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ORIGINAL PAPER

Transport engineering design of AND and NOR gates with a 1,4-2-phenyl-dithiolate molecule

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Abstract We have explored logical AND and NOR gate responses of a 1,4-2-phenyl-dithiolate molecule threaded by a magnetic flux ϕ in two-terminal junctions by using the Green's function method in the framework of a nearest-neighbor tight-binding approximation. Here, we put emphasis on the logical gate voltages, and obtain the electrical transmission and current-voltage characteristics with metal-molecule-metal (m-M-m) tunnel junctions. The hopping integral among two neighboring atoms in the molecule was quantitatively estimated by means of density functional theory (DFT) calculations. Our results show that the AND and NOR responses are explored through our molecular junction for a typical value of the magnetic flux. The numerical results may shed light on the next applications of molecular systems and make them a good, promising candidate for field-effect transistors.

Keywords Tunneling · Phenyl-dithiolate molecule · Green's function · Tight-binding method

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Introduction

Organic materials have recently attracted considerable attention from the fields of electronics, photonics, and especially an emerging field known as molecular electronics, and significant efforts are being made towards their integration in these fields. Molecules have unique properties that make them the most promising candidates for electronic devices. It is now conceivable for organic materials to open new avenues to cheap, low-weight, mechanically flexible, chemically inert, and bottom-up fabricated electronics devices.

The understanding of electron transport through a single molecule sandwiched between two external electrodes is a fundamental step in the development of molecular electronics devices; this is a molecular junction system, the so-called source-molecule-drain system [1, 2]. Therefore, electron transport through the molecular systems have been widely studied both experimentally and theoretically in recent years [3–6].

Conjugated molecules are more suitable than saturated ones for improving fabrications in molecular devices. This is because of the small energy gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) and also the easy tuning of electronic and optical properties.

1,4-*n*-phenyl-dithiolate is one of the organic molecules that is widely used in molecular electronics. This molecule is composed of a linear chain of n benzene rings with two sulfur atoms at its ends [7]. Reed et al. [8] have performed electronic properties of a 1,4-benzene-dithiolate molecule (a 1,4-*n*-phenyl-dithiolate molecule with $n = 1$). They

have found that in a 1,4-benzene-dithiolate molecule, the current–voltage characteristics show a non-ohmic relationship.

By applying one or two control voltages to the molecule, which modifies the relative phase, the electrical transport properties could be controlled. Furthermore, by tuning the magnetic flux, the so-called Aharonov–Bohm (AB) flux, which threads the molecule and also by changing the geometry, the transmission probability of an electron across the bridge can be modulated [9–12]. Maiti, with the help of the some mesoscopic metallic rings, designs some bridge systems that can act as different logic gates, which may be used in nanoelectronic circuits [13–16]. Baer et al. [17] have discussed increased conductivity due to coherent transfer in molecules in which the electron can pass through two routes, which by applying voltages to a molecule, like in FET or in XOR gates, the transmission could be controlled. In a previous paper [18], we studied a nanoscale logic NOR gate by applying magnetic flux inputs in a Z-shaped graphene nanoribbon composed of an armchair ribbon device sandwiched between two semi-infinite metallic zigzag ribbon leads. We have shown that the current and conductance are highly sensitive to both the magnetic fluxes subject to the device and the size of the system. In another work [19], we have investigated the XOR and OR gate responses, theoretically in a benzene molecule threaded by a magnetic flux and two gate voltages. The application of these results can be a base for the design of molecular electronics devices.

In the present work, we investigate the dependence of transport properties on the source-drain bias and gate voltage to address logic AND and NOR gates in both weak and strong couplings of bridge organic molecule to the leads. The 1,4-2-phenyl-dithiolate molecule is threaded by a magnetic flux ϕ and sandwiched symmetrically between the two metallic leads, which is kept at a certain source-drain bias. By applying two control gate voltages V_a and V_b to the molecule, considered as the two inputs of the logical gates, the transfer through the bridge could be controlled. The gate voltage is introduced as a capacitor composed of two parallel circular charged disks separated at a certain distance from each other. The axis of the capacitor is perpendicular to the transport direction.

The paper is organized as follows: In section "Theoretical framework", the quantum ring system is briefly defined and the proposed model for calculating the transmission and current–voltage characteristic is described. In section "Numerical results and discussions", the numerical results and discussion are presented. The last section of the paper is devoted to the discussion and conclusion of our findings.

Theoretical framework

All calculations in this work are done for the model shown in Fig. 1. The transmission and current–voltage characteristic are measured between two left and right metallic leads (denoted by L and R, respectively), which are attached to 1,4-2 phenyl-dithiolate molecule (denoted by M) via sulfur atoms (shown by red color). A uniform perpendicular magnetic field is applied on the molecule as shown in Fig. 1. The molecule is composed of two benzene rings with two sulfur atoms at both ends, symmetrically threaded by a magnetic flux ϕ due to the perpendicular magnetic field. In addition, two gate voltages gate-a and gate-b as V_a and V_b were applied in two lower arms of the two benzene rings in Figs. 1a, b. Also, we have applied two other gate voltages V_c and V_d in Fig. 1b, in the upper arms of the two ring molecules via the gate voltages gate-c and gate-d. The Green's function method is used to study the transport properties of a 1,4-2-phenyl-dithiolate molecule with different logical gates. We use a tight-binding model with the real hopping matrix elements as extracted by means of the density functional theory (DFT). In the formalism, we ignore the electron–phonon and electron–electron interactions. Also, for simplicity, the Zeeman splitting of energy levels has been neglected in this work.

The hopping integral between two nearest-neighbor atoms in the benzene molecule and also the twist angle (φ)

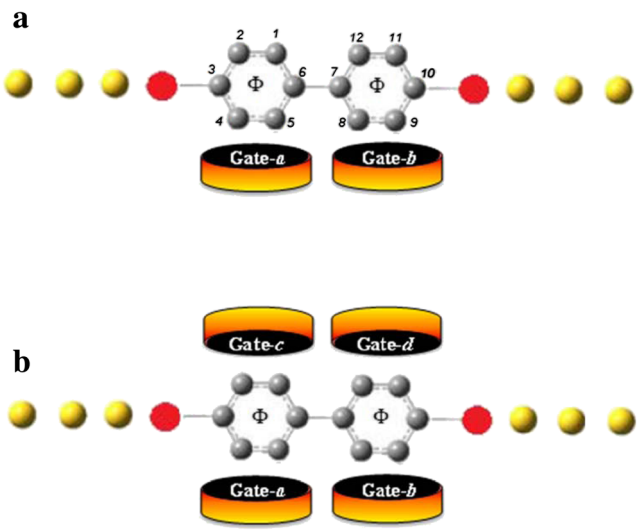

Fig. 1 Schematic view of a 1,4-2-phenyl-dithiolate molecule composed of two benzene rings and two sulfur atoms connected to two semi-infinite one-dimension metallic electrodes, namely, source and drain. Two gate voltages V_a and V_b were applied in two lower arms of the two benzene rings in (**a**) and (**b**). We also applied two other gate voltages V_c and V_d in (**b**) in the upper arms of the two benzene molecules

between two benzene rings were quantitatively estimated by means of a fully self-consistent DFT. The calculation has been performed with an efficient ab initio computer code, SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms), based on a flexible linear combination of atomic orbitals (LCAO) basis set, with essentially perfect $O(N)$ scaling [20–22]. We used a plane wave basis set with a MeshCutoff of 280.0 Ry, so the hopping integral between two nearest-neighbor atoms in the molecule can be expressed as [19]

$$t_{1,2} = \frac{E_{\mathrm{LUMO}} - E_{\mathrm{HOMO}}}{2}. \tag{1}$$

Here, the HOMO and LUMO energies refer to the 1,4-2-phenyl-dithiolate isolated molecule, and the hopping integral among the two neighboring atoms in the molecule is quantitatively estimated by means of DFT calculations. Also, by including the twist angle (ϕ) between two rings the hopping parameter of two neighboring atoms in two different rings can be written as

$$t_{6,7} = t_{1,2}\cos(\phi). \tag{2}$$

We obtain the electrical transmission properties and current–voltage characteristics using the Green's function method in the framework of a nearest-neighbor tight-binding approximation. The generalized Hamiltonian of the whole system can be described as

$$H_{\mathrm{system}} = H_{\mathrm{leads}} + H_{\mathrm{M}} + H_{\mathrm{contacts}}. \tag{3}$$

Here

$$H_{\alpha} = \sum_{i,j} \gamma_{i,j}^{\alpha} c_i^{\alpha\dagger} c_j^{\alpha}, \tag{4}$$

where α(=L, R and M) represents the Hamiltonian for the isolated left lead, right lead, and device, respectively. The matrix elements $\gamma_{i,j}^{\alpha} = \varepsilon^{\alpha}\delta_{i,j} - t_{\langle i,j\rangle}^{\alpha}$ contain of the local site energy and the nearest-neighbor coupling terms between atoms of the left or the right leads, the device, and device–lead interface. Here, $\langle\cdots\rangle$ stands for the summation on the nearest-neighbor atoms.

The Green's function of the central part in the subspace of **G** is [23, 24]

$$\mathbf{G}_{\mathrm{M}}(E) = [(E + i\eta)\mathbf{I} - \mathbf{H}_{\mathrm{M}} - \Sigma_{\mathrm{L}}(E) - \Sigma_{\mathrm{R}}(E)]^{-1}, \tag{5}$$

where η is an arbitrarily small number added into the above equation to incorporate the convergence conditions and **I** is the identity matrix. Also, $\mathbf{H}_{\mathrm{M}}$ is the Hamiltonian of the isolated molecule device. In this equation, Σ_j, $j \in$ (L, R) is the self-energy operator, which can be viewed as the effective Hamiltonian that arises from the coupling of device with the lead j. The self-energies of the metallic chain leads have non-zero matrix elements on the sites directly connected to the lead and is therefore local. This term modifies the energy eigenvalues of the molecule device [26].

With corresponding to Eq. 4, in the presence of an applied perpendicular magnetic field on the molecule, the Hamiltonian of the device can be expressed as

$$\mathbf{H}_{\mathrm{M}} = \sum_{i} \varepsilon_i c_i^{\dagger} c_i + \sum_{i,j} \left(t_{ij} e^{i\theta} c_i^{\dagger} c_j + \mathrm{h.c.} \right), \tag{6}$$

where $c_i^{\dagger}(c_i)$ is creation (annihilation) operator of an electron on site i. Here, t_{ij} is the hopping integral matrices between the nearest-neighbor carbon atoms in the system. In Eq. 6, the term involving ε_i describes the effect of site energy ε_{i0} and gate voltage V_g. In this model, we have applied different gate voltages V_a, V_b, V_c and V_d to the molecule and they operate on the nearest-neighbor atoms to the plates only, which we can show the on-site term as $\varepsilon_{i0} + V_a\delta_{ia} + V_b\delta_{ib}$. When the flux ϕ operates on the system, the phase factor is defined as a normalized flux by $\theta = 2\pi\phi/N\phi_0$, where N is the number of atoms in each ring.

In the absence of thermal effects and the charging terms, the transmission probability for electrons from the left lead to the right lead with energy E under the source-drain bias V_0 is related to Green's functions using Carolis formula [25]

$$T(E, V_0) = \mathrm{Trace}\left[\mathbf{\Gamma}_{\mathrm{L}}\mathbf{G}_{\mathrm{M}}\mathbf{\Gamma}_{\mathrm{R}}\mathbf{G}_{\mathrm{M}}^{\dagger}\right], \tag{7}$$

where

$$\mathbf{\Gamma}_{\mathrm{L(R)}} = i\left[\mathbf{\Sigma}_{\mathrm{L(R)}}(E + i\eta) - \mathbf{\Sigma}_{\mathrm{L(R)}}^{\dagger}(E + i\eta)\right], \tag{8}$$

reflects the coupling at energy E between the molecule and the left (right) lead. Also, the current–voltage characteristic through the organic molecule can be expressed by the relation

$$I(V_0) = \int_{E_{\mathrm{F}} - eV_0/2}^{E_{\mathrm{F}} + eV_0/2} T(E, V_0)\, dE, \tag{9}$$

where E_{F} is the equilibrium Fermi energy.

In the next section, we use the procedure outlined in this section to investigate the electrical transport behavior of a transmitted electron via the system when it is put in the presence of different gate voltages and a magnetic flux.

Numerical results and discussions

We consider the bridge system shown in Fig. 1a, b, which consists of a 1,4-2-phenyl-dithiolate molecule, threaded by a magnetic flux ϕ, is attached to two semi-infinite metallic electrodes. It is assumed that the two gate voltages V_a and V_b operate only on the nearest-neighbor atoms as shown in panel (a) of the figure. Also, panel (b) of Fig. 1 shows

two other gate voltages V_c and V_d, which are constant. The results are calculated for a typical value of the magnetic flux $\phi = \phi_0/2$, where $\phi_0 = ch/e$ is the elementary flux-quantum [19, 27–29]. This is a key controlling parameter for these calculations and we choose the unit $c = e = h = 1$ in our numerical calculations for simplicity.

All of the optimizations and electronic structure calculations of the molecule have been performed by using an efficient ab initio computer code, SIESTA package, which implements DFT with the pseudopotential approximation and a basis set of linear combination of atomic orbitals. The pseudopotentials were constructed using the Troullier and Martins [30] scheme to describe the valence electron interaction with the atomic core. A linear combination of numerical atomic orbitals is used to represent a double-ξ basis set with polarized functions (DZP). In order to obtain the Hamiltonian matrix elements, a grid in real space, which is obtained using a mesh cutoff of 280 Ry, is applied. Then, according to Eq. 1, we can obtain the hopping integral among two neighboring atoms in a ring of molecule equal to $t_{1,2} = 2.602t$ and the obtained C-C bond length is 1.95 Å. Also, by calculating the twist angle between two rings equal to 29 degrees, according to Eq.2 the hopping among the two neighboring atoms in two different rings is $t_{6,7} = 1.308t$. In the whole of this work, we take the transfer integrals as a unit energy (t) and also, for simplicity, all the on-site energies and the temperature are set to zero in the calculations.

Here, we present the results of the transmission and current–voltage characteristics and discuss the effect of the gate voltages on the transport phenomena in the nano-device. For this reason, we have chosen the leads to be made of the same uniform materials and the nearest-neighbor hopping strength (t_0) are fixed to 2.44 in unit of t. Also, the coupling between the molecule and leads are taken to be the same, but for two limiting cases depending on the strength of the coupling of the molecule to the left and right electrodes, $t_{\mathrm{DL}} = t_{\mathrm{DR}} = 2.5 \sim t$ for strong coupling and $t_{\mathrm{DL}} = t_{\mathrm{DR}} = 0.5 \ll t$ for weak coupling. Also, the Fermi energies are $E_{\mathrm{FL}} = E_{\mathrm{FR}} = 0$ for the left and right leads.

Figure 2 shows the transmission and current–voltage characteristics in the limit of weak and strong couplings. This figure is according to Fig. 1a in which two gate voltages are connected to one side of the molecule. We want to

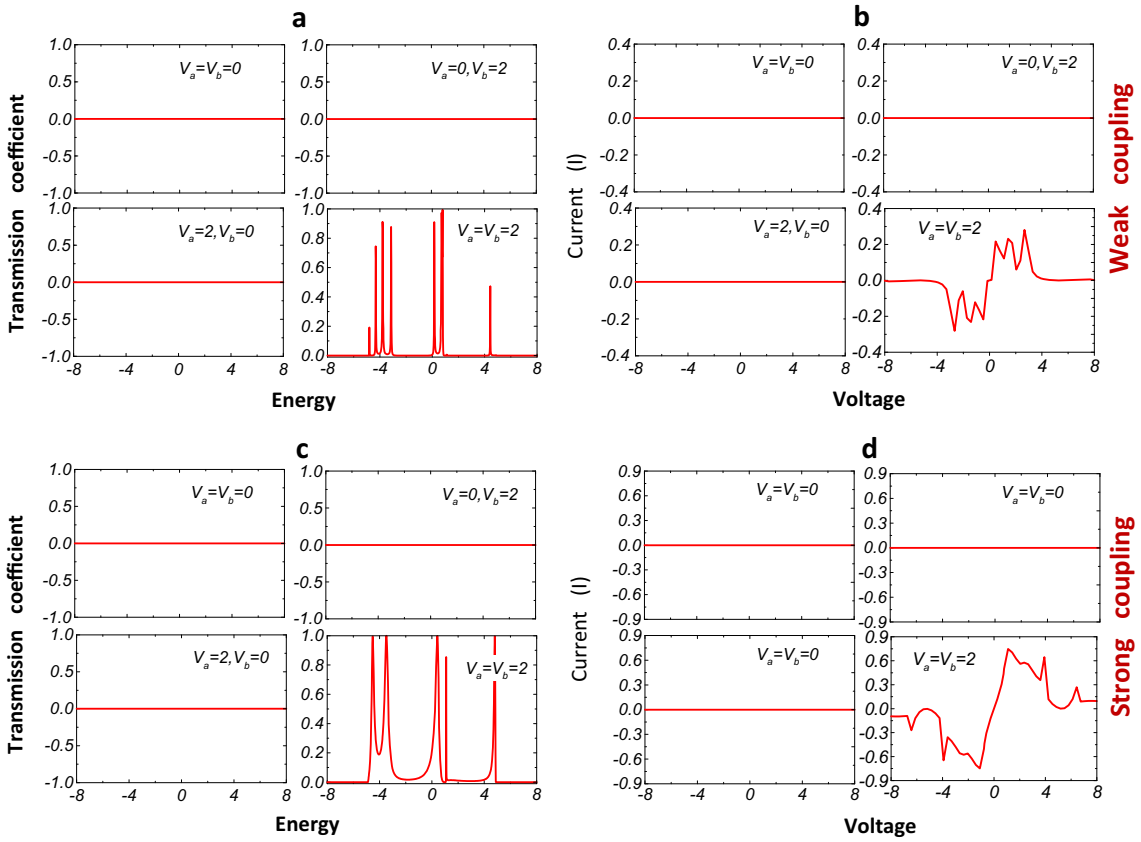

Fig. 2 This figure is according to Fig. 1a, which two gate voltages V_a and V_b are applied in two lower arms of the two benzene rings. The *curves* show that the electron transmission takes place through the molecule if both the inputs (gate voltages) are high, while if one of the inputs or both of them are low, the transmission is no longer possible. This feature obviously shows the AND gate behavior. The panels **a** and **c** are $T - E$ curves, and the panels **b** and **d** are $I - V$ characteristics in the weak coupling and strong coupling limit, respectively

address gate response in the bridge system. The input signals are now the gate voltages (V_a and V_b) and the output signals are the transmission and current carried through the device. In our numerical study, we choose two typical values for input signals, 2 for high and 0 for low value. Figure 2a shows the transmission T as a function of the energy E for the four different choices of the gate voltages V_a and V_b. It can be seen that when both of the two inputs V_a and V_b are small, i.e., ($V_a = V_b = 0$), and for the other two cases where any one of the two inputs to the gate is large and other one is small i.e., ($V_a = 0$ and $V_b = 2$) and ($V_a = 2$ and $V_b = 0$), the transmission probability of electrons through the molecule drops to zero for all energies. This means that an electron can not transmit from the source to the drain region. On the other hand, when both of the two inputs V_a and V_b are large, i.e., ($V_a = V_b = 2$), the transmission shows some sharp resonant peaks in particular energies. These correspond to the energy eigenvalues of the molecule, which indicate that the resonant peaks are induced by the confined quasibound states in the junction. Thus, we can express that the electron transmission takes place through the molecule if both of the inputs are high, while if one of the inputs or both of them are low the transmission is no longer possible. This feature obviously shows the AND gate behavior. The AND gate is an electronic circuit that gives a high output only if all its inputs are high. This means that the transmission through the molecule is possible if both the two inputs to the gate are high. By studying the current–voltage characteristics, all of these features of gate response become much more clearly visible. In Fig. 2b, the $I - V$ curves have been shown through the bridge system. It can be seen that when either of the two inputs are low ($V_a = V_b = 0$), or any one of the two inputs is high and the other is low ($V_a = 0$ and $V_b = 2$) and ($V_a = 2$ and $V_b = 0$), the current is zero for the entire range of the bias voltage in our molecular junction. Also, when both of the inputs are high, a remarkable current will be obtained. This behavior corresponds to the transmission coefficient shown in Fig. 2a, since the current is computed from the integration of the transmission function $T(E)$ (see Eq. 9). From these $I-V$ characteristics, the behavior of the AND gate response is clearly visible.

In Fig. 2c, d, we discuss the transmission coefficient and $I-V$ characteristics in the limit of strong-coupling. In this limit, the resonance peaks of transmission get broader compared to the weak-coupling limit and this broadening is due to the imaginary parts of the lead self-energies. Because the

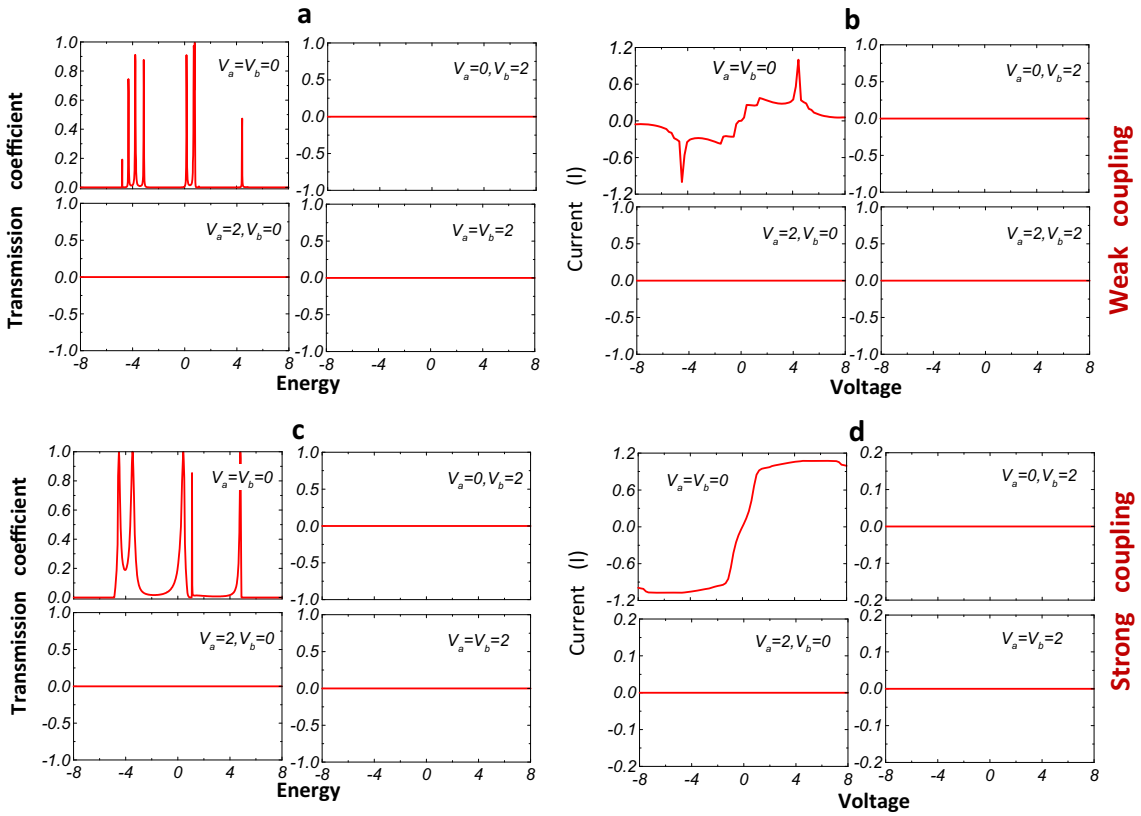

Fig. 3 This figure is according to Fig. 1b, which gate voltages V_a and V_b (V_c and V_d) are applied in two lower (*upper*) arms and of the molecule. The *curves* show that the molecule allows an electron to pass from the source to the drain only when both the two inputs (gate voltages) are low. All these features of electron transfer address an NOR gate response in the bridge system. The panels **a** and **c** are $T - E$ curves, and the panels **b** and **d** are $I - V$ characteristics in the weak coupling and strong coupling limit, respectively

self-energies modify the energy eigenvalues of the molecule in our molecular junction. Also, the results show that in the limit of strong coupling, the current achieves a larger amplitude than the weak-coupling limit. This is because in the strong-coupling limit all the energy levels get broadened, which provides a larger current passing through the molecule. These results show that by tuning the coupling strength of the leads to the molecule, we can obtain electron transmission through the molecule for a wider range of energies and achieve a large current amplitude for the same bias voltage. It is pointed out that all of the curves in Fig. 2, for the two limiting cases, clearly demonstrate the AND gate behavior.

According to Fig. 1b, Fig. 3 shows the transmission and current–voltage characteristics in the limit of weak and strong coupling in the molecular junction which the two gate voltages V_a and V_b (V_c and V_d) are connected to lower (upper) arms of the two rings. Now, we want to express the dependence of the two gate voltages in four different cases. The results show that the molecule does not allow the passing of an electron from the source to the drain when both of the inputs are high, i.e., ($V_a = V_b = 2$) and also for the other cases that either of the two inputs is high and the other is low ($V_a = 0$ and $V_b = 2$) and ($V_a = 2$ and $V_b = 0$). However, for the case that both of the inputs are low, i.e., ($V_a = V_b = 0$), the electron can transport through the molecule and the transmission spectra shows resonance peaks for some special energies in weak coupling limit. This feature clearly demonstrates NOR gate response in our molecular junction. The NOR gate is an electronic circuit that gives a high output if both of its inputs are low. This means that the outputs of all NOR gates are low if any of the inputs are high. Figure 3a, b shows the transmission and current in the limit of weak coupling and Fig. 3c, d is in the limit of strong coupling. All these features of electron transfer address an NOR gate response in the bridge system. The molecule allows an electron to pass from the source to the drain only when the symmetries of both the two rings are identically broken. It should be noted that in these cases, by applying the gate voltages, the symmetry of the upper and lower arms of the molecule is broken therefore the transmission curves indicate the resonance peaks for some particular energy values.

Conclusions

A compact realization of a logical AND as well as a logical NOR is proposed and quantitatively discussed by use of tight-binding simulations. A 1,4-2-phenyl-dithiolate molecule is placed between metal electrodes, where each of the two phenyl rings is threaded by a magnetic flux ϕ. The transmission characteristics of the resulting metal-molecule-metal tunnel junction are explored using a Green's function formalism within the tight-binding approach in the limit of coherent regime. All of the optimizations and electronic structure calculations of the molecule are performed by using an efficient ab initio computer code, SIESTA package. The transmission, and consequently the electric current, are found to be contingent on the simultaneous presence of high gate voltages at both phenyl rings. This is a representation of a logical AND. In an analogous manner, a logical NOR can be constructed. The application of the predicted results can be a base for the designing of molecular electronics devices.

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