (7) are solved self-consistently and the ground state of molecule is obtained in the presence of an EF (molecule relaxed in the presence of EF). For calculation of current we have used Green's function approach. Transmission coefficient as a function of energy in the presence and absence of magnetic field can be written as follows [7]:

$$T^{\sigma,\sigma'}(\varepsilon, V_B) = \text{Tr}[\Gamma_L^{\sigma} G^{\sigma'}(\varepsilon, V_B) \Gamma_R^{\sigma'} G^{\sigma}(\varepsilon, V_B)] \quad (8)$$

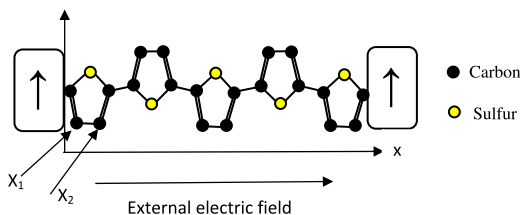


Fig. 1. The position of carbon atoms in a Pentathiophene molecule.

where  $G(\varepsilon)$  is Green's function of the system and is defined as

$$G^{\sigma,\sigma'}(\varepsilon, V_B) = [\varepsilon I - H_{PTM} - H_{EF}(V_B) - \Sigma_L^{\sigma} - \Sigma_R^{\sigma'}]^{-1} \quad (9)$$

The effect of coupling between molecule and electrodes is fully described by specifying self-energy terms. In the wide-band approximation,  $\Gamma_{L/R}$  is independent of energy and bias voltage and can be written as

$$\Sigma_{L/R}^{\sigma} = \frac{-i}{2} \Gamma_{L/R}^{\sigma} = \frac{-i}{2} (2\pi |\gamma_{L/R}|^2 \rho_{L/R}^{\sigma}) \quad (10)$$

where  $\gamma_{L/R}$  is the coupling between electrodes and molecule, which is an important parameter and could influence the shape of current–voltage curve [13–15].  $\rho_{L/R}^{\sigma}$  shows density of state in left/right electrode for electron with spin  $\sigma$ . The currents can be calculated using the Landauer–Büttiker formula

$$I^{\sigma,\sigma'}(V_B) = \frac{e}{h} \int_{-\infty}^{+\infty} T^{\sigma,\sigma'}(\varepsilon, V_B) [f_L(\varepsilon) - f_R(\varepsilon)] d\varepsilon \quad (11)$$

where  $f_{L/R}^m$  is the Fermi function of the left/right electrode with chemical potential  $\mu_{L/R} = \varepsilon_f \pm (eV_B/2)$  and Fermi energy  $\varepsilon_f$

$$f_{L/R}(\varepsilon) = [\exp[\beta(\varepsilon - \mu_{L/R})] + 1]^{-1} \quad (12)$$

Finally, TMR as a function of applied voltage is defined using the following equation:

$$TMR(V_B) = \frac{\sum_{\sigma} I^{\sigma,\sigma}(V_B) - \sum_{\sigma} I^{\sigma,-\sigma}(V_B)}{\sum_{\sigma} I^{\sigma,\sigma}(V_B)} \quad (13)$$

### 3. Result

Numerical calculations are carried out for a molecule with 5 rings (20 sites), the parameters for a Pentathiophene are chosen as,  $\varepsilon_0 = -4.3$  eV,  $t_0 = 2.5$  eV,  $t_1 = 0.675$  eV,  $\alpha = 4.65$  eV/Å,  $t' = \varepsilon' = 0.05 t_0$  and  $K = 21.0$  eV/Å<sup>2</sup>. These parameters are specifically chosen to reproduce previous results [16]. We have used the following set of parameters to describe cobalt electrodes:  $\rho^{\uparrow} = 0.1367$  (1/eV) and  $\rho^{\downarrow} = 0.5772$  (1/eV), and we set  $\gamma_L = \gamma_R = 0.2$ ,  $\varepsilon_f = -1$  eV,  $X_1 = 0.4$  Å and  $X_2 - X_1 = 1.4$  Å. In the presence of EF orbitals are affected differently by EF so the HOMO–LUMO gap is changed [16]. Fig. 2 shows the evaluation of HOMO–LUMO gap in the presence of external EF. With increasing of EF band gap decreases. Our results are in fair agreement with previous first-principle calculation [16]. Fig. 3 depicts the lattice distortion ( $y_i = u_{i+1} - u_i$ ) in different bias voltages. In Fig. 4(a) and (b) we represent respectively the net charge in the low and high voltage region. As we expected with increasing bias voltage electrons accumulate in the left side of molecule this phenomena has been

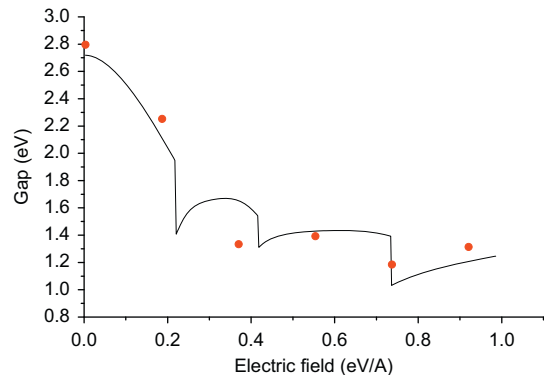


Fig. 2. Evaluation of HOMO–LUMO gap in the presence of external EF, the black solid line represents our calculation and the red circle is related to the previous first-principle calculation [16].

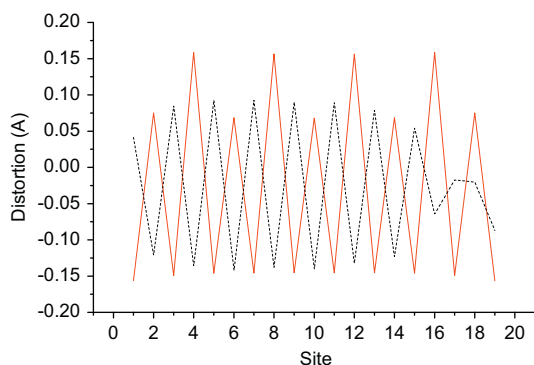


Fig. 3. Lattice distortion ( $y_i = u_{i+1} - u_i$ ) in different site (red solid line/ black dashed line) in the absence/presence of electric field (7 V).

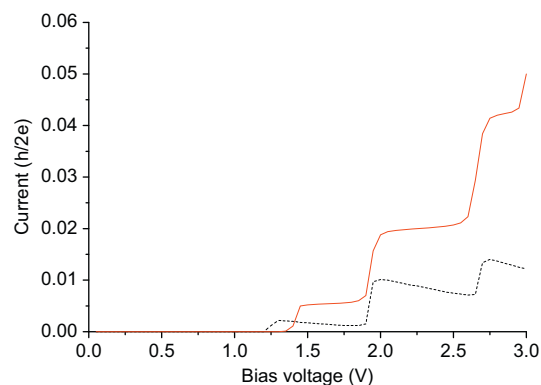


Fig. 5. Current as a function of bias voltage (red solid/black dashed line) in the absence/presence of electric field.

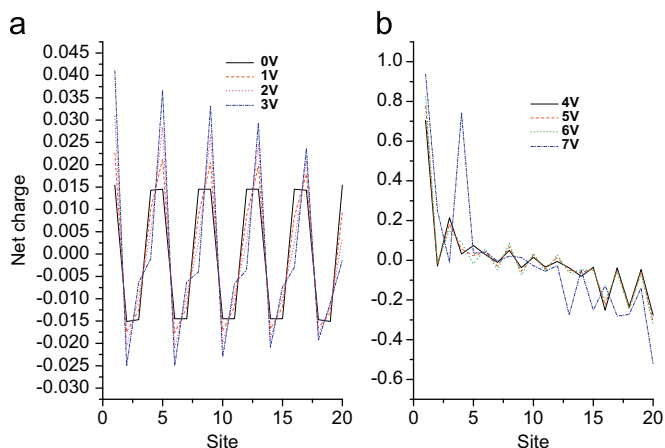


Fig. 4. Net charge on the carbon sites in different voltage for (a) low voltage regime and (b) high voltage regime.

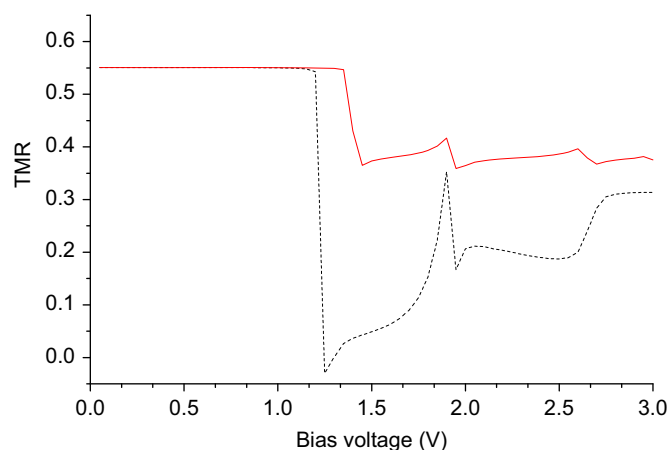


Fig. 6. TMR as a function of applied voltage, (red solid/black dashed line) in the absence/presence of electric field.

observed in the first-principle calculation [16]. Fig. 5 represents the current–voltage characteristic of molecule in the absence of magnetic field. If we do not consider the effect of external EF on the energy levels of molecule, with increasing of bias voltage energy-window opens and current increases in all voltages. However by taking into account the presence of EF along the molecule, the current decreases, which has been reported for in-plane electric field [17]. In the presence of EF the negative differential resistance (NDR) occurs, which has been observed theoretically in the previous work for polyhiophene [18] and other molecules [19]. In Fig. 6 we investigate the effect of this phenomenon on TMR. The interaction of EF with electrons is independent of spin so this effect decreases TMR. The major effect of EF is restricted in small voltage interval.

#### 4. Conclusion

In summary, based on Green's function formalism we have investigated the effect of presence electric field in the electronic and transport properties of a Pentathiophene molecule. Our calculations indicate that in the presence of electric field HOMO–LUMO gap, electron density, current and TMR change.

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