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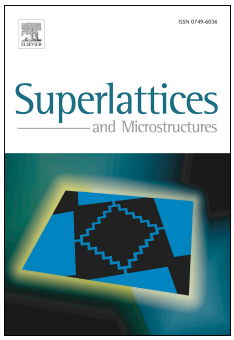

Theoretical study of electron transport throughout some molecular structures

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Theoretical study of electron transport throughout some molecular structures

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Abstract

The present work is a theoretical study of the electronic properties of some molecular structures. The system that takes into account in the study is left lead-donor-molecule-acceptor-right lead. The molecule, such as (phenyl, biphenyl, triphenyl, naphthalene, anthracene, and phenanthrene), is threaded by magnetic flux. This work contains two parts. First is computing density of states of the molecular structures as a closed system by density functional theory (DFT). Second is calculating the transmission probability and electric current of such molecular structures as an open system by steady-state theoretical model. Furthermore, the most important effects, taking into consideration are quantum interference, magnetic flux, and interface structure. Our results show that the connection of the molecule to the two leads, the number of rings, the magnetic flux, and the geometrical structure of the molecule play an important role in determining the energy gap of molecular structures.

Keywords: electron transport, single molecule, transmission probability, I-V characteristics.

1. Introduction

Single molecules as active electronic units have attracted huge attention in fabricating nanoelectronic devices [1-7]. During 1974s Aviram and Ratner [8] first studied theoretically the electron transport properties in molecular structures. The fundamental idea of such nanoelectronic devices is that the two metallic electrodes are separated by a gap preventing any transport of electrons. However, the insertion of a single molecule within this gap can operate as a bridge and thereby allow for crossing of electrons from one electrode to another. Many experiments have been carried out on electron transport through molecules inserted between two metallic electrodes [9, 10]. One of the most interesting advantages of these devices is its size. The small size of the devices, making the transfer of a single molecule of interest, particularly for information technology devices, as the demand for device miniaturization is growing rapidly. Obviously, in such small scales, quantum mechanical effects become crucial. This is due to the quantization of electronic spectrum with energy scale about eV [11]. Quantum interference effects can strongly influence electron transport properties at the molecular scale [2, 12-17].

Several studies that consider quantum interference effect in molecular structures have been published recently. The transmission properties and *I–V* characteristics of molecular structures connected to two metallic electrodes were investigated in terms of local molecular structures [18, 19]. In 2002, Baer and Neuhauser studied the quantum interference effect in a long alkene molecular wire and calculated transmission probability and *I-V* characteristics. They discuss possibility designing XOR switch based on the quantum interference effect [20]. In 2003, Liu et al. investigated a molecular wire containing a crown-6 molecule attached to sulfur atoms to two long atomic gold wires. They computed transmittance, a density of states and conductance by using DFT, they reveal the cationic binding suppresses conductance due to quantum interference effects [21]. Maiti calculated conductance and current by using of Green's function technique in four works with depending on quantum interference effects and molecule-to-electrode coupling strength. He studied different single polycyclic hydrocarbon molecules [22], single conjugated molecules [23], benzene-1, 4-dithiolate molecule and some other geometric structures[24] and single phenalenyl molecule [25]. In 2010, Rai et al. studied circular currents in many ring structures such as benzene, azulene, naphthalene, and anthracene and reveal that circular currents happen in such molecular structures [26]. Several efforts have already been made to interpret the electron transport properties throughout molecular structures. But the main motivation behind this work is explain effective factors on energy gap and electron transport properties of molecular structures as an open or closed system.