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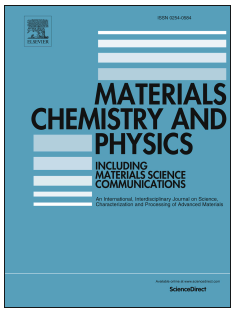

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Effect of the lateral linking groups on the switching behavior in single molecular device

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Abstract

We study the electronic transport properties of **biphenyl-2,2'-dithiol** molecule connected to graphene electrodes through different lateral linking groups by density functional theory and non-equilibrium Green's function. It is clearly found that the different lateral linking groups in molecule devices significantly influence the current and switching ratio. The linking groups $-NH_2$ and $-CH_3$ decrease the switching ratio. The linking groups $-BO_2$, -COOH and -OH enhance the switching ratio. The characteristics of the molecular switch are analyzed by transmission spectra in the different bias and the molecular projected self-consistent Hamiltonian at zero bias. Furthermore, the observed negative differential resistance effect in devices with $-NH_2$ and -OH in the oxidation state is explained by transmission spectra. The results suggest that the reasonable different lateral linking groups in the devices may significantly influence the current and switching ratio, displaying a potential application in future molecular circuit.

Keywords

Molecular device; Lateral linking group; Electronic transport; Switching behavior

Introduction

In recent years, with the increasing demands of miniaturization of microelectronic devices, silicon-based electronic devices have been facing the challenge due to Moore's Law. Many researchers focus on the nanodevices that show the strong stability and fast response[1,2]. A variety of functions in the molecular device, such as molecular switch[3-5], rectification[6,7], negative differential resistance(NDR) effect[8,9], field effect transistor[10] and spin filter[11,12], are investigated theoretically and experimentally. Molecular switch has an important potential application of the logical storage in the future[13,14].

The molecular switch is transferred between the "ON"(high conductance) and "OFF"(low conductance) states, which can control the strength of the current in the molecular circuit. A lot of trigger conditions induce the change of state, including the redox reaction[15,16], photoexcitation[17,18], electric field[19,20], the tip of scanning tunneling microscopy(STM)[21] and other external stimuli. Recently, photochromic molecules including azobenzene[22], diarylethenes[23], and spiropyran[24] are used to study the molecular switch, which can **be** reversible switched in different conductance states. The central molecule, electrodes and the lateral linking groups connecting molecule and electrodes influence the performance of molecular switch. Thus it is necessary to further understand the