



Electronic transport properties of a single chiroptical molecular switch with graphene nanoribbons electrodes



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ABSTRACT

Based on the nonequilibrium Green's function method and density functional theory calculations, we investigate the electronic transport properties of a single chiroptical molecular switch with two zigzag graphene nanoribbon electrodes. The molecule undergoing the switch can exhibit different chirality namely *cis*-isomer and *trans*-isomer by ultraviolet or visible irradiation. Theoretical results clearly reveal that these two isomers exhibit very different current – voltage characteristics, which can realize the switching behaviors when the molecule converts between *cis*-isomer and *trans*-isomer. Furthermore, the negative differential resistance behaviors also can be observed in these two isomers, suggesting potential applications of this type of junctions in future design of functional molecular devices.

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1. Introduction

Molecular devices which used molecules as electronic transport channels have attracted more and more attention due to their novel physical properties and potential application in nanoelectronic devices [1–4]. Several molecular devices with different functionalities have been designed and measured theoretically and experimentally in the past years, such as negative differential resistance (NDR), rectification, memory effects, amplification, switch and others [5–8]. As the basic element of logic in molecular devices, molecular switches, especially optical molecular switches, have been extensively investigated and discussed [9–12]. However, most mechanisms for optical molecular switch considered so far are based on the ring-opening reactions of the molecular bridge, such as diarylethene, naphthopyrans, dihydroazulenes and benzochromenes [13–19]. The greatest disadvantage of this mechanism is that the overall length of molecule is changed significantly when the molecule converts between two different isomers [20]. Recently, some experiments report that the thioxanthene-based molecule can exhibit different chirality, namely *cis*-isomer and *trans*-isomer, by ultraviolet or visible irradiation [21,22]. These two isomers only differ by the position of upper half [21,22]. The switching between the different chirality is very efficient and shows excellent reversibility, which make it usable as one of the candidates for light-driven molecular switches [21,22].

However, to our knowledge, the electronic transport properties of the thioxanthene-based molecule is not reported so far.

Moreover, following the progress in fabrication of graphene nanoribbons (GNRs) at room temperature, GNRs have become one of the most promising candidates for the next generation of electrodes materials [23–26]. Because GNRs electrodes did not have serious contact problems at the molecular scales comparing with the metallic electrodes materials like gold [27–31]. Therefore, in this paper, we investigate the switching behaviors of the thioxanthene-based molecule coupled to two GNRs electrodes by applying the nonequilibrium Green's function (NEGF) formalism combined with density functional theory (DFT).

2. Model and method

The molecular device for our theoretical study is illustrated schematically in Fig. 1. The pre-optimized thioxanthene-based molecule with different chirality, namely *cis*-isomer and *trans*-isomer, are sandwiched between two infinite 6-zigzag-graphene nanoribbon (named as 6-ZGNRs) electrodes. In our calculations, the amide end groups were used as linkages between the molecule and 6-ZGNRs electrodes. For each electrode, two layers of carbon atoms are included into the extended molecule region to screen the perturbation effect from the central scattering region and they are denoted as surface-atomic layers. In the calculations, the end of each zigzag-graphene nanoribbon is capped by H atoms to eliminate the dangling bonds.

The geometric optimizations and the electronic transport properties of the molecular devices are calculated by a developed

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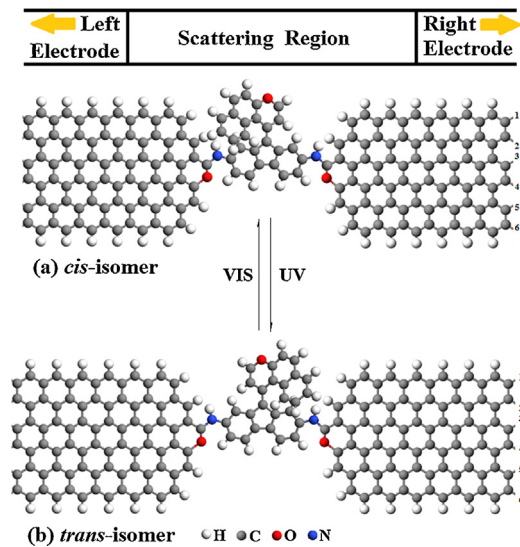


Fig. 1. Models of the molecular device for thioxanthene-based molecule connected to two 6-ZGNRs electrodes, with its different chirality, namely *cis*-isomer and *trans*-isomer, respectively.

first-principles software package Atomistix ToolKit [32,33], which is based on the DFT combined with self-consistent NEGF formalism. The main feature of the computational package is to model a nanostructure coupled to external electrodes with different electrochemical potentials and to realize the transport simulation of the whole two-probe system without inducing phenomenological parameters. Details of the method can be found in Refs. [32,33]. In the electronic transport calculations, the exchange-correlation potential is described by Ceperley – Alder local density approximation (LDA) [34]. The core electrons are modeled with Troullier – Martins nonlocal pseudopotential [35], while the valence electrons wave functions are expanded by a SIESTA basis set [36]. The double-zeta plus polarization (DZP) basis set is adopted for all atoms. The Brillouin zone is set to be $5 \times 5 \times 100$ points following the Monkhorst – Pack k-point scheme. The cut-off energy and the iterated convergence criterion for total energy are set to 150 Rydberg and 10^{-5} , respectively.

In NEGF theory, the transmission function $T(E, V)$ of the system is the sum of transmission probabilities of all channels available at energy E under external bias V [37]:

$$T(E, V) = \text{Tr}[\Gamma_L(E, V)G^R(E, V)\Gamma_R(E, V)G^A(E, V)], \quad (1)$$

where, $G^{R/A}$ are the retarded and advanced Green's functions, and coupling functions $\Gamma_{L/R}$ are the imaginary parts of the left and right self-energies, respectively. The self-energy depends on the surface Green's functions of the electrode regions and comes from the nearest-neighbor interaction between the extended molecule region and the electrodes.

For the system at equilibrium, the conductance G is evaluated by the transmission function $T(E)$ at the Fermi level E_F of the system:

$$G = G_0 T(E_F), \quad (2)$$

where, $G_0 = 2e^2/h$ is the quantum unit of conductance, h the Planck's constant, e is the electron charge.

The current through a molecular junction is calculated from the Landauer – Büttiker formula

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

where, f is the Fermi function, $\mu_{L/R}$ the electrochemical potential of the left/right electrode and the difference in the electrochemical potentials is given by eV with the applied bias voltage V , i.e.,

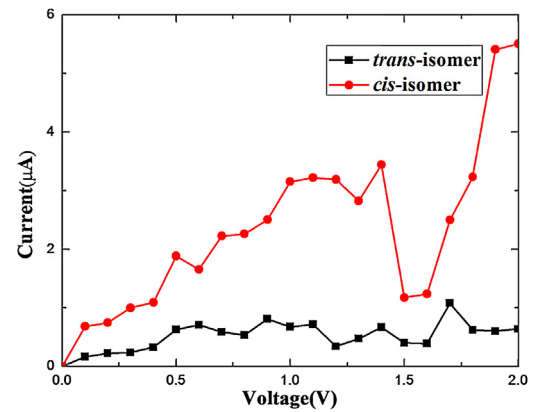


Fig. 2. The calculated $I - V$ characteristics of the molecule junction with 6-ZGNRs electrodes.

$\mu_L = \mu(0) - eV/2$ and $\mu_R = \mu(0) + eV/2$. Furthermore, $\mu_{L/R}(0) = E_F$ is the Fermi level.

3. Results and discussions

The calculated current – voltage ($I - V$) curves of the molecular device with different isomers under the bias voltage varying from 0 to 2.0V are given in Fig. 2. It should be pointed out that at each bias, the current is determined self-consistently under the non-equilibrium condition. As shown in Fig. 2, the calculated $I - V$ curves clearly demonstrate two following important features: (i) Although the two isomers only differ by the position of upper half, their conductance properties are drastically different. The current through the *cis*-isomer is evidently larger than that through the *trans*-isomer over the entire bias range. For example, the calculated current at 1.4 V is about 3.45 μA and 0.61 μA for the *cis*-isomer and *trans*-isomer, respectively. Thus, when the molecule in the device changes from the *cis*-isomer to *trans*-isomer under photoexcitation, the device is predicted to switch from ON (high conductance) to OFF (low conductance), and vice versa. The remarkable difference of current between the *cis*-isomer and *trans*-isomer under the applied bias can be quantified by the on – off ratio of the current defined as $\text{Ratio}(V) = I_{\text{cis-isomer}}(V)/I_{\text{trans-isomer}}(V)$. The calculated on – off ratio varies from around 2.3 to 9.4 in the bias range from 0 to 2.0V. The maximum on – off ratio can reach 9.4 at 1.2V, suggesting potential applications of this type of junctions in future design of light-driven molecular switches. (ii) The currents of two isomers with 6-ZGNRs electrodes both vary with the bias voltage in a complicated manner. The negative differential resistance (NDR) behaviors can be observed both in the *cis*-isomer and *trans*-isomer. For example, in the bias voltage region [1.4V, 1.7V], the current of *cis*-isomer decreases quickly as the bias voltage increases, leading to significant NDRs at these bias voltages. The maximum current of the *cis*-isomer is up to be about 3.4 μA at the peak position ($V_{\text{bias}} = 1.4\text{V}$), while the current reaches its minimum value 1.1 μA at the valley site ($V_{\text{bias}} = 1.5\text{V}$). Meanwhile, NDR also can be observed in the bias range of 1.1V to 1.8V for the *trans*-isomer. The maximum peak-to-valley ratio (PVR) is about 5 and 2 for *cis*-isomer and *trans*-isomer, respectively. The observed sequential NDR behaviors in the molecular device have important application in amplifier and logic gate.

To understand the nature of the observed switching behaviors, we calculate the zero-bias transmission spectra of the *cis*-isomer and *trans*-isomer with 6-ZGNRs electrodes in Fig. 3. In our calculation, the average value of the chemical potential of the left and right electrodes named average Fermi level is set as zero. The short vertical bars near the energy axes stand for the energy levels

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