

Journal of Nano Simulation

journal homepage: jons.du.ac.ir



Volume 1, Issue 1, Winter 2025, 16-21 DOI: 10.22128/jons.2025.969.1002

Electronic transport behavior of 4,5-bis(2,5-dimethylthiophen-3-yl)furan-2-amine (a Diarylethene) as optical molecular switch: A first-principles approach

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HIGHLIGHTS

G R A P H I C A L A B S T R A C T

- Transport properties of title compound molecular switch isomers are studied.
- DFT combined nonequilibrium Green's function (NEGF) technique is used in this study.
- Three different adsorption types including bridge, hollow, and top were investigated
- The effect of changing the electrode material on the conductivity was investigated.
- Title compound has been proposed as a potential molecular electronic device.



ARTICLE INFO

Article history: Received: 2025-03-03 Received in revised form: 2025-04-17 Accepted: 2025-05-24

Available online: 2025-06-23

Keywords: Switching behavior, Density functional theory, Diarylethene, Electronic transport, DFT-NEGF.

ABSTRACT

In this study, we studied the electronic transport properties of 4,5-bis(2,5-dimethylthiophen-3-yl)furan-2-amine (a Diarylethene) by nonequilibrium green's function (NEGF) joint with density functional theory (DFT). This molecule can be converted from closed-form to open form by ultraviolet irradiation or visible light. We have studied several parameters such as I–V characteristics, electronic transmission coefficients T(E), the effect of electrode materials (Au, Ag, and Pt) on electronic transport properties, on-off ratio and spatial distribution of molecular projected self-consistent Hamiltonian (MPSH) orbitals corresponding to the closed and open forms. The physical origin of switching behavior is interpreted based on the different molecular geometries, location and size of the frontier molecular orbitals and the HOMO–LUMO gap. The results showed that as the molecule changes from closed form to open form (closed \rightarrow open), conductivity changes from *on* state (high conductivity) to *off* state (low conductivity). We investigated the effect of different electrodes (Ag, Au, Pt) and various connection sites (hollow, top, bridge) on conductivity.

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1. Introduction

Over the last decade, the fast and growing development of electronic components technology, reduction in weight, volume, and the cost of production led to the manufacture of high-speed components in nanoscale. Nowadays, since the basis of electronic integrated circuits is based on complementary metal oxide semiconductor technology (CMOS) with a scale of several tens of nanometers, major problems occur, such as increased leakage current and increased heat in the components that affect their performance. Therefore, much attention has been drawn to other alternative technologies such as molecular electronics that can perform better and more successfully [1-4].

In general, molecular electronics can be considered as a molecule or a set of molecules that are located in an electronic component such as wire, switch, memory, etc. Many new physical attributes, for example negative differential resistance (NDR),[5] memory effects [6], switching properties [7-11], etc., are originate in different structures, containing organic compounds [12], carbon nanotubes [13], and DNA [14]. In this regard, the expansion of theoretical effort has contributed significantly to the basic understanding of molecular systems. Between these devices, the molecular switch attracts a lot of attention, because it plays a necessary part in the design of logic circuits and high-density optical memory [15-19].

Among the various types of nanoscale electronic devices, the most attention is paid to molecular switches because of their ease of addressability, rapid reply time, and appropriateness for dense phases and they have been studied by the methods of the first principles[20]. Molecular switches are flat in the *on* state and have a maximum overlap *of* the π -orbitals.

Molecules used as switches in molecular electronics must meet certain conditions. These molecules must have two different forms that are deformed by an external stimulus such as light, voltage, or pH. This deformation must be reversible.

4,5-bis(2,5-dimethylthiophen-3-yl)furan-2-amine optical molecular switch, which changes between open and closed forms under the excitation of light radiation (Figure 1) can be a good option for a molecular switch device, is one family member of diarylethenes [21]. Also, the investigation outcome of an experimental study of electron transfer in a diarylethene attached to Au atoms show that these compounds can be used as molecular switches[22].





Hence, in this work, we investigate the properties of electron transfer in a Diarylethene and its 3 derivatives in R position with two forms (open and closed), three kinds of adsorption and electrodes.

2. Model and computational methods

First, we optimized the geometry of two forms with one SH group as the linker by Gaussian 09 software [23] with B3LYP/6-311++g(d,p) basis set[24]. In this level ther is a good agreement between theoretical and with experimental values. Experimental outcomes have shown that the hydrogen atoms can poorly absorbed to the metal surface [25-26]. So we substituted sulfur atom for linkage hydrogen atom. In the next step, we placed the molecule between two parallel surfaces of the electrode with the most popular Y (1 1 1) surface [27-28] and with (6×6) periodic boundary conditions (see Figure 2) [29-30].



Figure 2 Schematic molecular junctions used in our calculations.

Au–S distances are set to 2.42, 1.9, 2.07 Å for the bridge, hollow, and top sites, respectively [26,31]. The Pt–S, and Ag–S distances are set to 2.41, and 2.46 Å for the hollow sites, respectively [32,33].

Due to the lack of computational resources, only the geometry of the atoms in the scattering region is optimized within a force convergence criterion of 0.02 eV/Å. Since the switching unit (convert closed form to open form) has distance from the electrode, the effect of structure optimization under bias is negligible [11,34-36].

The transport calculations from 0.0 to 3.0 V at 300 K were done using the Landauer–Büttiker formula in the TranSIESTA package [37].

$$I = \frac{2e}{h} \int T(E, V) [f(E - \mu_L) - f(E - \mu_R)] dE$$
(1)

The Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional is adopted for the generalized gradient approximation (GGA)[38]. We use a ξ plus single polarization (SZP) and double- ξ plus single polarization (DZP) basis sets for the electrons of electrode atoms and the organic atoms in the transport calculations, respectively. A k-grid sampling of 4×4×100 is used, together with a mesh cutoff energy of 150 Ry.

3. Results and discussion

The optimized structures of the 2-amino-4,5-bis(2,5-dimethylthiophen-3-yl) furan-3-carbonitrile in both forms are displayed in the Figure 3, and some selected geometric parameters (Å, 0) are listed in table 1.



		1		/	
Parameters ^a	closed	open	Parameters ^a	closed	open
Bond lengths (Å)					
C1-C2	1.448	1.366	C14-S18	1.777	1.750
C2-C3	1.345	1.455	C4-S18	1.880	1.747
C3-C4	1.541	1.377	C6-C20	1.433	1.479
C4-C5	1.548		C20-C21	1.355	1.361
C5-C6	1.543	1.375	C21-S23	1.777	1.749
C3-C13	1.435	1.471	C5-S23	1.877	1.747
C13-C14	1.354	1.361	C21-C24	1.494	1.498
C14-C15	1.494	1.498	C4-C27	1.547	1.497
			C5-C31	1.547	1.498
Bond angles (°)					
A(1,2,3)	125.3	136.4	A(3,4,27)	108.1	129.7
A(2,3,4)	115.3	125.3	A(4,5,6)	109.7	
A(2,3,13)	131.8	122.0	A(4,5,31)	113.5	
A(3,4,5)	109.7		A(4,5,23)	114.0	
A(3,4,18)	103.1	110.2	A(1,6,5)	117.2	125.0
A(3,13,14)	115.0	114.3	A(1,6,20)	130.5	122.4
A(13,14,15)	127.4	128.7	A(6,20,21)	115.1	114.4
A(13,14,18)	113.9	109.9	A(5,23,21)	91.5	92.8
Dihedral angles (°)					
D(1,2,3,4)	7.1	42.2	D(2,1,6,5)	9.0	49.3
D(1,2,3,13)	-175.4	-138.6	D(2,1,6,20)	-174.2	-132.6
D(2,3,4,18)	-161.5	-179.6	D(1,6,5,23)	-163.0	179.2
D(2,3,13,14)	167.9	179.8	D(1,6,20,21)	169.3	-179.3
D(3,13,14,15)	-179.0	-179.4	D(6,20,21,24)	-179.0	180.0
D(13,3,4,27)	-92.8	-177.5	D(20,6,5,31)	-94.0	-178.1
	2				

^a For atom numbering from Figure 3.

One of the effective factors in creating different behavior (switching behavior) is the change in the effective conjugation size of these two forms. As shown in Table 1, that the dihedral angles D(1,2,3,13) and D(2,1,6,20) are 138.6^o, 132.4^o and for 175.4^o, 174.2^o open and closed forms, respectively. The mentioned dihedral angles in the closed form are larger and closer to 180^o, which increases the π -electron conjugation and the π -overlapping[38].

is possible to be conjugated (conjugated form), while in the open form, conjugation is limited to the thiophene rings (cross-conjugated form). The voltage-current characteristics for both forms Au electrode in three mentioned adsorption sites are shown in Figure 4. Given the significant difference in conductivity between the two forms, conductivity for the open and closed form is plotted in two separate graphs.



Figure 3 Optimized geometry by B3LYP/6-311++G(d,p) for closed and open forms.

In the molecular devices with growing the efficient conjugation extent, the electric transport improved[39]. The photochromism of the title compound (a Diarylethene) occurs with a reversible photochemical breaking of the C4–C5 bond. The arrangement of the double bonds in the closed-form is such that it



Figure 4 The current-voltage (I–V) characteristics of the molecular switch in different site on Au (111) electrode: (a) closed form and (b) open form.

From this figure, it can be concluded that the current in the closed form is larger. For sample, the computed current in the hollow site at 1.8 V is at 6 μ A and 8939 μ A for the open and closed forms, respectively. The results showed that by changing the molecule (closed \rightarrow open), the conductivity changes from *on* state to *off* state. Figure 4 shows that maximum conductivity occurs in closed form with the hollow site. In all the three sites, with the growing of voltage, can be seen sharp changes in the range of 1.2 – 2.0 volts. According to this figure, the current-voltage curve of the bridge site is like to that in the hollow site.

We used the current ratio, *I*_{closed form}/*I*_{open form}, to check the current variations as a result of the isomer conversion (see Figure 5). It can be seen from Figure 5 that the switch behavior is clearly dependent on the adsorption types. As can be seen in Figure 5, the maximum current ratio (best switching efficiency) is about 3259.7 at 0.4 V in the hollow site. The lowest changes in the current ratio are observed in the bridge connection type.



Figure 5 The calculated current ratio of the molecular wires adsorbed at different sites on Au (111) electrodes.

According to this figure, the conductivity enhancement in the closed form is approximately 915–3260 times greater than that of the open form. This figure also shows that the most changes in the current ratio are in the hollow type. These ratios are smaller for the other two types (bridge and top) of connections and the least changes in the conductivity ratio are seen in bridge connection. The HOMO–LUMO gaps of the connection sites (hollow, top, bridge) for Au electrode increase in the order of hollow > top > bridge.

This difference of the HOMO–LUMO gaps can be interpreted by the levels of conjugation of connection sites. In addition, the eigenvalues of LUMO are much closer to Fermi level, than HOMO values are for all connectiones. This indicates that the LUMO plays an important role in facilitating tunneling in junctions based on all of the three connectiones, and in these systems currents through are driven by hole transport.

The previous studies have shown that the hollow site is the most popular based on energy [31,40,41] and considering that it has shown the best switch performance in this study, so we selected the hollow site to continue the study.

The difference in conductivity for these two forms can be justified on the basis of the transmission spectra (see Landauer-Bütiker formalism)[42]. The transmission spectra at zero-bias on Au (111) electrode with hollow site displayed considerable discrepancy between the open and the closed forms (see Figure 6). From Equation 1 it can be concluded that only electrons whose energy is near to the E_F play a necessary task in the current. Figure 6 showed that the transmission spectrum of the open form is smaller than closed the form.



Figure 6 The transmission spectra of the molecular switches at zero bias on Au (111) electrode with hollow site.

This system, the Fermi level E_F of the Au electrode aligns between HOMO and LUMO, therefore, the barrier for the electron transport is intensively relevant to the HOMO–LUMO gap. Figure 6 showed that the transmission bands of the title compound optical molecular switche in the closed form were closer than the open form respect the zero bias. Therefore, the HOMO–LUMO gap of the closed form is smaller than that of the open form. Also, when the system is in the open form, the value of the transmission coefficient is small than that of closed form in the energy region of [-2.0,2.0 eV]. As a result, the lack of significant peak in the region of [-2.0,2.0 eV] and the larger HOMO–LUMO gap due to the molecular structure changes accounts for the low conductivity in the open form.

In closed form the Fermi energy lies nearest the LUMO (there is a better interaction between LUMO molecular orbital and the atomic orbitals on the Au atoms), so the onset of current is due to electron transmission through the LUMO.

A clear understanding of this difference can be found in the spatial repartition of the molecular projected self-consistent Hamiltonian (MPSH) [43] As the distance between HOMO-LUMO increases and decreases, the electron transport augments and weakens, respectively. These orbitals for the closed form is nearer to the E_F compared to the open form, these values for open and closed form are -1.1615 eV, 0.8435 eV and -0.9169 eV, 0.9825 eV, respectively.

Figure 7 (the spatial distribution of the MPSH states) shows that HOMO and LUMO orbitals in the closed form are delocalized, have a large weight, and offer an additional comfortable way for electron transportation, while these orbitals in the open form are localized and have a little weight. It can be concluded that the smaller HOMO–LUMO gap and the bigger T(E) cause augment the conductivity of closed form.

Also, the electrode material can affect electron transfer in molecular devices. The calculated I–V characteristics of the molecular switch with three kinds of the electrode (Pt, Au, and Ag) are displayed in Figures 4 and 8.

From these graphs, it can be concluded that in this electron device with the change of electrode materials the current changed for both forms. It should be noted that at all three electrodes the current in the closed form is constantly less than the open form. The difference in current for the closed form is seen in voltages higher than 1.4 volt. For the closed and open forms the highest and lowest current were seen in Au and Pt electrodes, respectively.



Figure 7 The composition of molecular (MPSH) orbitals including the molecule–electrode interaction for (a) closed and (b) open forms at zero bias on Au (111) electrodes with hollow site.



Figure 8 The calculated I–V characteristics of the molecular switch on Ag and Pt electrode with hollow site: (a) closed and (b) open forms, (c) current switching ratio as a function of applied bias with different electrodes.

The calculated current ratio of the molecular switch at the Hollow site with three kinds of the electrode is shown in Figure 8c. It can be seen that the best performance of switch behavior is related to Au electrode.

3. Conclusion

The electronic transport properties of 4,5-bis(2,5-dimethylthiophen-3yl)furan-2-amine (a Diarylethene) have been studied. From the different molecular geometries, orbital localization and HOMO–LUMO gaps, I–V characteristics, *on-off* ratio, T(E), it can be concluded that there is a significant difference in the conductivity of these two (open and closed) forms, and this molecule can be used as a molecular switch. Also, the electron transport greatly changes with the change of electrode constituents (Pt, Au, and Ag) and varieties of adsorption (top, hollow, and bridge). The highest switching efficiency happened in the Au electrode with hollow site.

Acknowledgements

Authors are grateful to the Damghan University for financial support.

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