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Reversible switching in gold-atom–organic-molecule complex induced by reversible bond formation

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ABSTRACT

By applying nonequilibrium Green's functions in combination with the density-functional theory, we investigate the electronic transport properties of a molecule PTCDA sandwiched between two Au electrodes. The results show that the adsorption of an Au atom can modulate the conductance of the Au–PTCDA–Au junction remarkably. The reversible switching behavior can be found in this device, arising from the reversible bond formation between the Au adatom and the PTCDA molecule, which is in line with the experimental results. However, the switching behavior of the molecule PTCDA induced by reversible bond formation disappeared when the Au electrode is replaced by the armchair-edge graphene nanoribbons. That means the graphene electrodes with armchair termination deeply affect the electronic transport properties of the molecule PTCDA at small bias voltages.

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1. Introduction

The switching at single atoms or single molecules size plays an important role in future amplification, logic, and memory elements. Over the past ten years, the researchers all over the world do their best to design various molecular switching and to explore their inherent switching mechanism [1–3]. The early nano-scale switchings based on rotaxane and catenane were made by Heath's group in 1999 and 2000 [4,5]. Next, some oxidation and reduction induced switchings were made in experiment which offer us a new method to modulate the conductance of the molecular devices [6–9]. Subsequently, the current pulse was proved to be another effective way inducing the conductance switching [10,11]. Then, several typical

photochromism molecules including azobenzene, diarylethenes, and spiropyran were widely studied due to their rapid and reversible switching properties [12–14].

Although a large number of outstanding results about the molecular switching have been made, the researchers still try to find the simpler methods to control the conductance of a single molecule. Recently, Mohn and coauthors reported on a molecular switch that was based on the reversible bond formation between an Au adatom and an organic admolecule [perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA)] [15]. They found a switching between the bonded and the nonbonded configuration was accompanied by a change in the tunneling current of about 2 orders of magnitude. The results strongly suggested that the bond making and bond breaking can be used to modulate the conductance of some organic molecule and offer us a new and simple method to design the molecular switching.

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However, there still exist some points to confuse us. First, the PTCDA molecule was located on the surface of the Cu substrate in the experiment. When this molecule is sandwiched between the metal electrodes as a device, does the reversible bond formation still modulate its conductance? Secondly, what is the essential mechanism of the reversible bond formation to control the conductance of the molecule PTCDA? Thirdly, if the metal electrode is changed to other materials, whether the switching behavior of the molecule PTCDA induced by reversible bond formation still exists or not? To answer these questions, we theoretically investigate the electronic transport properties of a molecule PTCDA sandwiched between two electrodes as a molecular device. The results show that the switching behavior induced by reversible bond formation still exists when the molecule PTCDA connects to the Au electrode. However, when the molecule PTCDA connects to the armchair-edge graphene nanoribbon, the switching behavior disappears.

2. Models and formalism

The molecular devices we study are illustrated in Fig. 1. The molecule PTCDA is anchored to the Au electrodes or the armchair-edge graphene nanoribbons via the oxygen atoms [16,17]. The size of Au electrode is 3×3 with 9 atoms in one layer. The width of the armchair-edge graphene nanoribbon is 11 carbon dimmer lines with the smallest band gap. The device is divided into three regions: left electrode (L), right electrode (R), and central scattering region (C). The central scattering region contains a portion of the semi-infinite electrodes, thereby establishing the bonding between the molecules and the electrodes, the common Fermi level, and charge neutrality at equilibrium. Fig. 1(a) and (b) are the nonbonded configurations which the Au atom is supposed far away from the molecule PTCDA. Fig. 1(c) and (d) are the bonded configurations which the Au atom locates on the center of the molecule PTCDA. Bringing the Au atom closer to the molecule, the

molecule PTCDA bends a little due to the interaction between them.

The calculated method we adopt is an *ab initio* code package based on nonequilibrium Green's functions and density functional theory [18,19]. The exchange–correlation potential is described by the local density approximation (LDA), which works rather well for light elements and systems where electrons are delocalized. 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, $I(V_b) = \frac{2e}{h} \int_{\mu_L}^{\mu_R} (f_L - f_R) T(E, V_b) dE$, where $\mu_{L/R}$ is the electrochemical potentials of the left and right electrodes and $f_{L/R}$ is the Fermi distribution function [20]. With the applied bias potential V_b , the chemical potential of left electrode $\mu_L(V_b) = -eV_b/2$ and the chemical potential of right electrode $\mu_R(V_b) = +eV_b/2$. 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 $\Gamma_{L,R} = i(\sum_{L,R}^R(E) - \sum_{L,R}^A(E))$ is the coupling functions of the conductor to the left and right electrodes, $\sum_{L,R}^R(E)$ and $\sum_{L,R}^A(E)$ are the self-energy matrices used to include the effect of the left (right) semi-infinite electrode.

3. Numerical results and discussion

The transmission spectra of the Au–PTCDA–Au junctions or the GN(graphene nanoribbon)–PTCDA–GN(graphene nanoribbon) junctions at the equilibrium state are shown in Fig. 2(a) and (b), which is the most intuitive representation of quantum transport behaviors of the devices. In Fig. 2(a), A0 denotes the transmission spectrum of the

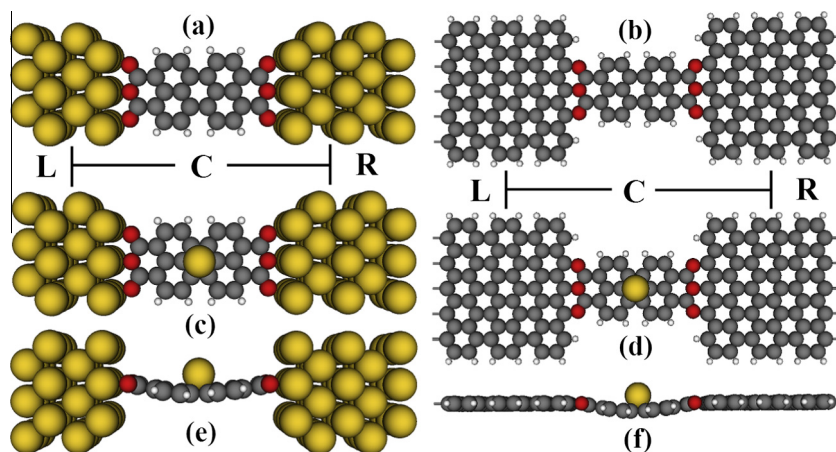


Fig. 1. Schematic diagram of the nonbonded configurations for (a) the Au–PTCDA–Au junction and (b) the GN–PTCDA–GN junction. The top view (c) and the side view (e) of the bonded configuration for the Au–PTCDA–Au junction. The top view (d) and the side view (f) of the bonded configuration for the GN–PTCDA–GN junction.

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