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Multi-terminal electron transport through single phenalenyl molecule: A theoretical study

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ABSTRACT

We do parametric calculations to elucidate multi-terminal electron transport properties through a molecular system where a single phenalenyl molecule is attached to semi-infinite one-dimensional metallic leads. A formalism based on the Green's function technique is used for the calculations while the model is described by tight-binding Hamiltonian. We explore the transport properties in terms of conductance, reflection probability as well as current–voltage characteristic. The most significant feature we articulate is that all these characteristics are very sensitive to the locations where the leads are connected and also the molecule-to-lead coupling strengths. The presence of other leads also has a remarkable effect on these transport properties. We study these phenomena for two-, three- and four-terminal molecular systems. Our numerical study may be utilized in designing tailor-made molecular electronic devices.

1. Introduction

Speed of growth of molecular electronics is being accelerated more and more as it has brought together scientists and engineers from various disciplines. The reason behind this attraction is inscribed into its smallness of size with wonderful electronic properties. In addition, several other properties such as magnetic, optical, etc., have been recognized in different molecules, which may be utilized in artificially tailored devices that are not possible with conventional materials [1]. The concept of electron transport which emerged first in the theoretical work of Aviram and Ratner [2] has opened a new era in the field of nanoscience. But at that time any type of measurement in such a small scale was a long-sought goal. Study at molecular scale level is not a simple one as we cannot avoid the effect of interface to the external electrodes. However, the progress in the theoretical works [3] was continuing, which bestowed inspirations to the experimentalists to take such task as a challenge. Now with the advancement in nanotechnology, it is possible to investigate several transport properties not only through a group of molecules [4] but also through a single molecule [5]. This single molecular electronics may play a key role in designing nanoelectronic circuits. For this we have to have a thorough understanding of the electronic transport processes at this molecular scale level [6–11]. Many problems are yet to be solved to make this field much more reliable. Therefore, the electron transport in molecular systems is an open area and detailed investigations of molecular transport are still needed.

All these works we have referred above are related to two-terminal electron transports. We can also analyze various transport phenomena of a multi-terminal system, which was first addressed by Büttiker [12]. The Büttiker formalism, which is an extension of the Landauer two-terminal conductance formula, is a very simple and elegant way to divulge the transport mechanism in terms of various transmission probabilities. There are several

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pioneering works [13–17] based on this formalism, which are very interesting from the theoretical as well as experimental point of view.

Several *ab initio* methods [18–21] are there which may be utilized to study electron transport properties through molecular junctions. At the same time, tight-binding model has been extended to density functional theory (DFT) for transport calculations [22]. But in case of molecular systems, the investigations based on this theory (DFT) have some quantitative discrepancies compared to the experimental predictions. Moreover, these *ab initio* theories are computationally very expensive. To avoid this we do model calculations by using a simple tight-binding framework.

In the present article we do a theoretical study of multi-terminal electron transport through a single phenalenyl molecule [23,24] attached to semi-infinite one-dimensional (1D) metallic leads. We do numerical calculations based on single particle Green's function formalism [25,26] to evaluate conductance, reflection probability and current–voltage characteristics. Quite interestingly, we show that the positions where the leads are connected to the molecule as well as the presence of other leads have eloquent effects on these transport properties. Moreover, these characteristics are also influenced significantly by the molecule-to-lead coupling strengths. These aspects can be utilized in designing nanoelectronic devices.

We organize the paper as follows. With a brief introduction (Section 1), in Section 2 we describe our model and the theoretical background. Results are analyzed in Section 3. Finally we conclude our results in Section 4.

2. Model and a view of theoretical formulation

In this section we focus our attention on the systems where a single phenalenyl molecule is attached symmetrically or asymmetrically to semi-infinite 1D metallic leads through thiol (SH bond) groups. The models are shown schematically in Fig. 1(a)–(c) where, the number of leads attached to the molecule is 2–4, respectively. To evaluate the conductance (g) and current (I) through this single molecular system we adopt the Green's function technique. For this, first we define the Green's function for the whole system as,

$$G = (E - H)^{-1} \tag{1}$$

where $E = \epsilon + i\eta$ with η arbitrarily very small number which can be set as zero in the limiting approximation. ϵ is the injecting electron energy. H is the Hamiltonian of the entire system which is of infinite dimension. So, the above equation deals with the inversion of an infinite dimensional matrix corresponding to the system consisting of a finite size molecule and semi-infinite leads. However, the full Hamiltonian can be partitioned into sub-matrices that correspond to the individual sub-systems like,

$$H = H_M + \sum_{p=1}^{N} \left(H_p + H_{pM} + H_{pM}^{\dagger} \right) \tag{2}$$

where H_M and H_p are the Hamiltonians of the molecule and lead-p, respectively. N is the number of leads to which the molecule is attached. H_{pM} represents the coupling matrix that will be non-zero only for the adjacent points in the molecular system (molecule with sulfur atoms) and the lead-p. Here all the leads are treated on an equal footing. Within the non-interacting picture, the tight-binding Hamiltonian of the molecular system can be manifested as,

$$H_M = \sum_i \epsilon_i c_i^{\dagger} c_i + \sum_{\langle ij \rangle} t \left(c_i^{\dagger} c_j + c_j^{\dagger} c_i \right) \tag{3}$$

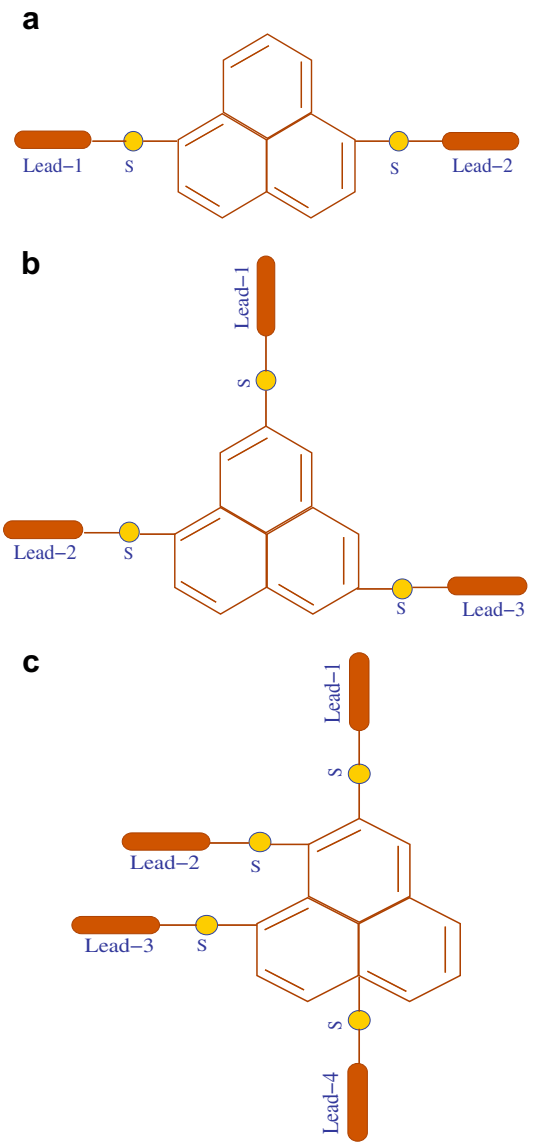

Fig. 1. Multi-terminal quantum system. A phenalenyl molecule is attached symmetrically or asymmetrically to semi-infinite 1D metallic leads through thiol (SH bond) groups in the chemisorption technique where sulfur (S) atoms reside and hydrogen (H) atoms remove. The filled yellow circles correspond to the location of S atoms. The number of leads attached to the molecule is 2, 3 and 4 as shown in (a), (b) and (c), respectively. Leads are denoted by lead-1, lead-2, lead-3 and lead-4. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)