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The charge transfer via a double helix DNA*

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This paper reports a double helix model of charge transfer in DNA molecule. The calculated results show that the transmission characteristics of DNA are not only related to the longitudinal transfer but also to the helicity of molecule. It finds that there are four transmission bands centred at 0.92, 3.07, 7.75 and 8.87 eV, also the width and intensity of bands corresponding to the helix direction are less than that of the longitudinal direction. With the increase of hopping energy, transmission bands become wide so that the transmission ability is enhanced.

Keywords: DNA, double helix model, charge transfer
PACC: 7200, 3470, 8715

1. Introduction

In recent years, charge transfer properties of DNA have attracted much attention among physics, chemistry, biology and so on. The advent of molecular electronics has sparked a lot of interest in the possibility to exploit DNA in functional nano-electronic devices.[1−7] Although the use of DNA molecules in nano-electronic circuits is very promising, their conductivity properties are still under intense debate.[8−10] Some reports consider that DNA may be a good linear conductor,[2,11] while other experimental measurements on single molecule showed that it seems to be an insulator,[3] even a superconductor at low temperature.[12] Recently, measurements of charge transfer through individual short DNA molecule indicate that it has a wide-band-gap semiconductor behaviour.[13,14] Therefore, a thorough understanding of the charge transfer properties of DNA is crucial in developing the future DNA-based nanoscale devices.

A number of theoretical models have been formulated to clarify the transmission properties of DNA molecule,[15−21] such as the fishbone model and the ladder model, etc. The fishbone model has one central conduction channel in which individual site represents a base-pair, but they are not interconnected along the backbone. And the ladder model is a planar projection of the DNA structure. It has two central branches, linked with one another, with interconnected sites where each represents a complete base and which are additionally linked to the upper and lower backbone sites. However, these models were not concerned with the double helix structure of DNA molecule. In this paper, we report on a double helix model of ploy(dG)-ploy(dC) DNA molecule and discuss the effects of two strands and helix structure on the properties of charge transfer.

2. Double helix model of charge transfer in DNA

DNA is a macromolecule consisting of a double helix with an aromatic π-stack core. Each chain is a linear polynucleotide consisting of four kinds of bases which is stacked on top of each other. The two chains are joined together by hydrogen bonds between pairs of nucleotides A–T and G–C. In Fig.1, each base is projected as a small ellipse with an arrow in the x–y plane, where $\theta_{\mathrm{A},n}$ and $\theta_{\mathrm{B},n}$ denote the angular displacements of the nth base belonging to two strands away from their equilibrium positions. The z-axis is a screw axis and perpendicular to the x–y plane. When the coordinate θ changes, the overlapping extent between adjacent bases will be affected so that the stacking energy changes. In addition, with the changing of the coordinate z, the neighbouring interaction of θ direction will alter.

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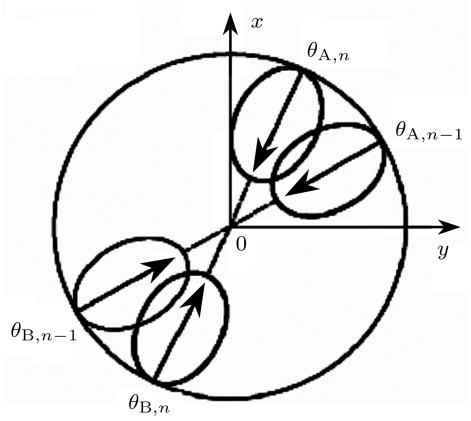


Fig.1. Schematic illustration of DNA structure.

In order to investigate the charge transport properties of DNA, the molecule is assumed to be connected to two semi-infinite electrodes. For simplicity, the structure change of DNA molecule is ignored in the course of charge transfer. For one strand of DNA, the coupling between base and electrode is related to the distance between them, which is related to two independent variables z and θ of bases. Therefore, when the charge injects into the DNA molecule, the transfer of θ direction can be treated as the analogous channel as one of the z direction. Considering the double strands structure of DNA, the charge transport system can be regarded as the parallel connection of four-dependent conducting channels connected to eight semi-infinite 1D electrodes. The model for transmission is illustrated in Fig.2. The Hamiltonian of the system can be expressed as

$$\begin{aligned} H = & H_{\rm mol} + H_{\rm leads} + H_{\rm coupl} \\ = & H_{\rm A} + H_{\rm B} + H_{\rm A-B} + H_{\rm leads} + H_{\rm coupl}, \end{aligned} \quad (1)$$

where $H_{\rm mol}$ is the Hamiltonian of the isolated molecule bridge, which comprises the Hamiltonian of two chains and the coupling interaction between them. $H_{\rm leads}$ and $H_{\rm coupl}$ represent the Hamiltonian of electrode and coupling between the electrode and molecule respectively.

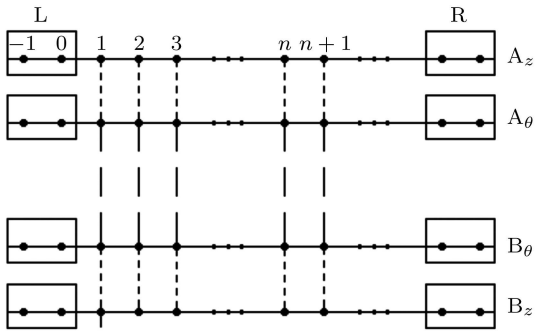


Fig.2. The Schematic illustration of the charge transport system.

The tight-binding Hamiltonian of each strand is expressed as

$$\begin{aligned} H_{\alpha={\rm A,B}} = & \ 2\sum_{n=1}^{N}[\varepsilon_n^{\alpha z} b_{\alpha,n}^{+} b_{\alpha,n} - (t_{n+1,n}^{\alpha z} b_{\alpha,n}^{+} b_{\alpha,n+1} + {\rm h.c.}) + \varepsilon_n^{\alpha\theta}\vartheta_{\alpha,n}^{+}\vartheta_{\alpha,n} \\ & -(t_{n+1,n}^{\alpha\theta}\vartheta_{\alpha,n}^{+}\vartheta_{\alpha,n+1} + {\rm h.c.}) - U_n^{\alpha}(z,\theta)(b_{\alpha,n}^{+}\vartheta_{\alpha,n} + {\rm h.c.})], \end{aligned} \quad (2)$$

where $b_{\alpha,n}^{+}(b_{\alpha,n})$ and $\vartheta_{\alpha,n}^{+}(\vartheta_{\alpha,n})$ are the creation (annihilation) operators of a charge at the site n. $\varepsilon_n^{{\rm A}_z} = 7.75\,{\rm eV}$ and $\varepsilon_n^{{\rm B}_z} = 8.87\,{\rm eV}$ are the on-site energy for charges at site $n(n = 1, \ldots, N)$ for base G and C at z direction respectively.[22] The rotational energy of the θ direction is less than the vibrational energy of the z direction, thus we take here $\varepsilon_n^{{\rm A}_\theta} = 3\,{\rm eV}$, $\varepsilon_n^{{\rm B}_\theta} = 1\,{\rm eV}$ (The effects of $\varepsilon_n^{{\rm A}_\theta}$ and $\varepsilon_n^{{\rm B}_\theta}$ will be discussed in Section 4.). $t_{n+1,n}^{\alpha z}$ and $t_{n+1,n}^{\alpha\theta}$ are the hopping energy between neighbouring sites n and $n{+}1$ for $1 \le n \le N-1$ at z and θ directions respectively. *Ab initio* calculations find that $t_{n+1,n}^{\alpha z}$ is ~ 0.1–$0.4\,{\rm eV}$,[22] we take $t_{n+1,n}^{{\rm A}_z} = t_{n+1,n}^{{\rm B}_z} = 0.2\,{\rm eV}$ in the present paper, and $t_{n+1,n}^{{\rm A}_\theta} = t_{n+1,n}^{{\rm B}_\theta} = 0.1\,{\rm eV}$. $U_n^{\alpha}(z,\theta) = 0.2\,{\rm eV}$ is the coupling energy between z and θ directions of one strand. The factor 2 in Eq.(2) and Eqs.(3–5) arise from the spin degeneracy.[17,23]

The coupling between A and B chain can be expressed as

$$\begin{aligned} H_{\rm A-B} = & -2\sum_{n=1}^{N}[U_n^{\rm AB}(z,z) b_{{\rm A}n}^{+} b_{{\rm B}n} \\ & + U_n^{\rm AB}(\theta,\theta)\vartheta_{{\rm A}n}^{+}\vartheta_{{\rm B}n} + {\rm h.c.}], \end{aligned} \quad (3)$$

where $U_n^{\mathrm{AB}}(z,z)$ and $U_n^{\mathrm{AB}}(\theta,\theta)$ are the coupling constants between A and B chain at z and θ directions respectively. Within the DNA double helix, the hydrogen bond locates at the plane perpendicular to the z-axis, which is ~ 0.4–$0.9\,\mathrm{eV}$,[24] therefore its effects on the energy of θ direction is larger than that of z direction. Furthermore, base A forms 2 hydrogen bonds with T on the opposite strand, and G forms 3 hydrogen bonds with C; we take $U_i^{\mathrm{AB}}(\theta,\theta) = 0.4\,\mathrm{eV}$, $U_i^{\mathrm{AB}}(z,z) = 0$.

The electrodes are described by the Hamiltonian

$$H_{\mathrm{leads}} = 2\sum_{n=-\infty}^{0}[\varepsilon_m a_n^+ a_n - t_m(a_n^+ a_{n+1} + \mathrm{h.c.})] + 2\sum_{n=N+1}^{\infty}[\varepsilon_m a_n^+ a_n - t_m(a_n^+ a_{n+1} + \mathrm{h.c.})], \tag{4}$$

where $\varepsilon_m = 5.36\,\mathrm{eV}$ is the on-site energy for electrode, which is equal to the platinum metallic work function, $t_m = 2.5\,\mathrm{eV}$ is the hopping energy for electrode.[20]

The coupling between the electrode and the DNA molecule end can be described by

$$\begin{aligned} H_{\mathrm{coupl}} = &-2(t_1 a_0^+ b_{\mathrm{A},1} + t_2 a_0^+ \vartheta_{\mathrm{A},1} + t_3 a_0^+ b_{\mathrm{B},1} + t_4 a_0^+ \vartheta_{\mathrm{B},1} + \mathrm{h.c.}) \\ &-2(t_1 a_{N+1}^+ b_{\mathrm{A},N} + t_2 a_{N+1}^+ \vartheta_{\mathrm{A},N} + t_3 a_{N+1}^+ b_{\mathrm{B},N} + t_4 a_{N+1}^+ \vartheta_{\mathrm{B,N}} + \mathrm{h.c.}), \end{aligned} \tag{5}$$

where $t_1 = t_3 = 0.4\,\mathrm{eV}$ is the hopping amplitude between electrode and DNA molecule along z direction,[20] while the hopping of θ direction can be set $t_2 = t_4 = 0.2\,\mathrm{eV}$.

3. Transmission coefficient

In order to evaluate the transport properties of the system, we have employed the transfer matrix method.[25] The Schrodinger equation $H\,|\Psi\rangle = E\,|\Psi\rangle$ becomes,

$$\begin{aligned} &t_{n+1,n}^{\mathrm{A}_z}\varphi_{n+1}^{\mathrm{A}_z} + t_{n-1,n}^{\mathrm{A}_z}\varphi_{n-1}^{\mathrm{A}_z} + \varepsilon_n^{\mathrm{A}_z}\varphi_n^{\mathrm{A}_z} + U_n^{\mathrm{A}}(z,\theta)\varphi_n^{\mathrm{A}_\theta} + U_n^{\mathrm{AB}}(z,z)\varphi_n^{\mathrm{B}_z} = E\varphi_n^{\mathrm{A}_z}, \\ &t_{n+1,n}^{\mathrm{A}_\theta}\varphi_{n+1}^{\mathrm{A}_\theta} + t_{n-1,n}^{\mathrm{A}_\theta}\varphi_{n-1}^{\mathrm{A}_\theta} + \varepsilon_n^{\mathrm{A}_\theta}\varphi_n^{\mathrm{A}_\theta} + U_n^{\mathrm{A}}(z,\theta)\varphi_n^{\mathrm{A}_z} + U_n^{\mathrm{AB}}(\theta,\theta)\varphi_n^{\mathrm{B}_\theta} = E\varphi_n^{\mathrm{A}_\theta}, \\ &t_{n+1,n}^{\mathrm{B}_z}\varphi_{n+1}^{\mathrm{B}_z} + t_{n-1,n}^{\mathrm{B}_z}\varphi_{n-1}^{\mathrm{B}_z} + \varepsilon_n^{\mathrm{B}_z}\varphi_n^{\mathrm{B}_z} + U_n^{\mathrm{B}}(z,\theta)\varphi_n^{\mathrm{B}_\theta} + U_n^{\mathrm{AB}}(z,z)\varphi_n^{\mathrm{A}_z} = E\varphi_n^{\mathrm{B}_z}, \\ &t_{n+1,n}^{\mathrm{B}_\theta}\varphi_{n+1}^{\mathrm{B}_\theta} + t_{n-1,n}^{\mathrm{B}_\theta}\varphi_{n-1}^{\mathrm{B}_\theta} + \varepsilon_n^{\mathrm{B}_\theta}\varphi_n^{\mathrm{B}_\theta} + U_n^{\mathrm{B}}(z,\theta)\varphi_n^{\mathrm{B}_z} + U_n^{\mathrm{AB}}(\theta,\theta)\varphi_n^{\mathrm{A}_\theta} = E\varphi_n^{\mathrm{B}_\theta}, \end{aligned}$$

where $\varphi_n^{\alpha z} = \langle \alpha z : n|\,\Psi\rangle$, $\varphi_n^{\alpha\theta} = \langle \alpha\theta : n|\,\Psi\rangle$.

The wavefunctions of sites $n+1$ and n are related to those of sites n and $n-1$ by a transfer matrix M_n,

$$\begin{pmatrix} \varphi_{n+1}^{\mathrm{A}_z} \\ \varphi_{n+1}^{\mathrm{A}_\theta} \\ \varphi_{n+1}^{\mathrm{B}_z} \\ \varphi_{n+1}^{\mathrm{B}_\theta} \\ \varphi_n^{\mathrm{A}_z} \\ \varphi_n^{\mathrm{A}_\theta} \\ \varphi_n^{\mathrm{B}_z} \\ \varphi_n^{\mathrm{B}_\theta} \end{pmatrix} = M_n \begin{pmatrix} \varphi_n^{\mathrm{A}_z} \\ \varphi_n^{\mathrm{A}_\theta} \\ \varphi_n^{\mathrm{B}_z} \\ \varphi_n^{\mathrm{B}_\theta} \\ \varphi_{n-1}^{\mathrm{A}_z} \\ \varphi_{n-1}^{\mathrm{A}_\theta} \\ \varphi_{n-1}^{\mathrm{B}_z} \\ \varphi_{n-1}^{\mathrm{B}_\theta} \end{pmatrix}, \tag{6}$$

where

$$M_n = \begin{pmatrix} \frac{E-\varepsilon_n^{\mathrm{A}_z}}{t_{n+1,n}^{\mathrm{A}_z}} & -\frac{U_n^{\mathrm{A}}(z,\theta)}{t_{n+1,n}^{\mathrm{A}_z}} & -\frac{U_n^{\mathrm{AB}}(z,z)}{t_{n+1,n}^{\mathrm{A}_z}} & 0 & -\frac{t_{n-1,n}^{\mathrm{A}_z}}{t_{n+1,n}^{\mathrm{A}_z}} & 0 & 0 & 0 \\ -\frac{U_n^{\mathrm{A}}(z,\theta)}{t_{n+1,n}^{\mathrm{A}_\theta}} & \frac{E-\varepsilon_n^{\mathrm{A}_\theta}}{t_{n+1,n}^{\mathrm{A}_\theta}} & 0 & -\frac{U_n^{\mathrm{AB}}(\theta,\theta)}{t_{n+1,n}^{\mathrm{A}_\theta}} & 0 & -\frac{t_{n-1,n}^{\mathrm{A}_\theta}}{t_{n+1,n}^{\mathrm{A}_\theta}} & 0 & 0 \\ -\frac{U_n^{\mathrm{AB}}(z,z)}{t_{n+1,n}^{\mathrm{B}_z}} & 0 & \frac{E-\varepsilon_n^{\mathrm{B}_z}}{t_{n+1,n}^{\mathrm{B}_z}} & -\frac{U_n^{\mathrm{B}}(z,\theta)}{t_{n+1,n}^{\mathrm{B}_z}} & 0 & 0 & -\frac{t_{n-1,n}^{\mathrm{B}_z}}{t_{n+1,n}^{\mathrm{B}_z}} & 0 \\ 0 & -\frac{U_n^{\mathrm{AB}}(\theta,\theta)}{t_{n+1,n}^{\mathrm{B}_\theta}} & -\frac{U_n^{\mathrm{B}}(z,\theta)}{t_{n+1,n}^{\mathrm{B}_\theta}} & \frac{E-\varepsilon_n^{\mathrm{B}_\theta}}{t_{n+1,n}^{\mathrm{B}_\theta}} & 0 & 0 & 0 & -\frac{t_{n-1,n}^{\mathrm{B}_\theta}}{t_{n+1,n}^{\mathrm{B}_\theta}} \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

When the DNA chain is connected to two semi-infinite electrodes, the global transfer matrix can be expressed as

$$\tilde{P} = M_{\mathrm{R}} \left(\prod_{n=N}^{1} M_n \right) M_{\mathrm{L}}, \tag{7}$$

where

$$M_{\mathrm{L}} = \begin{pmatrix} \frac{E-\varepsilon_m}{t_1} & 0 & 0 & 0 & -\frac{t_m}{t_1} & 0 & 0 & 0 \\ 0 & \frac{E-\varepsilon_m}{t_2} & 0 & 0 & 0 & -\frac{t_m}{t_2} & 0 & 0 \\ 0 & 0 & \frac{E-\varepsilon_m}{t_3} & 0 & 0 & 0 & -\frac{t_m}{t_3} & 0 \\ 0 & 0 & 0 & \frac{E-\varepsilon_m}{t_4} & 0 & 0 & 0 & -\frac{t_m}{t_4} \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{8}$$

$$M_{\mathrm{R}} = \begin{pmatrix} \frac{E-\varepsilon_m}{t_m} & 0 & 0 & 0 & -\frac{t_1}{t_m} & 0 & 0 & 0 \\ 0 & \frac{E-\varepsilon_m}{t_m} & 0 & 0 & 0 & -\frac{t_2}{t_m} & 0 & 0 \\ 0 & 0 & \frac{E-\varepsilon_m}{t_m} & 0 & 0 & 0 & -\frac{t_3}{t_m} & 0 \\ 0 & 0 & 0 & \frac{E-\varepsilon_m}{t_m} & 0 & 0 & 0 & -\frac{t_4}{t_m} \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{9}$$

The transmission coefficient at zero bias can be calculated by assuming that the plane waves propagate through four channels in the electrodes. Assume the wavefunctions $\varphi_{m,n} = \mathrm{e}^{\mathrm{i}kna} + \sqrt{R_m}\mathrm{e}^{-\mathrm{i}kna}$ for $n \leq 0, m = 1,2,3,4$ and $\varphi_{m,n} = \sqrt{T_m}\mathrm{e}^{\mathrm{i}kna}$ for $n \geq N+1$ in the left and right electrodes respectively,

where R_m and T_m are the reflection and transmission coefficients corresponding to single channel, the total transmission of system can be expressed as

$$T = T_1 + T_2 + T_3 + T_4. \tag{10}$$

4. Calculated results

In order to have a better physical understanding of charge transfer process for a ploy(dG)-ploy(dC) DNA molecule ($N = 30$ bp), Fig.3 shows the transmission spectrum based on the Eq.(10). The transmission spectrum is composed of two wide bands, which are $W_{\rm G} = W_{\rm C} = 0.8$ eV wide, centred at 7.75 and 8.87 eV respectively, plus two narrower bands, which are $W_{\rm C}^{\theta} = 0.4$ eV and $W_{\rm G}^{\theta} = 0.42$ eV wide, centred at 0.92 eV and 3.07 eV respectively. This illuminates that the transfer ability of double-strand DNA is stronger than that of single-strand.[26] The bands corresponding to base C are weaker than those of base G, and two wide bands are separated by an energy gap 0.33 eV, which is slightly less than the previous calculated results,[19] while the gap between two narrow bands is 1.66 eV. Two narrow bands do not centre at the on-site energies of θ direction, it results from the coupling between two strands. The width and intensity of transmission band of θ direction are less than those of z direction. Because the band of θ direction is located at the region of low energy, its role can not be ignored in charge transfer of DNA.

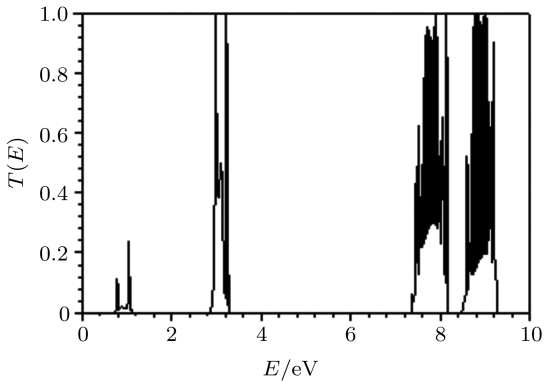


Fig.3. The transmission spectrum of DNA molecule at $t_{n+1,n}^{{\rm A}_z} = t_{n+1,n}^{{\rm B}_z} = 0.2$ eV, $\varepsilon_n^{{\rm A}\theta} = 3$ eV, $\varepsilon_n^{{\rm B}\theta} = 1$ eV, $U_i^{\rm AB}(\theta,\theta) = 0.4$ eV.

The transmission properties will be affected when the hopping energy of z direction changes (see Fig.4), which is related to the stacking energy. With the increase of hopping, the left two bands will be slightly affected and the right two bands widen so that the transmission ability becomes strong. When the hopping energy increases to 0.4 eV, two bands combine to form a very wide band so that the transmission ability enhances. These conclusions are consistent with the previous results.[19]

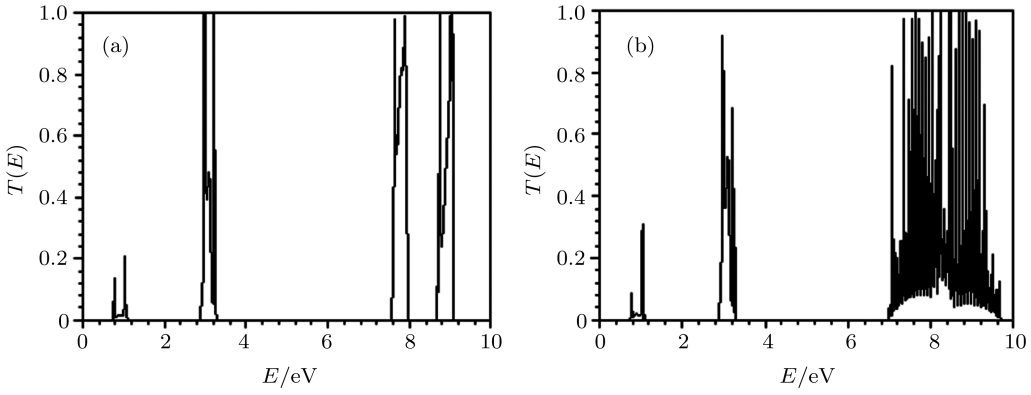


Fig.4. The transmission spectrum at different hopping energies along z direction, (a) $t_{n+1,n}^{{\rm A}_z} = t_{n+1,n}^{{\rm B}_z} = 0.1$ eV; (b) $t_{n+1,n}^{{\rm A}_z} = t_{n+1,n}^{{\rm B}_z} = 0.4$ eV.

Figure 5 shows the transmission curves at different couplings between two strands, which relate to hydrogen band. When the coupling increases, the left band moves to the left, while the second band moves to the right, and their intensities becomes weak. The result shows that the effect of hydrogen band on charge transfer is less than that of stacking energy. Therefore, charge transfer in DNA is mainly conveyed by π-stacking in agreement with the previous results.[18,27]

Figure 6 shows the transmission spectrum at different on-site energies of θ direction. When the on-site energy decreases, the intensity of two bands at left is weakened and the band gap becomes small, two bands combine to form a wide band at $\varepsilon_n^{A_\theta} = 1\,\mathrm{eV}$ and $\varepsilon_n^{B_\theta} = 0.5\,\mathrm{eV}$.

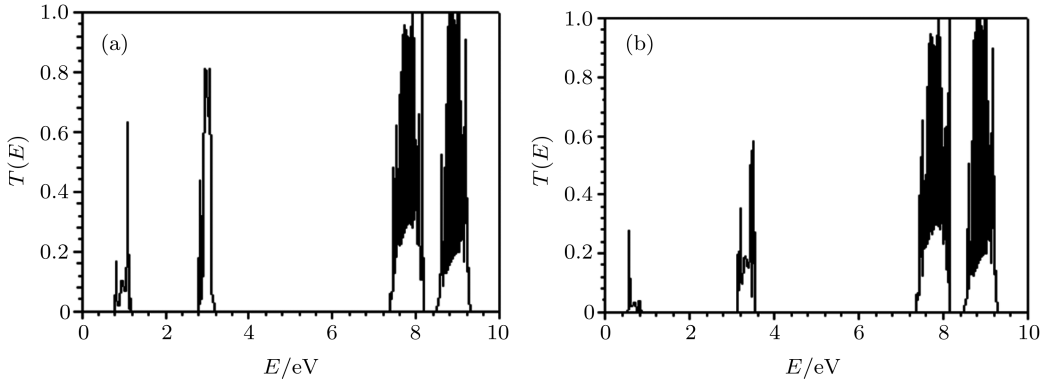


Fig.5. The transmission spectrum at different hydrogen bond energies, (a) $U_i^{AB}(\theta,\theta) = 0$; (b) $U_i^{AB}(\theta,\theta) = 0.9\,\mathrm{eV}$.

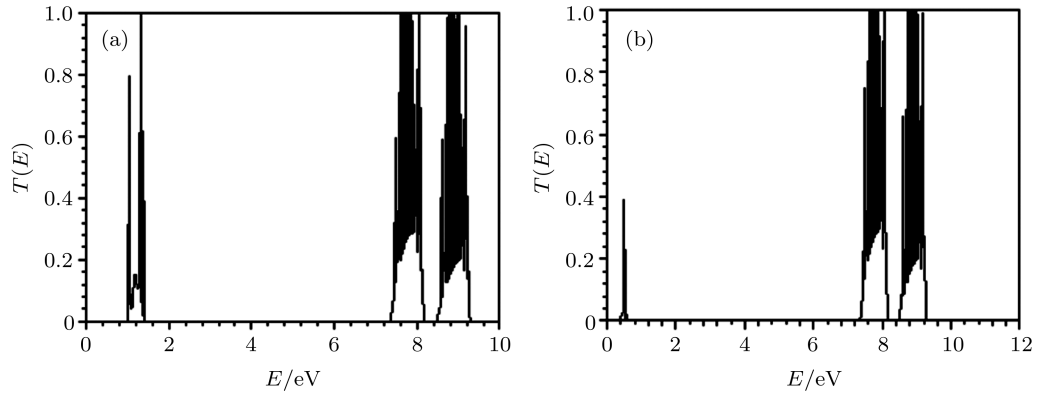


Fig.6. The transmission spectrum at different on-site energies of θ direction. (a) $\varepsilon_n^{A_\theta} = 1\,\mathrm{eV}$, $\varepsilon_n^{B_\theta} = 0.5\,\mathrm{eV}$; (b) $\varepsilon_n^{A_\theta} = \varepsilon_n^{B_\theta} = 0$.

5. Conclusion

In summary, we give the charge transfer model of a double helix DNA molecule. The calculated results show that the transmission characteristics of DNA are related to the z and θ direction, and the width and intensity of transmission band of the θ direction are less than those of the z direction, but its role can not be ignored. With the increase of hopping energy, transmission bands become wide so that the transmission ability enhances. On the other hand, the base dependence of the on-site energy and the hopping integral will result in the difference of transmission ability. This may provide a new sequence analysis method through transmission properties.

References

[1] Berlin Y A, Burin A L and Ratner M A 2000 *Superlattices and Microstructures* **28** 241
[2] Fink H W and Schonenberger C 1999 *Nature* **398** 407
[3] Storm A J, Noort J, Vries S and Dekker C 2001 *Appl. Phys. Lett.* **79** 3881
[4] Seeman N 2001 *Nano. Lett.* **1** 22
[5] Dong R X and Yan X L 2004 *Acta Phys. Sin.* **53** 4414 (in Chinese)
[6] Dong R X, Yan X L, Yu G F and Liu S G 2004 *Phys. Lett.* A **318** 600
[7] Yan X L, Dong R X and Lin Q D 2006 *Commun. Theor. Phys.* **46** 381
[8] Albuquerque E L, Vasconcelos M S, Lyra M L and Moura F A 2005 *Phys. Rev.* E **71** 021910
[9] Gao X T, Fu X, Song J, Liu D S and Xie S J 2006 *Acta Phys. Sin.* **55** 952 (in Chinese)
[10] Guo A M, Ma S S and Xu H 2007 *Chin. Phys.* 16

[11] Okahata Y, Kobayashi T, Tanaka K and Shimomura M 1998 *J. Am. Chem. Soc.* **120** 6165
[12] Kasumov A Y, Kociak M, Guéron S, Reulet B, Volkov V T, Klinov D V and Bouchiat H 2001 *Science* **291** 280
[13] Porath D, Bezryadin A, Vries S and Dekker C 2000 *Nature* **403** 635
[14] Yoo K H, Ha D H, Lee J O, Park J W, Kim J, Kim J J, Lee H Y, Kawai T and Choi H Y 2001 *Phys. Rev. Lett.* **87** 198102
[15] Liu X L, Xu H, Ma S S, Dong C S and Guo A M 2006 *Acta Phys. Sin.* **55** 5562 (in Chinese)
[16] Ma S S 2007 *Chin. Phys.* **16** 862
[17] Cuniberti G, Craco L, Porath D and Dekker C 2002 *Phys. Rev.* B **65** 241314
[18] Xiong G and Wang X R 2005 *Phys. Lett.* A **344** 64
[19] Roche S 2003 *Phys. Rev. Lett.* **91** 108101
[20] Macia E, Triozon F and Roche S 2005 *Phys. Rev.* B **71** 113106
[21] Yamada H 2004 cond-mat/ 0401351
[22] Zhang H Y, Li X Q, Han P, Yu X Y and Yan Y J 2002 *J. Chem. Phys.* **117** 4578
[23] Wang X F and Chakraborty T 2006 *Phys. Rev. Lett.* **97** 106602
[24] Marcus E 2006 *Vielberth Symposium on DNA Nanoelectronic* April 07-08, University of Regensburg
[25] Crisnati A, Paladin G and Vulpiani A 1993 *Products of Random Matrices* (Berlin: Springer) pp87–114
[26] Endres R G, Cox D L and Singh R R 2004 *Rev. Mod. Phys.* **76** 195
[27] Treadway C, Hill M G and Barton J K 2002 *Chem. Phys.* **281** 409