Chemical Physics 511 (2018) 27–32

Contents lists available at ScienceDirect

Chemical Physics

journal homepage: www.elsevier.com/locate/chemphys

Switching and oscillation of current along quinone based molecular device with graphene electrodes

Baoan Bian[a,*], Jingjuan Yang[a], Xiaoxiao Han[a], Peipei Yuan[a], Bin Liao[b]

[a] School of Science, Jiangnan University, Wuxi 214122, China
[b] College of Nuclear Science and Technology, Beijing Normal University, Beijing 100875, China

ARTICLE INFO

Keywords:
Molecular device
Electronic transport
Switching behavior

ABSTRACT

The electronic transport properties of quinone based molecular devices with zigzag graphene nanoribbon electrodes are investigated by using non-equilibrium Green's function and density functional theory. Although the devices with lateral linking groups -CONH and -NH_2 display different switching behavior, different lateral linking groups do not influence the presence of oscillated current. We discuss the switching effect, reversed current and oscillated current according to the transmission spectra and molecular projected self-consistent Hamiltonian. And the evolution of the frontier molecular orbital with the increase of bias is depicted to study effect of different linking group on the electron transmission. The results suggest that electron-withdrawing group -CONH is in favor of electron transmission and oscillated current originates from the change of molecule-electrodes coupling.

1. Introduction

Currently, molecular devices are designed to solve the problem that silicon-based microelectronics faced due to Moore's law. There are many interesting functions in molecular devices, such as switch [1,2], rectification [3,4], spin filtering [5,6], negative differential resistance (NDR) [7,8], memory effects [9,10] etc. The researches on molecular switching provide an important guidance to store digital information and route signals in molecular electronic logic circuits [11,12].

The molecular switching can be reversibly transformed between high conductance(ON) state and low conductance (OFF) state by photoexcitation/cite[13], redox reaction [14],scanning tunneling microscopy (STM) [15],electric field [16], pH value[17]. Many studies are carried out to further understand the switching mechanism. The substitution of atom and functional group in the molecules enhanced the switching behavior of molecular switching [18,19]. The lateral linking groups connected to molecule and electrodes influenced the performance of molecular switching due to the change of coupling between the molecule and electrodes [20]. It was reported that the switching behavior in the molecular device is influenced due to different substitution position of atom in the molecule [21]. Moreover, the electronic transport was investigated in the polyaniline-based molecular switching with gold and graphene electrodes [22,23].

Due to high carrier mobility, excellent mechanical strength and chemical stability, graphene has been applied to manufacture the molecular devices [24,25]. The theoretical investigations presented that the molecular switching based on graphene electrodes exhibited stable transmission properties and good conductivity [26]. Recently, diarylethenes based molecular switching with graphene electrodes has been fabricated, showing full reversibility and stability [27].

The quinone based molecular switching can reversibly transformed between the reduced hydroquinone (HQ) and oxidized quinone (Q) states by redox reactions, exhibiting the molecule-electrode binding geometry [28]. The first-principles calculations showed the oscillated current in the quinone based molecular switching with gold electrodes [29]. It is known that the linking groups influence the performance of molecular switching. The metaphenylene, paraphenylene and thienyl linkers modulate the conductivity of the molecular device due to the change of the degree of orbital hybridization with the metallic electrodes and the degree of orbital polarization [20]. The substituent of -NH_2 lowered the current switching ratio and the substituent of -NO_2 enlarged the current switching ratio in the molecular devices [19]. Therefore, in this work, we chose the electron-withdrawing group -CONH and electron-donating group -NH_2 as the lateral linking groups to study the switching behavior in the molecular device consisting of quinone based molecule and zigzag graphene nanoribbon(ZGNR) electrodes using a first-principles calculation. Compared with previous work, the different transmission spectra and oscillation of current are found in this work. And the results indicate that the lateral linking group influences the switching behavior.We discuss the effect of

* Corresponding author.
E-mail address: baoanbian@jiangnan.edu.cn (B. Bian).

https://doi.org/10.1016/j.chemphys.2018.05.027
Received 21 March 2018; Accepted 28 May 2018
Available online 29 May 2018
0301-0104/

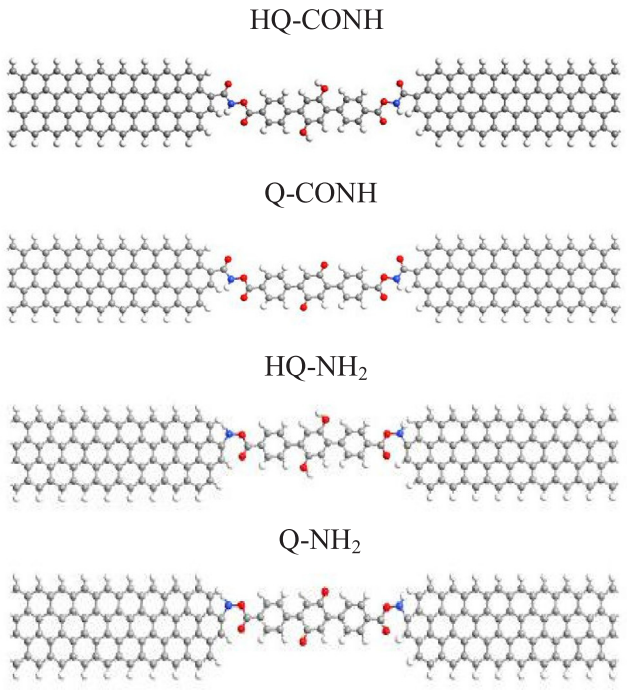

Fig. 1. Schematic diagram of molecular device. The gray, white, red and blue balls represent C, H, O, and N atoms respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

different linking group on the electron transmission according to the density of states, transmission spectra, molecular projected self-consistent Hamiltonian and evolution of the frontier molecular orbital.

2. Model and method

The designed moleculardevices are illustrated in Fig. 1. The pre-optimized the hydroquinone and quinone molecules are connected to zigzag graphene nanoribbons(ZGNRs) by different lateral linking groups -CONH and -NH_2. The molecular device is divided into three regions: left electrode, right electrode, and central scattering region. Along the transport direction, the semi-infinite electrodes are described by a supercell with three repeated ZGNR unit cells. The central scattering region consist of molecules and electrode extension considering the coupling between molecule and electrodes as well as electrode screening. The hydroquinone based and quinone based devices with -CONH and -NH_2 are called HQ-CONH, Q-CONH, HQ-NH_2 and Q-NH_2. We carry out the geometric optimization and electronic transport calculations for the present devices by density functional theory(DFT) and non-equilibrium Green's function(NEGF) as implemented in the Atomistix Toolkit (ATK)[30,31]package. It was reported that the difference between the generalized-gradient approximation (GGA) and local-density approximation (LDA) has only minor effect on the transmission spectrum [32]. Currently, the electronic transport properties in the molecular switching have been studied well by using LDA [33,34]. Thus in our calculations, we take the Perdew-Zunger functional within the local-density approximation (LDA.PZ)[35] as the exchange and correlation interactions. Double-zeta with polarization (DZP) basis set is taken for all atoms. In order to achieve a balance between calculation efficiency and accuracy, we take the k-point grid and the plane wave mesh cut-off as $1 \times 1 \times 400$ and 150 Ry,respectively.

The current through a molecular junction is calculated by the Landauer-Büttiker formula [36]:

$$I(V) = \frac{2e}{h}\int_{\mu_L}^{\mu_R}[f(E-\mu_L)-f(E-\mu_R)]T(E, V)dE \quad (1)$$

where f is the Fermi function, being with $\mu_{L/R}$ represents the electrochemical potential of the left/right electrode, and T(E,V) the transmission probability of electrons as a function of E and V. Furthermore,

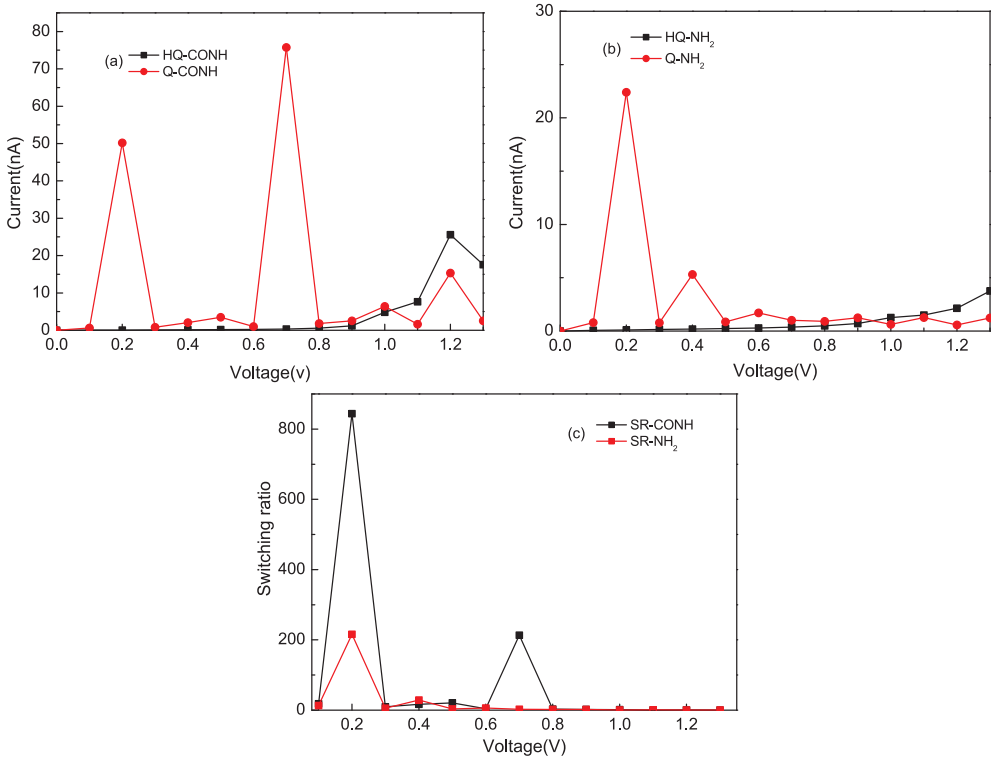

Fig. 2. (a), (b) The calculated I-V curves of the molecular switch with lateral linking groups of -CONH and -NH_2,respectively. (c) The switching ratio of current at different bias voltage.SR-CONH = $I_{Q-CONH}/I_{HQ-CONH}$ and SR-NH_2 = I_{Q-NH_2}/I_{HQ-NH_2}.