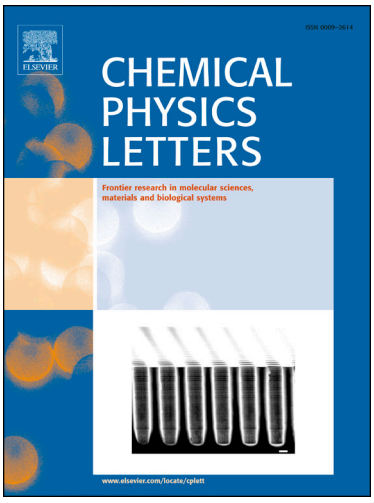

Research paper

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A first-principles study of aryloxyanthraquinone-based optical molecular switch7

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Abstract

We study the transport properties of 4-((9,10-dioxo-9,10-dihydroanthracen-1-yl)oxy) benzaldehyde molecular optical switch by the first-principles calculations. Our molecule can reversibly switch between trans and ana forms by visible or UV irradiation. We studied many properties such as, I–V characteristics, the effect of electrode materials on electronic transport properties, on-off ratio and spatial distribution of molecular projected self-consistent Hamiltonian orbitals corresponding to both forms. The physical behaviour of conductance interpret in terms of the HOMO–LUMO gap, the effective conjugation lengths, and size of the frontier molecular orbitals. Our results show, current through the ana form is higher than that the trans form.

Keywords: Nano-electronic device; Electronic transport; Non-equilibrium Green's function; Aryloxyanthraquinone.

1. Introduction

Photochromism is characterized by photo-induced reversible isomerization of one isomer to another isomer, which has a different absorption spectrum; different colors are created from compounds in crystal, amorphous or liquid phases. Under electromagnetic radiation (usually ultraviolet light), stable thermodynamic shape (A) transforms to a new colorful type (B) via photochemical reaction. Furthermore, the type (B) changes to the first shape (A) on a reverse direction via another light source like visible light or heat [1-3]. Photochromism delivers a suitable insight to the expansion of optical sensing applications [4],