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Effect of Backbone, Sequence, and Positional Disorders on Electrical Transport in Modified Poly(dA)–Poly(dT) DNA Wire

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Abstract

The effect of medium and thermal fluctuations on charge transport in two types of modified poly(dA)–poly(dT) DNA was studied by calculating the transmission probability and current–voltage (I–V) characteristics of a model DNA wire sandwiched between two metal electrodes. Modification was performed by randomly replacing several A–T base pairs with C–G or G–C base pairs along the DNA chain. The medium–DNA interaction was modeled as the backbone onsite energy disorder in the DNA tight-binding Hamiltonian. The helicity of the molecule was considered by incorporating twist-angle-dependent intrastand hopping amplitude in the model. Thermal fluctuation was modeled by varying the twist angles of each base in the DNA wire. Twist-angle disorder was influenced by temperature and frequency. The I–V results obtained by modeling the backbone disorder effect showed that the current decreased and the threshold voltage generally increased as disorder strength increased to a critical value. The current increased and the threshold voltage decreased as the disorder strength exceeded this critical value. However, certain values of the backbone disorder reduced the threshold voltage before the critical value was reached because the transmission bands shifted toward the Fermi energy. The results of thermal fluctuation modeling indicated that increasing thermal fluctuation (increasing temperature and decreasing frequency) degraded the electrical properties of the DNA modified with C–G base pairs but enhanced those of the DNA modified by G–C base pairs. This trend, however, did not always hold for all frequency values for the latter DNA type.

Keywords: DNA, electrical properties, backbone disorder, sequence disorder, thermal fluctuation

Introduction

Charge transport in DNA has been studied intensively and extensively given its role in numerous processes and the application of DNA in molecular electronics. DNA damage detection and repair [1-3] and molecular signaling [4,5] are some biological processes that involve charge transport. Nanowire templates [6,7], biosensors [8,9], and molecular transistors [10,11], as well as electrochemical sequencing [8], are molecular electronic applications that include charge transport.

Eley and Spivey proposed the first mechanism of charge transport in DNA [12]. They proposed that stacking between DNA bases could form a pathway for charge carriers through DNA. Research on charge transport in DNA performed after this proposal revealed that although DNA can carry electric charges, the conductivity of DNA is influenced by numerous factors. Some factors that can influence DNA conductivity include the disorder of the DNA base sequence [13-15], the disorder of base positions caused by thermal energy [8,15-19], and the disorder in the backbone molecules caused by the interaction between the environment medium and DNA, for example water molecules surrounding the DNA bind to the backbone molecules and introduce disorder to their structure [14,20-22]. These factors can explain why some DNA exhibit insulator properties, whereas other DNA exhibit conductor properties [23-30]. Moreover, several experiments have shown that the presence or absence of an adsorbed water layer on DNA, as well as humidity [31-34], buffer type [35], and temperature [35,36], can influence DNA conductivity. Given that DNA conductivity is influenced by numerous factors that can work together, theoretical studies can help in understanding the mechanism underlying the effects of these factors on charge transport in DNA.

This paper presents the results of computational studies that investigated the influence of sequence disorders, positional disorders, and environmental effects on DNA conductivity. Sequence disorder is simulated by replacing several bases in a poly(dA)–poly(dT) sequence with other bases, specifically, with G–C, or C–G base pairs.
Positional disorder is represented by changing DNA twist angles that are distributed in accordance with the equipartition theorem wherein distribution width or disorder strength is proportional to temperature. The twisting motions of bases can force the $p$ orbital between bases in or out of alignment. Finally, the influence of the environment or medium on DNA is modeled with the disorder of backbone onsite energies.

**Materials and Methods**

Computational Details. Our model consists of a DNA wire that is in contact with metallic electrodes on both ends. The DNA sequence is a poly(dA)–poly(dT) sequence and is modified by replacing 50 out of 102 AT base pairs with C–G (sequence A) or G–C (sequence B) base pairs that are randomly placed in the DNA chain. A charge can hop from the electrode to the bases in both strands. The charge can then migrate along the strands or hop from a base to its pair. The charge can also hop from a base to the nearest backbone site. It cannot, however, hop along backbone sites. The model is shown in Figure 1 and is called the ladder model [14,37].

The Hamiltonian of the DNA is as follows [37]:

$$ H = \sum_{i=1}^{L} \sum_{\tau=1,2} \left[ (\varepsilon_i^\tau + \phi_i^\tau) |i, \tau\rangle \langle i, \tau| + t_{i,i+1}^\tau \cos(\Delta_{i,i+1}^\tau) |i, \tau\rangle \langle i+1, \tau| + \sum_{q=u,d} \left( B_i^q |i, q\rangle \langle i, q| + h_i^q |i, q\rangle \langle i, q| \right) + I_{i,2}^2 |i, 1\rangle \langle i, 2| \right] + h. c., $$

with

$$ \phi_i^\tau = b_{i-1,i}^\tau (\cos \Delta_i^\tau - \cos \varphi_{eq}) + b_{i,i+1}^\tau (\cos \Delta_{i+1}^\tau - \cos \varphi_{eq}) $$

and

$$ \Delta_i^\tau = \varphi_{eq} - (\varphi_{i-1}^\tau - \varphi_i^\tau) $$

also

$$ \Delta_{i,i+1}^\tau = \varphi_{eq} - (\varphi_i^\tau - \varphi_{i+1}^\tau). \quad (1) $$

In Eq. (1), variables $\varepsilon$ and $B$ denote base and backbone onsite energies, respectively. The values of $\varepsilon$ are dependent on base type, as follows: $A = 8.22 \text{ eV}$, $C = 8.85 \text{ eV}$, $G = 7.84 \text{ eV}$, and $T = 9.06 \text{ eV}$ [37]. The value of $B$ can vary within the range of the uniform distribution $[Bn - W, Bn + W]$. Here $W$ is the width of the distribution or the strength of the backbone onsite energy disorder, and $Bn$ is the normal backbone onsite energy (9.36 eV) [37]. $L$ is the DNA sequence length, which is 102 base pairs. The symbols $i$, $\tau$, and $q$ are the site, base strand, and backbone strand indexes, respectively. Index $i$ ranges from 1 to $L$, whereas index $\tau$ has two values, 1 and 2, that denote the DNA strand. Index $q$ has two values, $u$ and $d$, which denote the upper and lower backbone strands, respectively. The hopping integrals $t$, $I$, and $h$ denote intrasstrand, intersstrand, and base–backbone charge-hopping probability, respectively. The values of the intrasstrand and intersstrand hopping integrals depend on the base pairs in the hopping direction. The values of the base–backbone hopping integrals depend on the bases paired to backbone sites. Given that DNA is a helix, the twist angle between neighboring bases in the same strand is represented by $\varphi_{eq}$, which is the twist angle at equilibrium. We also account for the effect of twisting-mode phonons on charge transport by using the variable $\varphi$, which is the deviation of the twist angle of a base from equilibrium position, and $b$, which is the charge–phonon coupling constant. Finally, $h. c.$ denotes the Hermitian conjugate. In our model, the influence of the twist phonon on the base onsite energies is given by the symbol $\phi$. The twist phonon also influences intrastrand hopping integrals. The values of hopping integrals and charge–phonon coupling constants can be seen in a previous publication [37]. Other parameters are the metal onsite energy, which is taken to be equal to the Fermi energy ($E_F$) 8.45 eV, and the metal–metal and metal–DNA hopping, which is 0.75 eV. The Fermi energy is selected as the average of the onsite base energies of A, T, G, and C bases to cover the whole energy spectrum of DNA bases. The metal–DNA hopping am-
plitude is independent of base type. The twist motions of the bases arise from thermal fluctuations [16,18], which are modeled by taking the values of $\varphi$ from a Gaussian distribution with average zero and standard deviation $\sqrt{T/\tau}$, where $T$ is temperature and $\tau$ is a variable proportional to the square of the twisting-mode frequency (ω) [37]. Standard deviation is derived from the equipartition theorem [16,18].

The transmission probability of the charges ($T(E)$) is then calculated by employing the transfer matrix and scattering matrix methods simultaneously as previously described [38]. The results for $T(E)$ are then averaged over 1,000 realizations of the twist-angle disorder to reduce the spurious effects of the random number generator. The transmission bands are calculated with respect to $E_F$. The current–voltage ($I$–$V$) curves are then calculated from $T(E)$ by using the Landauer–Büttiker formalism [39].

Results and Discussion

 Backbone Disorder Results. The $I$–$V$ characteristics calculated for $W$ values between 0 and 5 eV show that the saturation current initially decreases as $W$ increases (Figure 2). The current, however, increases as $W$ continues to increase. This trend was observed for sequences A and B and is reflected by theoretical $I$–$V$ curves generated by Guo et al. for the poly(dG)–poly(dC) sequence [21,22] and G4 DNA [22]. By using Lyapunov exponents, localization lengths, and density of states, Guo et al. and other research groups showed that the charge transport probability for poly(dG)–poly(dC) sequences and several other types of DNA increased as $W$ increased above a certain value [14,20,21]

The backbone disorder represents the influence of the medium on DNA. Given that backbone molecules are located on the outside of DNA, water molecules, oxygen molecules, and salt residues will adsorb and interact with backbone molecules rather than with bases [20]. These interactions will introduce disorder to backbone molecules [20]. Increasing backbone disorder means increasing the interaction between DNA and surrounding environment or medium. Our results show that increasing DNA–medium interaction increases the maximum current in the $I$–$V$ profile.

The increase in maximum current has been observed in experiments that compared the $I$–$V$ profiles of DNA in a vacuum and in ambient conditions [32,35]. The maximum current of DNA in ambient conditions is higher than that in a vacuum. The maximum current also increases with increasing relative humidity [32-34].

Figure 2. $I$–$V$ Characteristics of Sequences A (a–d) and B (e–h) when $W = 0, 1, 2, 5$ eV. The Insets in Each Panel Show Differential Conductance at Each $W$
These results were attributed to conduction through the adsorbed water layer on the DNA molecules. Other researchers observed an increase in maximum current with increasing sodium acetate salt concentration of a solution surrounding DNA molecules [34]. The increase in current was attributed to the condensation of salt residues on DNA molecules. Another experiment showed that oxygen hole doping can increase the maximum current of the DNA [31]. The increment in maximum current was attributed to the adsorption of oxygen on the DNA molecule.

These results agree with our $I$-$V$ results for $W$ values above 2 eV and may indicate that the interaction of DNA with $W$ values of more than 2 eV with the medium may be modeled as a backbone disorder. Although some researchers have argued that charges are conducted through the water layer as opposed through the DNA molecule, our results show that the backbone disorder caused by the hydration layer can increase maximum current. Therefore, our results hint at an alternative explanation for the increase in maximum current.

Threshold voltage also changes with increasing $W$. For example, the threshold voltage increases for small values of $W$ (less than 2 eV) but decreases for large values of $W$. Guo et al. [21, 22] observed that the threshold value of poly(dG)-poly(dC) and G4 DNA changed with $W$. In contrast to their results, which showed that the semiconductor underwent metallic transition above the critical $W$ value, our result continues to show a threshold voltage even as the threshold continues to decrease. We obtained different results because we selected different Fermi and backbone onsite energies for our model. Guo et al. selected the same value for $E_F$ and backbone onsite energy, whereas our $E_F$ and backbone onsite energy values differed by 0.91 eV. Our result diverges from the experimental results reported by Kleine-Ostmann et al., who found that threshold voltage and current increased with increasing humidity [32]. A gap opening mechanism likely existed in their experiment and was ignored in our model. On the other hand, in agreement with our results, the results reported by Jo et al. showed that the threshold voltage decreased and the current increased as humidity increases [34].

The $I$-$V$ curve profiles of the sequences also change with $W$. The profile for sequences A and B show two steps in the absence of a backbone disorder and only one step in the presence of a backbone disorder. We also observed that the saturation current of sequence A is larger than that of sequence B because the hopping parameter between G–T bases is larger than that between the G–A, C–T, and C–A base pairs. Although the saturation current of sequence A is larger than that of sequence B, the rate of change of the saturation current with $W$ is also faster than sequence B.

The differential conductance profiles (Figure 2 insets) show that differential conductance decreases as $W$ increases for small values of $W$ and increases for large values of $W$. The profiles also show that the number of peaks and gaps change with $W$. First, multiple peaks exist in the absence of $W$. The multiple peaks merge into one peak and then split to two or more overlapping peaks as $W$ increases. This trend may indicate that the original profile can be recovered with a sufficiently large value of $W$.

The decrease or increase in the differential conductance with $W$ is caused by the change in $T(E)$ profiles with $W$ (Figure 3). As $W$ increases from 0 eV, the transmission band widths and the transmission coefficients decrease. When $W$ continues to increase past a certain value, new bands with nonzero transmission coefficients appeared, and the bands begin to increase in width and in coefficient. Interestingly, the transmission bands shift two times from energies higher than the Fermi energy to energies lower than Fermi energy and back.

The change in transmission probability profiles with increasing $W$ is caused by the effect of backbone onsite energies on base onsite energies. In our model, the effect of backbone onsite energies on base onsite energies creates the effective base onsite energies \( \epsilon_i^{(r)} \).

\[
\bar{\epsilon}_i^{(r)} = \left( \epsilon_i + \frac{\hbar_i^2}{2m} \right) \quad (2)
\]

In Eq. (2), $E$ is the charge energy. This equation shows that the disorder introduced to the backbone will also affect effective base onsite energies. When $W$ is small, for example, when it is approximately 1 eV, the value of $B$ varies from 9.36 – 1 eV to 9.36 + 1 eV. This variation indicates that when $E$ is equal to $B$, the effective base energy becomes so large that transport is blocked. The transmission probability decreases, and the state with nonzero transmission probability shifts to less than the Fermi energy (8.45 eV) because only energies around base G, which are approximately 7 eV, are available for transport given that the base onsite energies of A, C, T, and G vary from 7 to 9 eV. When the value of $W$ exceeds 2 eV, the value of the effective base energy encompasses the whole range from 9.36 – 2 eV to 9.36 + 2 eV. This result indicates that energies near the limit of the distribution remain unfavorable for transport but that energies near 9.36 eV are now favorable for transport. This causes states with nonzero transmission probabilities to appear around the energy of backbone onsite energy above the Fermi energy.

The shifting of transmission probabilities across the Fermi energy causes the threshold voltage, as shown in Figure 3, to change with increasing $W$. When the transmission
The T(E) plot for Sequences A (a–d) and B (e–h) when $W = 1$, 2, 3, and 5 eV

![Image of T(E) plots](image)

Figure 3. T(E) for Sequences A (a–d) and B (e–h) when $W = 1$, 2, 3, and 5 eV

Band edge shifts closer to the Fermi energy, the threshold voltage will decrease and vice versa. The T(E) plot generated by Guo et al. shows that after passing the critical $W$, the transmission band emerges at the Fermi energy [21]. By contrast, our plot shows that the transmission band emerges at higher energies than the Fermi energy because of the different choice of backbone onsite energy and Fermi energy.

Given that the T(E) plot shows that the transmission bands shift across the Fermi energy when $W$ increases from 0 eV to 1 eV and from 1 eV to 2 eV, plotting the $I$–$V$ curves and T(E) with $W$ between these values is necessary to investigate how the shift happened. (Figure 4). The $I$–$V$ curves obtained when $W = 0$–1 eV show an interesting trend: both sequences show that the threshold voltage decreases for some values of $W$ before increasing again (Figures 4b and c insets). This trend can be explained by looking at the transmission plots (Figure 5) showing that at these $W$ values, transmission bands appear closer to the Fermi energy. The saturation current also does not show consistent behavior but fluctuates (Figures 4b and c) for some values of $W$ because of the fluctuation of the width of the transmission band and transmission coefficients. This trend of decreasing threshold voltage and saturation current for small $W$ has not been observed before with poly(dG)-poly(dC) sequence and G4 DNA [21,22]. Therefore, this effect is caused by the interplay between backbone and sequence disorders.

The $I$–$V$ curves obtained when $W$ is between 1 and 2 eV (Figure 6) show that the saturation current decreases, and then consistently increases. The insets in the figure show that the threshold voltage first increases and then falls. This behavior follows the behavior exhibited by the transmission bands (Figure 7). Specifically, the transmission coefficients decrease then increase with $W$. The transmission bands first emerge distant from the Fermi energy. As $W$ increases, however, new transmission peaks near the Fermi energy began to appear, and consequently the threshold voltage falls.

Temperature-Dependent Twist-Angle Disorder Results. The $I$–$V$ characteristic of sequence A obtained when $\omega = 3$ meV (Figure 8a) shows that as the temperature increases, the current decreases. Nevertheless, the current increases with temperature when voltage is less than 1 V. The current decreases as temperature increases when $\omega = 0.51$ meV (Figure 8c). In contrast to that for sequence A, the current for sequence B when $\omega = 3$ meV (Figure 8b) increases with increasing temperature. When the frequency decreases to $\omega = 0.51$ meV, the current increases when the temperature increases from 4.2 K to 77 K but then decreases afterward. Another effect of the increasing temperature on the $I$–$V$ characteristic is the smoothing of the profile. As shown in the panels in Figure 8, at low temperature, the $I$–$V$ profile exhibits two large and several small steps. As the temperature increases, the small steps are smoothed out until only the two large steps remain. The reduction in current with increasing temperature at voltages above 1 V and the increment in current in current with temperature otherwise continues to hold for sequence A at all frequencies used. The general trend exhibited by sequence B is that the current will increase...
with increasing temperature. At some frequencies there exists a temperature at which the $I-V$ profile reverses its trend. The behavior of current vs. temperature for sequence B at voltages below 1 V does not show the same trend at all frequencies but instead show varying degrees of fluctuation as the current increases. As inferred from Figure 8, the current of sequence A is considerably higher than that of sequence B as a result of the different types of replacement bases introduced into the sequences. Several bases in Sequence A have

Figure 4. $I-V$ Characteristics of (a) Sequence A at $W = 0$, 0.3, and 0.5 eV; (b) Sequence A when $W = 0.6$, 0.7, 0.9, and 1 eV; and (c) Sequence B when $W = 0$, 0.3, 0.5, 0.6, 0.7, 0.9, and 1 eV

Figure 5. T(E) Plots of Sequences A (a–e) and B (f–j) when $W = 0.3$, 0.5, 0.6, 0.7, and 0.9 eV
Figure 6. $I-V$ Characteristics of Sequences A (a) and B (b) when $W=1, 1.3, 1.5, 1.7$, and $2\text{ eV}$

Figure 7. T(E) plots for Sequence A (a–c) and B (d–f) When $W=1.3, 1.5, \text{ and } 1.7\text{ eV}$
been replaced with CG, and those in sequence B have been replaced with GC base pairs. The hopping parameter from A to G and T to C is comparable in our model and may cause wave interference from the two strands. Wave interference, in turn, reduces the current in sequence B. Meanwhile, in sequence B, the hopping parameter from A to C is drastically lower than that from G to T. Thus, the G–T strand has higher transport probability than the A–C strand. This characteristic would attenuate the wave interference from the A–C strand and increase the current of sequence A.

The increase in current with increasing temperatures for sequences A and B at voltages of less than 1 V and $T = 3 \text{ meV}$ can be seen clearly in the plot of differential conductance vs. temperature at 0.33 V (Figure 9). For sequence A, the current increases as the temperature increases monotonically (Figure 9a). For sequence B, the current generally increases as the temperature increases. This increase, however, is not monotonic because the current at 77 K is lower than that at 30 K.

We look at the T(E) plots for sequences A and B obtained when $T = 3 \text{ meV}$ (Figure 10) to understand the tendency of the current to increase/decrease with increasing temperature. Figures 10 a–e show that as temperature increases, the transmission probability for sequence A decreases. By contrast, Figures 10 f–j show that the transmission probability for sequence B generally stays constant but new transmission bands can appear at increasing temperatures. Thus, the current can increase with temperature for sequence B. The new transmission bands created at high temperature may result in the apparent reduction in threshold voltage for sequence B when $T = 3 \text{ meV}$ (Figure 8b). The transmission curve can also account for the differences between conductance results. The transmission value at 0.33 eV is increasing for both sequences, so the current at that value also generally increases.

Several researchers have reported that transport probability decreases as temperature increases [16,17,19]. We found the same results for sequence A. The same researchers found that thermal fluctuation enhances charge transport at low frequencies. Similarly, we found that thermal fluctuation enhances charge transport in sequence B at low frequencies. These researchers, however, did not observe that thermal fluctuation at high frequencies continue to enhance conductivity at high temperatures. Our result, however, appear to agree with the result reported by Yu and Song [18]. Thermal fluctuation may enhance transport in a sequence with low transmission probability (sequence B) but may impede transport in a sequence with high transmission probability (sequence A).

Vedala et al. observed that the current in a portion of the H5N1 gene decreased as the temperature increased [35]. They observed that as the temperature increased, the current decreased and the threshold voltage increased. Although our $I–V$ results for sequence A show the same trend at large voltages, our result differs from Vedala’s in that the threshold voltage actually decreases with increasing temperature. This difference at low voltage may be attributed to differences in the details in the sequence. The increase in current with increasing temperature may be due to the increase in transmission probability at high temperatures.
temperature observed for sequence B $T = 3$ meV has also been observed experimentally by Yoo et al. by using poly(dG)–poly(dC) and poly(dA)–poly(dT) DNA [36]. They also observed that at $T = 294$ K, the voltage gap disappeared, whereas we found that the voltage gap does not disappear although the current continues to increase at $T = 300$ K. Our result cannot explain their I–V result because they used a DNA sequence without a sequence disorder. Nevertheless, the trend of increasing current with temperature agrees with our $I–V$ result for sequence B.

Figure 9. $dI/dV$ as a Function of Temperature at 0.33 V when $\phi = 3$ meV for a. Sequence A and b. Sequence B

Figure 10. $T(E)$ of sequence A when $T = 3$ meV (a–e) and $T(E)$ sequence B when $T = 3$ meV (f–j) at several temperatures
The $I-V$ results obtained for both sequences at various frequencies and constant temperature are shown in Figure 11. At $T=30 \text{ K}$, increments in frequency caused the current in sequence A to increase (Figure 11a) but reduced the current in sequence B (Figure 11b). The $I-V$ result for sequence A shows that the current continues to increase with increasing frequency when the temperature is elevated to $T=300 \text{ K}$ (Figure 11c). The $I-V$ characteristic of sequence B at $T=300 \text{ K}$ (Figure 11d) shows that the current increases when the frequency increases up to a certain point, after which the current decreases with increasing frequency. The increase in current in sequence A with frequency holds for the other temperatures used in our study. The current in sequence B generally decreases with increasing frequency. This trend, however, may deviate at some temperatures. For example, the current may fluctuate with increasing frequency.

The differential conductance of sequences A and B at $T=30 \text{ K}$ and 0.33 V indicate that in general, current in the two sequences decreases with increasing frequency (Figure 12). The reduction in differential conductance with increasing frequency shown by sequence B is consistent with the behavior of the maximum current, which decreases with increasing frequency. By contrast, the maximum current in sequence A behaves as a function of frequency where the maximum current increases as frequency increases.

The T(E) plots of both sequences at $T=30 \text{ K}$ (Figure 13) show that the transmission probabilities for sequence A (Figure 13a–e) increase with increasing frequency. The value of the highest transmission probability for sequence B (Figure 13f–j) negligibly changes with increasing frequency but the number of states with nonzero transmission increase at low frequency. As the frequency increases, the number of states with nonzero transmission probability decreases, which caused the current to decrease. The transmission curve can also be used to explain the behavior of differential conductance as a function of frequency (Figure 12). At 0.33 eV, the transmission decreases with increasing frequency for both sequences. Thus, the differential conductance generally decreased with increasing frequency.

The trend exhibited by sequence A in this study, wherein the current and transmission probability increases with increasing frequency, agrees with the result of Zhu et al. [15], who found a similar trend for poly(dG)–poly(dC) DNA. They found that increasing the standard deviation of the twist-angle width decreases transmission. In our model, frequency is inversely proportional to standard deviation. Thus, a high frequency is indicative of a low deviation. The trend of sequence B observed in our study is in direct disagreement with that observed by Zhu et al. [15]. The difference between our results and those of Zhu et al. may be attributed to the enhancement of electrical transport by thermal fluctuations in the sequence with low transmission probability.

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Figure 12. $dI/dV$ as a Function of Frequency at 0.33 V when $T = 30 \text{ K}$ for a. Sequence A and b. Sequence B

Figure 13. $T(E)$ of Sequence A when $T = 30 \text{ K}$ (a–e) and $T(E)$ of Sequence B when $T = 30 \text{ K}$ (f–j) at Several Frequencies
Conclusions and Outlook

We studied the effect of backbone disorder and temperature and twist frequencies on charge transport in two poly(dA)-poly(dT) DNA sequences with different modifications. The sequences were modified by using G–C or C–G base pairs. Our results showed that above a critical value, backbone disorders can enhance the electrical properties of DNA. This enhancement is illustrated by the increase in maximum current and the reduction in threshold voltage. When the backbone disorder was less than its critical value, increasing the value of \( W \) decreased the maximum current but did not consistently increase the threshold voltage. Results showed that the effect of temperature and positional disorder on charge transport was heavily affected by the sequence disorder. The maximum current of one sequence consistently decreased as temperature increased and the frequency decreased, whereas that of the other sequence decreased only for some values of temperature and frequency. These behaviors showed that the effect of temperature and positional disorder on DNA electrical transport is secondary to sequence disorder.

Future research on the effects of backbone disorder should investigate DNA sequences with different types of base pair modifications and different sequence disorder concentrations to validate the generality of the phenomenon observed in this study. Studies on the temperature and twist-angle effect on sequences with different replacement bases and different numbers of replaced bases must be conducted to test the sequence dependence of the results reported here. This study has provided new insight on the influence of sequence disorder, medium, and twist-angle disorder on DNA conductance.

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