Quantum study of symmetrical/asymmetrical charge and energy transfer in a simple candidate molecular switch

Reza Safari1 · Hamid Hadi1,2 · Hamid Reza Shamlouei2

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Abstract
In this study, external electric field effect on some electronic/vibrational properties and molecular current–voltage characteristic curve (I-V curve) of a candidate field-effect molecular switch (for both isolated, M, and non-isolated, Au-M-Au, states) are studied, using quantum theory of atoms in the molecules (QTAIM) and Landau’s theory (LT). Analysis of these results shows that when the electric field intensity increases to 0.008 au, the switching mechanism (OFF/ON) occurs in this field-effect molecular switch. Moreover, the intra-molecular symmetrical/asymmetrical phenomenological coefficients (L_{sym} and L_{asym}) of this molecular switch are calculated, using the linear force-flux law (and Onsager phenomenological approach) and QTAIM. Analysis of these results shows that the sign and value of the L_{sym} and L_{asym} coefficients correspond to energy transfer (dissipation) schemes between different intra-molecular sections, induced by external electric field. These calculated phenomenological coefficients can (may) be used to predict and evaluate (manage) energy/heat fluxes in intra-molecular sections. Also, based on the results obtained in this study, it is predicted that this candidate field-effect molecular switch has acceptable performance in nanoelectronic circuits.

Keywords Molecular nanoelectronics · Molecular switch · Atoms in molecule theory (AIM) · Landau’s theory · Symmetrical/asymmetrical charge/energy transfer coefficients

Introduction
With the advent of nanotechnology, the process of downsizing electronic circuits/devices is advancing. In this regard, molecular electronic knowledge is of particular importance [1–13]. Usually, atomic scale study of molecular nanoelectronic systems requires the use of quantum mechanical knowledge [14–17]. For example, based on the quantum mechanical knowledge, the electronic/vibrational properties of the molecular nanoelectronic devices can be investigated [18–21]. Among molecular devices, field-effect molecular switches are of particular importance [22–28] because, by applying the external field, the switching mechanism (ON/OFF) in them can be managed and controlled. Thus, in this work, the external electric field effects on performance of a candidate field-effect molecular switch, Fig. 1 (in isolated, M, and non-isolated Au-M-Au states), are studied. In this regard, the electric current–voltage diagram (I-V characteristic curve) and the symmetrical/asymmetrical intra-molecular phenomenological coefficients of both isolated (M) and non-isolated (Au-M-Au) molecular switches are calculated, using Landau’s theory and quantum theory of atoms in molecules (QTAIM) [29–35].

Based on the QTAIM, the atomic kinetic energy (K), potential energy (V), and total electron energy (E), of a single nanoelectronic molecular system, are given by [36–40]:

$$K = \sum_{\Omega}^{N_{0}} K(\Omega)$$

$$V = \sum_{\Omega}^{N_{0}} V(\Omega); E = \sum_{\Omega}^{N_{0}} E(\Omega) = -2K$$

(1)

$$K(\Omega) = \frac{-h^{2}}{4m} \int_{\Omega} \int \left[ \psi \nabla^{2} \psi^{*} + \psi^{*} \nabla^{2} \psi \right] d\mathbf{r}$$

(2)
where $\psi$ and $\Omega$ are electronic wave function and atomic basins, respectively [41].

**Quantum computational details**

Geometry optimization and calculation of the structural and electronic/vibrational properties of the both (M) and (Au-M-Au) molecular switches have been carried out at DFT/UB3LYP/6-311G* level of theory, in the presence and absence of external electric field, using G09 program [42]. For the gold atoms of the electrodes, LANL2DZ pseudopotential is used. All QTAIM calculations are carried out using Bader’s AIM-PAC program package [43].

In addition, to predict the current–voltage characteristic curve (I-V curve) of this field-effect molecular switch, Landau’s theory (LT, Eq. (3)), is used:

$$I = \frac{2e}{h} \int T(E;V)[f(E - \mu_L) - f(E - \mu_R)]dE$$  \hspace{1cm} (3)$$

Here, $e$ is the electron charge, $h$ is Planck constant, $T(E,V)$ is the electron transfer coefficient due to the bias voltage effect ($V$), $f(E-\mu_L, E-\mu_R)$ is the Fermi-Dirac distribution function for electrochemical potential ($\mu_L, \mu_R$) for left and right electrodes [44]. Also, the temperature-independence direct-tunneling electric conduction ($G$) of a single molecule nanoelectronic system can be evaluated using Landau’s theory/formula, as:

$$G = \frac{1}{R} = \frac{2e^2\tau_e}{h}$$  \hspace{1cm} (4)$$

$$\tau = \exp(-\beta L)$$  \hspace{1cm} (5)$$

$$\beta = \left(\frac{2m^*\alpha \varphi}{\hbar^2}\right)^{\frac{1}{2}}$$  \hspace{1cm} (6)$$

where $\hbar$ is $\frac{h}{2\pi}$, $\varphi$ is the potential barrier height for tunneling through the HOMO or the LUMO level, which is equivalent to the energy difference between the Fermi energy and the molecular HOMO or LUMO level, $m^*$ is the effective mass of the electron ($m^* = 0.16m_0$, $m_0$ is the free electron mass), and $\alpha$ is the symmetry parameter in the potential profile, in this symmetric case, $\alpha = 1$ [39, 45, 46].

Also, since the $\varphi$ potential barrier plays an important role in the mechanism of electron transfer in molecular components [46], for the studied molecular switches studied in this work, three ranges were considered for the applied field intensity: 1-the low field intensity; $L_B (\varphi > 1 \text{ eV})$, 2-the threshold field intensity; $T_B (\varphi \approx 1 \text{ eV})$, and 3-the high field intensity; $H_B (\varphi < 1 \text{ eV})$ (Fig. 2).

**Results and discussion**

**I-Part one: isolated molecular switch(M)**

When an external electric field is applied on molecular switch studied in this work (Fig. 1), the atomic charge and energy are transferred between its different intra-molecular sections (or different atomic basins); these changes can be studied/analyzed using QTAIM. The external electric field effect on the frontier molecular orbitals (HOMO/LUMO), and the HLG gap ($E_{\text{HOMO}}-E_{\text{LUMO}}$), of the isolated molecular switch studied in this work (M, Fig. 1), are investigated, and sample of these results is shown in Fig. 3.

As shown in Fig. 2, the orbital spatial expansion shape and HLG gap, of the M molecular switch, are significantly dependent on the field intensity. This property indicates the observable and measurable response of the studied molecular switch to the properties of the applied field (such as field intensity direction). These electronic molecular (atomic) changes can indicate the increase of distribution (redistribution) of parallel and perpendicular charge/energy transfer

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Fig. 1 The isolated molecular switch (M) studied in this work

Fig. 2 External electric field intensity applied: low ($L_B$), threshold ($T_B$), and high ($H_B$) applied field intensity range (ON/OFF)
between different intra-molecular sections (atomic basins) in this molecule switch, induced by the applied external field.

In addition, the field effects on the molecular dipole moment tensors/vectors (as an index measuring the response to external electric field), of the molecular switch M, are investigated (Fig. 4).

Based on the results obtained here, the total electric dipole moment increases non-linearly with increasing electric field strength (Fig. 3). These significant molecular electronic changes may be related to effect of the external field on the expansion of the \( \pi \)-conjugated bond chain in this molecular switch.

In addition, analysis of the field effect results on other electronic properties (such as electron state density, DOS), and vibrational characteristics (such as vibrational frequencies, IR), of the molecular switch (M), show that these
properties/characteristics depend almost non-linearly on the electric field strength (Figs. 4 and 5).

Moreover, the external electric field effect on atomic electronic contour maps (such as topology graph of electron density ($\rho(r)$), Laplacian of electron density ($\nabla^2 \rho(r)$) and electronic kinetic energy ($K(r)$), of the molecular switch M, are studied, using quantum theory of atoms in molecules (QTAIM). Some of these QTAIM results are shown in Figs. 7, 8, 9, 10 and reported in Tables 1 and 2.

Analysis of these QTAIM results showed that the effect of the applied field on oxygen and sulfur atomic basins is greater than other atomic basins, such as hydrogen and carbon (Fig. 6).

Based on the results obtained here, the molecular switch (M) can be divided into intra-molecular acceptor/donor (n-like/p-like) sections. Consequently, it is possible to determine role of each intra-molecular sections (or atomic basins) in the intra-molecular charge/energy transfer mechanism.
I-V diagram and switching mechanism

In this study, based on Landau’s theory/formula (Eq. (4)), the molecular current–voltage characteristic curve (I-V curve) of the molecular switch (M) is calculated (Fig. 11).

As shown in Fig. 11, the current increases (almost non-linearly) with increasing the bias voltage. Hence, it is expected that at high field intensities ($80 \times 10^{-4}$ a.u.), and these molecular switch will be in the ON state.

Also, it can be predicted that the switching mechanism (and thus function of this field-effect molecular switch, M) is dependent on the molecular resonant structure and its changes, due to the application of external electric field (Fig. 12).
II-Part two: non-isolated molecular switch (E-M-E)

To investigate electrode effect on performance of the molecular switch M, this molecular switch is connected to the end gold atom electrodes (Au-M-Au, Fig. 13). Then, using DFT/QTAIM theories (at B3LYP 6-31G level of theory), and using LANLD2Z pseudopotential model, the external field effects on some electronic/vibrational properties of the Au-M-Au molecular switch are studied. In this regard, the effects of applying an external electric field on the HOMO/LUMO orbitals, I-V curve, electron density of state (DOS), and vibrational frequencies (IR) of the studied molecular switches (Au₄-M-Au₄/Au-M-Au) are investigated, in two ON/OFF states (Figs. 13, 14, 15, 16, 17, 18). Analysis of obtained all results (all not reported here for brevity) show that the presence of the gold electrode (Au-M-Au) has a significant effect on changing the electronic/vibrational properties of this molecular switch. These changes can be due to the participation of free electrons of gold metal atoms in the charge/energy transfer mechanism in the Au-M-Au molecular switch. Analysis of these results also show that with increasing field intensity (especially, fields with intensities greater than 60 × 10⁻⁴ a.u.), the electric current of the circuit increases significantly, and thus this molecular switch (Au-M-Au) is in the (ON) state (Figs. 14, 15, 16, 17, 18).

Another point which should be mentioned here is that QTAIM remains still able to partition a molecular system (into atomic basins or molecular sectional) with small violation of the virial theorem \( \left( \frac{V_{\text{elec}}}{K_{\text{elec}}} = -2 \right) \) [47]. Also, since application of the electric field displaces the electron density out of its equilibrium state and thus increases the potential energy, a directional deviation of the virial (−VT) from its
Fig. 12 Switching mechanism (ON/OFF) of the field-effect molecular switch (M)

Fig. 13 The non-isolated molecular switches (Au$_x$-M-Au$_y$/Au-M-Au) studied in this work (left) and external electric field effect on polarizability of these molecular switches (right)

Fig. 14 External field effect on current–voltage (I-V) curve of the non-isolated molecular switches studied in this work (Au$_x$-M-Au$_y$/Au-M-Au, Fig. 13) at low/L$_B$ and high/H$_B$ external bias
equilibrium value (2.00) is justified (Figs. 19). Thus, using QTAIM, the external electric field effect (with intensity $\varepsilon$) on the differential atomic kinetic energy, $\Delta K(\Omega, \varepsilon) = K(\Omega, \varepsilon) - K(\Omega, 0)$, of the gold electrode atomic basins ($\Omega$), of the non-isolated molecular switches studied in this work ($\text{Au}_4$-$\text{M}$-$\text{Au}_4$/Au-$\text{M}$-$\text{Au}$) are calculated, and sample of these results is shown in Figs. 20–21.

III-Part three: intra-molecular symmetrical/asymmetrical phenomenological coefficients

When a field-effect molecular device is placed in an external field, charge and energy can be exchanged/transfer between different atomic basins or different intra-molecular sections ($S_\Delta$) (Fig. 22).

Also, it is clear that the intra-molecular study of energy transfer/dissipation in single molecular nanoelectronic systems is of particular importance. So far, many attempts have been created to understand nanosize and molecular nanoelectronic systems’ thermal/electric (as thermoelectric) effects/phenomena [48–50]. The thermoelectric effects can cause energy transfer or dissipation in field-effect molecular systems. For example, when a current I passes through an n/p-type semiconductor device, heat is absorbed in the lower temperature junction and released at the higher temperature junction.

Similarly, thermoelectric-like effects (and their coefficients) can be defined in field-effect molecular systems with donor-like/acceptor-like sections. In this case, the local symmetrical heating (as Joule-like heating; $Q_J^\Delta$) and
Fig. 17  External electric field effect on molecular vibrational frequencies of the non-isolated molecular switch studied in this work (Au₄-M-Au₄)

Fig. 18  External electric field effect on the molecular electric dipole moment tensors/vectors and its components (in Debye), of the non-isolated molecular switches studied in this work (Au₄-M-Au₄/Au-M-Au, Fig. 13), at low (OFF) and high (ON) external bias

Fig. 19  Examination of the validity of the virial theorem for the Au₄-M-Au₄ and Au-M-Au molecular switches
the asymmetrical heating (as peltie-like heating; $Q^p$), and thus the overall heating/cooling ($Q$), of an intra-molecular thermoelectric-like device, are defined similarly as [50]:

$$\left\{ \begin{array}{l}
Q' = \frac{\alpha' + \alpha}{2} \\
Q^p = \frac{\alpha^2 - \alpha'}{2}
\end{array} \right. \Rightarrow Q = Q' + Q^p$$

(7)
Using QTAIM, the molecular switch (M) is divided into left (L; \(S_L\)) and right (R; \(S_R\)) intra-molecular sections (as n/p-like sections) (Fig. 22) which are used for the calculation of the symmetrical/asymmetrical energy transfer (dissipation) coefficients in this molecular switch. In this regard, using Onsager phenomenological approach, the general flux (such as heat, \(J_j\)) by different forces (such as external field, \(X_i\)) is given by the following:

\[
J_j = \sum_i L_{ij} \cdot X_i;
\]

here, \(L_{ij}\) is the phenomenological coefficients [51]. Thus, similar to n/p semiconductor thermoelectric systems, the intra-molecular \(L_{M_{\text{sym}}}^M\) and \(L_{M_{\text{asym}}}^M\) phenomenological coefficients, of each intra-molecular sections (\(S_L; S_R\)), can be defined as:

\[
\begin{align*}
L_{M_{\text{sym}}}^M(S_L; S_R) &\equiv \frac{L_{M_{\text{sym}}}^M(S_L; S_R) + L_{M_{\text{sym}}}^M(S_R; S_L)}{2} \\
L_{M_{\text{asym}}}^M(S_L; S_R) &\equiv \frac{L_{M_{\text{sym}}}^M(S_L; S_R) - L_{M_{\text{sym}}}^M(S_R; S_L)}{2}
\end{align*}
\]

(8)

Here, \(L_{M_{\text{sym}}}^M\) and \(L_{M_{\text{asym}}}^M\) are the overall intra-molecular phenomenological coefficients corresponding to the thermoelectric process with forward and reverse biases, respectively [52]. Based on the Eq. (8), the intra-molecular \(L_{M_{\text{sym}}}^M\) and \(L_{M_{\text{asym}}}^M\) phenomenological coefficients, of the molecular switches studied in this work (M, Au-M-Au, Au-M-Au), are calculated, and sample of these results is shown in Fig. 23.

Analysis of these results show that the molecular \(L_{M_{\text{sym}}}^M\) coefficient increases almost linearly with increasing the field intensity. But, the \(L_{M_{\text{asym}}}^M\) coefficients depend non-linearly on the electric field intensity (almost oscillate with intensity of the external field). These phenomenological coefficients, \(L_{M_{\text{sym}}}^M/L_{M_{\text{asym}}}^M\) can (may) be used to predict and thus evaluate (manage) energy/heat fluxes in intra-molecular sections of the field-effect molecular devices/switches.

**Conclusion**

In this study, the external field effect on the some electronic/vibrational properties and thus I-V curve of a candidate molecular switch (in isolated, M, and non-isolated, Au-M-Au states), at molecular/atomic scales, are studied, using QTAIM and Landau’s theory (without using numerical methods such as Green’s function). Analysis of the results showed that the application of an external electric field can cause the exchange of charge/energy between different atomic basins (or different intra-molecular sections), and consequently changes in atomic kinetic/potential energy of this field effect molecular switch. In addition, the effects of the electric field on these molecular switch show that the field strength (intensity) reaches 0.008 a.u, in which case this molecular switch is turned ON state. Moreover, the analysis of the results shows that gold electrode atoms play an important role in the local distribution of charge/energy (Laplacian) between different intra-molecular sections, and consequently the I-V curve/characteristics of this molecular switch. Also, in this quantum study, based on the linear force-flux law (Onsager phenomenological approach), the symmetrical (\(L_{M_{\text{sym}}}^M\)) and asymmetrical (\(L_{M_{\text{asym}}}^M\)) intra-molecular phenomenological coefficients, of this candidate molecular switch, are calculated, using QTAIM. The analysis of these results shows that the sign and the quantity of this intra-molecular phenomenological coefficients (\(L_{M_{\text{sym}}}^M\) and \(L_{M_{\text{asym}}}^M\)) depend on the charge/energy transfer mechanisms between different intra-molecular sections, induced by external electric field. Also, these results show that the \(L_{M_{\text{sym}}}^M\) increases nearly-linearly with electric field intensity, but the \(L_{M_{\text{asym}}}^M\) depends non-linearly on the electric field intensity. In this regard, it can be predicted that
when $L_{\text{asym}}^M$ increases (or $L_{\text{sym}}^M$ decreases), the electronic efficiency of the intra-molecular nanoelectronic devices increased. Therefore, using these intra-molecular phenomenological coefficients, it is possible to estimate the efficiency and effectiveness of intra-molecular field-effect molecular devices/switches.

**Author contribution** H. Hadi: Subject design, writing, and calculations. R. Safari: Subject design, writing/revising, and analysis of results. H.R. Shamlouei: writing and editing.

**Availability of data and material** The data and results of this computational study can be shared.

**Declarations**

**Competing interests** The authors declare no competing interests.

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