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# Controlled Electron Transport in the Thiophene Based Single Molecular Field Effect Transistor

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**Abstract :** The electronic transport properties of a gated single thiophenedithiol molecular device are studied by using non-equilibrium Green's function (NEGF) in combination with extended Huckel theory (EHT). The current-voltage characteristics and transmission spectra of the system are studied. We find that, positive or negative transverse gate bias $V_g$ will, respectively, raise or lower the Transmission Coefficients T(E) relative to the Fermi level ($E_F$). The results show that, depending on the applied transverse gate bias $V_g$, the magnitude of the source-drain current $I_{sd}$ varies over more than three times for same source-drain bias $V_{sd}$. This emphasizes that the external transverse gate electrode and gate field, can effectively tune the electronic transport properties of the molecular devices. Thus it reveals the importance of transverse electrodes in single molecular devices.

**Key words:** Molecular Electronics, Single Molecular Field Effect Transistor, Transverse Gate Field Effect, Extended Huckel Theory (EHT), Non Equilibrium Green's Function (NEGF).

## Introduction:

Device miniaturization is an inevitable trend in semiconductor industry development. Due to the nanometer scale and other potential superiorities, organic molecules have become one of the favorable candidates to substitute silicon-based semiconductor devices in the future. Molecular electronic devices offer the prospect of extending the semiconductor technological roadmap. The electronic transport properties of single molecules have attracted more and more attention for their possible uses as functional units for electronic devices. The most common and important function of single molecular devices is to control the charge transport properties effectively. At present, there are two main approaches to do this[1]. One is through the conformational changes in the molecules, and the other is through field-effect gating. The former one has been paying much attention and made progress in the past few decades[2,3,4]. Despite the fact that the conformational change in molecules can be performed by using the electric or light fields, its operating frequency is low. Nowadays, people are turning to the latter one for its high operation frequency and low power consumption.

Many field-effect transistor (FET) configurations have been achieved both experimentally[5-8] and theoretically[9-15]. Investigated electronic transport properties of a gated single 1, 3-benzenedithiol molecular device and influence of functional group of such devices using first principle's method[16,17]. Yet theoretical works in this respect are relatively lacking and few molecules have proved controllable by the transverse field with attractive I-V characteristics. It is therefore natural to seek new promising organic molecular devices with

favorable configurations and useable properties in the industry area. Among few molecules, Thiophene play a significant role, because of its conjugate nature and easily synthesized. But organic FET made up of a single unit of thiophenedithiol molecule is not widely reported. Therefore, the effect of gate field with respect to the single thiophenedithiol molecule is of great importance to the electronic transport properties of molecular devices of FET configuration and needs to be systematically investigated.

In this study, the semi empirical quantum transport method, which is applying non-equilibrium Green's function (NEGF) in combination with extended Huckel theory (EHT)[18], has been implemented to explore the electronic transport properties of a gated Au/S-Thiophene (Tp)-S/Au junction. The results show that the gate field has a crucial effect on the electronic transport properties of the molecular device.

**Computational scheme**

In this work, the computational scheme is carried out in two parts. First part is the geometry optimization of isolated thiophene molecule attached to the terminal groups sulfur. Second part is the calculation of transport properties of the optimized thiophenedithiol (Tp) molecule inserted between two Au(111)(3x3) source (LE) and drain (RE) electrodes through above mentioned terminal groups with a transverse gate electrode in a FET device configuration as shown in Fig. 1.

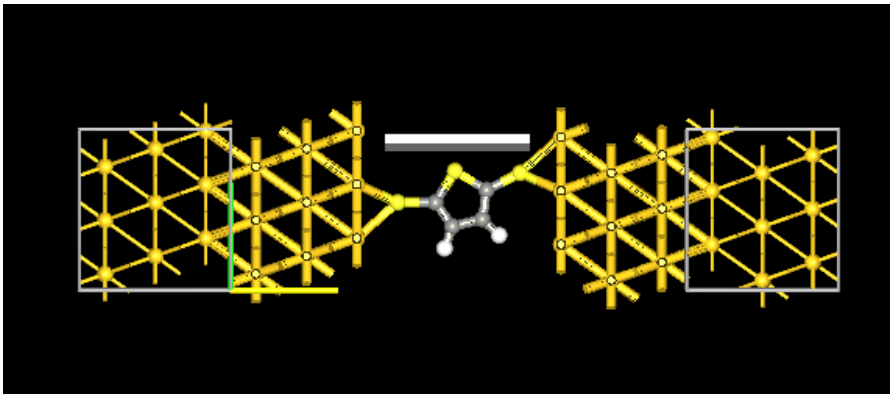

**Fig. 1. Schematic FET device configuration of a Thiophenedithiol (Tp) molecule sandwiched between left (source) and right (drain) Au electrodes through sulphur (S) atoms with transverse electrode. The gate voltage $V_g$ has no effect on the metallic electrodes. Color codes: Au (golden), C (gray), H (white), S (Yellow)**

The geometrical optimization and the electronic transport properties calculations are carried out by a package Atomistix ToolKit [19], which is based on the combination of extended Huckle theory (EHT) and Non-equilibrium Green's functions (NEGF) technique, and the method has been used by several groups for a variety of applications and has well documented. On NEGF theory, the molecular wire junction is divided into three regions: Left electrode (LE), scattering region (SR), and Right electrode (RE) as represented in Fig. 1. The scattering region contains parts of the electrodes include the screening effects in the calculations. To the left and right electrodes, we used 3 × 3 unit cells in the x and y directions to avoid the interaction between the molecules and the mirror image. The adsorption geometry is such that the molecules are located symmetrically at the top site of Au (111) surface. The Brillouin zone of the leads is sampled by 1 × 1 × 200 k points in the directions of x, y and z (z is the electron transport direction), which is enough to produce the results.

According to NEGF formulas, the source-drain current issued through the system is obtained by the Landauer – Buttiker formula,

$$I = \frac{2e}{h}\int_{\mu_L}^{\mu_R} T(E,V_{sd})[f(E-\mu_L) - f(E-\mu_R)]dE \quad (1)$$

where $\mu_{L(R)}$ are the chemical potentials of the left (right) electrode, f[E-$\mu_{L(R)}$] are the Fermi distribution functions of electrons on the left (right) electrode, and T (E, $V_{sd}$) is the transmission function through the device at energy E and source-drain bias $V_{sd}$ which can be obtained by the following formula,

$$T(E,V_{sd}) = Tr\left[\Gamma_L(E)G^R(E)\Gamma_R(E)G^A(E)\right] \quad (2)$$

where $G^R$ (E)and $G^A$ (E) are the retarded and advanced Green's functions of the scattering region, $\Gamma_{L(R)}=i[\Sigma^R_{L(R)}(E)-\Sigma^R_{L(R)}(E)]$ is the line width function, $\Sigma^R_{L(R)}(E) and \Sigma^R_{L(R)}(E)$ are the self-energies of the scattering region, which contain all the effects of the electrodes. The transmission coefficient T (E) can be decomposed into the contribution of an agent channel,

$$T(E) = \sum_n T_n(E) \quad (3)$$

For the system in equilibrium state, the equilibrium conductance can be obtained by the transmission coefficient T(E) at the Fermi level $E_F$,

$$G = G_o T(E_f) = G_o \Sigma T_n \quad (4)$$

where $G_o = 2e^2/h$ is the quantum conductance ($G_o$=7.7481x10$^{-5}$S).

The effect of the gate voltage ($V_g$) is taken into account by adding a constant shift to the scattering region [20-22].

## Results & Discussion

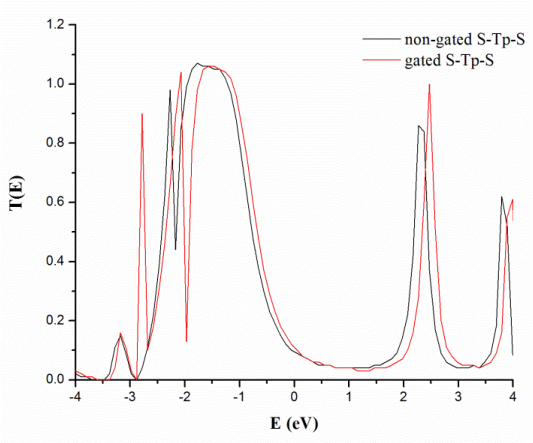


**Fig. 2. Transmission spectra T(E) for $V_{sd}$=0V at $V_g$=0V for non-gated and gated S-Tp-S device respectively are device shown for comparison.**

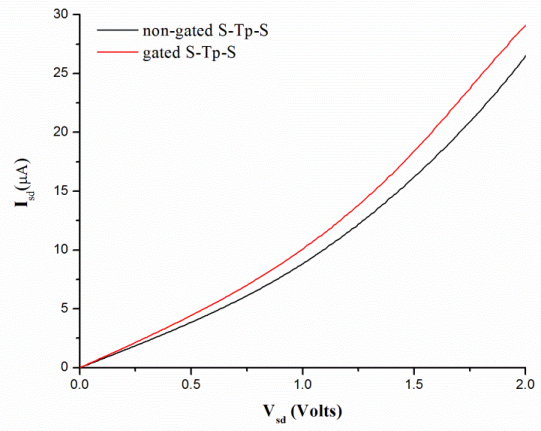


**Fig. 3. Drain current $I_{sd}$ as a function of source-drain voltage $V_{sd}$ at $V_g$=0V for non-gated and gated S-Tp-S respectively are shown for comparison.**

### Effect of Gate

To understand the influence of gate in molecular device conductance, we analyze transmission characteristics and $I_{sd}$-$V_{sd}$ characteristics of non-gated S-Tp-S device and gated S-Tp-S device. We studied zero bias transmission characteristics of non-gated and gated S-Tp-S device, which are shown in the Fig. 2. The gate voltage $V_g$ is set as 0V for gated device. The general shape of the zero transmission spectra for the two systems more or less resembles the same with the narrowest transmission peaks at either side of the Fermi Level. We observed that the HOMO is dominated in gated S-Tp-S system with a new peak developed in that region. Particularly, transmission peaks were shifted towards fermi level in HOMO region, leading to large transmission. This means that the conductance of gated S-Tp-S is higher than non-gated S-Tp-S, because the transmission channels near the Fermi levels dominate the electron transport. The calculated source-drain $I_{sd}$-$V_{sd}$ characteristics are shown in Fig. 3. The gate voltage ($V_g$) is set to 0 V and $V_{sd}$ is in a range from 0 to 2 V. The gated S-Tp-S system has the largest current than non-gated S-Tp-S system which is due to large transmission in HOMO region and the location of transmission channels near the Fermi level. Particularly at $V_{sd}$ = 3.0V, the current $I_{sd}$ varies by a magnitude of 3 μ A. This emphasizes the effect of gate electrode on molecular conductance.

To comprehend the effect of gate in molecular device conductance, we study $I_{sd}$-$V_{sd}$ characteristics of gated S-Tp-S device. The semi empirically calculated source-drain $I_{sd}$-$V_{sd}$ characteristics are shown in Fig 4. The gate voltage ($V_g$) is set to seven different values (-3.0, -2.0, -1.0, 0.0, 1.0, 2.0 and 3.0 V), and $V_{sd}$ is in a range from 0 to 2 V. We can observe a controllable gate-voltage dependence in this molecular junction. Particularly, the $I_{sd}$-$V_{sd}$ characteristics have several important features comparable with those of $V_g$ 0.0 V situations. When $V_{sd}$ is low, currents vary slightly with $V_g$ 0.0V situation. But the trend is reversed when $V_{sd}$ is

in high region. It is also obvious to see that the magnitude of current for $V_g$ = 3.0V is strikingly weak compared with that of the current for $V_g$ = -3.0V. It is also found that magnitude of current varies more than three times for same $V_{sd}$ over different $V_g$ bias. For example, particularly for $V_{sd}$ = 1.5V, the $I_{sd}$ is found to be 31.2 μA for V g = -3.0V and 8.71 μA for $V_g$ = 3.0V respectively, revealing the effect of gate field on molecular conductance.

**Effect of gate field**

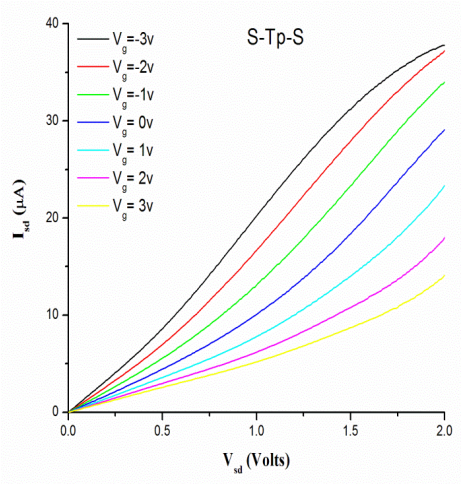


**Fig. 4. Drain current $I_{sd}$ as a function of source-drain voltage $V_{sd}$ for S-Tp-S device at different $V_g$ bias are shown for comparison.**

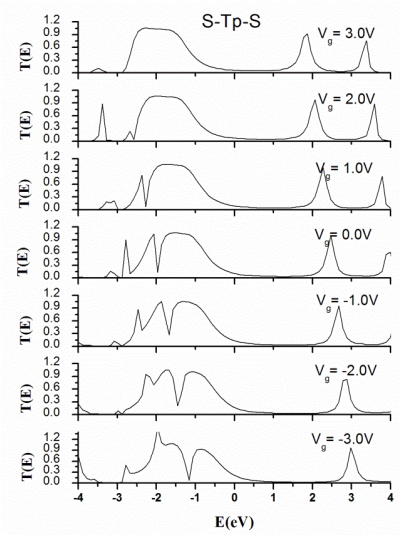


**Fig. 5. Transmission spectra T(E) for S-Tp-S device at $V_{sd}$ =0V at different $V_g$ bias are shown for comparison.**

Now to understand the I-V characteristics, we focus on the zero-bias transmission spectra T (E) as a function of energy E for gated S-Tp-S device for gate bias set to seven different values (-3.0, -2.0, -1.0, 0.0, 1.0, 2.0 and 3.0 V) are shown in Fig. 5. From Fig 5, we can see clearly the gated modulation on Transmission Coefficients T(E), which in turn leads to the change in conductance. A positive or negative $V_g$ will, respectively, raise or lower the T(E) of the molecule relative to the Fermi level ($E_F$). The Transmission coefficients T (E) at $E_F$ are 0.25, 0.17, 0.135, 0.11, 0.09, 0.075, and 0.065 for $V_g$ = -3.0, -2.0, -1.0, 0.0, 1.0, 2.0 and 3.0 V, respectively. Higher Transmission coefficient T(E) means largest current for $V_g$ = -3.0 V, which is in relevance with the $I_{sd}$-$V_{sd}$ characteristics of gated device. The Zero bias transmission coefficient T(E) for gate bias Vg= -3.0 V is large compared to all other $V_g$. This is due to the presence of large platform of highest occupied molecular orbital (HOMO) near the Fermi level $E_F$, is the main transmission channel in this device. The HOMO transmission peaks are getting shifted greater towards Fermi level when applied positive $V_g$'s than negative ones. For this reason, the magnitude of currents under positive $V_g$'s will be less than negative ones. Thus we show that the electronic transport properties of molecular devices can be effectively modulated by the external transverse gate electrodes, it makes a possibility of establishing FETs based on molecular devices.

## Conclusion

Using the extended Huckle theory (EHT) combined with a non-equilibrium Green's function (NEGF) approach, the electron transport properties of the non- gated and gated molecular junctions containing single Thiophenedithiol (S-Tp-S) molecule have been investigated. The theoretical results indicate that the transverse gate plays a crucial role in determining the overall conductivity of the gated molecular junctions. We find that, positive or negative $V_g$ will, respectively, raise or lower the Transmission Coefficients T(E) relative to the Fermi level ($E_F$). Results suggest that, negative gate voltages raise the conductance and positive ones lower the conductance. Finally, we show that depending on the applied transverse gate bias $V_g$, the magnitude of current $I_{sd}$ varies over more than three times under the same $V_{sd}$ bias range. This result gives us a right direction for designing single molecular FETs.

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