



Research paper

Displacement Effects on the Electrical Characteristics of a Single-Molecule Device

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Abstract

Background and Objectives: The displacement of molecules is one of the major fabrication faults in manufacturing molecular electronic devices. In this paper, we profoundly study the effect of displacement on the current-voltage, and conductance-voltage characteristics of the Au-Benzenedithiol-Au single-molecule device.

Methods: The *ab-initio* calculations on the isolated molecules were performed to obtain the basic single-level quantum-dot model parameters. These parameters were then used within the self-consistent field algorithm to calculate the electrical characteristics of the device.

Results: The maximum conductance occurs when the molecule is placed exactly in the midpoint of the distance between the two electrodes, where the electrostatic capacitance reaches its minimum. When the molecule deviates from this point, and approaches one electrode, the conductance is decreased, and asymmetric behavior emerges. A molecular rectifier can be manufactured by placing the molecule close to one electrode.

Conclusion: Although modern software packages may employ advanced and complicated models including the combination of the density functional theory (DFT) and non-equilibrium Green's function (NEGF) methods to obtain accurate results, they are demanding in computer memory and time. Moreover, understanding the physical quantities of the systems from large-scale matrices is often difficult. The single-level model is a computationally light method, which provides a profound understanding of the device characteristics since all quantities are presented by numbers.

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Introduction

Molecules, due to their advantages such as small size, chemical tunability, and self-assembly properties, are considered the main components of future electronic devices and systems [1]. The first molecular electronic device was proposed by Aviram and Ratner in 1974. During their theoretical calculations, they predicted that an organic molecule can act like a diode when attached to the electrodes. The proposed rectifier structure was similar to a P-N junction and consisted of electron donor and acceptor parts that were separated from each other

by a tunneling bridge [2]. But the main challenge was measuring the current and conductivity of individual molecules or a small group of them. This challenge was first overcome in 1997 by an experimental group at Yale University, led by Mark Reed. By using the mechanically controllable break junction (MCBJ) method, they succeeded in measuring the current in single molecules [3]. After this pioneering experiment, the measurement of molecular conformation, current and conductivity in molecular devices continued by many experimental research groups around the world [4]-[17]. Therefore, by

using various experimental procedures, including the spectroscopic, thermoelectricity, and break-junction methods, the researchers succeeded in fabricating single-molecule devices, and as a result investigated the effect of various factors such as the types of molecule-electrode contact (bonding and anti-bonding), the length of the molecular bonds, different molecular functional groups and environmental factors (solvent and temperature) that affect their conductivity [7]-[13]. In recent years, many researchers have measured charge transfer in single organic molecules or a small group of them [9]-[13]. In addition, theoretical models at the semi-empirical and quantum chemical levels were utilized to understand the conductivity in such molecules. These models include the non-equilibrium Green's function (NEGF) multi-level models, tight-binding (TB) model, density functional theory model (DFT), local density approximation (LDA) and first-principles approaches [18]-[32]. Conductance of molecular devices is a challenging concept in which not only the chemical nature of the molecule plays a role, but also external factors such as the geometry of the metal-molecule chemical bonds and the electrostatics of the environment are important [8]-[10]. Therefore, although the results of calculations and models generally determine the current-voltage behavior of the device, the values obtained from the *ab initio* methods are usually several tens of times higher than the measurements and practical observations [3], [21]. One reason is that the exact geometry of the electrodes made in practice is unknown. Additionally, modeling of the molecule-electrode interface is challenging. In the last few decades, the molecular structure of benzene has been considered a small molecule in electronics. Benzene, with the molecular formula C_6H_6 , is a planar molecule with a regular hexagonal structure in which each C-C-C bond angle is 120 degrees. Since each carbon atom is bonded to three other atoms, the orbitals are SP^2 type, and each carbon has an orbital perpendicular to the hexagonal plane; So, each orbital overlap with two neighboring orbitals to the same extent. Therefore, all six electrons are completely delocalized in the ring path, resulting in two donut-like electron clouds, one at the top and one at the bottom of the ring. This molecule can establish strong chemical bonds with the surface of gold electrodes by two thiol end groups [6]. In the manufacturing process of molecular devices, there is a possibility of deposition of a molecule in an inappropriate position between the electrodes. This paper aims to investigate the effect of the displacement of the molecule between two electrodes on the conductance of Au-1,4-benzenedithiol (BDT)-Au two-terminal device. Fig. 1 shows the BDT molecule between two gold electrodes. Changing the distance of the molecule to the source or drain changes its coupling to the electrodes (Fig. 2). Therefore, it is expected that the current and current-voltage characteristics of the device will be affected.

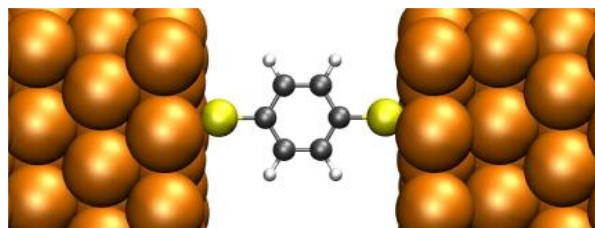


Fig. 1: BDT molecule between the source and drain electrodes.

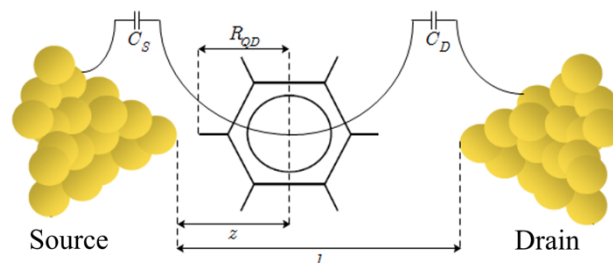


Fig. 2: Structure of the Au-BDT-Au molecular device. The source and drain contacts are modeled as the two plates of two planar capacitors.

In this research, we model the BDT molecule with a single-level quantum dot and investigate its displacement effect on the conductance of the Au-BDT-Au molecular device. Parameters in multi-level models are in the form of matrices, while they are in the form of numbers in single-level models. The single-level model is less complicated and accurate compared to other multi-level models, but because its parameters are numerical, it provides a better understanding of the physical behavior of the device in general. This paper is organized as follows. In the models and methods section, we briefly describe the single-level theoretical model, and in the discussion section, we analyze the effect of changing the position of the molecule on the device conductance, electrostatic capacitance, and molecule potential. Subsequently, we conclude in the last section.

Models and Methods

Although several mathematical and physical models and methods have been proposed for studying molecular devices, the results obtained using these models are often deviates from the measurements and experimental observations. Fig. 3 compares the practically measured current-voltage and conductance characteristics of the Au-BDT-Au device with the theoretical calculation results obtained from the multi-level DFT and NEGF model. This figure depicts that there is an impressive difference between theoretical and practical current values. To describe the electron transfer, we use the quantum dot (QD) model, which includes only one energy level. This is the simplest model to describe charge transfer in molecular devices, which includes the discrete nature of the energy spectrum of the molecule and ignores the effects related to the electrode-molecule contacts. In this model, the broadening of an energy level is approximated by the Lorentzian function as [20]:

$$g(\mathcal{E}) = \frac{2}{\pi} \frac{(\Gamma_S + \Gamma_D)/2}{(\mathcal{E} - \mathcal{E}_0)^2 + ((\Gamma_S + \Gamma_D)/2)^2} \quad (1)$$

where, Γ_S and Γ_D are the coupling energies of the source and drain electrodes to the molecule, respectively. The coupling energies are inversely related to the electron transfer rate, $\tau = \Gamma/\hbar$. In this paper we consider the coupling energies as follows:

$$\Gamma_S(z) = \Gamma_m \exp\left(-\frac{z - R_{QD}}{l/4}\right) \quad (2)$$

$$\Gamma_S(z) = \Gamma_m \exp\left(\frac{l - z - R_{QD}}{l/4}\right) \quad (3)$$

where, Γ_m denotes the maximum coupling energy, R_{QD} is the radius of the molecule, and z and l are the distance of the molecule from the source electrode, and the source-drain distance, respectively. The energy of the highest occupied molecular orbital (HOMO) of the molecule, \mathcal{E}_0 , the energy of the lowest unoccupied molecular orbital, \mathcal{E}_1 , and R_{QD} , and l have been calculated using the DFT at the B3LYP level of theory with 6-31G* basis set. These calculations for the isolated BDT molecule have been performed using the Gaussian-09 software. The electrochemical potential of the gold electrodes is $\mu = -5\text{eV}$ and the maximum coupling energy is $\Gamma_m = 0.1\text{eV}$.

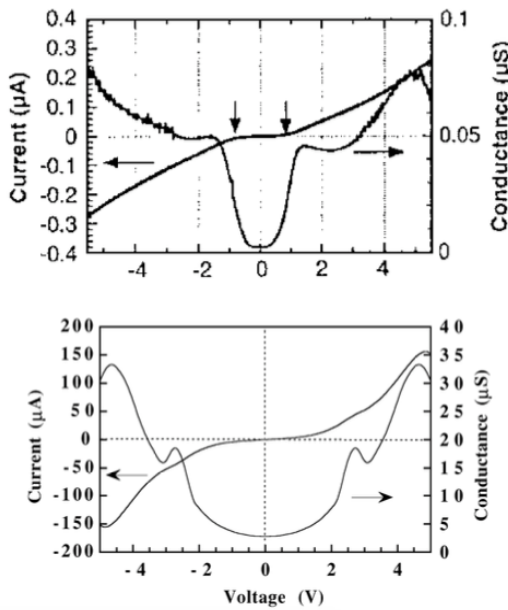


Fig. 3: The top figure depicts the measurement results [3], and the bottom figure shows the theoretical calculations [26] of the current-voltage and conductance of Au-BDT-Au device.

Table 1 lists the model parameters. According to the calculations, the electrochemical potential energy of the gold electrode is closer to the HOMO than to the LUMO, so it is expected that electron transfer will take place through the HOMO level.

Table 1: Model parameters used in this paper.

$\mathcal{E}_0(\text{eV})$	$\mathcal{E}_1(\text{eV})$	$l(\text{nm})$	$R_{QD}(\text{nm})$	$\mu(\text{eV})$	$\Gamma_m(\text{eV})$
-5.64	-0.36	5	1.5	-5	0.1

Moreover, in previous studies, it has been reported that the transfer in the Au-BDT-Au structure takes place through the frontier HOMO orbital [17]. Thus, it is reasonable to use one-level quantum-dot model.

After connecting the electrodes to the molecule, the Fermi energy level of the molecule is shifted by three mechanisms. The first mechanism is the state filling effect. Since initially the electrochemical potential of the electrodes is not equal to the Fermi energy of the molecule, some electric charge is transferred between the electrode and the molecule to equalize the Fermi energy level of the molecule to the electrochemical potential of the electrodes. Charge transfer in this case leads to the state filling effect. The second mechanism is the charging effect. Since the electron has an electric charge, the potential energy of the molecule changes due to electron transport. The third mechanism is the electrostatic effect of electrodes. Due to the fact that the molecule is located between two electrodes connected to the power source, the electric field created by the electrodes changes the energy level of the molecule. Therefore, the total change, U , in the energy level of the molecule includes the change due to charging effect, U_C , and the change caused by electrostatic effect, U_{ES} , which is $U = U_C + U_{ES}$. These energies can be approximated using the planar capacitor model. Considering the surface of gold electrodes and the molecule as parallel plates of a planar capacitor, the electrostatic capacitance is $C_{ES} = C_S + C_D$, as shown in Fig. 2. The charging energy of the molecule is given as [17]:

$$U_C = \frac{q^2}{C_{ES}} (N - N_0), \quad (4)$$

where, q is the elementary charge, N_0 denotes the number of electrons in the molecule before charge transfer, and N is the number of electrons after charge transfer, which can be calculated from the following equations.

$$N_0 = \int_{-\infty}^{+\infty} g(\mathcal{E}) f_m(\mathcal{E}) d\mathcal{E} \quad (5)$$

$$N = \int_{-\infty}^{+\infty} \frac{\Gamma_S f_S(\mathcal{E}, \mu_S) + \Gamma_D f_D(\mathcal{E}, \mu_D)}{\Gamma_S + \Gamma_D} g(\mathcal{E} - U) d\mathcal{E} \quad (6)$$

In (5) and (6), f_m , f_S and f_D are the Fermi-Dirac electron distribution functions of the molecule, source and drain electrodes, respectively. The current of the device is described by the self-consistent field (SCF) approach as follows [20],

$$I = \frac{q}{\hbar} \int_{-\infty}^{+\infty} g(\mathcal{E} - U) \frac{\Gamma_S \Gamma_D}{\Gamma_S + \Gamma_D} (f_S(\mathcal{E}, \mu_S) - f_D(\mathcal{E}, \mu_D)) d\mathcal{E} \quad (7)$$

The applied voltage, V_{DS} , changes the electrochemical potential energy levels of the source and drain electrodes as, $-qV_{DS} = \mu_D - \mu_S$.

The Fermi level of the molecule changes when the molecule moves between the source and the drain since the source and drain capacitors are changed. Thus, using the simple capacitor voltage divider circuit, the distant

dependent Fermi energy of the molecule is,

$$E_F(z) = -\frac{z}{l}(\mu_D - \mu_S) + \mu_S \quad (8)$$

The SCF algorithm, which provides the solution to the above equations is shown in Fig. 4.

SCF-Algorithm
Input V_{DS} , initial guess for U_{old}
loop: calculate N based on (6)
calculate U_{new} based on (4)
if $ U_{new} - U_{old} < \alpha$ then go to current
else
$U_{new} = U_{old} + \beta(U_{new} - U_{old})$
go to loop
current: calculate current using (7)
end

Fig. 4: The self-consistent field (SCF) algorithm for current calculation.

Results and Discussions

Considering the effects of the geometry of the metal-molecule chemical bonds and the electrostatic potential energy of the molecule, we investigate the effect of moving the BDT between the two electrodes on the three physical quantities; namely, the electrostatic capacitance, the potential energy of the molecule, and the device conductance.

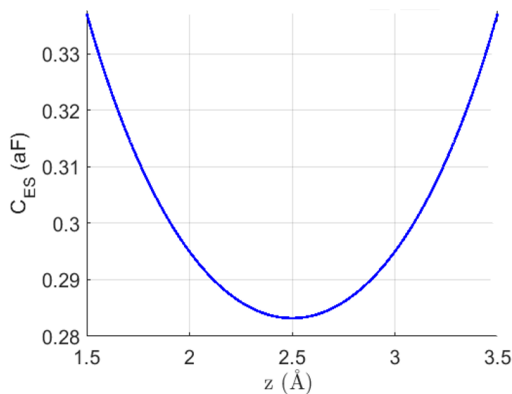


Fig. 5: The electrostatic capacitance vs. the distance of molecule from the source electrode, z .

A. The Potential Energy of the Molecule

Fig. 6 shows the change in the electrostatic potential of the molecule based on the change in the charging energy described by (4). when its distance from the source electrode changes from 1.5 Å to 3.5 Å. The results show that the electrostatic potential is not equal for the corresponding positive and negative voltages, when $z \neq l/2$. In the $R_{QD} < z < l/2$ range, the electrostatic potential in positive applied voltages has a greater value than in negative voltages. Because when the molecule is closer to the source, using (2) and (3) result in $\Gamma_S \gg \Gamma_D$. Consequently, for positive voltages, the charge transferred from the source to the molecule is greater than the charge transferred from the molecule to the drain per unit time, which ultimately causes the molecule to lose a small amount of charge. But in negative voltages, the charge transferred from the drain to the molecule is

less than the charge transferred from the molecule to the source per unit of time, and thus, the molecule loses a large amount of charge.

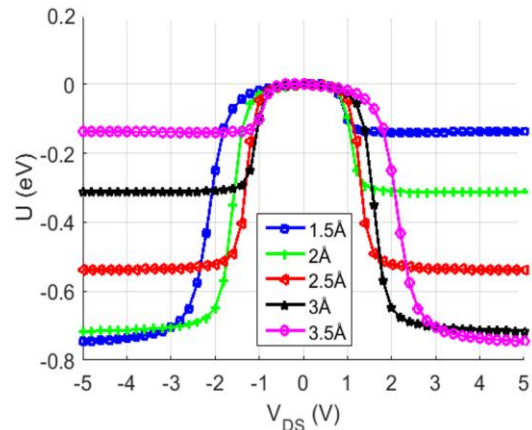


Fig. 6: The potential energy of the molecule vs. the distance of the molecule from the source electrode, z .

Based on the results depicted in Fig. 5 and using (8), it can be deduced that the electron transfer process in $V_{DS} > 0$ takes place in lower applied voltages. In the range $l/2 < z < l$ since $\Gamma_S \gg \Gamma_D$, the molecule loses more charge in $V_{DS} > 0$ than in $V_{DS} < 0$, and this process takes place in less negative voltages. Placing the molecule at $z = l/2$ results in $\Gamma_S = \Gamma_D$, and as a consequence, the amount of charge transferred from the molecule to the electrodes is equal in positive and negative voltages. The asymmetry properties suggest that by placing the molecule near one electrode, a molecular diode can be manufactured.

B. The Device Conductance

Fig. 7 and Fig. 8 depict the current-voltage and conductance-voltage characteristics of the Au-BDT-Au molecular device, when the distance of the molecule from the source electrode changes from 1.5 Å to 3 Å. It can be seen that when $z \neq l/2$, the electrical characteristics of the device are asymmetric and the asymmetry increases when the molecule deviates more from the middle point of the electrodes. As the molecule approaches the source, $R_{QD} < z < l/2$, the conductance is greater in the $V_{DS} > 0$ region than in $V_{DS} < 0$ region. Because, in $V_{DS} > 0$ region, the HOMO drops in the bias window in lower voltages and the conduction begins. The conduction starts when μ_D reaches the HOMO level at positive voltages, and when μ_S reaches the HOMO level at negative voltages. Fig. 8 shows that, in $R_{QD} < z < l/2$, the conductance peak is larger for $V_{DS} > 0$ than for $V_{DS} < 0$. Because, when the molecule moves in this region, $\Gamma_S \gg \Gamma_D$, and as a result, the electron transfer rate from the source to the molecule is higher than the electron transfer rate from the drain to the molecule, for $V_{DS} > 0$. Therefore, at positive voltages, the current reaches its maximum value with a greater slope. Instead, in the $l < z < l/2$ region, the conductance is higher at $V_{DS} > 0$ than at $V_{DS} < 0$. At $z = l/2$, the current-voltage (Fig. 7) and

the conductance-voltage (Fig. 8) characteristics are completely symmetric. The current-voltage and the conductance-voltage characteristics show that the maximum conductance occurs at $z = 1/2$, and it is decreased when the molecule approaches the source or the drain electrode. Fig. 7 depicts the turn-on voltage is $V_{on} \approx 1V$ at $z = 1/2$, which agrees with the measurement results [3] and first-principles calculations. Moreover, the conductance gap depicted in Fig. 8 is $V_{gap} \approx 2eV$, which is in agreement with the previous studies [3], [26].

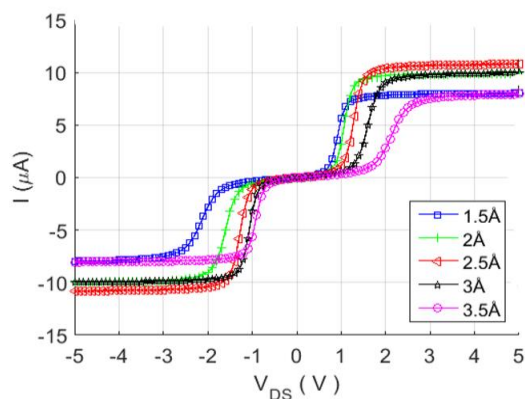


Fig. 7: The current-voltage characteristic of the device vs. the distance of the molecule from the source electrode, z .

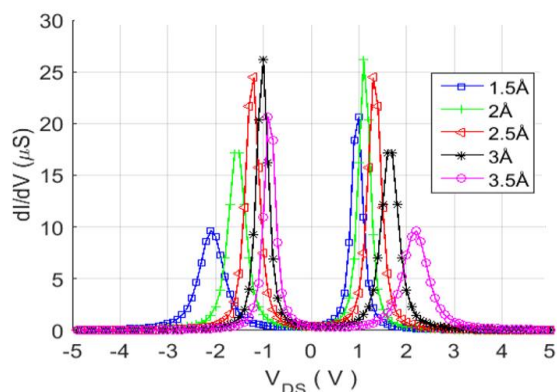


Fig. 8: The conductance-voltage characteristic of the device vs. the distance of the molecule from the source electrode, z .

Conclusions

In this paper, within the framework of the single-level quantum dot model, we have shown that the conductance of the Au-BDT-Au molecular device is maximized when it is placed at the midpoint of the distance between the source and the drain electrodes, where the electrostatic capacitance reaches its minimum. When the molecule approaches one electrode, the capacitance is increased, while the conductance is decreased. Moreover, the charge transferred through the HOMO is unequal in corresponding positive and negative voltages. In the symmetric distances from $z = 1/2$, the charge transfer is equal for corresponding negative and positive applied voltages. The turn-on voltage, $V_{on} \approx 1V$ and the conductance gap, $V_{gap} \approx 2eV$ are in agreement with other theoretical studies [26] and practical

measurements [3]. The results also indicate that displacing the molecule leads to rectification characteristics, which finds application in the manufacturing process of molecular diodes.

Author Contributions

The quantum chemical calculations have been done by E. Rahimi. Except that, all authors have contributed equally to developing the code, developing discussions, presenting the results and writing the article.

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Conflict of Interest

The authors declare no potential conflict of interest regarding the publication of this work. In addition, the ethical issues including plagiarism, informed consent, misconduct, data fabrication and, or falsification, double publication and, or submission, and redundancy have been completely witnessed by the authors.

Abbreviations

<i>DFT</i>	Density Functional Theory
<i>NEGF</i>	Non-Equilibrium Green's Function
<i>MCBJ</i>	Mechanically Controllable Break Junction
<i>BDT</i>	Benzenedithiol
<i>HOMO</i>	Highest Occupied Molecular Orbital
<i>LUMO</i>	Lowest Unoccupied Molecular Orbital
<i>SCF</i>	Self-Consistent Field
<i>TB</i>	Tight-Binding
<i>LDA</i>	Local Density Approximation
<i>QD</i>	Quantum Dot

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