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Conductance of three-terminal molecular bridge based on tight-binding theory*

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The quantum transmission characteristic of three-benzene ring nano-molecular bridge is investigated theoretically by using Green's function approach based on tight-binding theory with only a π orbital per carbon atom at the site. The transmission probabilities that electrons transport through the molecular bridge from one terminal to the other two terminals are obtained. The electronic current distributions inside the molecular bridge are calculated and shown in graphical analogy by the current density method based on Fisher–Lee formula at the energy points $E = \pm 0.42$, ± 1.06 and ± 1.5, respectively, where the transmission spectra appear peaks. We find that the transmission spectra are related to the incident electronic energy and the molecular levels strongly, and the current distributions agree well with Kirchhoff quantum current momentum conservation law.

Keywords: molecular bridge, transmission probability, molecular device
PACC: 6146, 0560, 7215

1. Introduction

Nano-molecular devices have been extensively investigated theoretically and experimentally since the concept of organic molecular electronics was proposed by Aviram and Ratner in the 1970s.[1] It is notable that the molecular devices become much more important components in fabricating smaller, faster and cheaper nano-electronic devices.[2] In the last decade, nanowires,[3] molecular memories,[4] nano-switching devices,[5] nano-logic gates,[6] molecular diodes[7] and transistors[8] have been proposed or researched. Recently, monovalent atomic wires,[9] the molecular wire current switch,[10] atomic bridge[11] and zero bias molecular conductance[12] have been reported. In particular, it is possible to fabricate molecular devices easily by the technology of the growth of single domain monatomic arrays[13] and the formation of pentacene.[14] Among them, the conductance properties of these molecular devices have been the focus of current researches,[15–21] since they are basic elements for understanding a variety of molecular electronic devices. In applications, it is very important to fabricate multi-terminal molecular devices, as a molecular bridge which can connect to a variety of devices in the nano-electronic circuits.

In this paper we present a model for a three-terminal molecular bridge consisting of 3 benzene rings with 14 carbon atoms, which has not been fully investigated theoretically so far. We study this problem in order to find and clarify new conductance characteristics and electron current distributions in such a nano-molecular bridge. The electronic transmission in a nano-scale molecular device should be described in a full quantum wave mechanical treatment, because some experiments suggested that electrons passing through a molecule do not behave like those in an ohmic resistor but show quantum features arising from the wave states of the electrons.[22] In this work, the electronic transmission spectra are obtained with the Green function method based on the tight-binding theory, in which only a π-orbital electron is considered for per carbon atomic site, and then the quantum current distributions inside the bridge are obtained by us-

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ing current density theory[23,24] at the energy points where the transmission spectra peaks appear clearly.

In addition, we also find that the quantum currents are not distributed on the segment evenly, and loop currents are not induced inside the molecular bridge.

2. Model and method

The molecular bridge model adopted in our study is composed of three benzene rings with 14 carbon atoms, and the bond length between the nearest atomic sites is 0.14nm. Three terminal sites of the bridge are connected to the atomic chain electrodes as shown in Fig.1. Each carbon atom in the benzene

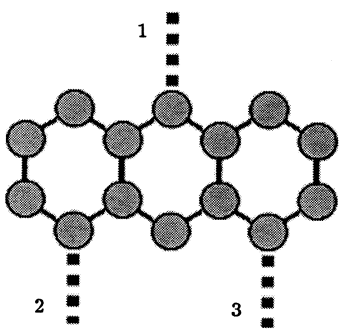


Fig.1. Three-terminal molecular bridge model.

rings has only one π-orbital electron of the 4 valence electrons. The electron transport in such a molecular bridge is primarily governed by the π-orbital electron,[25] so that we consider that it is sufficient to use the tight-binding theory with only one π orbital per atomic site. For the sake of simplicity, we neglect the electron–phonon coupling effect. This means that electronic transport is due to the elastic scattering and the coherence completely in the molecular bridge, and then the nearest neighbour hopping integral is taken into account only for the molecules and the leads. Thus the transmission probabilities $T_{\rm SD}(E)$ for electrons transmitting through the bridge are described precisely by Landauer–Büttiker theory,[26−29] i.e.

$$T_{\rm SD}(E) = {\rm Tr}[\Gamma_{\rm S} G^{\rm R} \Gamma_{\rm D} G^{\rm A}], \tag{1}$$

where $G^{\rm R(A)}$ is the retarded or the advanced Green's function of the whole system related to the incident electron energy E, which is defined by

$$G^{\rm R(A)} = \frac{1}{E - H_{\rm c} - \Sigma_1^{\rm R(A)} - \Sigma_2^{\rm R(A)} - \cdots - \Sigma_{\rm n}^{\rm R(A)}}. \tag{2}$$

In Eq.(2), $H_{\rm c}$ represents the Hamiltonian of the molecular part, and the retarded or the advanced self-energy $\Sigma_q^{\rm R(A)}$ (q=1, 2, 3) represents an effective potential arising from the interaction of the molecule with the electrode. $\Gamma_{\rm S(D)}$, the coupling between the lead and the atom site, is given by

$$\Gamma_{\rm S(D)} = {\rm i}\left[\Sigma^{\rm R}_{\rm S(D)} - \Sigma^{\rm A}_{\rm S(D)}\right]. \tag{3}$$

The self energy non-zero matrix elements corresponding to the sites attached to the S (D) leads are defined by

$$\Sigma^{\rm R(A)}_{\rm S(D)} = t'^2_{\rm S(D)} g^{\rm R(A)}_{\rm S(D)}, \tag{4}$$

where $t'_{\rm S(D)}$ and $g^{\rm R(A)}_{\rm S(D)}$ represent the coupling strength and the Green function for the leads, respectively. The latter is given as follows:

$$g^{\rm R(A)}_{\rm q} = \frac{E + {\rm i}\sqrt{4t_{\rm q}^2 - E^2}}{2t_{\rm q}^2}. \tag{5}$$

Here, q represents the nearest neighbouring sites, and $t_{\rm q}$ is the hopping integral between sites.

In order to design and fabricate molecular devices, it is also necessary to clarify the electronic current distribution: i.e., the magnitude and direction of the electronic current on each segment inside the molecular devices. In the framework of the quantum current density,[30−33] the quantum current from site i to site j is given by

$$I_{ij} = \frac{4e}{\hbar}{\rm Im}[\psi_i^* H_{ij} \psi_j], \tag{6}$$

where H_{ij} is the ij element of the Hamiltonian, and $\psi_{i(j)}$ is the electronic wavefunction at site $i(j)$. In our calculation the wavefunction $\psi_{i(j)}$ is expanded in terms of the molecular orbital $\phi_{\rm n}^{\nu}$ in the molecular region, i.e.

$$\psi_{\rm n} = \sum_{\nu} a_{\nu} \phi_{\rm n}^{\nu}, \tag{7}$$

where a_{ν} is the expanding factor. In the calculation, the strength of the bond current is expressed in units of $4e/h$.

3. Calculation and results

To investigate the dependence of the transmission spectra on the incident electron energy, the same atomic energy value is taken for each site. The hopping parameters (t) are taken as general because the elastic scattering is considered completely in the leads and the molecular body. The coupling between the atomic lead and the atomic site of the molecule, which is weaker than those between the neighbouring atoms

in the leads and in molecular body, is taken to be $t' = 0.6t$; then the energy is assumed to be stable at each atomic site. Thus the electronic transmission spectra obtained from terminal 1 to 2, 1 to 3 and 2 to 3 are shown in Figs.2, 3 and 4, respectively. From the results, some electronic transmission characteristics are clarified. (1) The transmission spectrum of Fig.2 is the same as that of Fig.3 due to the perfect symmetric geometry of the electronic channel. (2) The transmission spectra appear to be in the same category. The peaks appear at the same energy points from terminal 1 to 2 and 1 to 3 due to the symmetry. (3) The transmission probabilities from terminal 1 to 2 and 1 to 3 are 0.5, respectively, at energy points $E = \pm 0.42$, ± 1.5 as shown in Figs.2 and 3. However, the sum of both transmission probabilities is 1.0 at each peak. It means that the incident electrons transmit from the input to the two output terminals evenly. Namely, 50% of the incident electrons transmit to terminal 2, and the other 50% to terminal 3. (4) Assuming terminal 2 to be the incident one, the transmission spectrum from terminal 2 to 3 is quite different from what mentioned above in (3). There are only two peaks whose amplitudes are all 0.95 at $E = \pm 1.06$, which means that 95% of the incident electrons have transmitted to terminal 3, and only 5% transmit to terminal 1. (5) These transmission spectra also show that the incident electrons transmit through the molecular bridge hardly when the incident electronic energy is zero. It is obvious that this agrees well with the physical principle. Other low amplitudes appear due to the level difference between the incident electrons and the molecule.[34] In addition, the oscillatory feature of the electron transmission that is related to the quantized molecular level had been described in great detail in our previous paper.[35]

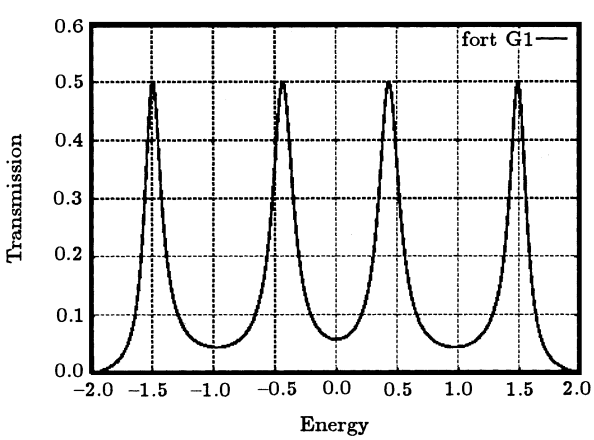


Fig.2. Transmission spectrum from terminal 1 to 2.

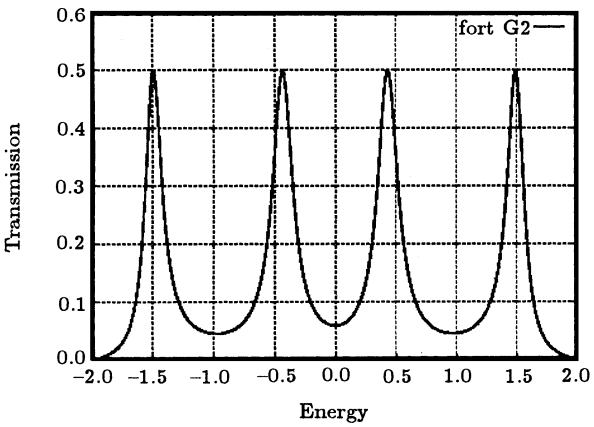


Fig.3. Transmission spectrum from terminal 1 to 3.

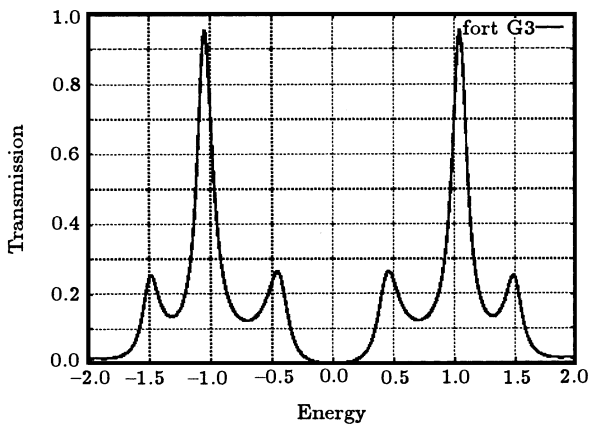


Fig.4. Transmission spectrum from terminal 2 to 3.

By using Eqs.(6) and (7), the quantum current distributions inside the bridge are calculated numerically and shown graphically at the energy points $E = \pm 0.42$, $E = \pm 1.06$ and $E = \pm 1.5$ where transmission probabilities are peaks. The directions and the amplitudes of the input, output and the bond current are shown in Figs.5 and 6, respectively. These results illustrate that the incident electrons transport directly from the input to the output terminals, and the bond currents arrowed on the segments have definite directions and the amplitudes.

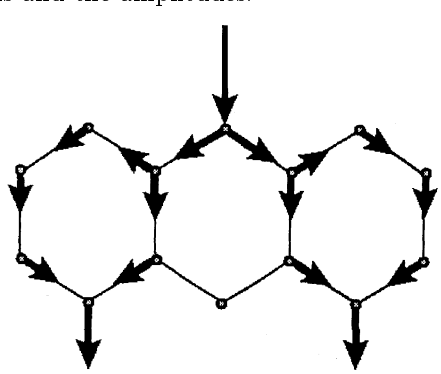


Fig.5. Current distributions at $E = \pm 0.42$ and $E = \pm 1.5$.

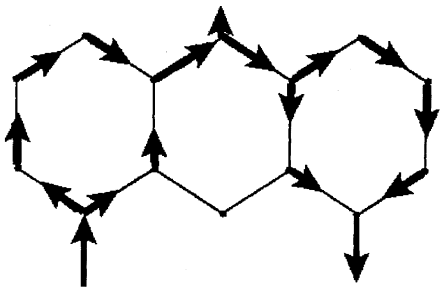


Fig.6. Current distributions at $E = \pm 1.06$.

The internal loop current which is induced in the phenalenyl molecular bridge[34] is not found in this molecular bridge since the transmission is symmetric. Finally, the input and the output currents are summed up at each atomic site, which agrees very well with the Kirchhoff quantum current momentum conservation theory.[36]

4. Conclusion

In this paper, the quantum transmission properties of the three-terminal molecular bridge have been investigated with the Green function method based on tight-binding theory, and the current distributions inside the molecular bridge have been clarified. We found that the transmission spectra depend significantly on both the electronic energy and the molecular level. Namely, each spectral peak appears at the energy point where the resonance happens between the incident electron and the molecular level. We also found that the quantum current direction and amplitude agree with the basic physical theory completely.

This theoretical result will be helpful to design, experiment, and fabrication of the molecular electronic devices. It is also useful to connect the manifold nano circuits. We hope that this theoretical approach will advance the further development of the nano molecular devices.

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