Enhancement of transport in DNA-like systems induced by backbone disorder

Ai-Min Guo, Shi-Jie Xiong, Zhi Yang, and Hong-Jun Zhu
National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China
(Received 11 September 2008; published 29 December 2008)

We report a theoretical study highlighting the fundamental effects of backbone disorder which simulates the environmental complications on charge transport properties of biological and synthetic DNA molecules. Based on effective tight-binding models of duplex DNA, the Lyapunov coefficient and current-voltage characteristics are numerically calculated by varying the backbone disorder degree. In contrast to the localization picture that the conduction of duplex DNA becomes poorer when the backbone disorder degree is increased, we find that the backbone disorder can enhance the charge transport ability of the DNA molecules when the environment-induced disorder surpasses a critical value, giving rise to a semiconducting-metallic transition. The physical origin for this is traced back to the antiresonant effects. These results provide a scenario to interpret a variety of transport behaviors observed in DNA molecules and suggest perspectives for future experiments intending to control the charge transport through DNA-based nanodevices.

DOI: 10.1103/PhysRevE.78.061922 PACS number(s): 87.14.gk, 72.15.Rn, 73.63.Nm

The DNA molecule, as the carrier of genetic code of all living organisms and as a promising candidate for molecular electronics, has attracted considerable attention among the physics, chemistry, and biology communities recently. Since the original statement proposed by Eley and Spivey that DNA could provide a natural pathway for conducting electrons [1], much progress on charge migration along duplex DNA has been achieved experimentally. On the one hand, photoinduced experiments have demonstrated that duplex DNA could serve as a molecular bridge for long-range electron transfer on the picosecond time scale [2], or contrarily that it is somewhat more effective than protein as a medium for electron transfer [3]. On the other hand, the results of direct charge transport measurements, mainly on poly(G)-poly(C) and λ-DNA molecules, are sometimes contradicting, indicating that they might be insulators [4–7], semiconductors [8–11], or conductors [12–16]. Such different transport behaviors stem from a wide range of experimental complications, including the DNA samples, counterions, humidity, interaction of DNA with substrate, and different situations of contacts between DNA and electrodes.

Theoretically, both *ab initio* calculations [17–25] and model-based Hamiltonians [26–45] are extensively adopted to interpret the diversity of the experimental results and to ascertain the underlying charge transport mechanisms. For instance, *ab initio* calculations predict that synthetic poly(G)-poly(C) is a semiconductor with a band gap ranging from 0.8 to 2.1 eV [45]. Different physical mechanisms, including hybridization between the base pairs and the sugar-phosphate backbone [28], interbase Coulomb repulsion [30], backbone-induced electronic effects [37], or dimensionality-induced effects [45], are put forward to account for the variability of band gap width within the framework of the tight-binding Hamiltonian and may give rise to semiconducting-metallic transition. Some consensus on the dominant mechanisms of charge migration along duplex DNA seems to be emerging currently [46]. The charge transport may result from either coherent tunneling (superexchange) [26,39] or incoherent hopping (phonon-assisted processes) [47].

Notwithstanding, to understand the diversity of the experimental data one should take into account three different contributions coming from the nucleobase system, the sugar-phosphate backbone, and the environment [28,32,34,37]. In fact, since the backbone phosphates are negatively charged and locate in the outer region of the double-helical structure, the backbone of duplex DNA will interact with the substrate on which many experiments are performed and its on-site energies can be modulated [5–7,13–15]. Additionally, in DNA's natural aqueous buffer solutions, the backbone phosphates have a propensity to attract counterions and polar water molecules which neutralize the phosphates and consequently change their vertical ionization potentials [20]. Even for a dried DNA in vacuum, its conformation can be quite different in various experiments because a few counterions or water molecules may still reside on the phosphates of the backbone after the drying process. Accordingly, it would be suitable to simulate the different experimental situations by choosing the on-site energies of the backbone satisfying a certain distribution function. In this paper, we report a theoretical study of the effects of the backbone energetics on the charge transport properties of poly(G)-poly(C), poly(A)-poly(T), human chromosome 22 (Chr22), and λ-DNA molecules. Our picture, similar to the antiresonant effects, suggesting that the backbone disorder can enhance the charge transport ability of the DNA molecules when the environment-induced disorder surpasses a critical value and will give rise to semiconducting-metallic transition, provides a scenario to interpret the wide spreading of the experimental results and may open perspectives for future experimental work which intends to control the charge transport through DNA-based nanodevices.

According to quantum chemistry studies on duplex DNA that the hydrogen bonding between complementary nucleobases is larger than the π stacking energies between successive base pairs, as a first approximation each Watson-Crick base pair can be treated as a single entity with a characteristic on-site energy [18,19,42]. Therefore a physically reasonable description of charge transport in duplex DNA would be the fishbone model [28]. The Hamiltonian is

$$\mathcal{H} = \sum_{n} [\varepsilon_n c_n^{\dagger} c_n - t_{n,n+1}(c_n^{\dagger} c_{n+1} + \text{H.c.})] + \sum_{n,p} \varepsilon_{np} b_{np}^{\dagger} b_{np} - \sum_{n,p} t_{np}(c_n^{\dagger} b_{np} + \text{H.c.}), \quad (1)$$

where $c_n^{\dagger}$ ($b_{np}^{\dagger}$) is the creation operator for a charge at the nth base pair (backbone) site, with index $n \in [1, N]$ labeling a nucleotide and index $p=\uparrow$ ($\downarrow$) labeling an upper (lower) backbone. ε_n and ε_{np} are the on-site energies of the nth base pair and nth backbone sites, respectively. $t_{n,n+1}$ is the hopping integral between neighboring base pairs, and t_{np} is the one between the base pair and backbone sites. A straightforward generalization of model (1) is the dangling backbone ladder model [34,48].

Let us first consider a homogeneous DNA chain with $\varepsilon_n = \varepsilon_d$, $\varepsilon_{n\uparrow} = \varepsilon_{n\downarrow} = \varepsilon_b$, $t_{n,n+1} = t$, and $t_{n\uparrow} = t_{n\downarrow} = t_b$. By using Bloch's theorem its energy spectrum can be calculated and is composed of highest occupied molecular orbital (HOMO) (E_-) and lowest unoccupied molecular orbital (LUMO) (E_+),

$$E_{\pm} \in \left[\frac{\varepsilon_b + \varepsilon_d}{2} - t \pm \sqrt{\left(\frac{\varepsilon_b - \varepsilon_d}{2} + t\right)^2 + 2t_b^2}, \frac{\varepsilon_b + \varepsilon_d}{2} + t \pm \sqrt{\left(\frac{\varepsilon_b - \varepsilon_d}{2} - t\right)^2 + 2t_b^2} \right], \quad (2)$$

which are separated by a band gap

$$\Delta_g = \sqrt{\left(\frac{\varepsilon_b - \varepsilon_d}{2} + t\right)^2 + 2t_b^2} + \sqrt{\left(\frac{\varepsilon_b - \varepsilon_d}{2} - t\right)^2 + 2t_b^2} - 2t.$$

Notice that for fixed t and t_b the band gap Δ_g increases with increasing the absolute value $|\varepsilon_b - \varepsilon_d|$, that might be a major factor for the difference between the band gap of the poly(G)-poly(C) and poly(A)-poly(T) [49]. Although considering a uniform charge distribution along the backbone sites can interpret the band gap opening of homogeneous DNA chains [28,37], it seems to be oversimplified to simulate the environmental complications as mentioned above. Therefore the most disordered case is employed to model the effects of the environment on the backbone sites, i.e., the on-site energy of the backbone ε_{np} is taken to be randomly distributed within the range $[\varepsilon_b - W/2, \varepsilon_b + W/2]$ and $\langle \varepsilon_{n\uparrow} \varepsilon_{n\downarrow} \rangle = \varepsilon_b^2$, with ε_b the center of the energy region and W the backbone disorder degree (we note that other distribution functions, e.g., Gaussian disorder and binary disorder, have been employed to model the environmental complications [34]). The on-site energies of the nucleobases and the base pairs are taken as the ionization potential, i.e., $\varepsilon_G = -0.56$ eV, $\varepsilon_A = -0.07$ eV, $\varepsilon_C = 0.56$ eV, $\varepsilon_T = 0.83$ eV, $\varepsilon_{GC} = (\varepsilon_G + \varepsilon_C)/2 = 0.0$ eV (reference point), and $\varepsilon_{AT} = (\varepsilon_A + \varepsilon_T)/2 = 0.38$ eV. The intrastrand hopping integral between like base pairs is chosen as 0.35 eV and between unlike base pairs 0.17 eV. The interstrand hopping integral is 0.3 eV. Since all the nucleobases are attached to the backbone sugars by identical C–N bonds, the hopping integral t_{np} is assumed to be $t_{n\uparrow} = t_{n\downarrow} = t_b = 0.7$ eV [28]. The parameters we used are consistent with the *ab initio* calculations [18,19,36].

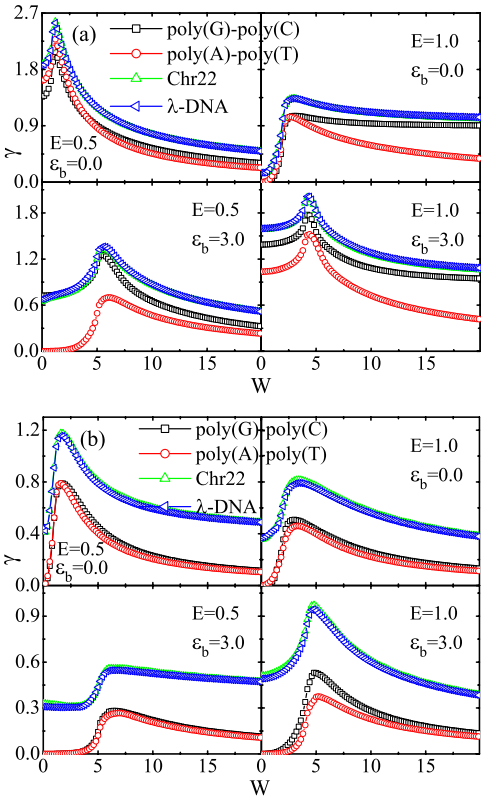

FIG. 1. (Color online) Lyapunov coefficient γ versus backbone disorder degree W for poly(G)-poly(C), poly(A)-poly(T), Chr22, and λ-DNA molecules with $E=0.5$, 1.0 eV and $\varepsilon_b=0.0$, 3.0 eV by considering (a) the fishbone model and (b) the dangling backbone ladder model.

By decimation of the upper and lower backbone sites the fishbone model (1) can be renormalized into an effective one-dimensional tight-binding Hamiltonian,

$$(\varepsilon_n^r - E)\psi_n = t_{n-1,n}\psi_{n-1} + t_{n,n+1}\psi_{n+1}, \quad (3)$$

with ψ_n being the amplitude of the wave function at the nth base pair site and

$$\varepsilon_n^r = \varepsilon_n - \sum_{p=\uparrow,\downarrow} t_p^2/(\varepsilon_{np} - E). \quad (4)$$

A similar procedure can also be implemented for the dangling backbone ladder model [34,48]. It is convenient to study the transport properties of these quasi-one-dimensional tight-binding models by using the transfer matrix method [50], which allows us to calculate the Lyapunov coefficient γ (the inverse of the localization length) of the duplex DNA. For a given energy E, γ reflects the level of backscattering events in the charge transport through the DNA chain.

In Fig. 1, we plot the Lyapunov coefficient γ for the poly(G)-poly(C), poly(A)-poly(T), Chr22, and λ-DNA molecules with $E=0.5$, 1.0 eV and $\varepsilon_b=0.0$, 3.0 eV, as a function of the backbone disorder degree W. It clearly appears that a general trend of γ versus W, as discussed below, is found for all periodic and aperiodic DNA sequences by taking into account either the fishbone model (a) or the dangling backbone ladder model (b). In all curves, the behavior of γ versus

W is not monotonic. There exists a crossover W_c for the backbone disorder degree that the Lyapunov coefficient increases with increasing W for $W<W_c$, whereas it decreases with increasing W for $W>W_c$. The crossover W_c is very sensitive to the parameters E and ε_b. As a matter of fact, the renormalized sites with on-site energy ε_n^r act as the potential barriers if $\varepsilon_n^r > E$ or as the potential wells if $\varepsilon_n^r < E$. By inspecting Eq. (4), one realizes that the charge transmission probability can be dramatically reduced at the sites with $|\varepsilon_n^r| \gg E$, i.e., the effective localized states that can strongly scatter the conduction states in the DNA chain should come from disordered backbone sites with ε_{np} in a neighborhood of E. As ε_{np} approaches E, provided that the range of this neighborhood is sufficiently small, the renormalized on-site energy ε_n^r approaches ∞ and the electrons (holes) will be completely reflected at site n. This is the so-called antiresonant effects [51]. For an electron with eigenenergy E propagating through the DNA chain, the wave function will be effectively eliminated at the base pair sites which connect the backbone sites with ε_{np} in the neighborhood of E. Therefore the average distance of two nearest backbone sites with ε_{np} in the neighborhood of E gives an approximate estimation of the localization length of the DNA chain. Consequently, when the values of E, ε_b, and ε_n are fixed, for $W<2|E-\varepsilon_b|$, the number of backbone sites with ε_{np} in this neighborhood will be enhanced by increasing W and leads to the decrease of the localization length at small W. On the other hand, when the backbone disorder degree is large enough that the energy range of ε_{np} covers this neighborhood ($W>2|E-\varepsilon_b|$), the number of backbone sites with ε_{np} in this neighborhood will be reduced by increasing W and can result in the enhancement of the localization length at large W. These results suggest that the backbone disorder-induced enhancement of transport has little to do with the particular form of the distribution functions of the backbone disorder, i.e., the charge transport ability of the DNA chains will increase with increasing W when the environment-induced disorder is sufficiently large; and one expects that the dependence of W_c on ε_b and E may be approximated as $W \sim 2|E-\varepsilon_b|$.

In Fig. 2, we plot the backbone disorder crossover W_c for the poly(G)-poly(C), poly(A)-poly(T), Chr22, and λ-DNA molecules with $E=-0.5$, 0.0, and 0.5 eV, as a function of the center of the energy region ε_b. As we can see, the behavior of W_c versus ε_b exhibits a general "∨" shape for all periodic and aperiodic DNA sequences by taking into account either the fishbone model (a) or the dangling backbone ladder model (b). The "∨" shapes will almost superpose with each other for different DNA sequences in some parameter ranges. This is not surprising because the renormalized on-site energy ε_n^r determines the crossover W_c when ε_{np} locates in the neighborhood of E and ε_n is negligible as compared with this ε_n^r. However, one observes distinct differences among the curves of W_c versus ε_b for different DNA chains with specific parameter values, e.g., the right parts of the curves with $E=-0.5$ for poly(G)-poly(C) and that for other DNA sequences by considering the fishbone model [Fig. 2(a), top panel]. This is mainly attributed to the different relative position of E in the energy spectra for different DNA chains. The crossover W_c will strongly deviate from $2|E-\varepsilon_b|$ if the eigenenergy E is quite close to the outer band edge, i.e.,

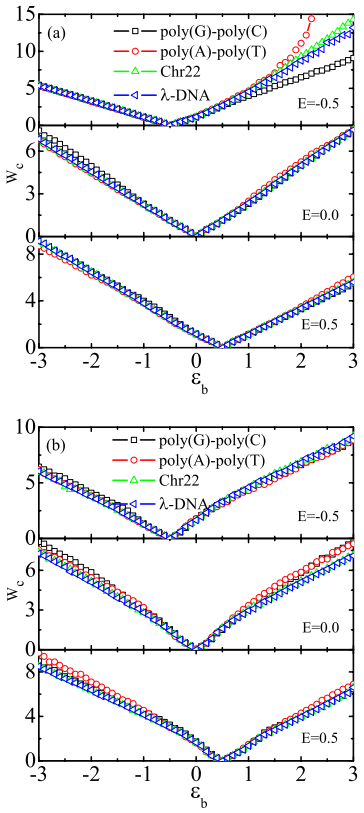

FIG. 2. (Color online) Backbone disorder crossover W_c versus center of the energy region ε_b for poly(G)-poly(C), poly(A)-poly(T), Chr22, and λ-DNA molecules with $E=-0.5$, 0.0, and 0.5 eV by considering (a) the fishbone model and (b) the dangling backbone ladder model.

E_{+max} and E_{-min} of Eq. (2). Due to this reason, the expression $W \sim 2|E-\varepsilon_b|$ mentioned above holds only for a small value of $|E-\varepsilon_b|$, whereas the deviation of W_c to $2|E-\varepsilon_b|$ increases with increasing $|E-\varepsilon_b|$ for a large value of $|E-\varepsilon_b|$. Therefore, for a critical value of the Fermi energy, one concludes that the backbone disorder-induced enhancement of transport is a generic feature for DNA chains with various nucleotide arrangement by properly modulating the environmental complications.

To directly and quantitatively explain the large scatter of the experimental results within the antiresonant effects, we numerically calculate the transmission coefficient and the current-voltage (I-V) characteristics by considering the fishbone model [28], of which the results are in good agreement with the experiments [52]. The duplex DNA is assumed to be connected in between two semi-infinite one-dimensional electrodes with on-site energies $\varepsilon_m = \varepsilon_{GC}$ and hopping integral $t_m = 4$ eV. Then, the I-V characteristics can be evaluated by using the standard Landauer-Büttiker formula:

$$I = \frac{2e}{h} \int_{-\infty}^{+\infty} T(E)[f_L(E) - f_R(E)]dE, \tag{5}$$

where $f_{L/R}(E) = \{1 + \exp[(E \mp eV/2 - E_F)/k_B T]\}^{-1}$ is the Fermi distribution function, and $T(E)$ is the transmission coefficient of the system which is related to the Landauer conductance

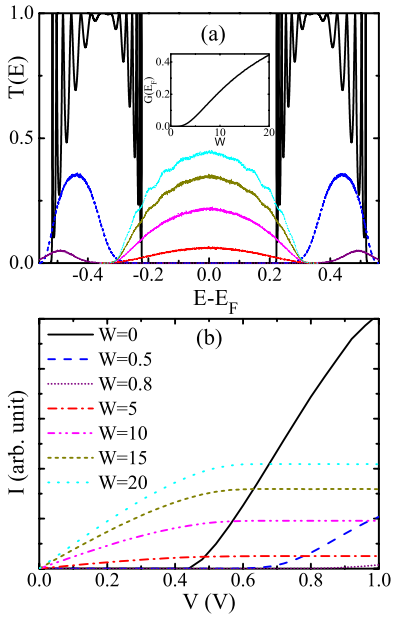

FIG. 3. (Color online) (a) Energy-dependent transmission coefficient $T(E)$ and (b) the corresponding current-voltage characteristics for poly(G)-poly(C) with various backbone disorder degrees W. Inset: The Landauer conductance at the Fermi energy $G(E_F)$ (in units of $2e^2/h$) versus W. Here the Fermi energy is set to locate in the middle of the band gap for the homogeneous poly(G)-poly(C) chain (E_F=0.0 eV) [28,37] and will not be changed with W since the on-site energy of the backbone is assumed to be randomly distributed around zero. Other parameters are $\varepsilon_{GC}=\varepsilon_b$=0.0 eV, t =0.15 eV, t_b=0.24 eV [28], and N=15. The results are averaged over 200 000 configurations.

$G(E)=G_0T(E)$ with G_0 the quantum conductance [31]. E_F and V are, respectively, the equilibrium Fermi energy and applied voltage. The temperature T is set to 4 K. To minimize the contact effects, we assume an appropriate coupling $\tau=\sqrt{t\times t_m}$ between the electrodes and the duplex DNA [53].

Figure 3 shows the transmission coefficient $T(E)$ and current-voltage characteristics for the short poly(G)-poly(C) with several backbone disorder degrees W by adopting the values $\varepsilon_{GC}=\varepsilon_b$=0 eV, t=0.15 eV, and t_b=0.24 eV [28]. The results are averaged over 200 000 configurations. In Fig. 3(a), it can be seen that there are three main bands in the transmission spectra, symmetrically distributed around the Fermi energy, and one is at the center and the other two are on both sides. One notices the following features by increasing the backbone disorder degree W: (1) The width and transmission coefficient of two side bands gradually decrease and finally vanish, which is consistent with the localization picture. (2) The right (left) side transmission band is shifted towards higher (lower) energies. (3) The central transmission band is absent at small W and will emerge around the Fermi energy by increasing W, consistent with the experimental results as well as the *ab initio* calculations that the environmental factors can lead to impurity states in the band gap [10,46]; and its transmission coefficient is progressively enhanced. Since electrons around the Fermi energy determine the charge transport properties of the duplex DNA, it would be useful to plot the Landauer conductance versus W at the Fermi energy. As we can see, the Landauer conductance $G(E_F)$ increases with increasing W [Fig. 3(a), inset]. This may give a qualitative explanation for the experimental observation that the conductivity of the DNA chains increases with increasing the salt concentration and pH, and a larger current is observed at ambient conditions than in vacuum conditions [54]. In addition, one can further observe the backbone disorder-induced semiconducting-metallic transition in short DNA molecules by increasing W, as it is further illustrated in Fig. 3(b). The threshold voltage increases with increasing W in the case of small W, whereas it vanishes in the case of large W; and the current is significantly enhanced by increasing W at low bias. This physical scenario illustrates the different transport behaviors of the poly(G)-poly(C) observed in Refs. [14,52]. The experimental measurement in Ref. [14] was performed on a mica surface with roughness 0.8 Å and the backbone disorder will be stronger, leading to the linear I-V curves at low bias. The experiment of Ref. [52] was carried out by suspending the DNA molecules between two metal nanoelectrodes by electrostatic trapping and the backbone disorder will be weaker, and consequently the poly(G)-poly(C) behaves as a semiconductor. This physical scenario may also elucidate the different current amplitude [14] and the variation of the voltage gap width [52] observed in the same experiments, since the backbone disorder is very sensitive to the sample preparation and surrounding environment. Our results also tend to support the experimental observation that the DNA molecules show different I-V curves by modulating the relative humidity [55].

In summary, we numerically investigate the charge transport properties of the poly(G)-poly(C), poly(A)-poly(T), human chromosome 22, and λ-DNA molecules induced by the backbone disorder which simulates the environmental complications. The negatively charged backbone locates in the outer region of the double-helical structure and its on-site energies are very sensitive to the sample preparation and surrounding environment. Our results show that the backbone disorder plays an important role in the charge transport efficiency of DNA molecules with various nucleotide arrangement, leading to the enhancement of transport when the environment-induced disorder surpasses a critical value. This physical picture can interpret the variety of transport behaviors observed in DNA molecules. Since the backbone disorder-induced enhancement of transport is a generic feature for the fishbone model as well as for the dangling backbone ladder model, we expect that the environmental disorder may enhance the charge transport ability of other quasi-one-dimensional materials, such as carbon nanotubes and graphene nanoribbons, which are subjected to the disordered side sites (like the substrate) by random interactions. This may need to be further corroborated.

This work was supported by the State Key Programs for Basic Research of China (Grant Nos. 2005CB623605 and 2006CB921803), and by National Foundation of Natural Science in China Grant Nos. 10874071 and 60676056

[1] D. D. Eley and D. I. Spivey, Trans. Faraday Soc. **58**, 411 (1962).
[2] M. R. Arkin, E. D. A. Stemp, R. E. Holmlin, J. K. Barton, A. Hörmann, E. J. C. Olson, and P. F. Barbara, Science **273**, 475 (1996).
[3] F. D. Lewis, T. Wu, Y. Zhang, R. L. Letsinger, S. R. Greenfield, and M. R. Wasielewski, Science **277**, 673 (1997).
[4] E. Braun, Y. Eichen, U. Sivan, and G. Ben-Yoseph, Nature (London) **391**, 775 (1998).
[5] P. J. de Pablo, F. Moreno-Herrero, J. Colchero, J. Gómez Herrero, P. Herrero, A. M. Baró, P. Ordejón, J. M. Soler, and E. Artacho, Phys. Rev. Lett. **85**, 4992 (2000).
[6] A. J. Storm, J. van Noort, S. de Vries, and C. Dekker, Appl. Phys. Lett. **79**, 3881 (2001).
[7] Y. Zhang, R. H. Austin, J. Kraeft, E. C. Cox, and N. P. Ong, Phys. Rev. Lett. **89**, 198102 (2002).
[8] H. Cohen, C. Nogues, R. Naaman, and D. Porath, Proc. Natl. Acad. Sci. U.S.A. **102**, 11589 (2005).
[9] M. S. Xu, R. G. Endres, S. Tsukamoto, M. Kitamura, S. Ishida, and Y. Arakawa, Small **1**, 1168 (2005).
[10] E. Shapir, H. Cohen, A. Calzolari, C. Cavazzoni, D. A. Ryndyk, G. Cuniberti, A. Kotlyar, R. Di Felice, and D. Porath, Nature Mater. **7**, 68 (2008).
[11] S. Roy, H. Vedala, A. D. Roy, D.-H. Kim, M. Doud, K. Mathee, H.-K. Shin, N. Shimamoto, V. Prasad, and W. Choi, Nano Lett. **8**, 26 (2008).
[12] H. W. Fink and C. Schönenberger, Nature (London) **398**, 407 (1999).
[13] P. Tran, B. Alavi, and G. Gruner, Phys. Rev. Lett. **85**, 1564 (2000).
[14] L. Cai, H. Tabata, and T. Kawai, Nanotechnology **12**, 211 (2001).
[15] A. Y. Kasumov, M. Kociak, S. Guéron, B. Reulet, V. T. Volkov, D. V. Klinov, and H. Bouchiat, Science **291**, 280 (2001).
[16] B. Xu, P. Zhang, X. Li, and N. Tao, Nano Lett. **4**, 1105 (2004).
[17] J. P. Lewis, P. Ordejón, and O. F. Sankey, Phys. Rev. B **55**, 6880 (1997).
[18] A. A. Voityuk, J. Jortner, M. Bixon, and N. Rösch, J. Chem. Phys. **114**, 5614 (2001).
[19] Y. J. Yan and H. Y. Zhang, J. Theor. Comput. Chem. **1**, 225 (2002).
[20] R. N. Barnett, C. L. Cleveland, U. Landman, E. Boone, S. Kanvah, and G. B. Schuster, J. Phys. Chem. A **107**, 3525 (2003).
[21] E. B. Starikov, Philos. Mag. Lett. **83**, 699 (2003).
[22] R. Di Felice, A. Calzolari, and H. Zhang, Nanotechnology **15**, 1256 (2004).
[23] H. Mehrez and M. P. Anantram, Phys. Rev. B **71**, 115405 (2005).
[24] J. Ladik, A. Bende, and F. Bogar, J. Chem. Phys. **127**, 055102 (2007).
[25] A. A. Voityuk, J. Chem. Phys. **128**, 115101 (2008).
[26] J. Jortner, M. Bixon, T. Langenbacher, and M. E. Michel-Beyerle, Proc. Natl. Acad. Sci. U.S.A. **95**, 12759 (1998).
[27] Y. A. Berlin, A. L. Burin, and M. A. Ratner, Chem. Phys. **275**, 61 (2002).
[28] G. Cuniberti, L. Craco, D. Porath, and C. Dekker, Phys. Rev. B **65**, 241314(R) (2002).
[29] M. Unge and S. Stafström, Nano Lett. **3**, 1417 (2003).
[30] J. Yi, Phys. Rev. B **68**, 193103 (2003).
[31] S. Roche, D. Bicout, E. Maciá, and E. Kats, Phys. Rev. Lett. **91**, 228101 (2003).
[32] Y. Zhu, C.-C. Kaun, and H. Guo, Phys. Rev. B **69**, 245112 (2004).
[33] H. Yamada, E. B. Starikov, D. Hennig, and J. F. R. Archilla, Eur. Phys. J. E **17**, 149 (2005).
[34] D. Klotsa, R. A. Römer, and M. S. Turner, Biophys. J. **89**, 2187 (2005).
[35] R. Gutiérrez, S. Mandal, and G. Cuniberti, Nano Lett. **5**, 1093 (2005).
[36] K. Senthilkumar, F. C. Grozema, C. F. Guerra, F. M. Bickelhaupt, F. D. Lewis, Y. A. Berlin, M. A. Ratner, and L. D. A. Siebbeles, J. Am. Chem. Soc. **127**, 14894 (2005).
[37] E. Maciá and S. Roche, Nanotechnology **17**, 3002 (2006).
[38] R. Gutiérrez, S. Mohapatra, H. Cohen, D. Porath, and G. Cuniberti, Phys. Rev. B **74**, 235105 (2006).
[39] X. F. Wang and T. Chakraborty, Phys. Rev. Lett. **97**, 106602 (2006).
[40] E. M. Conwell, S. M. Bloch, P. M. McLaughlin, and D. M. Basko, J. Am. Chem. Soc. **129**, 9175 (2007).
[41] E. Díaz, A. Sedrakyan, D. Sedrakyan, and F. Domínguez-Adame, Phys. Rev. B **75**, 014201 (2007).
[42] E. Maciá, Phys. Rev. B **76**, 245123 (2007).
[43] C.-T. Shih, S. Roche, and R. A. Römer, Phys. Rev. Lett. **100**, 018105 (2008).
[44] J. A. Berashevich, V. Apalkov, and T. Chakraborty, J. Phys.: Condens. Matter **20**, 075104 (2008).
[45] A.-M. Guo and S.-J. Xiong, Phys. Lett. A **372**, 3259 (2008).
[46] R. G. Endres, D. L. Cox, and R. R. P. Singh, Rev. Mod. Phys. **76**, 195 (2004).
[47] M. Bixon and J. Jortner, Chem. Phys. **319**, 273 (2005).
[48] G. Cuniberti, E. Maciá, A. Rodriguez, and R. A. Römer, in *Charge Migration in DNA: Perspectives from Physics, Chemistry and Biology*, edited by T. Chakraborty (Springer-Verlag, Berlin, 2007).
[49] M. Taniguchi and T. Kawai, Phys. Rev. E **70**, 011913 (2004).
[50] B. Kramer and A. MacKinnon, Rep. Prog. Phys. **56**, 1469 (1993).
[51] X. R. Wang, Yupeng Wang, and Z. Z. Sun, Phys. Rev. B **65**, 193402 (2002).
[52] D. Porath, A. Bezryadin, S. de Vries, and C. Dekker, Nature (London) **403**, 635 (2000).
[53] E. Maciá, F. Triozon, and S. Roche, Phys. Rev. B **71**, 113106 (2005).
[54] H. Vedala, S. Roy, M. Doud, K. Mathee, S. Hwang, M. Jeon, and W. Choi, Nanotechnology **19**, 265704 (2008).
[55] T. Kleine-Ostmann, C. Jördens, K. Baaske, T. Weimann, M. Hrabe de Angelis, and K. Koch, Appl. Phys. Lett. **88**, 102102 (2006).