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Theoretical studies on electronic transport properties of 2,5-dimercapto-pyridazin molecular junctions: influence of CO and H_2O molecules

Ying-Feng Zhang, Xiao-Hua Yi, Zheng Zhang, Jun-Xia Sun and Zong-Liang Li*

College of Physics and Electronics, Shandong Normal University, Jinan, 250014, the People's Republic of China

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Abstract. Based on first-principles calculations, the electrode force acted on 2,5-dimer capto-pyridazin molecular device is studied. The pressing effects of CO and H_2O molecules on the 2,5-dimercapto-pyridazin molecular junctions are also studied at B3LYP level to simulate the effects of little ambient molecules on the functional molecular junctions. The electronic transport properties of 2,5-dimercapto-pyridazin molecular junction with the pressing of CO and H_2O molecules are studied by employing elastic scattering Green's function method. The numerical results show that the 2,5-dimercapto-pyridazin can be squeezed out of the electrode gap when the electrode distance is compressed to 1.02 nm. It is need about 1.5 nN stretching force to break down the 2,5-dimercapto-pyridazin molecular junction, which agrees with the experiment probes very well. The 2,5-dimercapto-pyridazin molecule is bent by the pressing of CO or H_2O molecule, and is pushed to the edge of Au (111) triangles with the terminal S atoms first to the bridge and then to the top positions of Au (111) triangles, until at last one terminal S atom is pushed out of Au (111) triangle. The pressing of CO and H_2O molecules to the molecular junctions will enhance the couplings between molecule and electrodes, which further enhances nonresonant transmission of the molecular junctions.

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Key words: molecular device; 2,5-dimercapto-pyridazin molecule; electronic transport properties; effect of small ambient molecule.

1 Introduction

Due to its high efficiency, low energy consumption and high integration density, the single molecular devices have been paid more and more attention to in the studies in recent

*Corresponding author. *Email address:* lizongliang@sdnu.edu.cn (Z.-L. Li)

years. Various kinds of nano-structures like atomic wires [1], short organic molecular wires [2,3,4], long-chain polymers [5], carbon nanotubes [6] and fullerenes [7] have been investigated experimentally, and many valuable properties have been found. Most of the studies in this area are focused on the spatial structure, electrical transport properties, negative differential resistance, rectification or switching properties of the molecular devices, and so on. Both experimental and theoretical works have proved that the electronic transport properties and functional performance of the molecular devices are determined by many factors [5,8-28], for instance, molecular structure [9], contact configuration [19], positions of the terminal atoms on the metal surfaces [11], distance between the electrodes [20], pressure of the electrodes [10,15], ambient [12,13,18], etc..

In experimental measurement, molecular junctions may be probed in different circumstance, such as solution or gas, etc. It is inevitable that the irregular movements of the ambient molecules may push the functional molecule out of the electrode gap. Thus in this article, the effects of small ambient molecules on the geometric structures and electronic transport properties of organic molecular junctions are investigated. Based on the *ab initio* calculation, the presses of small ambient molecules such as CO and H_2O on 2,5-dimercapto-pyridazine molecular junctions are simulated, and the electronic transport properties with different pushing displacements are discussed applying elastic scattering Green's function method. The studies not only reveal that the pushing of the small ambient molecules can break down organic molecular junctions, but also are helpful to understand gas sensitivity or humidity sensitivity of molecular device.

2 Theoretical details

A molecular junction consists of a functional molecule and two gold electrodes. In order to simulate the 2,5-dimercapto-pyridazin molecular junction [29], we sandwiched the molecule between two gold atom clusters to form gold-molecule-gold extended molecule. By this way, the influence of electrodes on the functional molecule can be approximately considered, because the gold atom clusters which consist of the gold atoms nearby the functional molecule can screen the influence of the other gold atoms which are far away from the molecule. The schematic structure of 2,5-dimercapto-pyridazin molecular junction is shown in Fig. 1, where the terminal S atoms on the hollow position of Au (111) surfaces/triangles. In the calculation, we changed the electrode distance and relaxed the functional molecule by performing geometric optimization at B3LYP level with Lanl2DZ basis set in Gaussian03 packages [30]. The distance with the lowest energy corresponds to the equilibrious electrode distance. At equilibrious distance, the pressing of small ambient molecule on the molecular junction was simulated by moving the small ambient molecule close to the functional molecule gradually, which are also simulated at B3LYP level with Lanl2DZ basis set in Gaussian03 packages [30].

The electronic transport properties of molecular junctions are studied applying elastic scattering Green's function method based on the general Green's function formalism of