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Effect of Nitrogen on Negative Differential Conductance in Polythiophene

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Abstract: Polythiophene is a highly conductive molecule which possesses thermal and chemical stability showing great performance in electrical devices. Polythiophene also shows an uncommon highly demanding electrical property named negative differential resistance which is a decrease of electron current with increase of applied voltage. To address this issue, in this work we study theoretically electron transport properties of a polythiophene molecular bridge sandwiched between two metal leads in the presence of Nitrogen atom as a substitute for one or two of the Carbon atoms in the molecule. The results based on Green's function formalism show that the presence of Nitrogen reduces the electron transmission coefficient. On the other hand, Nitrogen can lead to amplification of negative differential resistance. Strength of the resistance is affected by the positions and number of Nitrogen atoms in the system. Therefore, choosing right positions for locating impurities is very important. We found that by substituting a Carbon atom with Nitrogen in some positions the system shows notable negative differential resistance. Besides, when two Carbon atoms are replaced by Nitrogen atoms there are some special locations that not only the system shows negative deferential resistance but also it works as an electronic molecular switch which is highly demanding in electronic industry.

Keywords: Green's Function Method, Molecular Device, Negative Differential Resistance, Polythiophene

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1. INTRODUCTION

To meet today's technological needs; minimization of the device size has prompted tremendous interest especially in nanoelectronic industry [1-5]. Extensive efforts have been paid to investigate and reveal electron transport properties through single molecule devices. Making stable molecular junctions as well as controlling the electrical properties of the junctions is highly demanded for the electronic applications.

Among various molecules, benzene rings [6], organic molecules [7,8] and polymers [9], phenyl rings and polythiophene [10,11] are widely considered as basic building blocks of molecular junctions. Various experimental and theoretical studies of transport properties through molecular junctions have indicated many interesting phenomena such as shot noise [12,13], spintronic characteristics [14-16], thermoelectric characteristics [17], excellent thermoelectric properties [18], electromechanical switching, and negative differential resistance (NDR) [19-21].

A nonlinear transport phenomenon, an increase in the source-drain bias in particular voltage ranges leading to decreasing electronic current, is known as negative differential resistance (NDR) [22]. The NDR behavior have been offered in lots of physical phenomena such as redox reactions [23,24], phonon blockade[25], polaron [19], chemical reaction [26], charge reduction [23], localization and delocalization of orbitals [27], etc. It has been shown that substituting nitro and amino groups on the central ring in a phenylene ethynylene trimer leads to NDR behavior [27]. Farajian et.al. reported the NDR behavior in a seven thiophene molecular field effect transistor by using density functional theory [28]. Effective confinement of π electrons due to the presence of sulfur atom induces NDR behavior in polythiophene as reported by Liu et.al [29]. In the research, the NDR behavior was found to be a result of electron hopping energy changes between carbon atoms neighboring the sulfur atom in polythiophene. Given that the hopping energy is an intrinsic property of the two atoms, changing it seems difficult and largely unworkable. Motivated by this fact, we study the nitrogen atom substituted for carbon in a polythiophene molecule at different sites. The energy hopping changes between carbon atoms and nitrogen causes the NDR behavior. This is an intrinsic property that exists in this molecular junction without the induction of any conformational changes and unreasonable change of hopping energy; therefore, it deserves an independent study. This paper is organized as follows: section 2 gives details on the Hamiltonian of polythiophene and computational method. The results are presented in section 3, where we show the dependence of transport properties on existence of nitrogen as well as the location of it and explain the NDR behavior.

2. METHOD and MODEL

The system considered in this probe, as it is demonstrated in Fig.1, is a polythiophene molecule which is made up of four loops of thiophene molecules

connected to two one dimensional semi infinite metal electrodes. We assume one of the Carbons of the molecule is replaced by Nitrogen as an impurity.
The Hamiltonian of system is given by:

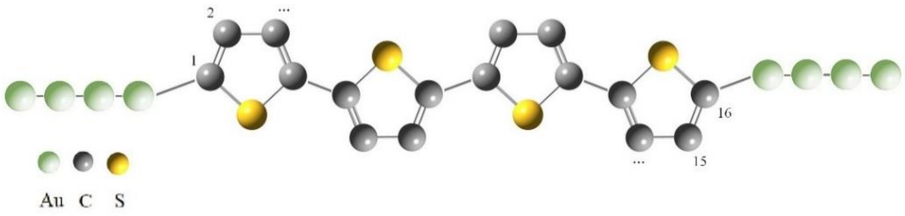


Fig. 1. (Colour on-line). Scheme diagram of the structure of a polythiophene sandwiched between metal leads.

The Hamiltonian of system is given by:

$$H = H_M + H_{coup} + H_{L/R}, \tag{1}$$

here, H_M , H_{coup} and $H_{L/R}$ is the Hamiltonian of the polythiophene molecule, the Hamiltonian of coupling between the electrodes and the polythiophene molecule and the Hamiltonian of left/right electrode, respectively. The electron-phonon interaction based on the Su–Schrieffer–Heeger (SSH) model [30] includes the effect of the sulfur atoms by electron hopping between carbon atoms on both sides of the sulfur atom. The Hamiltonian of polythiophene can be written as [10, 29]:

$$\begin{aligned} H_M &= \sum_n (\varepsilon_0 c_n^\dagger c_n - t_n (c_{n+1}^\dagger c_n + h.c.)) + \frac{1}{2} K \sum_n (u_{n+1} - u_n)^2 \\ &+ \sum_n [\varepsilon_\Delta^S (c_{4n}^\dagger c_{4n} + c_{4n-3}^\dagger c_{4n-3}) - t_\Delta^S (c_{4n-3}^\dagger c_{4n-3} + h.c.)], \end{aligned} \tag{2}$$

,

$$(3) t_n = t_0 - \alpha\left(u_{n+1} - u_n\right) - t_e \cos\left(n\pi/2\right)$$

where ε_0 is the on-site energy of carbon atoms, t_n is the hopping energy of carbon atoms between sites n+1 and n. α is electron-phonon coupling constant. The displacement coordinate of the nth site from its minimum energy values, u_n , that can be obtained via the Hellman–Feynman theorem can be used for calculation the lattice distortion $(u_{n+1} - u_n)$ [10]. Moreover, t_e is nondegeneracy parameter of polythiophene molecule. Also, $c_n^\dagger(c_n)$ reveals the creation (annihilation) operator of an electron at the nth site. K describes the elastic constant. t_Δ^S and ε_Δ^S are electron hopping between sulfur and carbon at 4n-3 and 4n sites and effective confinement energy of electrons from the sulfur atom, respectively. In this work we have set the SSH model's parameters as: $t_0 = 2.5eV$, $t_\Delta^s = 0.125eV$, $\varepsilon_\Delta^S = 0.125eV$,$\varepsilon_\Delta^S = 0.125eV$,$\varepsilon_\Delta^S = 0.125eV$, $t_e = 0.27eV$, $\alpha = 0.44eV/A^{o2}$ and $K = 21.0eV/A^{o2}$ [29]. The parameters are considered such that the band gap of polythiophene gained by the model agrees with the one measured experimentally [31]. Moreover, we choose the lattice distortion parameters $(u_{n+1} - u_n)$ in agreement with the ones obtained in ref. 10 by Liu *et al.* and here n indicates the number of site in the structure.

We explain two identical metal electrodes by a one-dimensional single electron tight binding model

$$H_{L/R} = \sum_n [\varepsilon_n d_n^\dagger d_n + t_m \left(d_{n+1}^\dagger d_n + h.c.\right)], \tag{4}$$

here, ε_m and t_m are on-site energy of a metal atom and nearest neighbor hopping energy of metal sites, respectively. Here, $d_n^\dagger(d_n)$ denotes the creation (annihilation) operator of an electron at the nth site in metal electrodes. The Hamiltonian of coupling between the electrodes and the polythiophene molecule (H_{Coup}) is similar to the Hamiltonian of two electrodes except that $t_m = t_{ML} = t_{MR} = \beta\left(t_f + t_0\right)$ where $\beta = 0.25$ is the molecule-metal binding parameter and we consider $t_f = 3eV$ [10]. Notice that, the electrodes are connected to central chain via sites 1 and 16.

The transmission coefficient of electron through the polythiophene molecule junction can obtain by Green's function method. We consider that the metal electrodes are consisted of infinite number of unit cell (0, 1, 2,…,n). In order to acquire the total Green's function, the retarded Green's function of the left and right electrodes should be calculated as follows, [32,33]

$$g_{N+1,N+1}^R = [(E + i\eta)I - H_{0,0}^R - H_{0,1}^R \Lambda^R]^{-1}, \tag{5}$$

$$g_{0,0}^L = [(E + i\eta)I - H_{0,0}^L - H_{0,1}^L \tilde{\Lambda}^L]^{-1}, \tag{6}$$

where η is a positive infinitesimal number and I is the unit matrix. $H_{0,0}^q$ and $H_{0,1}^q$ $(q = L, R)$ are the Hamiltonian of unit cell in the electrode and the coupling matrix between two neighboring unit cells, respectively. $g_{N+1,N+1}^R$ and $g_{0,0}^L$ indicate the Green's function of the right and left electrodes, respectively.

Moreover, $\Lambda^R(\tilde{\Lambda}^L)$ presents the transfer matrix which is calculated by using the iterative procedure as follows,

$$\Lambda^q = K_0^q + \tilde{K}_0^q K_1^q + \tilde{K}_0^q \tilde{K}_1^q K_2^q + \ldots + \tilde{K}_0^q \tilde{K}_1^q \tilde{K}_2^q \ldots K_n^q \tag{7}$$

$$\tilde{\Lambda}^q = K_0^q + K_0^q \tilde{K}_1^q + K_0^q K_1^q \tilde{K}_2^q + \ldots + K_0^q K_1^q K_2^q \ldots \tilde{K}_n^q \tag{8}$$

where recursive formulation can be used for calculation of K_l and $\tilde{K}_l$

$$K_i^q = (I - K_{i-1}^q \tilde{K}_{i-1} - \tilde{K}_{i-1} K_{i-1}^q)^{-1} (\tilde{K}_{i-1}^q)^2 \tag{9}$$

$$\tilde{K}_i^q = (I - K_{i-1}^q \tilde{K}_{i-1} - \tilde{K}_{i-1} K_{i-1}^q)^{-1} (\tilde{K}_{i-1}^q)^2 \tag{10}$$

$$K_0^q = [(E + i\eta)I - H_{0,0}^q]^{-1} (H_{0,1}^q)^\dagger \tag{11}$$

$$(12)\,\tilde{K}_0^q = [(E + i\eta)I - H_{0,0}^q]^{-1} (H_{0,1}^q).$$

Until $K_n, \tilde{K}_n \le \delta$ with δ arbitrarily small is obtained, this process is repeated. Then, we can calculate the left and right electrodes Green's function (layer by layer from *l=N* to *l=2*) as follows

$$g_{l,l}^q = [(E + i\eta)I - H_{l,l}^q - H_{l,l+1}^q g_{l+1,l+1}^q (H_{l,l+1}^q)^\dagger]^{-1}, \tag{13}$$

Finally the total retarded (advanced) Green's function can be written as

$$G^r(E) = [G^a(E)]^\dagger = ((E + i\eta)I - H_c - \Sigma_L - \Sigma_R)^{-1}, \tag{14}$$

where Σ_q exhibits the self-energy matrix which indicates the interaction of the molecular region with left and right electrodes and can be calculated as

$$\Sigma_q = H_{cq}^\dagger g_q^r H_{cq}, \tag{15}$$

where H_{cq} is the interaction Hamiltonian matrix between the molecule (channel) region and the electrode *q*. $T(\varepsilon, V)$ is transmission coefficient which can reveal electrons transport properties through the polythiophene at the energy level ε with a finite bias voltage V and can be obtained as:

$$T(\varepsilon, V) = Tr\left(\Gamma_L G^r \Gamma_R G^a\right) \tag{16}$$

with $\Gamma_q(\varepsilon) = -2\,\mathrm{Im}\left(\Sigma_q(\varepsilon)\right)$ is the broadening matrix that explains the effects of reservoir electrodes on the central molecule. The junction current calculated based on the NEGF formalism by the Landauer-Buttiker equation that can be given by [34]:

$$I = \frac{2e}{h}\int T(\varepsilon,V)[f_L(\varepsilon,V) - f_R(\varepsilon,V)]d\varepsilon \tag{17}$$

the term involving $f_L(\varepsilon,V)$ and $f_R(\varepsilon,V)$ denotes the Fermi-Dirac distribution function for left and right metallic electrode at energy ε level with a certain bias voltage V.

3. NUMERICAL RESULTS and DISCUSSION

Based on numerical method presented in sec 2, we study I-V characteristics of nitrogen-doped polythiophene attached to Au leads. We assume that a Nitrogen atom is doped in various positions of the molecule (n=1,.., 16) as an impurity and study the effect of existence of the impurity on transmission coefficient and current of electrons passing between Source and drain via the molecular bridge. Here, the Fermi energy is considered to be zero and we assume that the temperature of the system is T=11K unless mentioned otherwise.

In order to study the electronic properties of molecular bridges, sandwiched between source and drain, first of all we explore transmission coefficient of electrons tunnelling through the bridge and afterwards we study I-V characteristics of the system.

In Figs. 2(a) and (b), we plot the transmission coefficient of electrons for a pure polythiophene molecular bridge as a function of energy of electrons. Also, Figs. 2 (c) and (d) illustrate density of states of electrons associated with Figs. 2(a) and (b), respectively. As it is illustrated in the figures, there is a clear consistency between behaviour of electron transmission and the density of states. In fact, comparing DOS curves with the transmission ones shows that whenever there is no available room for electrons in the bridge to pass through (i.e. DOS=0), a gap appears in the transmission curve (T=0). Moreover, as it is demonstrated in the figure by substituting a Carbon atom with Nitrogen atom the DOS of the system reduces and accordingly the probability of transmission of electrons declines. Furthermore, as the electron current directly is related to the electron transmission coefficient, we predict that the I-V characteristics shows a step-like behaviour which is because of the gap intervals in the transmission curves versus the electron energy. Moreover, as shown in Fig. 2(b) when the molecule has a Nitrogen impurity, the transmission coefficient decreases and the peaks of the plot get narrow and short comparing to the pure polythiophene molecule which is in consistent with the behaviour of the DOS of the electrons. This means that one should expect a decrement in current of electrons in the presence of impurity which can in some especial conditions lead to negative deferential resistance where by increasing the applied voltage the current of the system decreases.

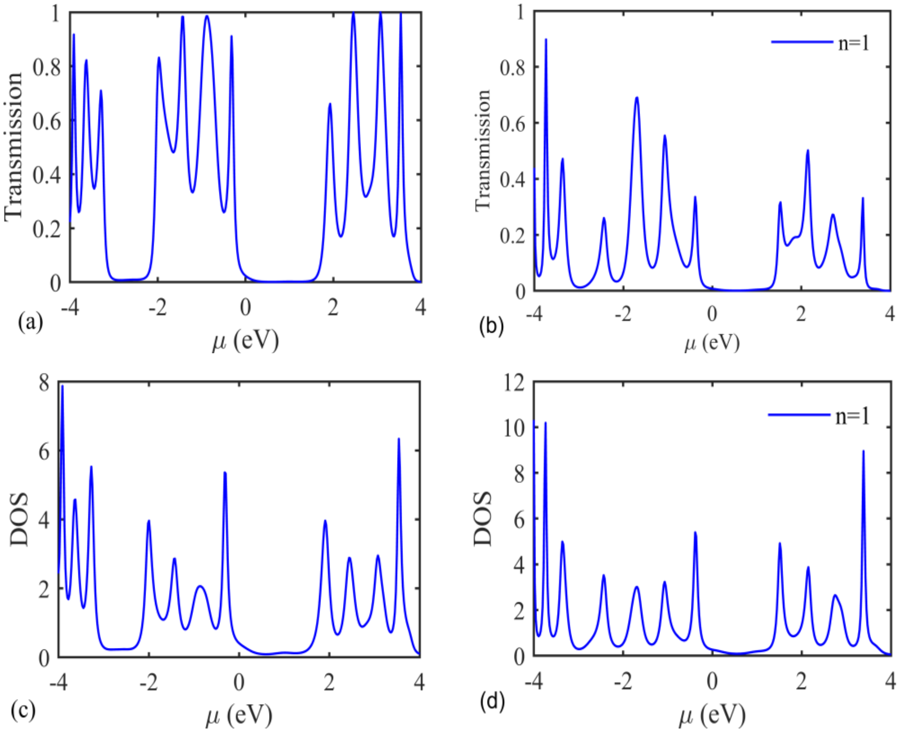


Fig. 2. Transmission function (a and b) and density of states of electrons (c and d) versus electrons energy (a and c) without impurity and (b and d) with impurity located on n=1.

In Fig. 3, to see the effect of existence of the Nitrogen atom on electronic properties of the molecular bridge we plot local density of states of electrons (LDOS) for the first position of the bridge (n=1) when (a) there is no impurity, and (b) the Carbon atom on n=1 position is substituted by Nitrogen atom. As it is clearly shown in the figure by substituting the impurity the LDOS decreases in most of energies which means that the impurity demolishes some of the available states of the n=1 position for electrons to pass through and this will affect the strength of flow of electron through the system.

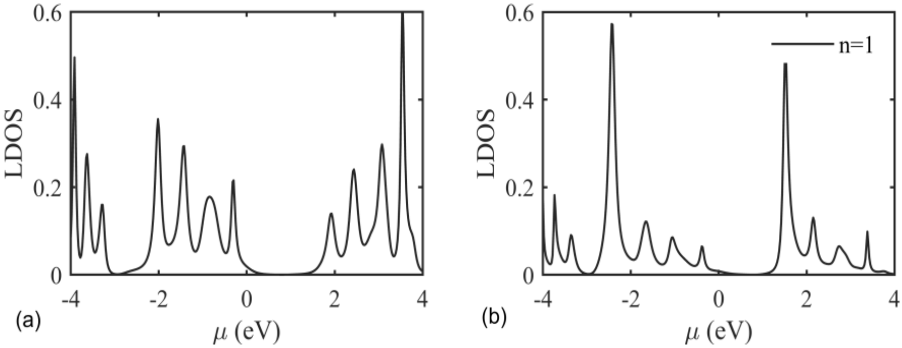


Fig. 3. Local density of states (LDOS) of the multi polythiophene molecular bridge versus energy of incoming electrons for polythiophene (a) without and (b) with Nitrogen atom on site n=1.

In Figs. 4 the I-V characteristics of the polythiophen molecule connected to the Au-leads is plotted in the absence of Nitrogen impurity. As it is shown in the figure by increasing the source-drain voltage the current shows a step-like increase and its maximum value reaches to about 30 μA. Also, when the voltage varies between 1.5eV and 1.8eV or between 2eV and 2.5eV there is a slight minus slope in the curve which means that in these ranges of voltages the system shows a weak NDR behavior. However, to see the effect of higher temperatures in Fig. 4 we also consider the I-V characteristics of the system in T=300K which shows that the behavior of the system does not change dramatically by increasing the temperature

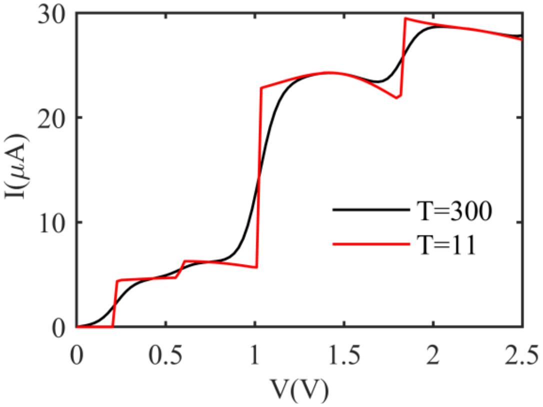


Fig. 4. (Colour on-line) I-V characteristics of polythiophene molecular bridge in T=11K and T=300K.

In order to study the effect of existence of the Nitrogen impurity and its position on NDR effect we plot I-V characteristic of the system when one of the carbon atoms is substituted with a Nitrogen atom on various sites of the polythiophene molecule in Fig. 5. In Figs. 5(a), (b), (c) and (d) we plot current versus voltage for n=1, 7, 10, and 14, respectively. As it is illustrated in the figure, doping Nitrogen reduces the strength of the current passing through the molecule. Moreover, the results show that the position of doped Nitrogen has dramatic impact on the current and also negative differential resistance. In fact, when the position of the Nitrogen impurity gets closer to the drain we need to apply stronger source-drain voltage to get the NDR effect. Moreover, to show the NDR behavior of the system more clear we plot differential resistance, dI/dV, versus the voltage in the inset and find that, the most powerful differential resistance can be obtained for n=14 which is -20 $\mu A/V$ for V=2.4V.

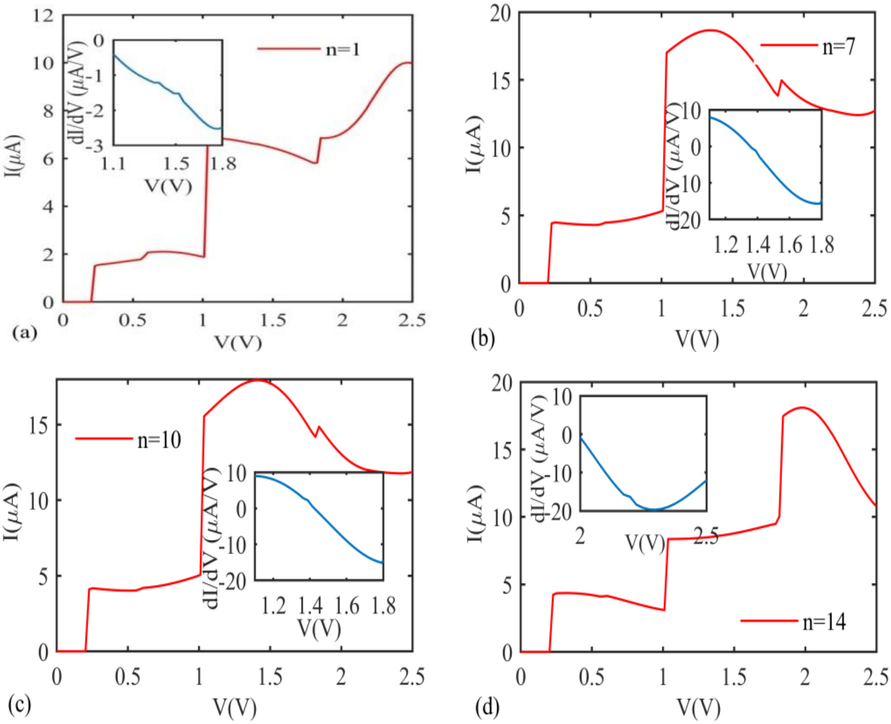
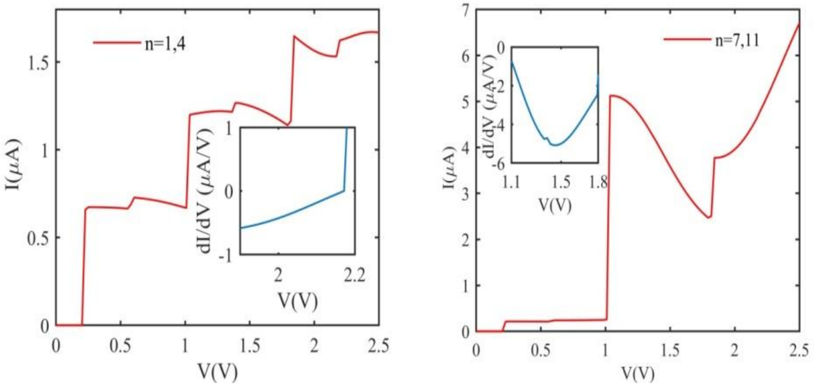


Fig. 5. (Colour on-line) I-V characteristics in the presence of impurity on (a) n=1, (b) n=7, (c) n=10, and (d) n=14. The insets show the differential resistance, dI/dV versus the bias voltage (V).

To study the effect of doping two impurity atoms in the I-V characteristics of polythiophene molecular bridge we plot current versus applied voltage in Fig. 6 for (a) n=1,4 and (b) n=7,11. The insets show the differential resistance versus the applied voltage. As it is clearly shown in the figures adding extra impurity reduces the current strength. Also, in the case of existence of two Nitrogen atoms the strength of NDR effect become weak comparing to the case in which the structure has just one Nitrogen impurity. On the other hand, the comparison between Fig. 6(b) and Fig. 5(b) shows that when we add another impurity on n=11, the NDR effect can be obtained in lower voltages which is not the case when we consider the Nitrogen atom is located on n=1, 4. This shows that the location of impurity can totally affect the results. Moreover, as it is illustrated in Fig. 6(b) the system is approximately off (the amount of current is very low) up to V=1v and as soon as the voltage gets higher than this value the system suddenly let the electrons pass the molecular bridge. This means that one can use the polythiophene molecular bridge with two Nitrogen impurities placed at n=7,11 as a molecular electronic switch which is highly demanding in electronic industry.

At the end it is worth to mention that to study the NDR behavior of the polythiophene molecular bridge in the presence of Nitrogen atom we have tried different possible positions for the impurity as well as different number of impurities. The results presented in this paper are the most noteworthy ones.



(a) (b)

Fig. 6. (Colour on-line I-V characteristic when there are two Carbon atoms are substituted with Nitrogen atoms on (a) n=1, 4 and (b) n=7,11.

4. CONCLUSION

Using Green's function formalism, we have studied the charge transport properties in a polythiophene molecule connected to two external metal leads. We investigate the effect of substituting carbon atom with Nitrogen atom on the electron transmission through the molecular bridge. It is found that local density of states of electrons on the location of impurity reduces. Therefore, the electron transmission coefficient reduces by substituting Carbon atom with Nitrogen impurity. However, the existence of impurity leads to an important phenomenon named negative differential resistance. We have studied the effect of position of the substituted atoms as well as the number of Carbon atoms replaced with Nitrogen and found that when there is an impurity on sites n=14 the system shows negative differential resistance which is noticeably strong. Moreover, when there are two impurities on n=7,11 one can see that the current is close to zero in voltages less than 1V and as soon as the voltage gets upper than 1V, the current suddenly increases. Therefore, the polythiophene molecular bridge can be used as an electronic molecular switch which can be tuned by external voltage.

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