Organic Electronics 27 (2015) 92–100

Contents lists available at ScienceDirect

Organic Electronics

journal homepage: www.elsevier.com/locate/orgel

Negative differential resistance, rectifying performance and switching behaviour in carbon-chain based molecular devices

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ARTICLE INFO

Article history:
Received 13 May 2015
Received in revised form
5 September 2015
Accepted 9 September 2015
Available online 19 September 2015

Keywords:
Mono atomic carbon chains
I–V characteristics
Transmission spectrum
NEGF-DFT
Rectification ratio
Multi switching

ABSTRACT

Using non equilibrium Green's function formalism coupled with density functional theory, we carry out electronic transport calculation in two types of molecular devices, one constructed by linear monoatomic carbon chain (···C–C–C–C ···) and the other by two carbon chains capped with a phenyl ring (···C–C–Ph–C–C···), sandwiched between two z-shape electrodes, constructed by zigzag-armchair-zigzag (zz-ac-zz) graphene nanoribbons (GNRs). The potential difference between the z-shape contacts can be varied by employing an external d.c. voltage source. Thus, one may observe the variation of conductivity through the channels. The current–voltage (I–V) characteristics of the proposed resistors show N-type negative differential resistance (NDR), within a particular voltage region. The figure of merit or PVR (peak to valley) ratio (I_{peak}/I_{valley}) gets significantly increased, on capping the chains with phenyl ring. A higher value of PVR in I–V characteristics enhances the possibility of applications utilizing NDR. The calculated I–V characteristic is asymmetric and the rectification ratio is found to be 7, in case of the linear carbon chain.

The rectification ratio $R(V) = I(V)/I(-V)$ is an important parameter which determines, its suitability as rectifying device. It has been demonstrated that on varying the conformation of the phenyl ring with respect to the plane of electrodes, the transport properties of the system can be modulated. Interestingly, I–V characteristics are asymmetric and show dual NDR peaks in perpendicular conformation of the phenyl ring, with respect to the electrodes in the (···C–C–Ph–C–C···) system. The figure of merit is found to be respectively 8 and 51 for the first and second NDR regions. The later value is extremely high, making it an excellent candidate for potential applications. Moreover, the multi peak NDR device may be widely used in multiple-valued logics. Only a limited number of multiple NDR peak molecular-based nano systems have so far been reported, which are quite complex; by contrast the present system seems to be quite simple. The physical phenomenon of NDR was explained in the light of molecular projected self-consistent Hamiltonian (MPSH) and also the evolution of the frontier molecular orbitals (HOMO–LUMO) as well as transmission under various external bias voltages.

1. Introduction

As electronic devices are getting miniaturized, silicon-based technology is fast approaching its physical and technological limits. Beyond a certain scale, silicon based devices will definitely cease to operate, as quantum effects set in, in that domain. Molecular electronics seems to be a promising alternative for future [1] nanoelectronics. The advantages of using molecular based devices are, high packing density, faster response time, less operational power and high efficiency. Molecular electronics usually addresses the issue of molecular junction transport, where the molecule acts as a barrier for incoming electrons. From the point of view of applications; it is of great interest in the context of studying transport characteristics through molecules and molecular systems. They may act as building blocks and play a crucial role in the development of nanoelectronics. The first suggestion of electronic transport through molecules was reported in 1970's [2,3]. Dithiol-benzene (DTB) molecule coupled to Au(111) gold surfaces [4] has been a prototype of standard model system for initial theoretical studies [5–14]; by virtue of the stability of thiol-terminated organic molecules employing gold electrodes.

During the last few years, electronic transport through various

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http://dx.doi.org/10.1016/j.orgel.2015.09.014
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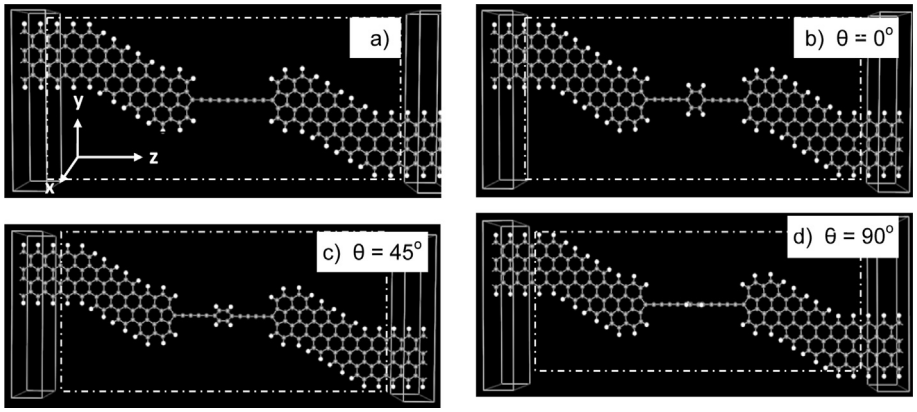

Fig. 1. Schematic representation of device models used to predict transport properties of the systems with a) A ten carbon atom long chain; b) two carbon chain capped system with phenyl ring coplanar with the plane of electrodes; c) two carbon chain capped system with phenyl ring making an angle of 45° to the plane of electrodes; d) carbon chains capped system with the phenyl ring at right angle to the plane of electrodes. The portion inside the dotted line rectangle shows the scattering region. The difference in the electrostatic potential between the electrodes generates the current. The scattering region (shown by dotted rectangle) includes the carbon chain system and the surface layers. The direction of electron transport is along carbon atomic chain, labelled as z.

systems has been extensively studied [15–34]. The current–voltage (I–V) behaviour of these systems reveals several interesting and useful physical features which can be utilized in fabrication of future novel nano devices. Various molecular devices such as switching [35,36], dual-conductance transport [37], molecular rectification [38–41], and negative differential resistance (NDR) [42–45] have been reported in the past. Prominent among these is negative differential resistance (NDR), which involves rise and fall in current, as the bias voltage is steadily increased. NDR has found applications in a vast range of devices; including logic circuits, memory, switching, amplification and many others.

Linear atomic carbon chains are generally classified as cumulenes (with equal double bonds between carbon atoms) and polyyne (alternate single and triple bond) regarded as one dimensional molecular wires. They have long been anticipated as active component of molecular devices, due to their theoretically predicted extraordinary physical and chemical properties [46]. Until 2009, the experimental studies of carbon chains were limited due to lack of reliable and effective ways of producing them; owing to their high reactivity. By irradiating energetic electrons on GNR inside a transmission electron microscope, Jin et al. [46] in 2009 reported the production of 2.1 nm carbon atomic chains consisting of sixteen atoms. The average bond length in such *sp*-hybridized carbon chain is smaller than the sp^2-hybridized GNR edge. Shorter bond length implies more valance electrons distributed around bonds; there by increasing the bond strength. These rigid carbon chains may be regarded as ultimate basic components of molecular device. Difference in electronic character of electrodes results in remarkably different transport behaviour. Since the bands near the Fermi level mainly arise from the π-orbital of the carbon atom, the transport is dominated by the π-electron, which is delocalized, in real space.

In this study, we present DFT-calculation based findings regarding the conductance of a) mono atomic ten carbon atoms long chain, b) two carbon chains capped with a phenyl ring each linking a pair of z-shape electrodes constructed by zigzag-armchair-zigzag (zz-ac-zz) graphene nanoribbons (GNRs). The electronic transport is determined by the electronic structure of the system and the scattering at contact–channel interface. The conformation of molecule generally affects the conduction behaviour [47]. It is of interest to calculate the transport parameters in coplanar and perpendicular conformations of the phenyl ring and

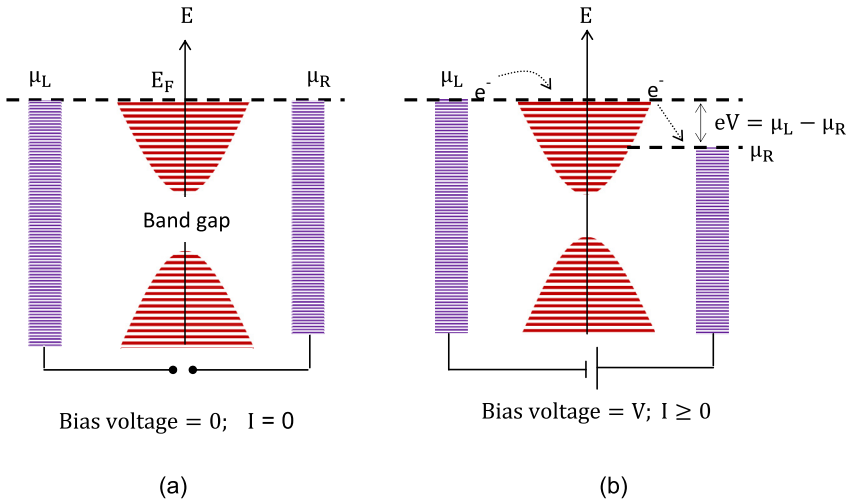

Fig. 2. Cartoon of the junction setup. The density of states (DOS) of the molecular system is shown between the electrodes. (a) At zero bias, the chemical potentials of both the electrodes match the fermi level of the system so the transmission is zero; (b) at finite bias due to potential gradient, the electrons transmit from left to right electrode via the molecular levels within the bias window $\Delta\mu = \mu_L - \mu_R$.