

Electrical transport through two-dimensional DNA nanostructure

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Abstract. In this work, we numerically investigate the transport properties of a square lattice built from disordered deoxyribonucleic acid sequence. To do so, we used an effective tight-binding model to describe the electronic structure, while the current is obtained within a Green's function framework. We show that the self-assembled DNA structures based-on the disordered sequences display currents, which, by increasing the size of the systems, quickly go to undetectable experimental current values.

1. Introduction

The field of deoxyribonucleic acid (DNA) nanotechnology aims to generate nanomaterials for the construction of electronic devices. Seeman [1,2] developed a self-arrangement of branched artificial DNA, where four single strands of DNA were hybridized to form a stable four-way cross. Based-on these results, regular two-dimensional structures of self-assembled DNA have been reported in the literature [3–7]. These assemblies have been used to construct complex 2D structures with high nanoscale precision [8–11] and are promising to control topography at the nanoscale regime with a much higher resolution than conventional lithography.

The transport properties of DNA [12–14] and self-assembled DNA may be affected by a large variety of effects, either environmental like interaction with substrates, sample dryness, or intrinsic like nucleotide sequencing [15–17]. Here, we contribute to the discussion by putting the current-voltage characteristic for a naturally occurring DNA (*i.e.* λ -DNA) sequence as a particularly well-suited reference for self-assembled DNA experiments.

2. Theoretical formulation

In this study, we describe the transport properties of a self-assembled DNA molecule according to a heuristic tight-binding models where the self-assembled DNA molecule is coupled to two electrodes, as shown in Figure 1. The model, a double-strand chain of nucleotides, contains parameters for the description of the longitudinal and transverse base to base hopping terms which take into account the size difference between pyrimidines (C, T) and purines (A, G). The Hamiltonian of DNA, can be written in Equation (1).



$$H_{\text{DNA}} = \sum_{l=1}^N \sum_{\alpha=1}^2 (\varepsilon_{l\alpha} |l, \alpha\rangle \langle l, \alpha| - t_{l,\alpha}^{\rightarrow} |l, \alpha\rangle \langle l+1, \alpha| - t_{l,\alpha}^{\downarrow} |l, \alpha\rangle \langle l, \alpha+1|) + \text{h.c.} \quad (1)$$

The onsite energies $\varepsilon_{l\alpha}$, are taken to be the effective primary ionization energies of the base nucleotides, *i.e.* $\varepsilon_A = 8.24$ eV, $\varepsilon_T = 9.14$ eV, $\varepsilon_C = 8.87$ eV and $\varepsilon_G = 7.75$ eV. Both strands of DNA are modelled explicitly and the different diagonal overlaps of the larger purines and the smaller pyrimidines are despised by the low energy of inter-strand couplings [18, 19]. The intra-strand couplings are $t_{l,\alpha}^{\rightarrow(\leftarrow)} = 0.35$ eV between identical bases and 0.17 eV between different bases. Perpendicular couplings to the backbone sites are $t_{l,\alpha}^{\downarrow(\uparrow)} = 0.7$ eV.

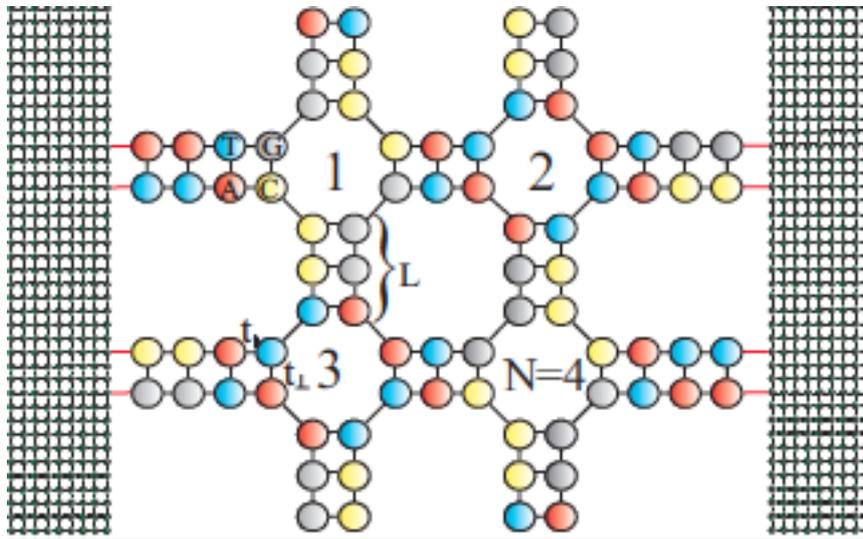


Figure 1. Schematic representation of a ladder-type model for electronic transport along self-assembled DNA between two semi-infinite source(L) and drain(R) contacts as indicated. The nucleotide base pairs sequence is indicated by circles, representing the four possible effective nucleotides. Different colors indicate different nucleotides: Adenine (Red), Thymine (blue), Cytosine (yellow) and Guanine (gray). The possible electronic pathways are shown as lines.

The transmission probability $T(E)$ between the electrodes can be evaluated by Equation (2).

$$T(E) = \text{Tr} [\Gamma_L G^r \Gamma_R (G^r)^\dagger], \quad (2)$$

where G^r is the Green's function between the electrodes L and R. The electrode-DNA coupling τ depends on the geometry of the chemical bond [20], we use $\tau = 0.35$ eV, comparable as the inter-chain DNA couplings [21, 22]. To calculate G^r , we determinate g , the electrodes Green's Function, by a recursive method [23]. In the low-temperature limit the electronic current can be expressed as [24] (see Equation (3)).

$$I = -\frac{2e}{h} \int_{\mu_L}^{\mu_R} T(E) dE. \quad (3)$$

The use of this model has grown in interest in the last decade [25], because, despite the simplified mathematics structure, it allows studied the electronic and transport properties of systems with more than 10000 sites in contradistinction to *ab-initio* approaches.

3. Results and discussion

Two-dimensional DNA models offer the opportunity to construct materials with nanometric precision, allowing them to be considered as possible components of functional devices. However, the main difficulty lies on their characterization. Their collective properties will depend on their arrangement as well as their dimensions. Figure 2 shows the effect of the size (D) of the auto-arrangement (square mesh) and the separation (L) between the chains that make the auto-arrangement over the current. The red curve represents a system with $L = 10$ bps; the black curve is a system with $L = 20$ bps and the blue curve a system with $L = 25$ bps. For the λ -DNA case, regardless of the separation L , at a voltage $V_D = 2$ eV, the current increases with increasing size D . For any size D , for any L the current decreases exponentially with size D . For sizes higher than $D = 120$ base pairs (40 nm), the current is below pA , being experimentally difficult to measure.

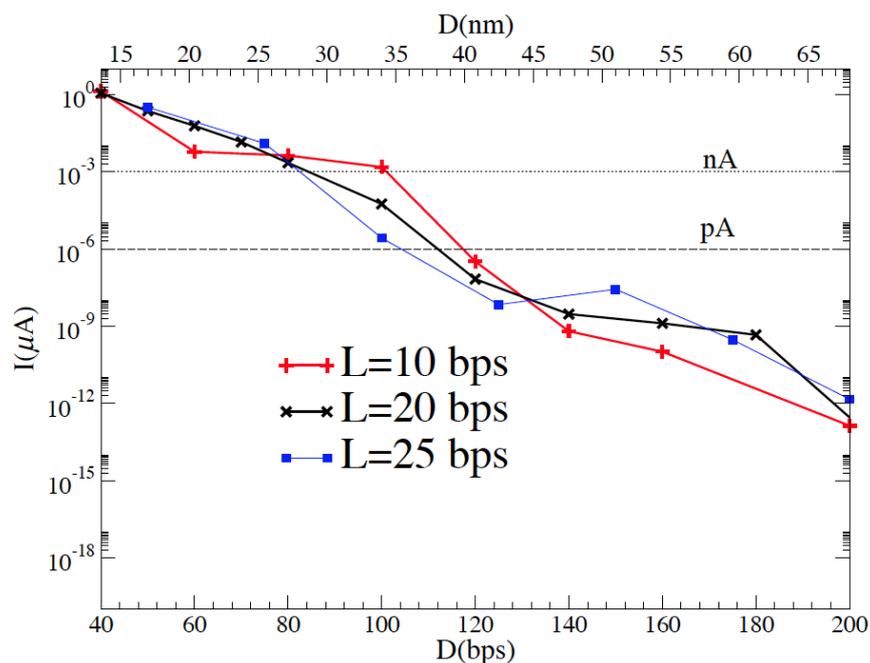


Figure 2. Schematic representation of a ladder-type model for electronic transport along self-assembled DNA between two semi-infinite source and drain contacts as indicated. A third (gate) terminal modulates the conductance of the molecule.

Self-assembled DNA as nano-devices largely depends on how the device is coupled to the contacts. We are assuming that all horizontal chains are coupled to the contacts through the 3' and 5' terminations. For λ -DNA, increasing the number of channels decreases the current regardless of chain separation. In the case of $L = 10$ bps (20-channel) disordered self-assembled DNA have currents of the order of nA. Thus, in the disordered system, a greater relocation of the wave function to all energies and displays.

4. Conclusions

The electronic and transport properties of self-assembled DNA systems remain unexplored, despite the tradition of investigating the transport properties of DNA strands. Thus, we present results on transport properties in self-assembled DNA systems.

The devices investigated in the present work provide a reference for the systematic investigation of possible DNA applications in nanoelectronics. I-V characteristic spectrum,

for $\lambda - DNA$ sequence, shows as the current decreases exponentially with the size of systems. Percolation mechanisms that depend on the competition between the location length and the distance between the self-assemblage intersections are observed.

Acknowledgments

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