Effects of contact and efficient charge transport in G4-DNA molecules

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We report a theoretical study highlighting the fundamental effects of contact between molecule and electrodes and of the off-diagonal disorder on the transport properties of guanine-quadruplex DNA (G4-DNA) molecules. On the basis of the effective tight-binding model which simulates charge transport through G4-DNA, the transmission coefficient and localization length are numerically calculated by using the transfer-matrix method. In contrast to the physical intuition that a strong coupling at the molecule-metal interface will lead to a large conductance, we find that the averaged transmission coefficient is decreased by increasing the coupling when the coupling strength surpasses a critical value and the optimal configuration of contact for efficient charge transport through G4-DNA is obtained. In addition, the localization length of G4-DNA, especially at band centers, is much larger than that of poly(G)-poly(cytosine) molecules, suggesting that G4-DNA is potentially better as a conducting molecular wire than double-stranded DNA molecules. Several effectively delocalized states can be found in realistic G4-DNA molecules at low temperatures. These results may provide perspectives for experimental work aimed at controlling charge transport through DNA-based nanodevices.

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Double-stranded DNA (dsDNA), as one of the leading candidates for molecular electronics, has attracted extensive interest among the physics, chemistry, and biology communities during the past few decades. Direct charge transport measurements of single dsDNA, however, revealed that its transport behavior is very sensitive to sample preparations and to environmental conditions,[1] and its performance as an intrinsic conductor is still questioned.[2] Besides the Watson-Crick double-helical conformation, other DNA derivatives constructed from guanine (G) nucleotides, especially the G-quadruplex DNA (G4-DNA), have been widely investigated recently, owing to their peculiar structural and self-assembling properties.[3] The unique structure of the G4-DNA consists of stacked G quartets, where each G quartet is a planar aggregate of four hydrogen-bonded G nucleotides arranged in a squarelike configuration.[3] The G4-DNA can be formed spontaneously in many G-rich sequences, including telomeres, ribosomal DNA, minisatellites, and immunoglobulin heavy-chain switch regions,[4,5] while the long uniform samples can be synthesized from poly(G)-poly(C) molecules (C: cytosine).[6] The G4-DNA is of particular importance in the telomeric regions of all eukaryotic chromosomes as a target for anticancer agent[7,8] and is argued to play a regulatory role in gene transcription based on the genome-wide analysis.[9]

Besides the physiological aspects, the G4-DNA is currently attracting attention in the Nanotechnology Research Community and may be a better candidate than the dsDNA as a conducting molecular wire.[10] This envisaged characteristic of the G4-DNA is proposed on the basis of its peculiar structural features which are expected to improve the charge transport through DNA-based nanodevices. (i) Because of the densely stacked G quartets which form a quadruple-helical conformation, the structure of the G4-DNA is extremely stable under physiological conditions as revealed by NMR spectroscopy and x-ray crystallography.[11,12] In addition, it is observed by atomic force microscopy and gel electrophoresis that the G4-DNA exhibits higher rigidity and larger persistence length than the dsDNA when deposited onto substrate or heated in aqueous solution for one hour.[6] The G4-DNA is completely insensitive to deoxyribonuclease I which efficiently degrades the native dsDNA.[6] (ii) G-rich DNA sequences, due to the lowest ionization potential of G base among the nucleobases, show efficient long-range charge-transfer properties.[13] Additionally, according to Bloch's theorem, the electronic wave functions in perfectly ordered crystals are extended. Therefore, it is reasonable to assume that the G4-DNA, including the G nucleotides only, should exhibit much higher charge transport efficiency over longer distances as compared with the dsDNA. (iii) The stacking distance and the twist angle between two neighboring G quartets being, respectively, 3.25 Å and 30°, smaller than in the dsDNA, might imply a better π-π coupling along the stacking direction of the G4-DNA. This has been recently demonstrated by using the self-consistent charge-density-functional tight-binding method.[14] On the other hand, the G4-DNA can be viewed as comprising of four parallel π stacks, which are two times larger than that of the dsDNA, implying that the channels for conducting charges in the G4-DNA are two times larger than in the dsDNA. These suggest that the G4-DNA has a better "π way" which is favorable for conducting charges through the superposition of π orbitals along DNA molecules. Because of these appealing structural traits, the electronic structure of the G4-DNA has been investigated based on the density-functional theory (Refs. 3 and 15) and the polarizability has been demonstrated in the G4-DNA by using the electrostatic force microscopy.[10] All these may reveal a higher conductivity of the G4-DNA as compared with the dsDNA, which needs to be further corroborated theoretically or experimentally.

In the present paper, we numerically investigate the effects of contact between the molecule and electrodes and of off-diagonal disorder on charge transport properties of the G4-DNA by employing an effective tight-binding model with parameters determined in first-principles calculations.[16,17] Since the backbone is believed to have little effect as a transmission channel in dry DNA,[18,19] as a first approximation it is neglected completely. Therefore, a physically

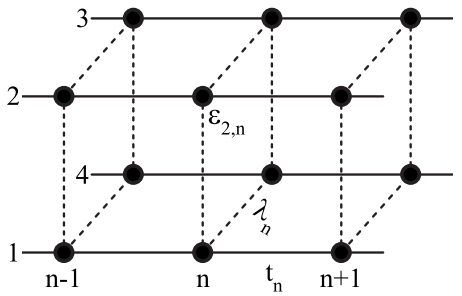

FIG. 1. Schematic illustration of G4-DNA. The circles represent the G bases and the solid (dashed) lines denote the intrachain (interchain) hopping integral.

reasonable description of charge transport through the G4-DNA is then given by an effective tight-binding Hamiltonian

$$\mathcal{H} = \sum_{n}^{} \sum_{j=1}^{4} [\varepsilon_{j,n} c_{j,n}^{\dagger} c_{j,n} - t_n (c_{j,n}^{\dagger} c_{j,n+1} + \text{H.c.})] - \sum_{n=1}^{N} \sum_{\langle i,j \rangle} \lambda_n (c_{i,n}^{\dagger} c_{j,n} + \text{H.c.}), \quad (1)$$

where each lattice site represents a G base for $n \in [1, N]$. The operator $c_{j,n}^{\dagger}(c_{j,n})$ creates (annihilates) a charge at the nth site of the jth chain of the G4-DNA ($1 \leq n \leq N$), of the left electrode ($n \leq 0$), and of the right electrode ($n \geq N+1$). $\langle \cdots \rangle$ denotes the nearest-neighbor sites. For the G4-DNA, the on-site energy is evaluated by ionization potential of the G base as $\varepsilon_{j,n} = \varepsilon_G = 7.75$ eV,[16] t_n is the intrachain hopping integral between the nth and $n+1$th G quartet, and λ_n is the interchain hopping integral with $\lambda_n = \lambda = 0.4$ eV (Ref. 17) (see Fig. 1). For the electrodes, the on-site energy and the hopping integral are taken as $\varepsilon_m = \varepsilon_G$ and $t_m = 4$ eV, respectively. The coupling parameter between the G4-DNA and the electrodes is denoted by τ. Since the G4-DNA is flexible and has structural fluctuations at finite temperature, the intrachain hopping integral may be expressed as[20]

$$t_n = t(5.84 \cos \theta_n - 4.84), \quad (2)$$

where θ_n is the relative twist angle deviated from its equivalent value between the nth and $n+1$th G quartet. Each θ_n is an independent random variable that follows a Gaussian distribution with average $\langle \theta_n \rangle = 0$ and standard deviation $\sqrt{\langle \theta_n^2 \rangle} = W$.[21,22] Here, W is the disorder degree measuring the structural fluctuations.

In the site representation, the Schrödinger equation $\mathcal{H}|\Psi\rangle = E|\Psi\rangle$ corresponding to Eq. (1) becomes

$$\begin{pmatrix} \boldsymbol{\Psi}_{n+1} \\ \boldsymbol{\Psi}_n \end{pmatrix} = \begin{pmatrix} \mathbf{M}_n & -\frac{t_{n-1}}{t_n} \mathbf{I}_4 \\ \mathbf{I}_4 & \mathbf{0}_4 \end{pmatrix} \begin{pmatrix} \boldsymbol{\Psi}_n \\ \boldsymbol{\Psi}_{n-1} \end{pmatrix}$$

with $\boldsymbol{\Psi}_n = (\psi_{1,n}, \psi_{2,n}, \psi_{3,n}, \psi_{4,n})^T$, $\mathbf{I}_4$ and $\mathbf{0}_4$ being the 4×4 identity and zero matrices, respectively, and

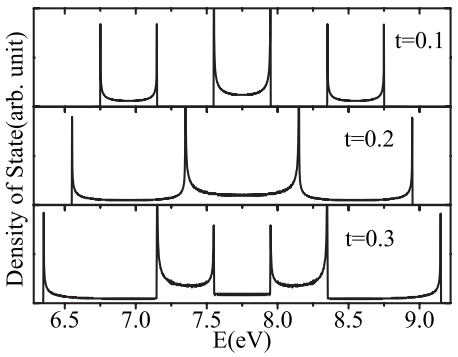

FIG. 2. Density of states for homogeneous G4-DNA with several intrachain hopping integrals t. The length is sufficiently large ($N=3750$) so that the results are irrespective of N.

$$\mathbf{M}_n = \begin{pmatrix} \frac{\varepsilon_{1,n} - E}{t_n} & \frac{-\lambda_n}{t_n} & 0 & \frac{-\lambda_n}{t_n} \\ \frac{-\lambda_n}{t_n} & \frac{\varepsilon_{2,n} - E}{t_n} & \frac{-\lambda_n}{t_n} & 0 \\ 0 & \frac{-\lambda_n}{t_n} & \frac{\varepsilon_{3,n} - E}{t_n} & \frac{-\lambda_n}{t_n} \\ \frac{-\lambda_n}{t_n} & 0 & \frac{-\lambda_n}{t_n} & \frac{\varepsilon_{4,n} - E}{t_n} \end{pmatrix}.$$

Here, $\psi_{j,n}$ is the amplitude of the wave function at the nth site of the jth chain and T denotes the transpose. Then the amplitude of the wave function at two ends of the G4-DNA is related by

$$\begin{pmatrix} \boldsymbol{\Psi}_{N+1} \\ \boldsymbol{\Psi}_N \end{pmatrix} = \mathbf{T}_N \begin{pmatrix} \boldsymbol{\Psi}_1 \\ \boldsymbol{\Psi}_0 \end{pmatrix}, \quad (3)$$

where $\mathbf{T}_N$ is the total transfer matrix.

Let us first consider a homogeneous G4-DNA chain with $W=0$. In this case, the Hamiltonian given by Eq. (1) can be diagonalized to yield the dispersion relation analytically,

$$(E - \varepsilon_G + 2t \cos k)^2 (E - \varepsilon_G + 2t \cos k - 2\lambda) \times (E - \varepsilon_G + 2t \cos k + 2\lambda) = 0, \quad (4)$$

where the exponent "2" in the first factor indicates that there exist two superposed energy bands within the range $[\varepsilon_G - 2t, \varepsilon_G + 2t]$. By inspecting Eq. (4), one realizes that for $\lambda > 2t$ the energy spectrum is composed of three isolated subbands of width $B_w = 4t$ and the three subbands will be merged into a single band when $\lambda \leq 2t$. These features are further illustrated in Fig. 2, where the density of states for the G4-DNA is plotted with several values of t and $N=3750$. We emphasize that the results are irrespective of N because the length is sufficiently large. One observes six Van Hove singularities in the energy spectrum of the G4-DNA as expected.

To understand the DNA's transport features, however, one should explicitly take into account the effects of contact between the molecule and the electrodes. For instance, several transport experiments have reported that chemical bonding between DNA and metal electrodes can enable one to obtain

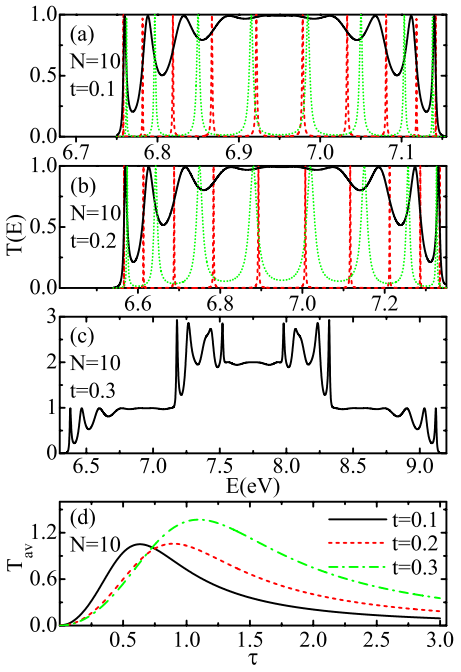

FIG. 3. (Color online) Energy-dependent transmission coefficient $T(E)$ for homogeneous G4-DNA with (a) $t=0.1$ eV, (b) $t=0.2$ eV, and (c) $t=0.3$ eV. The solid, dashed, and dotted curves represent the transmission coefficient with $\tau=\sqrt{t\times t_m}$, $\tau=0.1$ eV, and $\tau=2.5$ eV, respectively. (d) shows the averaged transmission coefficient T_{av} versus τ with several values of t.

reproducible results and to achieve higher conductance,[23,24] while others have laid down the molecules directly on the electrodes. For this situation, one may simulate the effects of contact on the transport properties of the G4-DNA by varying the coupling parameter τ at the DNA-metal interface.[25] At zero temperature, the transmission coefficient can be calculated by using the multichannel Landauer-Büttiker formula[26]

$$T(E)=\sum_{i,j=1}^{4} T_{i,j}, \tag{5}$$

where $T_{i,j}$ is the transmission probability for a charge injected into the ith chain of the left electrode and transmitted to the jth chain of the right electrode.

Figures 3(a) and 3(b) show the transmission coefficient $T(E)$ of a single band for the G4-DNA with several values of t and τ, while Fig. 3(c) plots $T(E)$ over the whole energy spectrum of the G4-DNA with $t=0.3$ eV and $\tau=\sqrt{t\times t_m}$. As can be seen from Figs. 3(a) and 3(b), a certain number of resonances $[T(E)=1]$ are found within the single band for whatever the values of τ and the energies of these resonances are very sensitive to τ. One may attribute this to the fact that the coupling parameter can rearrange the energy levels of the nanostructured system comprising of the G4-DNA and the electrodes. Additionally, one observes that a strong coupling will sometimes damp the transmission probability in the energy spectrum. This is due to the interference effects between the G4-DNA molecular bands and the electronic structure of the electrodes at the DNA-metal interface. From Fig. 3(c) we can see that the maximum of the transmission coefficient can reach two (three) in certain energy range because the states with eigenenergy E in this range are twofold (threefold) degenerated [see Eq. (4)].

In order to further illustrate the effects of contact on the transport properties of the G4-DNA, we have calculated the averaged transmission coefficient as

$$T_{\mathrm{av}}=\frac{1}{\Omega}\int_{\Omega} T(E)dE, \tag{6}$$

where Ω represents the energy range determined by Eq. (4). Figure 3(d) shows the averaged transmission coefficient T_{av} for the G4-DNA with several values of t, as a function of the coupling strength τ. It is clear that the behavior of T_{av} versus τ is not monotonic. A turning point τ_c is observed in all curves that the averaged transmission coefficient increases with increasing τ for $\tau<\tau_c$ and decreases with increasing τ for $\tau>\tau_c$. The dependence of T_{av} on τ, which may exist in one-dimensional (1D) or quasi-1D systems, is due to the aforementioned interference effects. We find that the optimal configuration of contact for efficient charge transport through the G4-DNA is determined by $\tau_c=\sqrt{t\times t_m}$, consistent with the results obtained in single-stranded DNA molecules.[25]

In what follows, we will discuss the transport properties of the G4-DNA by calculating the localization length Λ with $t=0.2$ eV (Ref. 17) and $W\neq 0$. For long G4-DNA with the off-diagonal disorder, the Lyapunov exponents (LEs) can be calculated by using the standard method of **QR** decomposition, viz., the transfer matrix $\mathbf{T}_N$ [see Eq. (3)] can be factored into an orthogonal matrix **Q** and an upper triangular matrix **R** with positive diagonal elements. Then the LEs are defined as the positive logarithms of the diagonal elements of **R**.[27] To avoid the terrible overflow of multiplication of transfer matrices, we perform the additional Gram-Schmidt reorthonormalization after every ten transfer-matrix multiplications.[28] This method is equivalent to direct diagonalization of the Hermitian matrix $\mathbf{T}_N^{\dagger}\mathbf{T}_N$ and has been widely used to calculate the transport properties of other quasi-1D and two-dimensional (2D) systems.[27–29] The smallest LE is the most physically significant quantity which determines the conductance of the system and whose inverse is the localization length.[28] The rescaled localization length is defined as $\frac{\Lambda}{N}$: the states are extended if $\frac{\Lambda}{N}$ increases with increasing N or are localized if $\frac{\Lambda}{N}$ decreases with increasing N. For a finite system, however, one can define an effective delocalization:[30] a state with localization length larger than the system size can be regarded as effectively delocalized.

In Fig. 4(a), we plot the localization length Λ for the G4-DNA with several off-diagonal disorder degrees W as a function of the energy E. As a comparison, Fig. 4(b) shows Λ versus E for the poly(G)-poly(C), which is one of the most conductive dsDNA molecules and can be simulated by the two-leg ladder model with the on-site energy $\varepsilon_C=8.87$ eV.[30–36] From the tight-binding calculation, whatever the value of W is, three identical bumps, corresponding to the energy bands, are found in the energy spectrum of the G4-DNA, while two identical bumps are observed in the energy spectrum of the poly(G)-poly(C). The localization

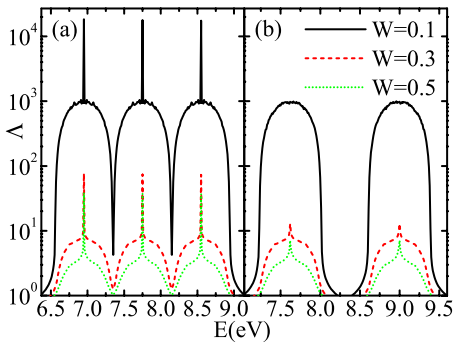

FIG. 4. (Color online) Energy-dependent localization length Λ for (a) G4-DNA and for (b) poly(G)-poly(C) in the presence of off-diagonal disorder with strength $W=0.1,0.3,0.5$ and length $N=10^6$.

length is decreased by increasing W over the whole energy spectrum for both DNA molecules as expected. However, we always see a peak at the center of each bump for the G4-DNA, where the localization length is much larger than that of other energy states. We emphasize that these peaks will not vanish even if the results are averaged over configurations of off-diagonal disorder. This anomalously large localization length may be related to the chiral symmetry which is conserved for the G4-DNA in the case of off-diagonal disorder.[37,38]

Figures 5(a) and 5(b) show the rescaled localization length Λ/N versus length N at the center of the left bump (see Fig. 4) for the G4-DNA and for the poly(G)-poly(C) with several off-diagonal disorder degrees W, respectively. For all values of W, the rescaled localization length always decreases with increasing N. This indicates that all the states are localized by weak off-diagonal disorder for both DNA molecules in the thermodynamic limit. On the other hand, the dependence of the logarithm of Λ/N on the logarithm of N can be linearly fitted by using the least squares, i.e.,

$$\log_{10}(\Lambda/N) = \beta + \alpha \log_{10} N. \tag{7}$$

The fitting parameters α and β for the G4-DNA at $E=6.95$ eV and for the poly(G)-poly(C) at $E=7.62$ eV are plotted in Figs. 5(c) and 5(d), respectively, as functions of the off-diagonal disorder degree W. Since the parameter α is -1.00 within the numerical accuracy for both DNA molecules [Fig. 5(c)], the localization length is independent of N and is approximated to be $\Lambda=10^{\beta}$ for a certain W. By inspecting Fig. 5(d), one notices that the localization length decreases with increasing W and will saturate at some point for both DNA molecules because the localized electronic wave function will no longer feel any intrachain structural fluctuations when the off-diagonal disorder degree is sufficiently large. For a given W, the localization length at the band center of the G4-DNA is about one order of magnitude larger than that of the poly(G)-poly(C). To further substantiate the aforementioned point, it would be important to perform the dependence of the localization length on the hopping integrals because other first-principles calculations have reported different and smaller hopping integrals.[39–41] Figures 5(e) and 5(f) show the localization length Λ versus t at the

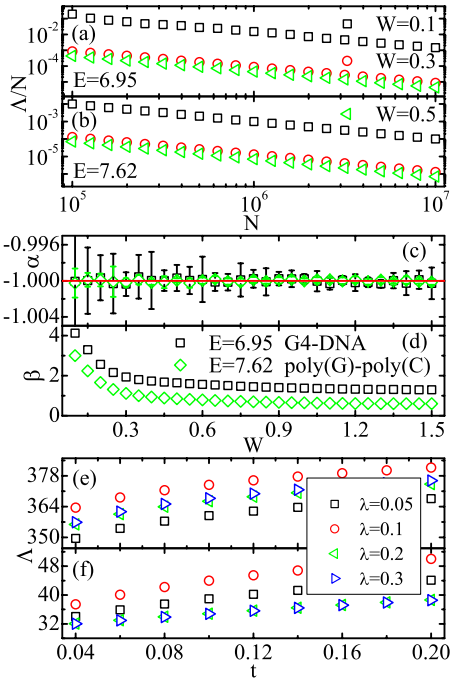

FIG. 5. (Color online) Rescaled localization length Λ/N versus length N for (a) G4-DNA at $E=6.95$ eV and for (b) poly(G)-poly(C) at $E=7.62$ eV in the presence of off-diagonal disorder with strength $W=0.1$, 0.3, and 0.5. (c) and (d) show the corresponding fitting parameters α and β, respectively, as functions of W for both DNA molecules. The solid line represents the constant value $\alpha=-1.00$. The results are averaged over at least five configurations of off-diagonal disorder. (e) and (f) show the localization length Λ versus t at the left band center [the energy of which depends on λ and can be obtained from Eq. (4) or equivalently from Fig. 4] for G4-DNA and for poly(G)-poly(C), respectively, with different values of λ and $W=0.2$.

center of the left band for both DNA molecules with several values of λ and $W=0.2$, which corresponds to the typical value of off-diagonal disorder degree for the dsDNA molecules at low temperature (~ 10 K).[22] It clearly appears that the localization length of the G4-DNA is much larger than that of the poly(G)-poly(C) for all values of λ and t. On the other hand, since the structure of the G4-DNA is much more stable,[6] the minimum localization length of the G4-DNA at the band center is estimated to be $\Lambda > 349$ [see Fig. 5(e)], greater than the representative sample size obtained in the experiment.[6] Therefore, we come to the conclusion that there exist several effectively delocalized states in the realistic G4-DNA molecules at low temperatures.

In conclusion, we adopt a tight-binding model to simulate the charge transport through the G4-DNA molecules. Based on the effective tight-binding model with parameters fitted from first-principles calculations, the transport properties of the G4-DNA are numerically investigated by taking into account the effects of contact between the molecule and the electrodes and of the off-diagonal disorder. Our results clearly show that the coupling at the DNA-metal interface plays an important role in the charge transport efficiency of the G4-DNA. The optimal condition of contact for efficient charge transport through the G4-DNA is determined by τ_c

$=\sqrt{t \times t_m}$. The averaged transmission coefficient increases with increasing τ if $\tau < \tau_c$ and decreases with increasing τ if $\tau > \tau_c$. On the other hand, the transport properties of the G4-DNA are also investigated in the presence of off-diagonal disorder by calculating the localization length. We find that the localization length at the center of each energy band for the G4-DNA is anomalously large, due to the chiral symmetry. The localization length of the G4-DNA is much larger than that of the poly(G)-poly(C) molecules, suggesting that the G4-DNA is potentially a better candidate as a conducting molecular wire than the dsDNA molecules. Additionally, the states at the band centers of the realistic G4-DNA molecules are effectively delocalized at low temperatures. These results may open perspectives for future experimental work which intends to control the charge transport through DNA-based nanodevices.

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