Effective models for charge transport in DNA nanowires

R. Gutierrez[a] **and G. Cuniberti**

[a]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

The rapid progress in the field of molecular electronics has led to an increasing interest on DNA oligomers as possible components of electronic circuits at the nanoscale. For this, however, an understanding of charge transfer and transport mechanisms in this molecule is required. Experiments show that a large number of factors may influence the electronic properties of DNA. Though full first principle approaches are the ideal tool for a theoretical characterization of the structural and electronic properties of DNA, the complexity of this molecule make these methods of limited use. Consequently, model Hamiltonian approaches, which filter out single factors influencing charge propagation in the double helix are highly valuable. In this chapter, we give a review of different DNA models which are thought to capture the influence of some of these factors. We will specifically focus on static and dynamic disorder.

1. Introduction

The increasing demands on the integration densities of electronic devices is considerably limiting conventional semiconductor-based electronics. As a result, new possibilities have been explored in the last decade. They have led to the emergence of molecular electronics, which is basically relies on the idea of using single molecules or molecular groups as basic elements of electronic devices [1]. A new conceptual idea advanced by molecular electronics is the switch from a top-bottom approach, where the devices are extracted from a single large-scale building block, to a bottom-up approach in which the whole system is composed of small basic building blocks with recognition and self-assembly properties.

A molecule that has recently attracted the attention of both, experimentalists and theoreticians, is DNA. The observation of electron transfer between intercalated donor and acceptor centers in DNA oligomers in solution over unexpected long length scales [2], led to a revival of interest in the conduction properties of

this molecule. Though the idea that DNA might be conducting is rather old [3], there were no conclusive proofs that it could support charge transfer over long distances. This is however a critical issue when considering e. g., damage repair during the replication process [4]. Apart from the relevance of these and similar experiments for biology and genetics, they also suggested that by appropriately tuning the experimental conditions, DNA molecules might be able to carry an electrical current. Further, DNA oligomers might be useful as templates in molecular electronic circuits, by exploiting their self-assembling and self-recognition properties [5–8]. These possibilities have become more realistic in the last years. Nowadays, it is possible to carry out transport experiments on single molecules connected to metallic electrodes. Though many technical and theoretical problems have still to be surmounted, electronics at the molecular scale will be a leading field during the next century.

However, despite the many expectations put on DNA as a potential ingredient of molecular electronic circuits, transport experiments on this molecule have revealed a very intriguing and partly contradictory behavior. Thus, it has been found that DNA may be insulating [9,10], semiconducting [11] or metallic [12,13]. These results demonstrate the high sensibility of DNA transport experiments to different factors affecting charge motion, like the quality of the contacts to the metal electrodes, the base-pair sequence, the charge injection into the molecule or environmental effects (dry vs. aqueous environments) among others.

Theoretically, knowledge of the electronic structure of the different building units of a DNA molecule (base pairs, sugar and phosphate groups) is essential for clarifying the most effective transport mechanisms. First principle approaches are the most suitable tools for this goal. However, the huge complexity of DNA makes *ab initio* calculations still very demanding, so that only comparatively few investigations have been performed [14–21]. Further, environmental effects such as the presence of hydration shells and counterions make *ab initio* calculations even more challenging [15,16].

In this chapter, we will review a complementary (to first principle approaches) way to look at DNA, namely, model Hamiltonians. They play a significant role in filtering out possible charge transfer and transport mechanisms as well as in guiding the more involved first principle investigations. We are not aiming at a thorough review of Hamiltonian-based theories. In fact, since the authors belong to the "physical community", model approaches for charge transfer formulated in the "chemical community" will not be the scope of this chapter. The interested reader can consult e. g., Refs. [22–27]. In the next two sections, we discuss models describing the influence of static disorder and dynamical effects, on charge propagation in DNA. For the sake of the presentation, we discuss both
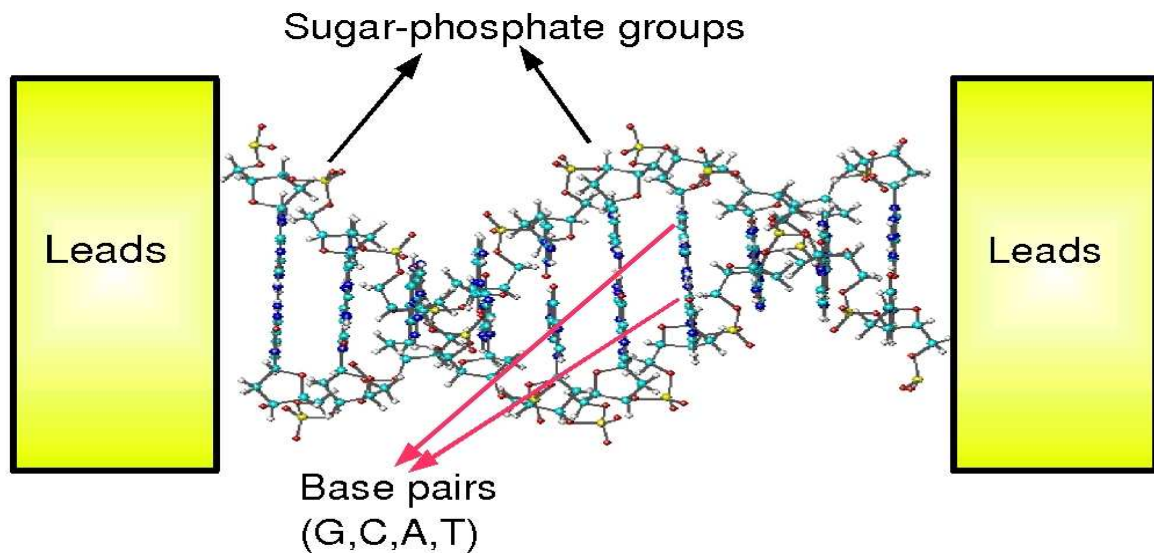
Fig. 1. Schematic representation of a double-stranded DNA oligomer with an arbitrary base-pair sequence and connected to left and right electrodes.

factors in different sections. Nevertheless, the reader should be aware that an interplay between them is expected to be closer to reality.

2. Static Disorder

DNA oligomers consist of four building blocks (oligonucleotides): adenyne (A), tymine (T), cytosine (C) and guanine (G). As is well-known, they have specific binding properties, i. e., only A-T and G-C pairs are possible, see Fig. 1. Sugar and phosphate groups ensure the mechanical stability of the double helix and protect the base pairs. Since the phosphate groups are negatively charged, the topology of the duplex is only conserved if it is immersed into an aqueous solution containing counterions (Na^+, Mg^+) that neutralize the phosphate groups. Thus, experiments on "dry" DNA usually means that the humidity has been strongly reduced, but there are still water molecules and counterions attached to the sugar-phosphate mantle.

The specific base-pair sequence is obviously essential for DNA to fullfil its function as a carrier of the genetic code. However, this same fact can be detrimental for charge transport. The apparent random way in which the DNA sequence is composed, strongly suggests that a charge propagating along the double helix may basically feel a random potential leading to backscattering. It is well-known that in a one-dimensional system with uncorrelated disorder all electronic states are completely localised (Anderson localization). How-

ever, correlated disorder with e. g., power-law correlations [28] may lead to delocalised states within some special energy windows in the thermodynamic limit. As a result, for a fixed disorder strength an insulator to metal transition can be obtained at some critical value of the so-called scaling exponent α. This quantity describes the correlation properties of a random process [29,28], specifically, the length-dependence of the position autocorrelation function: $C(l) \sim l^{-\alpha}$. Thus, $\alpha = 0.5$ corresponds to a pure random walk, while other values indicate the presence of long-range correlations and hence, the absence of relevant length scales in the problem (self-similarity).

Some of the main issues to be addressed when investigating the role of disorder in DNA are, in our view, the following: (i) Is the base-pair sequence in DNA completely random (Anderson-like) or do there exist (long- or short-ranged) correlations? (ii) A measure for the degree of confinement of the electronic wave function is given by the localization length ξ [30], which can be calculated using transfer-matrix techniques [28,30]. Are the resulting localization lengths larger or smaller than the actual length L of the DNA segments studied in transport experiments? For $\xi \gg L$ the system may appear as effectively conducting, despite the presence of disorder, though in the thermodynamic limit all states may remain localised. To clear these issues requires a close cooperation between experimentalists and theoreticians. In what follows we review some theoretical studies addressing these problems.

The simplest way to mimic a DNA wire is by assuming that after charge injection, the electron (hole) will basically propagate along one of the strands (the inter-strand coupling being much smaller), so that one-dimensional tight-binding chains can be a good starting point to minimally describe a DNA wire. Roche [31] investigated such a model for Poly(GC) and λ-phage DNA, with on-site disorder (resulting from the differences in the ionization potentials of the base pairs) and bond disorder $\sim \cos \theta_{n,n+1}$ related to twisting motion of nearest-neighbor bases along the strand, $\theta_{n,n+1}$ being independent Gaussian-distributed random variables. Poly(GC) displays two electronic bands, thermal fluctuations reduce the transmission peaks and also slightly, the band widths. The effect of disorder does not appear to be very dramatic. In the case of λ-phage, however, the transmission peaks are considerably diminished in intensity and in number with increasing chain length at zero temperature, since only few electronic states are not backscattered by the random potential profile of the chain. Interestingly, the average Ljapunov exponent, which is related to the localization length, increases with increasing temperature, indicating that despite thermal fluctuations many states are still contributing to the charge transport.

In an early paper Roche *et al.* [32] used so called rescaling coefficients, which give a measure for the existence of long-range correlations in disordered sys-

tems. Their results show that e. g., DNA built from Fibonacci sequences has a very small Hurst exponent (indicating strong correlations). Uncorrelated random sequences show a strong fragmentation and suppression of the transmission with increasing length, while in correlated sequences several states appear to be rather robust against the increasing rate of backscattering. Hence, it may be expected that correlated disorder will be more favorable for long-distance carrier transport in DNA wires.

Another typical example of correlated disorder was presented by Alburquerque *et al.* [33] within a one-dimensional tight-binding model. The authors investigated the quasi-periodic Rudin-Shapiro sequence as well as the human genome Ch22. As expected, the transmission bands became more and more fragmented with increasing number of nucleotides. Though for very long chain lengths all electronic states did tend to be completely localised, long-range correlations yielded large localization lengths and thus transport may still be supported for special energy points on rather long wires.

Zhu *et al.* [34] formulated an effective tight binding model including only HOMO and LUMO of poly(GC) together with onsite Coulomb interactions. Onsite and off-diagonal disorder, related to fluctuations of the local electrostatic potential[35] and to twisting motion of the base pairs at finite temperatures, respectively, were also included. The main effect of the Coulomb interaction was to first reduce the band gap, so that the system goes over to a metallic state, but finally the gap reappears as a Coulomb-blockade gap. Twisting disorder was apparently less relevant for short wires and low temperatures.

Caetano and Schulz [36] investigated a double-strand model with uncorrelated disorder along the single strand, but taking into account the binding specificity of the four bases when considering the complementary strand (A-T and G-C). Participation ratios $P(E)$ were computed, which give a measure of the degree of localization of electronic states. $P(E)$ is e. g, almost zero for localised states in the thermodynamic limit. The results suggest that inter-strand correlations may give rise to bands of delocalised states, with a participation ratio that does not appreciably decay with increasing length.

A very detailed study of the localization properties of electronic states in two minimal models of different DNA oligomers (poly(GC), λ-DNA, telomeric DNA) was presented by D. Klotsa *et al.* [37]: a fishbone model [38–40] and a ladder model. Both models fullfil the minimal requirement of showing a band-gap in the electronic spectrum, mirroring the existence of a HOMO-LUMO gap in isolated DNA molecules. However, the ladder model allows for an inclusion of interstrand effects as well as to include the specific base-complementarity typical of the DNA duplex, an issue that can not be fully captured by the first model. The authors were mainly interested in environmental-induced disorder.

Hence, they assume that only the backbone sites were affected by it, while the nucleotide core was well screened. Nevertheless, as shown by a decimation procedure [37], disorder in the backbone sites can induce local fluctuations of the onsite energies on the base pairs (gating effect). Uniform disorder (where the onsite energies of the backbones continuously vary over an interval $[-W, W]$, W being the disorder strength) is shown to reduce continuously the localization length, as expected. For binary disorder (onsite energies take only two posible values $\pm W/2$), as it may arise by the binding of counterions to the backbone sites, the situation is similar up to some critical disorder strength W_c. However, farther increase of W leads to an unexpected behavior: the localization length on the electronic side bands is suppressed but a new band around the mid-gap with *increasing* localization length shows up. Thus, disorder-induced delocalization of the electronic states is observed in some energy window. This result, obtained within a simple model, may be supported by first principle calculations [41] which clearly show that the environment can introduce additional states in the molecular band gap and thus effectively reduce it.

Most of the foregoing investigations consider onsite disorder, only. The influence of off-diagonal short range correlations was investigated by Zhang and Ulloa [42] in λ-DNA. They showed that this kind of disorder can definitely lead to the emergence of conduction chanels in finite systems. For some special ratios of the nearest-neighbor hopping amplitudes, there may even exist extended states in the thermodynamic limit. As a consequence, the authors suggested that λ-DNA may show a finite current at low voltages.

3. Dynamical Disorder

In the last section, we presented several studies related to the influence of static disorder on the charge transport properties of different DNA oligomers. Here, we address a second aspect of high relevance, namely the impact of dynamical disorder related to structural fluctuations, on charge propagation. Considering the relative flexibility of DNA, one may expect that vibrational modes may have a strong influence on the charge motion via a modification of electronic couplings.

The considerably small decay rates found in electron-transfer experiments [2] have led to the proposal that, besides unistep superexchange mechanisms, phonon-assisted hole hopping might also be of importance [25]. The hole can occupy a specific molecular orbital, localised on a given molecular site; it can also, however, extend over several molecular sites and build a (small) polaron, which is basically a lattice deformation acompanying a propagating charge. It results from the energetic interplay of two tendencies: the tendence to delo-

calise the charge, thus gaining kinetic energy, and the tendence to localise it with a consequent gain in elastic energy. The softness of the DNA molecule and the existence of modes that can appreciably affect the inter-base electronic coupling (like twisting modes or H-stretching bonds), makes this suggestion very attractive [43,44]. Conwell and Rakhmanova [44] investigated this issue using the Su-Heeger-Schrieffer (SSH) model [44], which is known to entail a rich nonlinear physics and that it has extensively been aplied to study polaron formation in conducting polymers. The SSH model deals classically with the lattice degrees of freedom while treating the electrons quantum mechanically. The calculations showed that a polaron may be built and be robust within a wide range of model parameters. The influence of random base sequences was apparently not strong enough to destroy it. Thus, polaron drifting may constitute a possible transport mechanism in DNA oligomers.

The potential for the lattice displacements was assumed in the previous work to be harmonic. Inter-strand modes like H-bond stretching are however expected to be strongly anharmonic; H-bond fluctuations can induce local breaking of the double-strand and have thus been investigated in relation to the DNA denaturation problem [45]. To investigate this effect, Komineas et al. [46] studied a model with strong anharmonic potentials and local coupling of the lattice to the charge density. The strong nonlinearity of the problem led to a *dynamical* opening of bubbles with different sizes that may eventually trap the polaron and thus considerably affect this charge transport channel.

Zhang and Ulloa [47,48] studied a simple model that describes the coupling of torsional excitations (twistons) in DNA to propagating charges and showed that this interaction leads to polaron formation. Twistons modify the inter-base electronic coupling, though this effect is apparently less strong than e. g., in the Holstein model [49], because of the strong nonlinearity of the twistons restoring forces as well as of the twiston-electron coupling. For small restoring forces of the twisting modes and in the non-adiabatic limit ("spring constant" much bigger than electronic coupling), the inter-base coupling is maximally perturbed and an algebraic band reduction is found, weaker than the exponential dependence known from the Holstein model. Thus, it may be expected that the polaron will have a higher mobility along the chain.

The oservation of two quite different time scales ($5\,ps$ and $75\,ps$) in the decay rates of electron transfer processes in DNA, as measured by femtosecond spectroscopy [50], was the main motivation of Bruinsma *et al.* [51] to investigate the coupling of the electronic system to collective modes of the DNA cage. For this, they considered a tight-binding model of electrons interacting with two modes: a twisting mode which mainly couples to the inter-base π-orbital matrix elements, and a linear displacement coupling to the onsite energies of the

radical and acting as a local gating of the latter. In the strong-coupling, high-temperature limit, the hopping matrix elements can be treated perturbatively and build the lowest energy scale. Transport has thus hopping-like character. In analogy with electron transfer theories, the authors provide a picture where there are basically two reaction coordinates related to the above mentioned linear and angular modes. The strong thermal fluctuations associated with the twisting motion are shown to introduce two time scales for electron transfer that can be roughly related to optimal (short) and non-optimal (long) relative orientation of neighboring base pairs.

In several papers, Hennig *et al.* [52–54] formulated a model Hamiltonian where only the relative transverse vibrations of bases belonging to the same pair are included. Their calculations showed the formation of stable polarons. Moreover, the authors suggested that poly(GC) should be more effetive in supporting polaron-mediated charge transport than poly(AT), since for the latter the electron-lattice coupling was found to be about one order of magnitude smaller. Though the authors remarked that no appreciable coupling to twisting distortions was found by their semiempirical quantum chemical calculations, this issue requires further investigation in view of the previously presented results [47,48,51]. Disorder did not apparently have a very dramatic influence in this model; the localization length only changed quantitatively as a function of the disorder strength [54].

Asai [55] proposed a small polaron model to describe the experimental findings of Yoo *et al.* [12] concerning the temperature dependence of the electric current and of the linear conductance. Basically, he assumed that in poly(GC) completely incoherent polaron hopping dominates while in poly(AT) quasi-coherent hopping, i. e., with total phonon number conservation, is more important. As a result, the temperature dependence of the above quantites in both molecules is considerably different. This model was formulated for an infinite system. It is however not clear, how finite size effects may affect the results.

Complementary to the foregoing research which mainly addressed individual vibrational modes of the DNA cage, other studies have focused on the influence of environmental effects. Basko and Conwell [56] used a semiclassical model to describe the interaction of an injected hole in DNA which is placed in a polar solvent. Their basic conclusions pointed out that the main contribution was given by the interaction with water molecules and not with counterions; further, polaron formation was not hindered by the charge-solvent coupling, the interaction rather increased the binding energy (self-localization) of the polaron by around half an eV, which is much larger than relevant temperature scales. Li and Yan [57] as well as Zhang *et al.* [58] investigated the role of dephasing reservoirs in the spirit of the Büttiker-D'Amato-Pastawski model [59,60]. Zhang *et*

al. showed that a change in the length scaling of the conductance can be induced by the dephasing reservoirs as a result of incoherent phonon-mediated transport, a result known from electron transfer theories [61]. In a similar way, Feng and Xiong [62] considered gap-opening as resulting from the coupling to a set of two-level systems which simulate low-lying states of the bosonic bath. Gutierrez *et al.* [39,40] have discussed electron transport in a "broken"-ladder model in presence of a strong dissipative environment simulated by a bosonic bath. It was found that the environment can induce virtual electronic states inside the molecular band gap and thus lead to a change in the low-energy transport properties of the system. Especially, the $I - V$ curves become metallic-like at low voltages as a result of phonon-assisted hopping. We note that these latter results are quite similar to that found in *ab initio* calculations, showing that water states can appear inbetween the $\pi - \pi^*$ gap [63], thus effectively reducing the HOMO-LUMO band gap of DNA molecules.

We finally mention that the role of nonlinear excitations (solitons, breathers) in the process of denaturation of DNA double strands [45,64,65] and in the transmission of "chemical" information between remote DNA segments [66] have been early addressed in the literature. Since these approaches are not directly connected with the issue of charge transport in short DNA wires between electrodes, we do not go into further details. They may however open a new interesting mechanism for transport and deserve a more careful investigation.

4. Conclusions

Though big progress has been achieved in the past decade to clarify the relevant transport mechanisms in DNA oligomers, a coherent, unifying picture is still lacking. The experimental difficulties to give reliable transport characteristics of this molecule make the formulation of model Hamiltonians quite challenging. The theoretical research presented in this chapter shows that charge transport in DNA is considerably influenced by both static and dynamical disorder. Long-range correlated disorder can play a role in increasing the localization length beyond the relevant molecular length scales addressed in experiments, thus making DNA to effectively appear as a conductor. This effect may be supported or counteracted by thermal fluctuations arising from internal (vibrations) or external (solvent) modes and leading to increased charge localization or to coherent or incoherent transport.

The presented models only focus on the equilibrium, low-bias limit of transport. However, real transport experiments probe the molecules at finite voltages and hence, non-equilibrium effects have to be also considered. This makes of course the mathematical treatment as well as the physical interpretation more

involved. Considerable efforts to deal with this issue have been made in the last times [67,68]; to address them goes however beyond the scope of this chapter.

5. Acknowledgments

REFERENCES

1. *Molecular Electronics II*, ed. by A. Aviram and M. Ratner, (Johns Hopkins University Press, 1999); *Molecular Electronics III*, ed. by J. R. Reimers, C. A. Picconatto, J. C. Ellenbogen, and R. Shashidhar, Ann. NY Acad. Sci. **1006** (2003).
2. C. J. Murphy, M. R. Arkin, Y. Jenkins, N. D. Ghatlia, S. H. Bossmann,N. J. Turro, and J. K. Barton, Science **262**, 1025 (1993).
3. D. D. Eley and D. I. Spivey, Trans. Faraday Soc. **58**, 411 (1962).
4. E. C. Friedberg, Nature **421**, 436 (2003).
5. C. Dekker and M. Ratner, Physics World (August 2001).
6. K. Keren, R. S. Berman, E. Buchstab, U. Sivan, and E. Braun, Science **302**, 1380 (2003).
7. M. Hazani, F. Hennrich,M. Kappes, R. Naaman, D. Peled,V. Sidorov, and D. Shvarts , Chem. Phys. Lett. **391**, 389 (2004).
8. M. Mertig, R. Kirsch, W. Pompe, and H. Engelhardt, Eur. Phys. J. D **9**, 45 (1999).
9. E. Braun, Y. Eichen, U. Sivan, and G. Ben-Yoseph, Nature **391**, 775 (1998).
10. A. J. Storm, J. V. Noort, S. D. Vries, and C. Dekker, Appl. Phys. Lett. **79**, 3881 (2001).
11. D. Porath, A. Bezryadin, S. D. Vries, and C. Dekker, Nature **403**, 635 (2000).
12. K.-H. Yoo, D. H. Ha, J.-O. Lee, J. W. Park, J. Kim, J. J. Kim, H.-Y. Lee, T. Kawai, and H. Y. Choi , Phys. Rev. Lett. **87**, (2001).
13. B. Xu, P. Zhang, X. Li, and N. Tao, Nano letters **4**, 1105 (2004).
14. R. D. Felice, A. Calzolari, and E. Molinari, Phys. Rev. B **65**, 045104 (2002).
15. R. N. Barnett, Ch. L. Cleveland, A. Joy, U. Landman, and G. B. Schuster, Science **294**, 567 (2001).
16. F. L. Gervasio, P. Carolini, and M. Parrinello, Phys. Rev. Lett. **89**, 108102 (2002).
17. E. Artacho, M. Machado, D. Sanchez-Portal, P. Ordejon, and J. M. Soler, Mol. Phys. **101**, 1587 (2003).
18. S. S. Alexandre, E. Artacho, J. M. Soler, and H. Chacham, Phys. Rev. Lett. **91**, 108105 (2003).
19. J. P. Lewis, P. Ordejon, and O. F. Sankey, Phys. Rev. B **55**, 6880 (1997).
20. E. B. Starikov, Phil. Mag. Lett. **83**, 699 (2003).
21. H. Wang, J. P. Lewis, and O. Sankey, Phys. Rev. Lett. **93**, 016401 (2004).
22. *Long-Range Charge Transfer in DNA I and II*, Vol. 237 of *Topics in Current Chemistry*, edited by G. B. Schuster (Springer, Berlin, 2004), .
23. A. Nitzan, Annual Reviews of Physical Chemistry **52**, 681 (2001).
24. A. Nitzan and M. Ratner, Science, **300**, 1384 (2003).
25. J. Jortner, M. Bixon, T. Langenbacher, and M. E. Michel-Beyerle, Proc. Natl. Acad. Sci. USA **95**, 12759 (1998).
26. J. Jortner and M. Bixon, Chemical Physics **281**, 393 (2002).

27. Y. A. Berlin, A. L. Burin, L. D. A. Siebbeles, and M. A. Ratner, J. Phys. Chem. A **105**, 5666 (2001).
28. P. Carpena, P. Bernaola-Galvan, P. C. Ivanov, and H. E. Stanley, Nature **418**, 955 (2002).
29. C.-K. Peng, S. V. Buldyrev, A. L. Goldberger, S. Havlin, F. Sciortino, M. Simons, and H. E. Stanley, Nature **356**, 168 (1992).
30. P. Phillips, *Advanced Solid State Physics*, Boulder, CO, Westview Press (2003).
31. S. Roche, Phys. Rev. Lett. **91**, 108101 (2003).
32. S. Roche, D. Bicout, E. Macia and E. Kats Phys. Rev. Lett. **91**, 22810 (2003).
33. E. L. Alburquerque, M. S. Vasconcelos, M. L. Lyra, and F. A. B. F. de Moura, Physical Review E **71**, 21910 (2005).
34. Y. Zhu, C. C. Kaun, and H. Guo, Phys. Rev. B **69**, 245112 (2004).
35. C. Adessi, S. Walch, and M. P. Anantram, Phys. Rev. B **67**, 081405(R) (2003).
36. R. A. Caetano and P. A. Schulz, `cond-mat/0409245` (2004).
37. D. Klotsa, R. A. Röemer, and M. S. Turner, `q-bio.GN/0504004` (2005).
38. G. Cuniberti, L. Craco, D. Porath, and C. Dekker, Phys. Rev. B **65**, 241314 (2002).
39. R. Gutierrez, S. Mandal, and G. Cuniberti,, to appear in Nano Letters (2005).
40. R. Gutierrez, S. Mandal, and G. Cuniberti, to appear in Phys. Rev. B (2005).
41. A. Huebsch, R. G. Endres, D. L. Cox, and R. R. P. Singh, Phys. Rev. Lett. **94**, 178102 (2005).
42. W. Zhang and S. E. Ulloa, Phys. Rev. B **69**, 153203 (2004).
43. P. T. Henderson, D. Jobes, G. Hampikian, Y. Kan, and G. B. Schuster, Proc. of Natl. Acad. Sci **96**, 8353 (1999).
44. E. M. Conwell and S. V. Rakhmanova, Proc. of Natl. Acad. Sci. **97**, 4556 (2000).
45. M. Peyrard and A. R. Bishop, Phys. Rev. Lett. **62**, 2755 (1989).
46. S. Komineas, G. Kalosakas, and A. R. Bishop, Physical Review E **65**, 061905 (2002).
47. W. Zhang, A. O. Govorov, and S. E. Ulloa, Phys. Rev. B **66**, 060303(R) (2002).
48. W. Zhang and S. E. Ulloa, Microelec. Journal **35**, 23 (2004).
49. T. Holstein, Ann. Phys. N.Y. **8**, 325 (1959).
50. C. Wan, T. Fiebig, S. O. Kelley, C. R. Treadway, and J. K. Barton, Proc. of Natl. Acad. Sci **96**, 6014 (1999).
51. R. Bruinsma, G. Gruener, M. R. D'Orsogna, and J. Rudnick, Phys. Rev. Lett. **85**, 4393 (2000).
52. D. Hennig, Physical Review E **64**, 041908 (2001).
53. F. Palmero, J. F. R. Archilla, D. Hennig, and F. R. Romero, New J. Phys. **6**, 13 (2004).
54. H. Yamada, `cond-mat/0406040` (2004).
55. Y. Asai, J. Phys. Chem. B **107**, 4647 (2003).
56. D. M. Basko and E. M. Conwell, Phys. Rev. Lett. **88**, 098102 (2002).
57. X. Q. Li and Y. Yan, Appl. Phys. Lett. **79**, 2190 (2001).
58. H. Y. Zhang, X.-Q. Li, P. Han, X. Y. Yu, and Y.-J. Yan , J. Chem. Phys. **117**, 4578 (2002).
59. M. Büettiker, IBM J. Res. Develop. **32**, 317 (1988).
60. J. L. D'Amato and H. M. Pastawski, Phys. Rev. B **41**, 7411 (1990).
61. D. Segal, A. Nitzan, W. B. Davies, M. R. Wasielewski, and M. A. Ratner, J. Phys. Chem. B **104**, 3817 (2000).
62. J.-F. Feng and S.-J. Xiong, Physical Review E **66**, 021908 (2002).
63. R. G. Endres, D. L. Cox, and R. R. P. Singh, Rev. Mod. Phys. **76**, 195 (2004).
64. J.-X. Xiao, J.-T. Lin, and G.-X. Zhang, J. Phys. A: Math. Gen. **20**, 2425 (1987).
65. L. V. Y. adn A. V. Savin and L. I. Manevitch, Physical Review E **66**, 016614 (2002).
66. Z. Hermon, S. Caspi, and E. Ben-Jacob, Europhys. Lett. **43**, 482 (1998).

67. Y.-C. Chen, M. Zwolak, and M. D. Ventra, Nano letters **5**, 621 (2005).
68. A. Pecchia, A. Di Carlo, A. Gagliardi, S. Sanna, Th. Frauenheim, and R. Gutierrez, Nano letters **4**, 2109 (2004).