The dramatic changes in the DNA Conductance with stretching: Structural Polymorphism at a critical extension : Supporting Information

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Section I

Charge Transfer Rate between the Base and Electrode

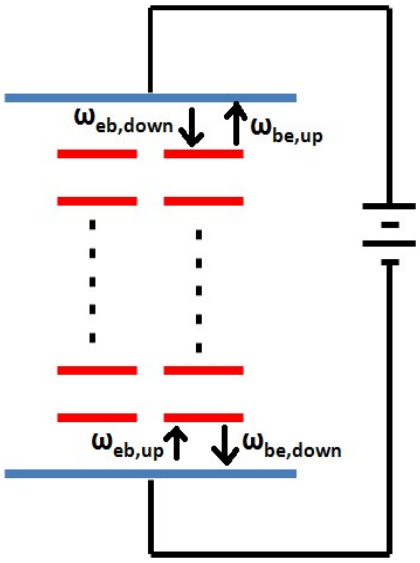

Figure S1. Different charge hopping rates from the DNA base to the electrode and from the electrode to the base. Red lines are representatives of the bases and the blue lines represent the electrode. The black arrows indicate the hopping events with the corresponding rates written along its side.

We have assumed that the rates $\omega_{be,up}$ ($\omega_{be,down}$) and $\omega_{eb,up}$ ($\omega_{eb,down}$) are very high (low) while $\omega_{be,down}$ ($\omega_{be,up}$) and $\omega_{eb,down}$ ($\omega_{eb,up}$) are very low (high) for electron (hole) transport in comparison to the inter-base rates.

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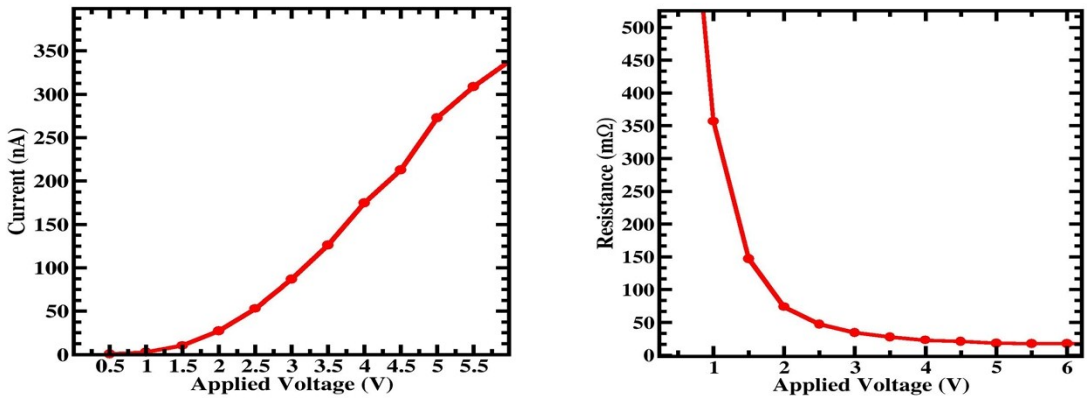
Section II

V-I characteristics for the unstretched DNA

We calculated the I-V characteristics of the dsDNA in its unstretched condition as shown in Figure below S2(a). We also plotted the resistance as a function of applied voltage in Figure S2(b). Up to the cutoff voltage of 1.5 V the DNA conductance is below 6.6×10^{-9} A/V. Above this point the current increases rapidly until it starts to saturate above 5V.

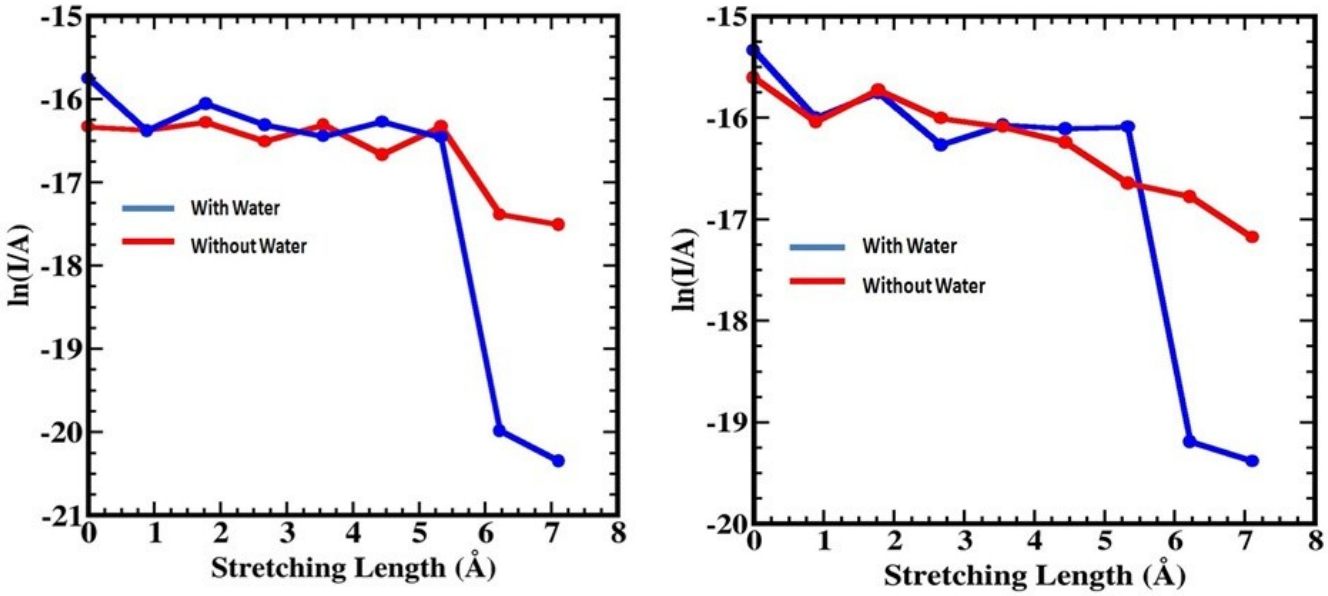


(a) (b)

Figure S2. Current through the unstretched DNA (a) and resistance (b) as a function of the applied voltage. Up to the cutoff voltage of 1.5 V the DNA hardly conducts, indicting high resistance value. Then the current increases rapidly and starts saturating after 5V, resulting a sharp drop of resistance to a much lower value of 20 mΩ.

Section III

Effect of Solvation on DNA conductance

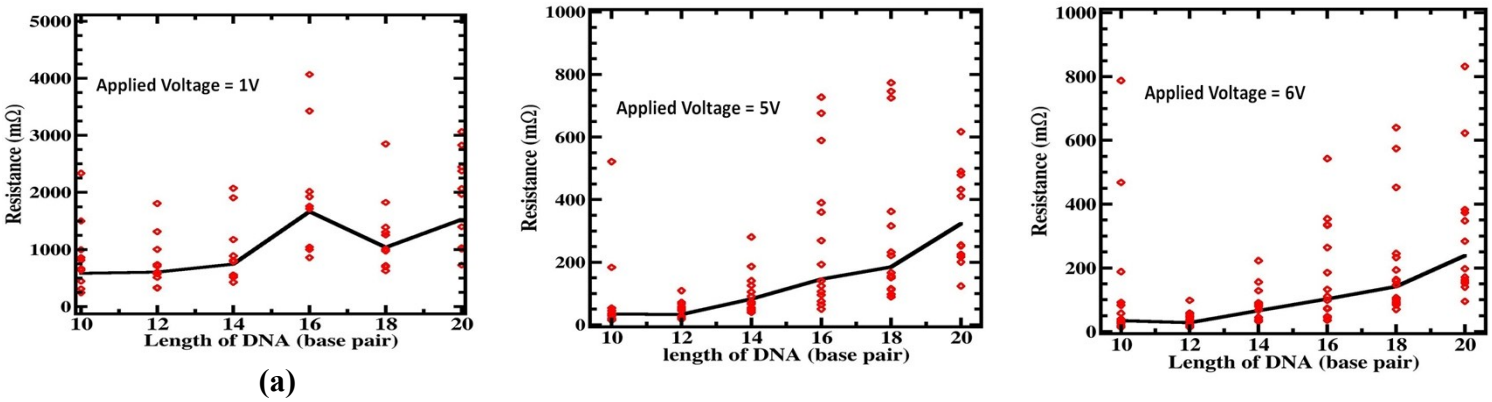


(a) **(b)**

Fig. S3. Logarithm of current as a function of end to end distance of the DNA for 5'end1-5'end2 pulling. Required DFT calculations for the calculation of current were done using mo62x/6-311g level of theory (a) and b3lyp/6-311g level of theory (b). The current show sharp jump when the PCM model was included in the DFT calculation to include the effect of surrounding water (blue lines). The jump in current is not so prominent when PCM model was not considered (red lines).

Section IV.

Resistance vs. DNA length plot for various applied Voltage



(a) **(b)** **(c)**

Fig. S4. Intrinsic resistance of the DNA as a function of DNA length for various applied voltage. The red dots represent the individual case studied and a mean line in black is drawn to guide the eyes.

Section V.

Inclination angle between DNA base pairs

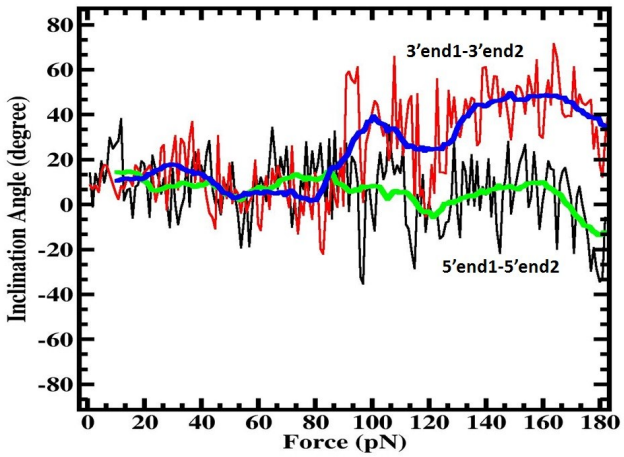


Fig. S5. Inclination angle between the DNA base pairs at the terminal of the DNA as a function of applied force for 5'end1-5'end2 and 3'end1-3'end2 pulling respectively. All the individual case studied are shown in red and black lines. Mean lines are (blue and green) drawn to guide the eyes.

Section VI.

Effect of External Reorganization Energy

To determine the effect of external reorganization energy on the calculated current, we repeated our calculations for various values of the external reorganization energy. We assumed that the external reorganization energy is independent of the hopping pairs. The results for the 5'end1-5'end2 case are presented in figure S6 below, where it is clear that the introduction of external reorganization energy does not affect the behavior of current as a function of end-to-end length of the dsDNA, it only reduces the value of the current.

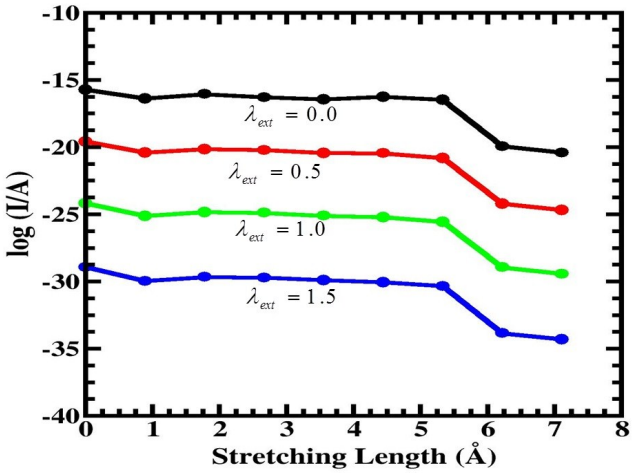
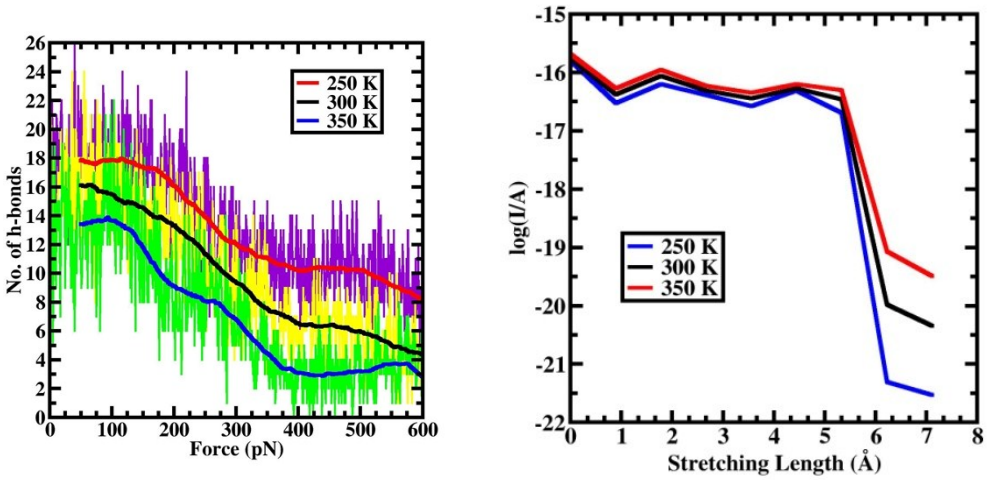


Figure S6. Logarithm of current as a function of end to end distance (5'end1-5'end2 case) of the DNA for various values of external reorganization energy. The External reorganization energy does not affect the behavior of current, it only reduces its magnitude.

Section VII.

Effect of Temperature on Current Calculation



(a) **(b)**

Figure S7. Number of hydrogen bonds as a function of applied force on DNA for 5'end1-5'end2 pulling case for three different temperature (a). Both the original (thin lines) and the running averaged data (thick lines) are shown. Current through the DNA as a function of the stretching length for pulling from 5'end1-5'end2 ends at different temperature (b).

Section VIII.

Effect of Small Bias

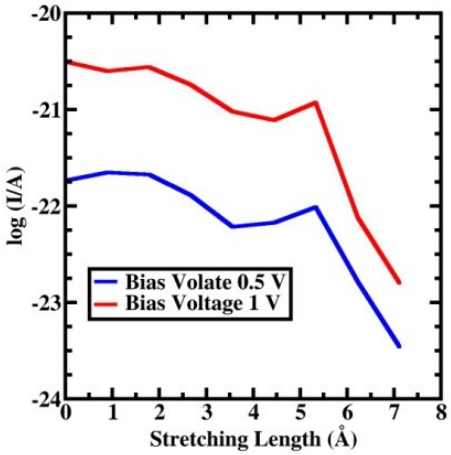


Figure S8. Current through the DNA as a function of the stretching length for 5'end1-5'end2 pulling case for different bias voltage.

Section IX.

Effect of the DNA Sequence

To determine whether the results of our calculation depend on the sequence of the DNA, we performed additional pulling simulations (5'-5') with DNA sequences d(ATATATATATAT) and d(CGCGCGCGCGCG), which differ substantially from the case, d(CGCGAATTCGCG), considered in the main text. The resulting hydrogen bond profiles (which are the measure of the structural changes of the DNAs) as plotted in Figure S9. It is clear from Figure S9 that the shape of the h-bond profile is quite similar for all three cases. In all three cases the significant change in the hydrogen bonds occurs at a force of 150 pN. Of course the absolute values are different. Thus we can conclude that the conductance jump is governed by the changes in the number of h-bonds as a function of applied force, not the absolute value. Thus we conclude that the results reported in the text should be independent of the specific sequence.

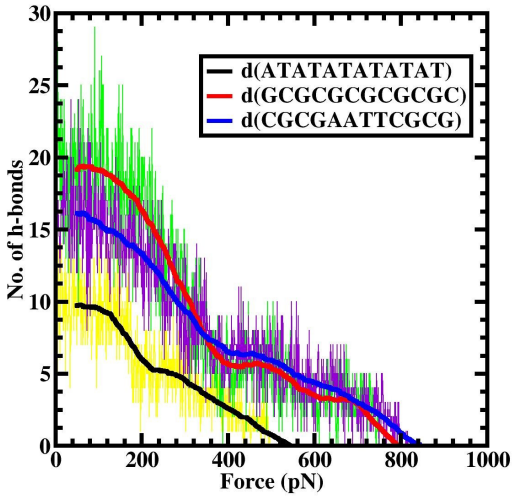


Figure S9. Number of hydrogen bonds as a function of applied force (5'end1-5'end2 pulling case) for three different DNA sequences . Both the original (thin lines) and the running averaged data (thick lines) are shown.

Section X.

Effect of longer DNA

The calculation of the current through the DNA was carried out assuming that the charge transport through the DNA happens via incoherent hopping of charge through the bases. Since the DNA we have studied is short in length (12bp), the transport of charge may have some tunneling effect. To check the

validity of the main conclusion of the paper (critical stretching length), we performed additional calculations for the 5'-5' pulling case with a 20 base pair long dsDNA, where the charge transport is dominated by the hopping mechanism. We see that the conductance jumps with a small stretching of almost 11 %. Consequently, we conclude that the results we show for the 12 base pair DNA remains valid for this longer dsDNA fragment.

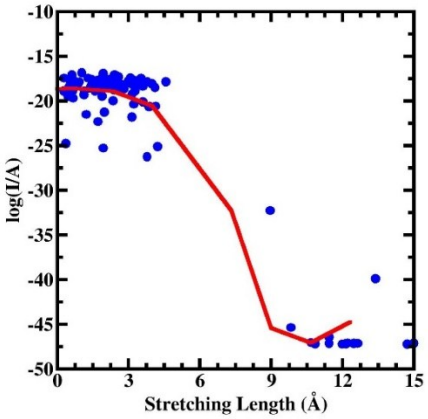


Fig. S10. Current through the 20 bp long DNA as a function of the stretching length for pulling from 5'end1-5'end2 ends. Actual values of current for all individual cases studied are shown in blue dots. A mean line in red is drawn to guide the eyes. Jump in current is seen for a stretching of ~11%. Similar current jump was also observed in 12bp dna (see Figure 4(a) in the main text) at a stretching of 17%.