



Negative differential resistance and stable conductance switching behaviors of salicylideneaniline molecular devices sandwiched between armchair graphene nanoribbon electrodes



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ABSTRACT

By applying nonequilibrium Green's functions in combination with the density-functional theory, we investigate the electron transport properties of the salicylideneaniline molecule sandwiched between two armchair graphene nanoribbon (AGNR) electrodes. It shows that the width of the AGNR electrodes plays a significant role in the transport properties of the salicylideneaniline molecular junctions. The current–voltage characteristics of the salicylideneaniline molecule sandwiched between 8AGNR electrodes can perform a stable conductance switching behavior at the bias region [1.2 V, 1.6 V] when the molecule translates between the *trans*-enol form and the *trans*-keto form. When the electrodes change to 7AGNR, a remarkable negative differential resistance behavior can be found in the salicylideneaniline molecular device at the *trans*-keto form. That means the salicylideneaniline molecule can perform different functions when it connects to the different AGNR electrodes.

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1. Introduction

Design and building functional devices by using the molecules or a few atoms are the ultimate goal of future molecular electronics, motivated by the prospect of using them to miniaturize the traditional electronic devices [1–5]. To achieve this aim, more and more efforts were putted to develop capabilities to measure, control, and understand electronic transport mechanisms of molecular junctions. Up to now, plenty of molecular devices have been discovered with striking functional properties. Among them, several atomic scale junctions consisting of the functional molecules showed highly nonlinear current–voltage characteristics, such as negative differential resistance (NDR) [6–9], current switching [10–13], electrostatic rectification [14–16], and spin filtering [17–19]. These interesting and important nonlinear properties have profound potential for future atomic-scale circuits.

Recently, a novel two-dimensional material-graphene has

aroused an all round interest due to its unique electronic structures and transport characteristics [20,21]. One-dimensional graphene nanoribbons (GNRs) which cut off from the graphene are expected to have potential applications in the future molecular electronics. The edge styles (zigzag or armchair) were found to play a pivotal role in the observed charge-transport behavior of these GNRs [22,23]. Various molecular devices based GNRs have been fabricated and more theoretical investigations regarding its transport properties have been reported. The perfect spin-valve and spin-filter effects had been found in zigzag graphene nanoribbon (ZGNR)-carbon wire junctions in 2010 [24]. The oscillatory conductance was also found in atomic carbon wire-graphene junctions for even-odd number of carbon atoms [25]. Then, the negative differential resistance behavior was explored from the electronic transport properties of zigzag graphene nanoribbons (GNRs) with two kinds of triangular defects [26]. Recently, excellent rectifying behaviors similar to macroscopic p-n junction diodes had been found in a donor–acceptor molecule between two armchair graphene nanoribbons (AGNR) [27].

In this work, we explore the electronic transport properties of a salicylideneaniline molecule sandwiched between two AGNRs by using a first-principles approach. Salicylideneaniline is a photochromism molecule and has long been proposed as an example of

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molecular switching activated by photoinduced hydrogen atom transfer in the experiment [28,29]. It shows that the current–voltage characteristics of the devices depend on the width of the AGNR remarkably. The NDR behavior and stable conductance switching behavior are found in salicylideneaniline molecular devices between the 7-AGNRs or the 8-AGNRs, respectively.

2. Model and method

The molecular devices we study are illustrated in Fig. 1. Only the left end of the salicylideneaniline molecule covalently connects to the left AGNR electrode. The device is divided into three regions: left electrode, right electrode, and central region. The central region contains two units of the AGNR on each side, thereby establishing the bonding between the molecules and the electrodes, the common Fermi level, and charge neutrality at equilibrium. After the *trans*-enol (E-OH) form of salicylideneaniline in the ground state absorbs one photon, the excited-state intramolecular rapid proton-transfer process from the oxygen to the nitrogen atom occurs [30,31]. Then it can undergo a torsion and transform into a photochromic product *trans*-keto (E-NH) form [32]. For simplicity, the *trans*-enol (E-OH) form and the *trans*-keto (E-NH) form of salicylideneaniline molecules switching between the 8-AGNRs are named M1 and M2, respectively. The *trans*-enol (E-OH) form and the *trans*-keto (E-NH) form of salicylideneaniline molecules switching between the 7-AGNRs are named M3 and M4, respectively.

The structural relaxation and electronic transport properties calculation are performed by using an *ab initio* code package Atomistix ToolKit (ATK) based on nonequilibrium Green's functions and density functional theory [33,34]. The Perdew-Burke-Ernzerhof (PBE) formulation of the generalized gradient approximation (GGA) is used as the exchange-correlation functional. The Hamiltonian, overlaps, and electronic densities are evaluated in a real space grid defined with a plane wave cut off of 150 Ry to achieve a balance between calculation efficiency and accuracy. The geometries are optimized until all residual force on each atom is smaller than 0.05 eV/Å. The nonlinear current through the contact is calculated by using the Landauer formula $I(V_b) = \left(\frac{2e}{h}\right) \int_{\mu_L}^{\mu_R} (f_L - f_R) T(E, V_b) dE$, where $\mu_{L/R}$ is the electrochemical potentials of the left and right electrodes, $T(E, V_b)$ is the bias-dependent transmission coefficient, and $f_{L/R}$ is the Fermi distribution function [35]. With the applied bias potential V_b , the chemical potential of left electrode $\mu_L(V_b)$ equals to $-eV_b/2$ and the

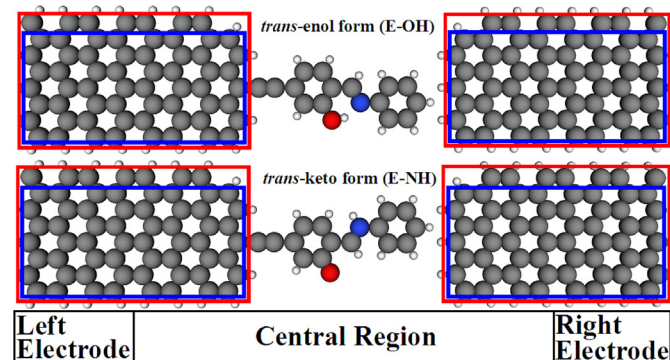


Fig. 1. Schematic views of salicylideneaniline molecular devices sandwiched between the 7-AGNRs (blue rectangular box) or the 8-AGNRs (red rectangular box). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

chemical potential of right electrode $\mu_R(V_b)$ equals to $+eV_b/2$. The energy region of the transmission spectrum that contributes to the current integral in the Landauer formula is referred to the bias window $[-V_b/2, +V_b/2]$. The transport coefficient $T(E, V_b)$ can be calculated using the well-known formula, $T(E, V_b) = \text{Tr}[\Gamma_L(E)G^R(E)\Gamma_R(E)G^A(E)]$, where $G^R(E)$ and $G^A(E)$ are the retarded and advanced Green's functions, respectively, and $\Gamma_{L,R} = i(\Sigma_{L,R}^R(E) - \Sigma_{L,R}^A(E))$ is the coupling functions of the conductor to the left and right electrodes, $\Sigma_{L,R}^R(E)$ and $\Sigma_{L,R}^A(E)$ are the self-energy matrices used to include the effect of the left (right) semi-infinite electrode.

3. Results and discussion

The current–voltage characteristics for M1 and M2 in a bias range from 0 to 2.0 V, and M3 and M4 in a bias range from 0 to 2.5 V are shown in Fig. 2. Most strikingly, the electronic transport properties of salicylideneaniline molecules sandwiched between the 8-AGNRs or the 7-AGNRs are different from each other. In Fig. 2 (a), the currents of M1 are always zero in a bias range from 0 to 1.6 V. Then, they increase with bias gradually. When the salicylideneaniline molecule transforms into the *trans*-keto (E-NH) form, the currents of M2 are also zero in a bias range from 0 to 0.6 V. However, they will increase at first abruptly after 1.0 V and then become gradual from 1.2 to 2.0 V. Therefore, there is a switch from the high conductance to the low conductance in bias region from 1.2 to 1.6 V when the molecule changes from the *trans*-enol form to the *trans*-keto form under photoexcitation. In order to compare the electronic transport abilities of M1 and M2, we calculate the current switching ratios as a function of bias (the insert figure). The figure indicates the current switching ratios in bias region from 1.2 to 1.6 V are high (up to 2 orders of magnitude) and stable. That means the salicylideneaniline molecule doesn't losing its functionality once connected to an electrode and can be made as a switchable molecular device. In Fig. 2(b), the currents for M3 always are zero in a bias range from 0 to 2.0 V. Then, they increase with bias gradually. When the salicylideneaniline molecule transforms into the *trans*-keto (E-NH) form, the currents for M4 are also zero in a bias range

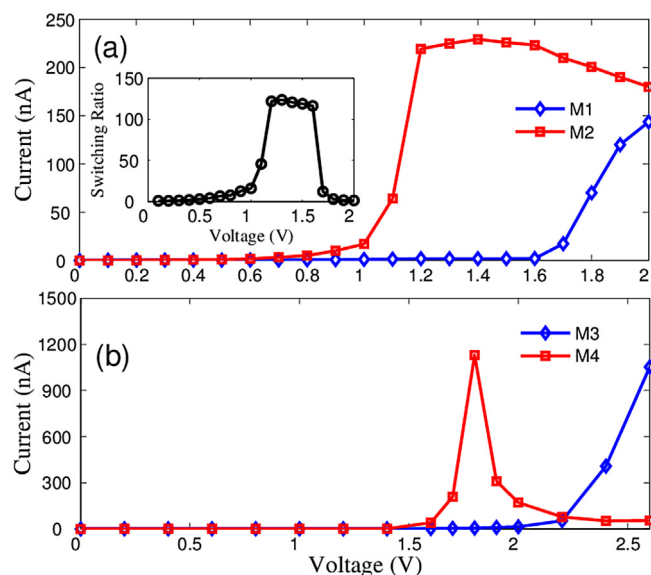


Fig. 2. Calculated current as a function of applied bias for M1, M2, M3 and M4, respectively. The insert figure is the current switching ratios (I_{M2}/I_{M1}) as a function of bias.

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