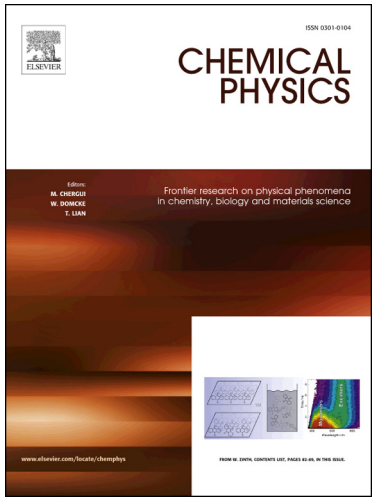

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Effect of different substitution position on the switching behavior in single-molecule device with carbon nanotube electrodes

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Abstract

We investigate the electronic transport properties of dihydroazulene(DHA) and vinylheptafulvene(VHF) molecule sandwiched between two carbon nanotubes using density functional theory and non-equilibrium Green´s function. The device displays significantly switching behavior between DHA and VHF isomerization. It is found the different substitution position of F in the molecule influences the switching ratio of device, which is analyzed by transmission spectra and molecular projected self-consistent Hamiltonian. The observed negative differential resistance effect is explained by transmission spectra and transmission eigenstates of transmission peak in the bias window. The observed reverse of current in VHF form in which two H atoms on the right side of the benzene ring of the molecule are replaced by F is explained by transmission spectra and molecule-electrode coupling with the varied bias. The results suggest that the reasonable substitution position of molecule may improve the switching ratio, displaying a potential application in future molecular circuit.

Keywords

Molecular switch; Electronic transport; Switching behavior

Introduction

With the development of silicon-based microeletronics ,more and more researches found the limitations of this approach due to the difficulties of the production process and the laws of physics, looking for new methods. Molecular electronics is a new method that can desigen molecular electronic devices by organic molecules and not be affected by Moore's Law. Recently, a variety of different functional molecular devices have been studied and prepared successfully, such as molecular switch[1-3], negative differential resistance[4,5], spin filtering[6,7], molecular rectifier[8,9], etc. Molecular switch as an essential part of the molecular electronic device attracts great attention.

The molecular switch is a class of bistable quantum system, which can switch between the two states reversibly. One of the states is high conduction (ON) state, allowing current flow through molecular electronic logic circuits and another is low conduction (OFF)state, preventing current transmission. The transformation between two states in the molecular switch is achieved by light[10], the redox process[11], the electric field[12] and other external trigger conditions. Photoexcitation is a stable and rapid way to achieve change of molecular structure. At present, the studies on molecular switch mainly are focused on the electron transport properties of azobenzene[13,14] and diarylethene[15,16]. The azobenzene molecule can be switched between the “trans” and “cis” forms by the light stimulus. The open and closed isomers of diarylethene molecule have obvious switching properties under light