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Charge Transfer Through Single- and Double-strand DNAs: Simulations Based on Molecular Dynamics and Molecular Orbital Methods

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Abstract

To elucidate the difference in charge transfer through single- and double-strand DNAs, we performed simulations based on classical molecular dynamics (MD) and semiempirical molecular orbital (MO) methods. Stable structures of DNA strands in water were determined by MD simulations and their energy levels and distributions of frontier MOs that mediate charge transfer were analyzed by the MO calculations. The transfer integrals for a hole or an electron between the neighboring DNA bases were estimated from the energy levels of frontier MOs. We obtained the current-voltage characteristics for single- and double-strand DNAs that are qualitatively in agreement with the experimental results.

1. Introduction

In genome research, it is crucial to accurately determine the sequence of DNA bases within a realistic time. As a basic technology for detecting the sequence, several types of DNA chips have been developed. Although the fluorescence-type DNA chip is more popular than the electrochemical DNA chip, the fluorescence-type chip is less practical because of its low detection accuracy, the large size of detection device required and the long detection time. The electrochemical DNA chip detects DNA base sequences based on the change in charge conductivity through DNA. Because it can detect the sequence more accurately than the fluorescence-type and the detection device can be more compact, it is expected that the electrochemical DNA chip will be commercially available sooner. However, since the mechanism of charge transfer through DNA and its dependence on the DNA sequence are not yet clarified in experimental or theoretical studies, the elucidation of the mechanism is essential to the development of more accurate electrochemical DNA chips.

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On a DNA chip, the single-strand DNA having a complementary base-sequence to the single-strand DNA stuck on the chip can form a double-strand DNA, while other single-strand DNAs cannot. As a result, many single-strand DNAs remain on the DNA chip. In an experimental study [1], double-strand DNAs were found to conduct much greater electric current than single-strand DNAs. However, the underlying mechanism that manifests such a large difference in electric current between single- and double-strand DNAs has not been clarified.

In the present study, we attempt to elucidate the difference in charge transfer property of single- and double-strand DNAs by using simulations based on molecular dynamics (MD) and molecular orbital (MO) methods. We first investigated the structures of single- and double-strand DNAs in water using classical MD simulations. For the structures obtained by MD as well as the standard B-form structures, the energy levels and distributions of frontier MOs that mediate charge transfer were analyzed by the semiempirical MO calculations, accounting for the electric field of solvent water molecules, counter ions and DNA backbones around the base pairs. The transfer integral for charge transfer between the neighboring DNA bases was estimated from the energy levels of frontier MOs, and finally the hole- and electron-conductivities through single- and double-strand DNAs were evaluated by the current-voltage analysis simulator recently developed in our laboratory [2].

2. Method of molecular simulations

2.1. Structure optimization for single- and double-strand DNAs

We first constructed the standard B-form DNA structures for the following six types of DNAs with 12 bases or base-pairs by using the molecular modeling software HyperChem [3].

- a. Single-strand DNA with 12 Guanine (G) bases
- b. Single-strand DNA with 12 Cytosine (C) bases
- c. Single-strand DNA with 12 Adenine (A) bases
- d. Single-strand DNA with 12 Thymine (T) bases
- e. Double-strand DNA with 12 G-C base pairs
- f. Double-strand DNA with 12 A-T base pairs

Counter ions Na^+ were added to the phosphate groups of DNA backbones; their positions were optimized by the AMBER force field [4]. The positions of all atoms in DNA were subsequently fully optimized by the AMBER force field in water. The effects of ambient water molecules were accounted for in the continuous solvation model HCT [5] implemented in the molecular mechanics (MM) and MD calculation program TINKER [6]. Starting with these optimized structures, MD simulations were performed in water at room temperature (300 K). The time step of MD simulation was one femtosecond and the total time of MD simulation was one nanosecond.

2.2. MO calculations and estimation of charge transfer integrals for DNA

Charge transfer in DNA is thought to take place through the DNA bases. To estimate the charge transfer integrals between the neighboring DNA bases, we calculated the electronic properties of stacking models with two DNA bases. The charge transfer occurs between the neighboring bases as shown in Fig. 1, in which the arrows indicate the directions of charge transfer. It is noted that the DNA backbones are substituted with hydrogen atoms, their positions optimized by MO calculations. This is because we must perform MO calculations for several tens of thousands of DNA stacking models, and the MO calculations including DNA backbones and counter ions cannot be carried out in a realistic time. We thus constructed 11 types of stacking models for single-strand DNA and 56 types of stacking models for double-strand DNA based

on the standard B-form structures as well as those determined by MD simulations for the six types of DNA strands having 12 bases or base-pairs. The electronic properties for these stacking models were obtained by the semiempirical MO program package MOPAC [7]. In the MO calculations in water, we used the PM3 Hamiltonian [8] and the continuous solvation approximation based on COSMO method [9]. To include the effect of DNA backbones and counter ions on the electronic property of base-stacking models, we performed MO calculations, accounting for the external electric field of ambient water molecules, counter ions, and DNA backbones around the base pairs.

Next, we outline the method for estimating charge transfer integrals between DNA bases in the generalized Mulliken-Hush (GMH) theory [10–12]. Assume H is the Hamiltonian of the system (donor + acceptor) and Φ is the wavefunction. Then

$$H|\Phi\rangle = \varepsilon|\Phi\rangle \quad (1)$$

Expand $|\Phi\rangle$ in the $\{|D\rangle, |A\rangle\}$ basis; where $\Psi_D = |D\rangle$ and $\Psi_A = |A\rangle$

$$|\Phi\rangle = C_1|D\rangle + C_2|A\rangle \quad (2)$$

The equation (1) is expressed as:

$$(H|D, H|A) \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \varepsilon(|D, |A\rangle) \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} \quad (3)$$

Multiply from the left with $\begin{pmatrix} \langle D| \\ \langle A| \end{pmatrix}$ to get

$$\begin{pmatrix} H_D & H_T \\ H_T & H_A \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \varepsilon \begin{pmatrix} C_1 \\ C_2 \end{pmatrix}, \quad (4)$$

where

$$H_D = \langle D|H|D\rangle \quad (5)$$

$$H_A = \langle A|H|A\rangle \quad (6)$$

$$H_T = \langle A|H|D\rangle \quad (7)$$

This eigenvalue has nonzero value if the determinant is zero

$$\begin{vmatrix} H_D - \varepsilon & H_T \\ H_T & H_A - \varepsilon \end{vmatrix} = 0 \quad (8)$$

this determinant leads to eigenvalues as

$$\varepsilon = \frac{(H_D + H_A) \pm \sqrt{(H_D - H_A)^2 + 4H_T^2}}{2}. \quad (9)$$

It is considered that the charge transfer from donor to acceptor becomes more facile when the difference in energy between donor and acceptor becomes smaller by the structural change of DNA and/or the external electric field of surrounding Na^+ ions and ambient waters. Hence we assume $H_D = H_A = E_0$ in Eq. (9) to obtain

$$\varepsilon = E_0 \pm H_T, \quad (10)$$

and then

$$\begin{cases} \varepsilon_1 = E_0 + H_T \\ \varepsilon_2 = E_0 - H_T \end{cases}. \quad (11)$$

Finally we obtain H_T as follows,

$$H_T = \frac{\varepsilon_1 - \varepsilon_2}{2}, \quad (12)$$

where ε_1 and ε_2 are, respectively, the eigenvalues of donor and acceptor.

For the DNA strands with A and T bases, the electron transfer from A to T contributes to the change conductivity [13]. Therefore, ε_1 and ε_2 are the energy levels of LUMO+1 and LUMO (lowest unoccupied MO), respectively, and H_T is described as

$$H_T = \frac{1}{2} \times [E_{\text{LUMO}+1} - E_{\text{LUMO}}]. \quad (13)$$

On the other hand, for the DNA strands consisting of G and C bases, the hole transfer contributes to the change conductivity [14,15], primarily because the HOMO energy level of G is higher than those of A, T and C. Thus G easily becomes a hole trapping site. For the charge transfer in DNA consisting of G and C, ε_1 and ε_2 are the energy levels of HOMO (highest occupied MO) and HOMO-1, respectively, and we obtained Eq. (14).

$$H_T = \frac{1}{2} \times [E_{HOMO} - E_{HOMO-1}] \quad (14)$$

Therefore, we can estimate the charge transfer integrals based on Eqs. (13) and (14) from the energy levels of frontier MOs.

In the present study, we obtained the energy levels of frontier MOs for the stacking models of DNA bases to estimate the charge transfer integrals based on Eqs. (13) and (14), because the charge transfer thorough DNA is expected to take place through the stacking DNA bases. In the MO calculations, we considered the effect of the external electric field of ambient water molecules, counter ions and backbones around the DNA bases. As shown in Fig. 2, the direction of the external electric field is determined by the direction from the center of the donor base to the center of the acceptor base. The external electric field was varied from -2.0 to 2.0 V/Å to determine its value that makes the difference in the energy between HOMO and HOMO-1 (or LUMO and LUMO+1) minimal. We used this external-field value in estimating the charge transfer integral, because the charge transfer becomes more facile as the potential difference between donor and acceptor becomes smaller. The site energy of each base was taken to be equivalent to the LUMO energy. Based on these transfer integrals and site energies, we investigated the current (I)-voltage (V) characteristic by using the previously developed I-V simulator [2]. In simulating DNAs composed of G and C bases, the hole is a carrier for charge-transfer, so that we set the HOMO level of G (-8.0 eV) as Fermi energy. On the other hand, for DNAs with A and T bases, electron is mainly transferred, so that we set the LUMO level of A or T (-0.1 eV) as Fermi energy in the I-V simulations.

In a previous study, Adessi et al. [16] showed that the counter ions electrostatically change the potential of base pairs. Mehrez and Anantram [17] considered only the base pairs to determine the charge hopping parameters between bases. We assumed that the neglect of counter ions and backbones has no significant effect on the charge transfer properties because the charge transfer in DNA is generally considered to occur through the overlap of π -orbitals of stacked DNA bases. The electrostatic interactions of counter ions and PO_4 parts of DNA backbones are long-range effects, so that the electronic properties of base pairs are affected by these electrostatic interactions. In the present study, we accounted for these interactions by introducing the external electric field in MO calculations.

3. Results and Discussion

3.1. I-V characteristic for standard B-form structures of DNAs

The saturation currents for the standard B-form structures of G-C double-strand, and G and C single-strands are compared in Table 1. The saturation current of G-C is found to be larger than those of G and C single-strands. This result is qualitatively in agreement with the experimental result [1] showing that double-strand DNAs conduct greater electric current than single-strand DNAs. In fact, the saturation currents for G-C and G are almost the same, while that for C is about 1/7 of those for G-C and G, as indicated in Table 1. These differences may be explained by the difference in the ionization potential (IP) between G and C bases. The values of IP are 8.64 (G) and 9.02 eV (C), respectively, so that the hole is more readily trapped at G than at C [2]. In the G-C double-strand adopted in the present study, each strand has only one kind of base: G or C. Therefore, in the G-C, the hole transfers through only the G strand, resulting in the saturation currents for G-C and the single-strand G being similar to each other.

As for the saturation currents for the standard B-form structures of A-T double-strand, and A and T single-strands, the saturation current of A is about 300 times that of A-T and 10^6 times

that of T. This result is inconsistent with the experimental result [1]. For the DNA constructed with A and T, the electron is expected to transfer through the DNA bases through LUMO distribution. We thus investigated the LUMO distributions for the 12 types of A-T base pairs extracted from the standard B-form double-strand with 12 A-T base pairs. Depending on the structures of A-T base pairs, the LUMO distributions change, so that the LUMO is not localized at only one strand. This result is completely different from that for the G-C base pairs where the HOMO is localized at only G strand. As a result, in the standard B-form A-T double-strand, the electron transfer between the different strands occurs frequently, so that the saturation current of A-T becomes smaller than that of the single-strand A.

It should be noted that the results for the standard B-form DNA fail to account for the dynamical change in DNA structure. In the next subsection, we investigate how the change in DNA structure affects the charge transfer in DNA.

3.2. I-V characteristic for DNA structures obtained by MD simulations

To elucidate the effect of structural change on the I-V characteristic of DNA, we investigated the structures of the above-mentioned 6 types of DNAs by using the MD simulations based on AMBER force field. For the structures obtained by MD, the I-V characteristic was analyzed in the same way as for the standard B-form DNAs discussed in section 3.1.

Figure 3 shows the structures obtained by the 1 ns MD simulations at 300 K in aqueous environment represented by the continuous solvation model HCT [5]. To facilitate the visualization of DNA structure, the Na^+ counter ions are not shown in Fig. 3. From Figs. 3(a), 3(b), 3(c) and 3(d), it is found that the single-strand DNAs largely deform their structures to be a ball-like shape, with the stacking structure between the neighboring bases almost disappearing. On the other hand, the structures of G-C and A-T double-strands tend to keep their chain-like structures, as shown in Figs. 3(e) and 3(f). In the double-strand DNAs, each base forms hydrogen bonds with the complementary base, resulting in more rigid structures than those in the single-strand DNAs. The single-strand DNAs are also less stable from the viewpoint of chemical reactivity, because the bases in the single-strand DNA have sites for establishing hydrogen bonds to other molecules, such as water.

Comparison between the structures of G-C (Fig. 3(e)) and A-T (Fig. 3(f)) double-strands reveals that the G-C stacking structure is more rigid than the A-T structure, because the A-T base pairs are largely deformed at both edges of the double-strand. This result can be explained by the difference in the hydrogen bonding strengths of the G-C and A-T base pairs. In our previous MO calculations [18] based on the *ab initio* MP2/6-311G(2df, pd) method, the hydrogen bonding energies in G-C and A-T pairs are -28.88 and -14.94 kcal/mol, respectively.

From the structures obtained by the MD simulations, we constructed the stacking models of DNA bases and investigated their electronic properties by semiempirical MO (MOPAC-PM3) calculations. The charge transfer integrals H_T estimated from the Eqs. (13) and (14) are tabulated in Tables 2, 3 and 4. The average H_T values for all types of intrastrand and interstrand base-stacking models obtained by the present simulations are qualitatively in agreement with the previous results obtained by Mehrez and Anantram [17]. As for the single-strand DNAs, the A strand has larger average H_T than the other single-strands (Table 2). However, the minimum H_T of A is very small (0.0001 eV), so that the saturation electron-current of A is smaller than that of the T single-strand, as shown in Table 1. The minimum H_T of the C single-strand is also so small (0.0002 eV) that the saturation hole current of C is much smaller than that of the G single-strand. From these facts, we concluded that the conductance of hole or electron in the single-strand DNAs is related to the magnitude of the minimum H_T . On the other hand, the conductance in the double-strand DNAs cannot be explained only by the magnitude of H_T , because there are many paths for charge transfer.

In recent theoretical studies [19,20], electric coupling matrix for hole transfer between adjacent Watson-Crick pairs in DNA was investigated by using the GMH method and many types of MO calculations. It was concluded that semiempirical MO methods (MNDO, AM1 and PM3) fail to provide acceptable values of the electric coupling matrix in the DNA base stacks. However, these studies did not consider the effect of the external electric field of ambient water molecules as well as the counter ions. Therefore, it cannot be concluded whether or not the charge transfer integrals between DNA bases including the external electric field can be estimated by semiempirical MO calculations. It should be noted that the magnitude of the charge transfer integrals is significantly reduced by the external electric field.

Based on these values of the transfer integrals and the sites energies, the I-V characteristics were obtained by using the I-V simulator [2]. The I-V curves of G-C and A-T double-strands are shown in Figs. 4(a) and 4(b). The saturation currents of the single-strand G, C, A and T are smaller than those of the double-strand DNAs as shown in Table 1. This result is qualitatively consistent with the experimental result [1].

As for the DNA strands constructed with G and C bases, the saturation currents of G-C and G are nearly the same (Table 1). The result indicates that the hole transfers through both the G-C and G are the same as described in section 3.1. The effect of the structural change on the I-V characteristic is displayed in Table 1; the saturation current of G-C (G) is reduced to about 1/25 (1/20) by the structural change from the standard B-form to the MD structure. Therefore, it can be concluded that the structural change during the hole transfer through the G-C double-strand must be considered for obtaining realistic I-V characteristic.

As for the A-T, A, and T strands, Table 1 shows that the saturation current of A-T is about 500 and 50 times greater than those of A and T, respectively. As shown in Figs. 3(c) and 3(d), the structures of the A and T single-strands are largely deformed to the ball-like structure, so that the electron transfer through A and T are largely reduced. The saturation current of A-T double-strand is also reduced to 1/8800 by the structural change. The structural change is generally large for A-T as shown in Fig. 3(f), so that the reduction in the current is greater than that for the G-C double-strand. Therefore, we conclude that the effect of structural change on the I-V characteristic is larger for the single-strand DNAs than it is for the double-strand DNAs.

3.3. Dependence of I-V characteristic on the structure of G single-strand

In order to elucidate what type of DNA structure is more preferable for hole transfer, we investigated the dependence of the saturation current on the structure for the flexible single-strand G. Figure 5 shows the change in the stacking distances between neighboring bases for the single-strand G. The changes in average, minimal and maximum stacking distances are plotted for each structure obtained by the MD simulation. The minimal and average distances are almost constant, while the maximum distance changes drastically. Therefore, it is expected that only a few stacking distances are changed largely by the MD simulation.

We chose several structures with a large change in the maximum stacking distance and investigated their I-V characteristics. They are nine types of structures at 0, 10, 20, 40, 70, 320, 360, 620 and 820 ps of MD simulation. The values of hole transfer integrals H_T for each stacking model, saturation current and distance between the contacts are listed in Table 5. The distance between the contacts is estimated from that between the 3' and 5' ends of the single-strand, because the contacts are attached to these ends in our developed I-V simulator.

From the comparison of the average and minimal values of H_T and the saturation current shown in Table 5, it is concluded that the structure with larger minimal H_T has greater saturation current, while there is no well-defined relation between the average H_T and the saturation current. In other words, the G single-strand having a base stacking with small H_T has smaller

saturation current. It is thus expected that the saturation current is drastically reduced, even if only one base stacking with smaller H_T exists in the G single-strand. On the other hand, the values of average H_T and distance between contacts seem to have no relation with the size of saturation current, as shown in Table 5. Therefore, we concluded that the base stacking with small H_T becomes a bottleneck of hole transfer in the single-strand G, resulting in the large reduction of the hole current.

4. Conclusions

In the present study, we investigated the structures and electronic properties of single- and double-strand DNAs by using the classical MD based on AMBER force field and semiempirical MO (MOPAC-PM3) methods. Based on the energy levels and distributions of frontier MOs, the current-voltage (I-V) characteristics of these DNA strands were analyzed by the I-V simulator program we developed [2]. In the MO calculations, we considered the electric field of solvent water molecules and counter-ions to obtain realistic charge transfer integrals between bases. Furthermore, to elucidate the effect of structural change on the I-V characteristic of the single- and double-strand DNAs, the I-V characteristic was investigated for the standard B-form structures as well as for the deformed realistic structures obtained by the MD simulations.

The results indicate that the single-strand DNAs are largely deformed from the B-form structure, so that their saturation currents are significantly reduced in the MD structures. On the other hand, the double-strand DNAs tend to keep their chain-like structures to maintain large saturation currents. The computed I-V characteristics for the MD structures of single- and double-strand DNAs are qualitatively in agreement with the experimental results [1] showing the electric current through double-strand DNAs are greater than those in single-strand DNAs. It is also elucidated that the occurrence of base stacking with small H_T in the G single-strand drastically reduces the conductance of hole current.

Acknowledgments

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Figure 1.

DNA base-stacking models for estimating charge transfer integral between bases; (a) for double-strand DNAs, both inter-strand and intra-strand charge transfers are considered, (b) for single-strand DNAs, only intra-strand charge transfer is considered. The arrows indicate the direction of charge transfer.

Figure 2.
Direction of external electric field for A-T base pair headed from the center of A to that of T.

Figure 3. Structures of single- and double-strand DNAs obtained by the MD simulations (300K, 1ns) based on AMBER force field; (a) single-strand G, (b) single-strand C, (c) single-strand A, (d) single-strand T, (e) double-strand G-C, and (f) double-strand A-T.

Figure 4. I (current)-V (bias) curves for G-C and A-T double-strand DNAs having the structures shown in Figs. 3(e) and 3(f).

Figure 5. Change in stacking distance between the neighboring bases for the single-strand G during MD simulation.

Table 1
Saturation currents (A) of single- and double-strand DNAs for the standard B-form and the MD simulated structures

DNAs	Double-strands		Single-strands			
	G-C	A-T	G	C	A	T
B-form structure	2.3×10^{-14}	1.2×10^{-8}	1.8×10^{-14}	3.2×10^{-15}	3.3×10^{-6}	2.2×10^{-12}
MD structure	9.3×10^{-16}	1.4×10^{-12}	8.9×10^{-16}	1.7×10^{-18}	2.8×10^{-15}	2.8×10^{-14}

Table 2

Charge transfer integrals H_T (eV) for single-strand A, T, G and C DNAs, whose structures were obtained by MD simulations

Stacked bases	A	T	G	C
1–2	0.0001	0.0009	0.0046	0.0012
2–3	0.0003	0.0028	0.0120	0.0029
3–4	0.0037	0.0094	0.0050	0.0028
4–5	0.0335	0.0063	0.0023	0.0043
5–6	0.0020	0.0019	0.0023	0.0045
6–7	0.0200	0.0018	0.0290	0.0002
7–8	0.1065	0.0058	0.0296	0.0036
8–9	0.0007	0.0055	0.0206	0.0016
9–10	0.2140	0.0080	0.0032	0.0028
10–11	0.0138	0.0066	0.0039	0.0008
11–12	0.0033	0.0037	0.0051	0.0049
Average	0.0362	0.0048	0.0107	0.0027
Maximum	0.2140	0.0094	0.0296	0.0049
Minimum	0.0001	0.0009	0.0023	0.0002

Table 3
Charge-transfer integrals H_T (eV) for A-T double-strand, whose structure was obtained by MD simulations. Intra A and Intra B are the intra-strand stacked bases in the A and B strand, respectively; Inter A and Inter B are the inter-strand stacked bases as shown in Fig. 1. W-C is the Watson-Crick base pair

Stacked bases	Intra A	Intra B	Inter A	Inter B	W-C
1-2	0.0032	0.0039	0.0020	0.0026	0.0168
2-3	0.0023	0.0033	0.0000	0.0051	0.0022
3-4	0.0018	0.0038	0.0006	0.0016	0.0040
4-5	0.0051	0.0174	0.0025	0.0031	0.0037
5-6	0.0024	0.0018	0.0029	0.0023	0.0010
6-7	0.0129	0.0146	0.0027	0.0027	0.0014
7-8	0.0024	0.0038	0.0028	0.0019	0.0030
8-9	0.0031	0.0029	0.0022	0.0001	0.0094
9-10	0.0031	0.0026	0.0007	0.0009	0.0020
10-11	0.0034	0.0027	0.0034	0.0017	0.0019
11-12	0.0024	0.0033	0.0029	0.0084	0.0062
12	-	-	-	-	0.0010
Average	0.0038	0.0055	0.0020	0.0027	0.0044
Maximum	0.0129	0.0174	0.0034	0.0084	0.0168
Minimum	0.0018	0.0018	0.0000	0.0001	0.0010

Table 4
Charge-transfer integrals H_T (eV) for G-C double-strand, whose structure was obtained by MD simulations

Stacked bases	Intra A	Intra B	Inter A	Inter B	W-C
1-2	0.0138	0.0109	0.0049	0.0019	0.0049
2-3	0.0077	0.0028	0.0009	0.0022	0.0016
3-4	0.0053	0.0052	0.0003	0.0036	0.0021
4-5	0.0016	0.0022	0.0034	0.0003	0.0013
5-6	0.0193	0.0065	0.0022	0.0026	0.0018
6-7	0.0028	0.0150	0.0047	0.0012	0.0068
7-8	0.0033	0.0223	0.0010	0.0028	0.0029
8-9	0.0016	0.0019	0.0001	0.0027	0.0042
9-10	0.0055	0.0101	0.0041	0.0028	0.0039
10-11	0.0074	0.0101	0.0020	0.1093	0.0042
11-12	0.0081	0.0031	0.0047	0.1158	0.0051
12	-	-	-	-	0.0062
Average	0.0069	0.0082	0.0025	0.0223	0.0037
Maximum	0.0193	0.0223	0.0049	0.1158	0.0068
Minimum	0.0016	0.0019	0.0001	0.0003	0.0013

Table 5

Changes in charge-transfer integrals H_T (eV), saturation current and the distance between the contacts during MD simulation for the single-strand G

MD Time (ps)	0	10	20	40	70	320	360	620	820
H_T 1-2	0.0326	0.0085	0.0040	0.0042	0.0059	0.0099	0.0020	0.0025	0.0007
2-3	0.0326	0.0034	0.0243	0.0064	0.0133	0.0034	0.0055	0.0054	0.0109
3-4	0.0327	0.0096	0.0394	0.0045	0.0110	0.0013	0.0027	0.0044	0.0022
4-5	0.0326	0.0021	0.0111	0.0054	0.0050	0.0100	0.0042	0.0019	0.0010
5-6	0.0327	0.0204	0.0461	0.0038	0.0051	0.0009	0.0077	0.0012	0.0061
6-7	0.0327	0.0073	0.0027	0.0047	0.0072	0.0094	0.0043	0.0304	0.0171
7-8	0.0327	0.0040	0.0095	0.0047	0.0023	0.0145	0.0073	0.0198	0.0251
8-9	0.0326	0.0317	0.0047	0.0158	0.0350	0.0403	0.0186	0.0298	0.0060
9-10	0.0326	0.0036	0.0015	0.0027	0.0015	0.0061	0.0028	0.0027	0.0038
10-11	0.0326	0.0101	0.0154	0.0007	0.0053	0.0023	0.0057	0.0059	0.0043
11-12	0.0326	0.0051	0.0053	0.0072	0.0023	0.0246	0.0047	0.0129	0.0069
HT Average	0.0326	0.0096	0.0149	0.0054	0.0085	0.0111	0.0059	0.0106	0.0076
H_T Maximum	0.0327	0.0317	0.0461	0.0158	0.0350	0.0403	0.0186	0.0304	0.0251
H_T Minimum	0.0326	0.0021	0.0015	0.0007	0.0015	0.0009	0.0020	0.0012	0.0007
Current ($\times 10^{-16}$ A)	180	10.6	10.2	4.91	8.74	1.86	11.8	3.62	4.44
Distance (Å)	42.94	41.47	30.06	41.60	33.58	31.43	32.82	27.38	28.43