

## The properties of electron transport through CNT/*trans*-PA/CNT system

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(Received 4 October 2005 ; in final form 28 May 2006)

### Abstract

Using a tight-binding model and a transfer-matrix technique, we numerically investigate the effects of the coupling strength, and the length of the molecule on the electronic transmission through a CNT/(single) molecule/CNT system. With *trans*-polyacetylene (*trans*-PA) as the molecule sandwiched between two semi-infinite carbon nanotube(CNT), we rely on *Landauer* formalism as the basis for studying the conductance properties of this system. Our calculations show that the conductance is sensitive to the CNT/molecule coupling and that it exponentially decreases with the increase in the length of the molecule, as expected.

**Keywords:** molecular wire, t-matrix, carbon nanotube, electronic transmission, Landauer formalism

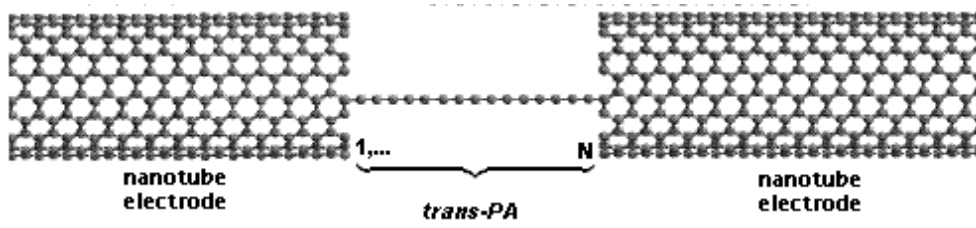
### 1. Introduction

Smaller, faster and cheaper electronic devices drives a race of increasing pace for the miniaturization of transistors. Such an activity has provided an interplay between fundamental and applied research giving rise to the fields of mesoscopic and nanophysics.

Since the original proposal of a molecular rectifier [1], significant progress on electronic transport across a single molecule has been demonstrated experimentally only in this decade. Technologically, this was first achieved by using a scanning tunneling microscope (STM) tip above molecules laid on a metallic substrate [2-4]. In a typical experimental setup however, a molecular bridge connects two electrodes acting as the electron donor and acceptor reservoirs. Despite this conceptual separation of molecular device into its constituents, what is measured is the conductance across the whole of the system. This implies that besides the intrinsic molecular ability to convey charge, the coupling of the molecular bridge to the electrodes is significant. The molecular orbitals of the molecule when it couples to the electrodes provide favourable pathways for electrons. Small conjugated polymers, as the molecular bridges, can easily be processed to afford functional electronics, such as field effect transistors(FETs) [5,6]. It is shown that *trans*-PA has considerable potential applications as an alternative conductor [7]. The possibility of the semiconductor-to-

metal transition [8] and the capability of becoming a very conductive material have been the reason for the experimental and theoretical investigations on the physical properties of *trans*-PA in comparison with the other conducting polymers. Several studies on the structural, electronic and conduction properties of *trans*-PA have been published [9-14]. Most studies have focused on the understanding of how the details of *trans*-PA electronics structures, the nature of electronic states, the impurities and solitons affect the conduction properties of *trans*-PA along the molecular wires. However, there are other important factors whose influence on the conductance of molecular wires, with *trans*-PA as the molecule, have not yet been fully studied. This has been our motive for the work presented in this paper. As a model, we numerically investigate the effects of some of the features of the CNT/*trans*-PA/CNT structure (figure 1) on the electronic transport. It is shown that single-walled carbon nanotubes (SWNT) can be used as quasi one-dimensional electrodes to construct CNT/(single) molecule/CNT system with a molecular scale width and channel length, such as single electron molecular transistors [15-17].

A typical CNT/conjugated polymer/CNT structure may be constructed through a reproducible method as cutting of metallic SWNTs to form small gaps within the tubes and with control over the gap size down to ~3nm. The cutting depends on the electrical break-down of individual



**Figure 1.** A schematic representation of the CNT/*trans*-PA/CNT structure as described in the text.

SWNTs between the two metal electrodes [18], and the size of the cut was found to be controllable by changing the length of the SWNTs [19]. Conjugated polymers were then deposited to bridge the gap in the vapor or solution phase, forming the smallest CNT/conjugated polymer/CNT system with an effective channel length down to  $\sim 3$ nm. Here, we model the electrodes as the open-ended single-walled carbon nanotubes (SWNTs). CNTs support up to two channels for electrons with energy around the equilibrium Fermi energy and have a complex topology. They are known to exhibit a wealth of properties depending on their diameter ( $\sim$ nm), chirality (orientation of graphite sheet roll up) and whether they consist of a single cylindrical surface (single-wall) or more (multi-wall) [20].

The procedures we have applied in this work are based on two powerful numerical methods particularly suitable to treat the electron transmission through the large system: the *Landauer* formalism and transfer-matrix(t-matrix) technique, where the solution of the Schrödinger equation is obtained by means of a product of  $2 \times 2$  matrices.

The outline of the paper is as follows: In Sec.(2) our methodology to calculate the t-matrices, the electronic density of states(DOS) and the transmission coefficient is described. The results and discussion are presented in Sec. (3) followed by a summary and conclusions in Sec. (4).

## 2. Methodology

We use the following generalized Hamiltonian for the description of the CNT/molecule/CNT structure;

$$H = H_{CNT} + H_{SSH} + H_C, \quad (1)$$

where  $H_{CNT}$ ,  $H_{SSH}$  and  $H_C$  describe the semi-infinite CNT nanocontacts, the SSH Hamiltonian for the *trans*-PA molecule and the couplings of the contacts to the molecule, respectively. The CNT is described with a tight-binding Hamiltonian with only one  $\pi$ -orbital per atom. This Hamiltonian can describe reasonably well the band structure of a nanotube especially near the Fermi level which is zero in this case since the onsite energy is assumed to be zero and each orbital is half-filled;

$$H_{CNT} = \sum_j \varepsilon_j c_j^\dagger c_j - \sum_j t_{j+1,j} (c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}), \quad (2)$$

where  $c_j$  ( $c_j^\dagger$ ) is the annihilation (creation) operator of an electron at  $j$ th site. For the semi-infinite CNT

contacts we set  $\varepsilon_j = \varepsilon_0$  for all  $j$  and  $t_{j,j\pm 1} = t_{CNT}$  between all  $j$  and  $j \pm 1$  for nearest-neighbor hoppings.

$H_{SSH}$ , is described within the tight-binding approximation [21] and is one of the well-known frameworks for studying the conduction and structural properties of *trans*-PA [8,22]. As we have shown [22], the electronic part of  $H_{SSH}$  is as follows;

$$H_{SSH} = - \sum_n t_{n+1,n} (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1}), \quad (3)$$

in which  $t_{n+1,n}$  is the nearest-neighbor hopping integral and is given as;

$$t_{n+1,n} = t_0 + \alpha(u_n - u_{n+1}), \quad (4)$$

where  $t_0$  is the hopping integral of an undimerized chain,  $\alpha$  the electron-phonon coupling constant and  $u_n$  the displacement of the  $n$ th carbon atom from its equilibrium position. The reference energy is chosen such that the carbon on-site energy is zero. For perfectly dimerized *trans*-PA  $u_n$  and bandgap are given as  $u_n = (-1)^n u_0$  and  $2\Delta_0 = 8\alpha u_0$ , respectively.

Throughout this study for  $2\Delta_0 = 1.4$ eV, we shall use the parameters of Ref. [21], so  $\alpha = 4.1$ eV/ $\text{Å}$  and  $t_0 = 2.5$ eV. These correspond to an equilibrium dimerization amplitude  $u_0 \approx 0.04$  Å. For  $H_C$  we have;

$$H_C = -t_C (c_L^\dagger c_1 + c_1^\dagger c_L + c_R^\dagger c_N + c_N^\dagger c_R), \quad (5)$$

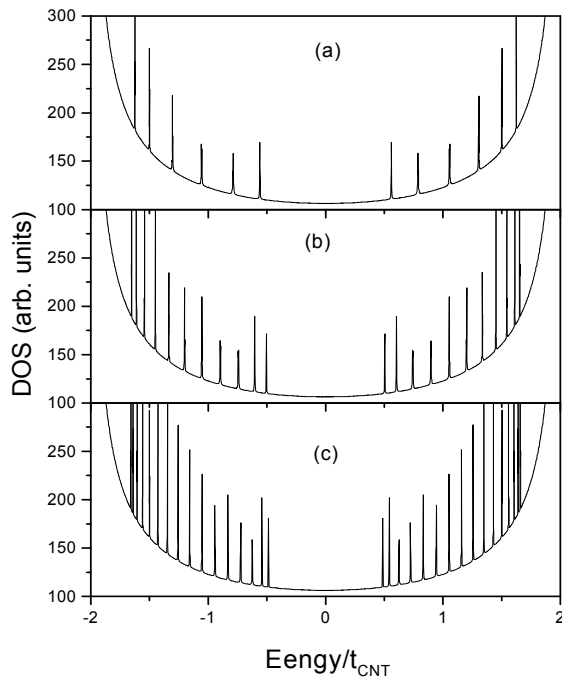
where we take the couplings to be identical on both sides of the molecule and of strength  $t_C$ .

Here we present a brief description of the t-matrix technique and *Landauer* formalism which we employed to calculate the electronic transmission through the CNT/*trans*-PA/CNT system. Let us consider a one-dimensional system in which both diagonal and off-diagonal terms are present in the Hamiltonian;

$$H = \sum_i [|i\rangle \varepsilon_i \langle i| + t_{i,i+1} |i\rangle \langle i+1| + t_{i,i-1} |i\rangle \langle i-1|], \quad (6)$$

where  $\varepsilon_i$  is the on-site energy of the site  $i$  and  $t_{i,i\pm 1}$  are the nearest-neighbor hopping integrals between the sites  $i$  and  $i \pm 1$ . The electronic properties of this system is then studied through the following Schrödinger equation;

$$t_{i,i-1} \psi_{i-1} + (\varepsilon_i - E) \psi_i + t_{i,i+1} \psi_{i+1} = 0, \quad (7)$$



**Figure 2.** A plot of the electronic DOS vs the dimensionless parameter  $\text{Energy}/t_{\text{CNT}}$  for the CNT/trans-PA/CNT system with the parameters of  $t_{\text{CNT}}=3\text{ eV}$  and  $t_c=0.3\text{ eV}$  as described in the text. Plots (a)-(c) show the results for the molecules with 11, 21 and 31 atoms, respectively.

in which  $\psi_i$  is the wave amplitude at site  $i$ . eq.(7) can be rewritten in the matrix form as follows;

$$\begin{pmatrix} \psi_{i+1} \\ \psi_i \end{pmatrix} = \begin{pmatrix} E - \varepsilon_i & -t_{i,i-1} \\ t_{i,i+1} & 0 \end{pmatrix} \begin{pmatrix} \psi_i \\ \psi_{i-1} \end{pmatrix} = M_i(E) \begin{pmatrix} \psi_i \\ \psi_{i-1} \end{pmatrix}, \quad (8)$$

where  $M_i(E)$  is the local t-matrix associated with

site  $i$ . Defining  $M(E) = \prod_{i=1}^N M_i(E)$  as the global t-

matrix of the system, the eq. (8) is generalized as follows;

$$\begin{pmatrix} \psi_{N+1} \\ \psi_N \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} = \prod_{i=1}^N M_i(E) \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix}, \quad (9)$$

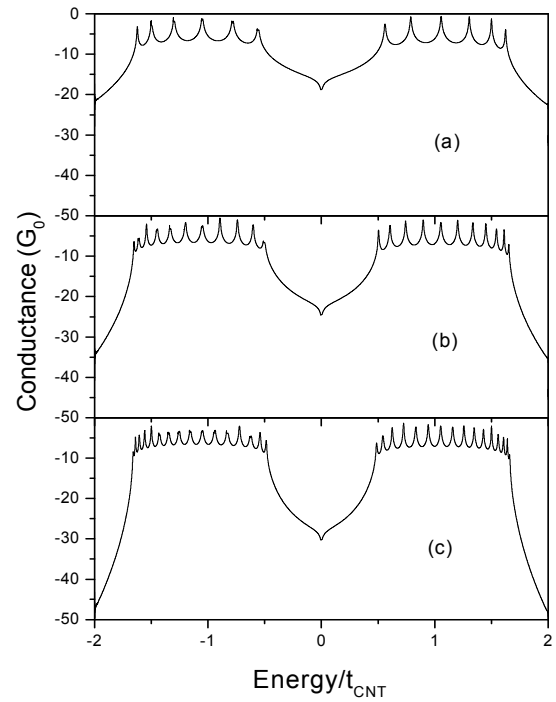
where;

$$M(E) = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}. \quad (10)$$

We see that t-matrices depend on energy,  $E$ . If the eigenenergies are known, then the whole eigenfunctions will easily be calculated from the t-matrices. Now we proceed to the calculation of the transmission coefficient  $T(E)$ , whose magnitude is directly related to the conductance through the *Landauer* formula [23];

$$G = \frac{2e^2}{h} T(E). \quad (11)$$

In the absence of a non-coherent elastic transport [24], inelastic scattering and electron-electron correlations,



**Figure 3.** Conductance in units of  $G_0$  vs the dimensionless parameter  $\text{Energy}/t_{\text{CNT}}$  for the CNT/trans-PA/CNT system with  $t_{\text{CNT}}=3\text{ eV}$  and  $t_c=0.3\text{ eV}$  corresponding to the figure 2. Plots (a)-(c) show the conductance of the system for the values of the molecular length 11, 21 and 31 atoms, respectively.

*Landauer* theory provides a general framework for calculations of the electronic current through mesoscopic conductors that are coupled to ideal single or multi-channel quasi-one dimensional leads. It relates the electronic current to the transmission probability for an electron incident from the source lead to scatter elastically through the conductor and into the drain.

Connecting the molecular chain to two semi-infinite CNT nanocontact,  $T(E)$  is identical to the probability that an incident electron with energy  $E$  in the left-hand CNT emerges in the right-hand one. Using Eq.(9), the transmission coefficient  $T(E)$  is given by [2,25,26];

$$T(q) = \frac{4(1-q^2)}{(Z+qY)^2 + (1-q^2)X^2}, \quad (12)$$

where the dimensionless parameters  $q$ ,  $X$ ,  $Y$  and  $Z$  are given as follows;

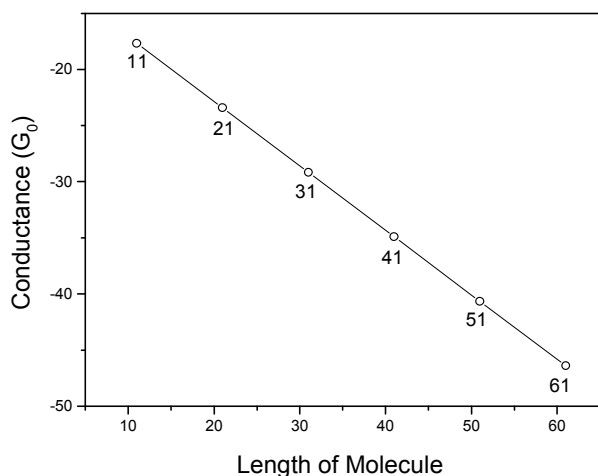
$$q = 1 - \frac{E}{2t_{\text{CNT}}}; \quad X = m_{22} + m_{11} \quad (13)$$

$$Y = m_{22} - m_{11}; \quad Z = m_{21} - m_{12}$$

where  $t_{\text{CNT}}=3\text{ eV}$  are the hopping integral of semi-infinite leads in the system and  $m_{ij}(i, j=1,2)$  are the matrix elements of the global t-matrix,  $M(E)$ , of the system.

### 3. Results and discussion

Considering the remarks in Sec.(2) and calculating the eigenvalues, one may write the following expansion for

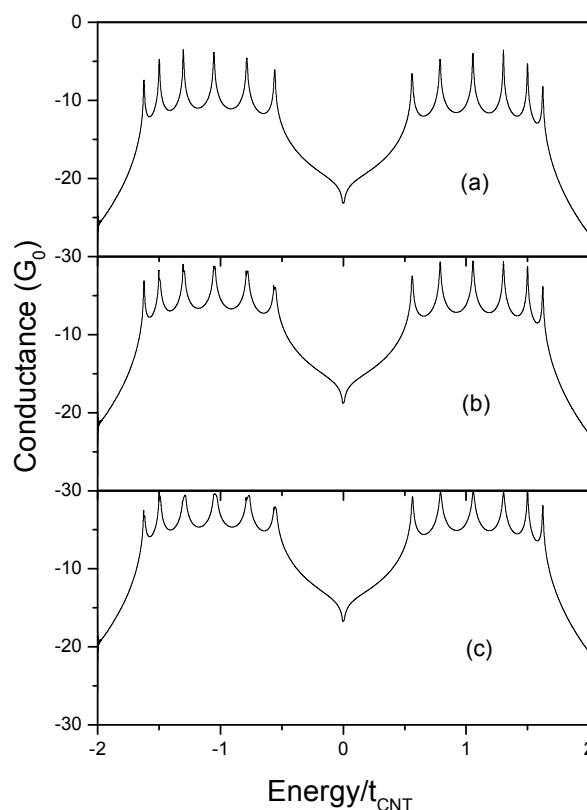


**Figure 4.** A plot of the exponential decrease of the conductance as a function of length of the molecule for  $t_c = 0.3$  eV and the molecules with 11, 21, 31, 41, 51 and 61 atoms.

the electronic density of states (DOS) of the former structures[14];

$$\rho(E) = \begin{cases} \frac{1}{E_{i+1} - E_i} & \text{if } i=1 \text{ and } \frac{N}{2} + 1 \\ \frac{1}{E_i - E_{i-1}} & \text{if } i = \frac{N}{2} \text{ and } N \\ \frac{1}{2} & \text{otherwise} \\ \frac{1}{E_{i+1} - E_{i-1}} & \end{cases} \quad (14)$$

Setting the CNT/molecule coupling,  $t_c = 0.3$  eV and hopping integrals between  $\pi$ -electrons in carbon nanotubes,  $t_{CNT} = 3$  eV figures 2(a)-(c) illustrate the electronic DOS for the CNT/*trans*-PA/CNT structures for the *trans*-PA molecules with 11, 21 and 31 atoms, respectively. Figure 3(a)-(c) show the corresponding conductance in units of  $G_0$  with the same parameters in figure 2. From figure 3 we see that when the length of the molecule increases, the conductance decreases. We find that the decrease of the conductance follows an exponential law as introduced by *Magoga* and *Joachim*[27]. To illustrate the exponential behaviour, we have shown in figure 4 the variations of the conductance as a function of the length of six molecules with 11, 21, 31, 41, 51 and 61 atoms, respectively. In this figure the same parameters as the ones in figure 3 have been used for the calculations of the conductance at the given energy, i.e. the Fermi energy. Another feature of the conductance spectra in figure 3 is the presence of resonance peaks which arise when the energy  $E$  coincides with an eigenenergy of the *trans*-PA molecule. The results show that the density of resonances scales as the molecule size. We have also repeated the calculations for different values of the CNT/molecule coupling,  $t_c$ . Increasing  $t_c$  leads to a significant increase of the conductance and our results suggest that for the large coupling, i.e.



**Figure 5.** Conductance in units of  $G_0$  vs the dimensionless parameter  $\text{Energy}/t_{CNT}$  for the CNT/*trans*-PA/CNT system with  $t_{CNT} = 3$  eV. Plots (a)-(c) show the results for the molecule with 11 atoms and  $t_c = 0.1, 0.2$  and  $0.3$  eV, respectively.

$t_c \geq 2$  eV, the interaction between the electrodes and *trans*-PA molecule are so strong that the molecule loses its identity to the extent that the conductance through the molecule can no longer be considered as a tunneling process.

#### 4. Summary and conclusions

In this paper we investigate in detail some of the properties of the conductance in a CNT/molecule/CNT structure with a *trans*-polyacetylene(*trans*-PA) as the molecule. Our calculations are performed on the basis of well-known procedures. We used a tight-binding model for the nanotube electrodes as well as SSH Hamiltonian for *trans*-PA molecule. Using the transfer-matrix technique, we calculate the conductance within the *Landauer* formalism. We focus on the effects of the dependence of the conductance on the length of *trans*-PA molecule and the CNT/molecule coupling strength. Our results show the strong dependence on the conductance to the strength of the CNT/molecule coupling and the exponentially decrease of the conductance as the length of the molecule increases. Further investigations of the effects of other parameters of the system, such as the role of soliton distributions on the conductance, are being carried out and the results will be presented in the near future.

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