Supporting Information for
Anisotropic Charge Transport in Nanoscale DNA Wire

Saientan Bag[#], Tathagata Biswas[#], Manish Jain and Prabal K Maiti[*]

Center for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560012

Section I: Internal Reorganization Energy between the DNA bases

DNA Base 1	DNA Base 2	Internal Reorganization Energy (eV)
Guanine	Guanine	0.68
Cytosine	Cytosine	0.43
Guanine	Cytosine	0.50
Cytosine	Guanine	0.61

Table S1: Computed internal reorganization energy between different DNA bases.

Section II: Fixing the value of chemical potential of gold electrode in hopping calculation

The value of chemical potential (μ) can be set by ensuring that there is no net flow of charge at the interface when no voltage is applied. This condition can be mathematically written as

$$\int_{-\infty}^{\infty} exp\left[-\frac{(E-E_b-\lambda)^2}{4\lambda k_B T}\right] f_{FD}(E,\mu)dE = \int_{-\infty}^{\infty} exp\left[-\frac{(E_b-E-\lambda)^2}{4\lambda k_B T}\right](1-f_{FD}(E,\mu))dE$$

The equation above is numerically solved to find out the value of μ relative to the DNA base energy level E_b.

*maiti@iisc.ac.in
[#] equal contribution

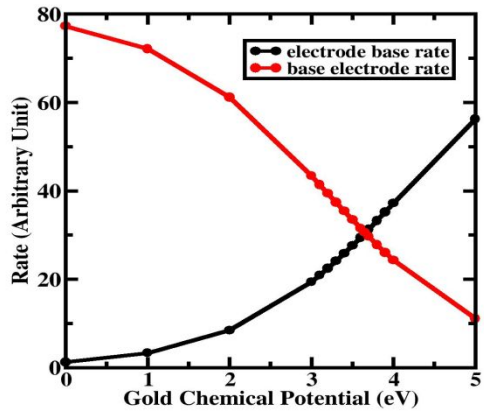

Fig. S1. Hopping rates from the electrode to the DNA base and DNA base to the electrode as a function chemical potential of gold electrode. Two curves intercepts at a value of chemical potential equal to 3.65 eV.

Section III: Fixing the value of chemical potential of gold electrode in tunneling calculation

The value of chemical potential μ can be found by demanding zero net current between the gold and the DNA interface when no voltage is applied. For the current due to hole transport, the above condition turns out to be the following

$$\int_{-\infty}^{\infty} f(E,\mu)T(E,E_{homo})dE = \int_{-\infty}^{\infty}(1-f(E,\mu))T(E_{homo},E)dE$$

E_{homo} is the HOMO energy of the DNA base and f is the fermi function. Here $T(E, E_{homo})$ is the transmittance of the electron form the energy state E to the energy state E_{homo}.

$$\text{Since, } T(E,E_{homo}) = T(E_{homo},E) = \delta(E - E_{homo})$$
$$f(E_{homo},\mu) = 1 - f(E_{homo},\mu)$$
$$E_{homo} = \mu$$

Section IV: Choice of the parameters in the hopping model

Parameter	λ_{eb} and λ_{be}	λ_{ext}	μ	C	φ
Value	0.5 eV	0 eV	3.65 eV	0.05	0.8

Table S2: Value of parameter used in the semi-classical hopping calculations.

The hopping model was analysed for the ranges of the parameters value and robustness of the model was verified with respect to change of the parameter in that range. Here, we briefly describe the philosophy behind the choice of parameters used.

The parameter φ related to the voltage drop across the junction, has to be between 0 and 1. "1" means no voltage drop and "0" means complete drop. We have chosen "0.8" which means 20% drop over two junctions. We checked the electrode to base rate (and also base to electrode) for different φ in that range and observed just decay (increases) in rate with the increase in φ and nothing else. Similarly, the parameter λ_{ext} also decreases in current as we have found earlier[1]. λ_{be} is also known to fall within 0 to 1 eV and previously taken to be ~0.5 eV in the work of Livshits et al.[2] . So, the φ, λ_{ext}, and λ_{be} , together set the magnitude of the electrode to base rate which is later normalized by parameter "C" to get the experimental observed ratio between the base to base and base to electrode right as mentioned in the main text.

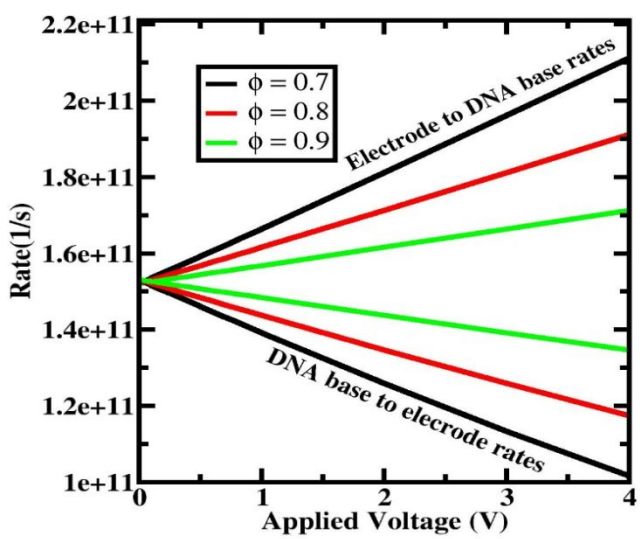

Fig S2: Electrode to DNA base and DNA base to electrode rates for different φ's with the specific choice of

other parameters.

The electrode-base transfer rate works as a bottleneck of the transport (for semi-classical case) as long as the electrode-base transfer rate is less efficient than the base-base transfer rate. The relative values of the conductance for different DNA attachments with the electrode remain unchanged even if the exact value of the charge transport efficiency ratio (between base-base and base-electrode) is not exactly 40. Therefore, the experimental observation of less efficient electrode-base transfer rate is important rather than the exact empirically derived number. So, the assumption regarding the density of state and the interaction energy is justified when one is looking for the relative conductance between different kinds of electrode attachment.

Section V: Average value of the parameters in the Tight Binding Hamiltonian

Parameter	$\langle\varepsilon_{11}\rangle$	$\langle\varepsilon_{12}\rangle$	$\langle\varepsilon_{21}\rangle$	$\langle\varepsilon_{22}\rangle$	$\langle\alpha_{12}^{1}\rangle$	$\langle\alpha_{12}^{2}\rangle$	$\langle\beta_{1}\rangle$	$\langle\beta_{2}\rangle$	$\langle\gamma_{1}\rangle$	$\langle\delta_{1}\rangle$
Average Value	-5.92 eV	-5.93 eV	-5.93 eV	-5.92 eV	0.08 eV	0.08 eV	0.03 eV	0.03 eV	0.01 eV	0.01 eV

Table S3: Average value of parameters used for the tight binding Hamiltonian.

Section VI: Orbital-resolved density of states (DOS)

Orbital-resolved DOS for electrode-base system is calculated where of 3' end of the Guanine base is connected with the electrode. In the following figure, we have shown the contributions coming from the different parts of the electrode-base system to different eigenstates that are close to the Fermi level (FL).

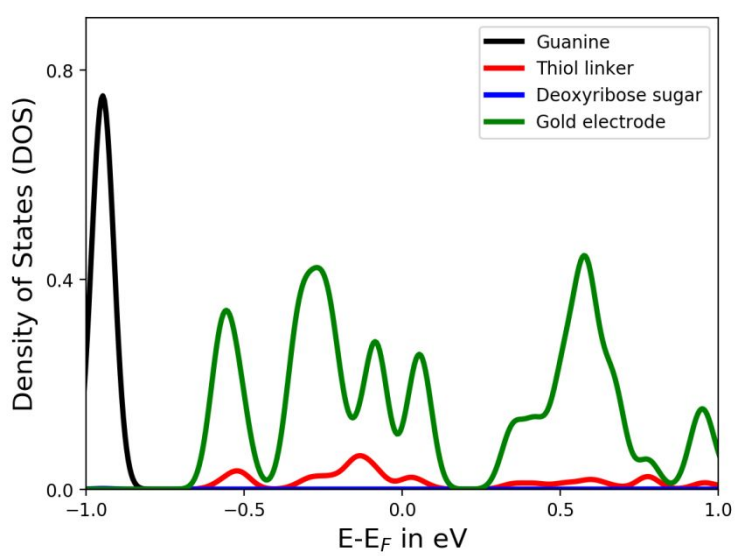

Figure S3: Orbital-resolved Density of States (DOS) for the 3' connection of the Guanine base with Gold electrode. Guanine base (black), Thiol linker (red), Deoxyribose sugar (blue) and Gold electrode (yellow) contributions to the eigenstates close to the FL has been shown.

In Fig. S3, we have resolved the Density of States (DOS) into contributions coming from Guanine base, Thiol linker, Deoxyribose sugar and Gold electrode parts of the system. It is evident from Fig. S3 that the HOMO and LUMO states of the system doesn't have any contribution from the Guanine base molecular orbitals. Those orbitals only have significant contribution to the eigenstates that lies ~1 eV below the FL, hence doesn't play any significant role in the electrode-base transfer. These findings are in perfect agreement with the conclusions already mentioned in the manuscript.

Section VII: Sample Input Files

sample_input_siesta: Sample input file for structural relaxation calculation, performed using SIESTA code

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%endblock Kgrid_Monkhorst_Pack


MeshCutoff         200 Ry

MaxSCFIterations     500
DM.MixingWeight      0.1
DM.NumberPulay       5
DM.Tolerance         1.d-4
```

sample_input_qe: Sample input file for obtaining Kohn-Sham wavefunction, performed using Quantum Espresso code.

```
&control
    calculation = 'scf',
    restart_mode='from_scratch',
    prefix='DNA',
    pseudo_dir = '../pp',
    outdir='./temp',
/
&system
       ibrav = 0,
         nat = 241,
        ntyp = 6,
     ecutwfc = 50,
 occupations = 'smearing',
    smearing = 'fd',
     degauss = 0.001,
   celldm(1) = 1.88972687777,
/
&electrons
    mixing_mode = 'plain'
```

```
    mixing_beta = 0.3
    electron_maxstep=300
    conv_thr =  1.0d-10
/
CELL_PARAMETERS (alat= 1.88972687777)
   21.435878560      -0.168228072      -0.146103223
   -0.168421603      21.433603860      -0.142969503
   -0.288469136      -0.283765035      42.381708137
ATOMIC_SPECIES
Au   82.94  Au_oncv.UPF
 S   16.94  S_oncv.UPF
 O    8.94  O_oncv.UPF
 C    6.94  C_oncv.UPF
 N    7.94  N_oncv.UPF
 H    1.94  H_oncv.UPF
ATOMIC_POSITIONS {crystal}
 C     0.488249033       0.435184149       0.293690254
 C     0.440415329       0.432178623       0.266224300
 C     0.472446461       0.426971429       0.234186491
 H     0.409570004       0.390672037       0.269806508
 H     0.409891359       0.473722892       0.266385118
 S     0.416309501       0.410375616       0.200865992
 H     0.506563530       0.388389788       0.234219852
 H     0.498679258       0.470474613       0.228418699
 H     0.523375120       0.398007778       0.289986663
 H     0.514352606       0.480738795       0.294034780
 H     0.480013577       0.578411940       0.412694262
 O     0.460916652       0.549988230       0.397294777
 C     0.478684351       0.487743974       0.403738729
 H     0.460828011       0.472079685       0.427015419
 H     0.530530264       0.482502732       0.403762394
 C     0.448768303       0.446551025       0.377902137
 H     0.470537115       0.399666092       0.377439332
 O     0.383740680       0.439836064       0.384189398
 C     0.347191629       0.465469235       0.359355160
 H     0.325866891       0.426520593       0.344800375
 N     0.295389457       0.498187666       0.372655661
 C     0.292697116       0.557704721       0.386139157
 H     0.335353579       0.586374404       0.389469025
 N     0.236411090       0.572644668       0.395382958
 C     0.199898784       0.520362602       0.388310120
 C     0.134116526       0.507165006       0.392840456
 O     0.091358171       0.539137610       0.402433098
 N     0.120674694       0.443008282       0.383646231
 H     0.074811141       0.431456232       0.386492599
 C     0.161306826       0.400707512       0.371235178
 N     0.138922942       0.341940067       0.363462685
 H     0.100534361       0.324633584       0.374143243
 H     0.172889253       0.311164124       0.358241728
 N     0.220352660       0.413986414       0.365694142
 C     0.236157055       0.473118969       0.374606893
 C     0.454347863       0.474385420       0.344515521
 H     0.494628835       0.507916477       0.343064861
 C     0.391746029       0.507136945       0.340518016
 H     0.395506890       0.554001595       0.351840358
 H     0.377172907       0.511888644       0.315516252
 O     0.461223850       0.423177626       0.323507920
 Au   -0.000353071      -0.000654450      -0.000584959
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Au	0.100367787	0.000494109	0.051222765
Au	0.000673933	0.100262997	0.051191415
Au	0.001606484	0.001443455	0.103892612
Au	0.101991974	0.101820741	0.104674113
Au	0.102437751	0.002896349	0.156075130
Au	0.002905808	0.102244478	0.155986850
Au	-0.000837808	0.199216162	-0.000188976
Au	0.099636544	0.299335614	0.000466483
Au	0.100709843	0.200160869	0.051490967
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Au	0.002121868	0.201413882	0.104668492
Au	0.102144421	0.301092377	0.105019609
Au	0.103106707	0.202357319	0.156653477
Au	0.003110245	0.302483952	0.156438982
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Au	0.101530497	0.501600393	0.105371756
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Au	0.001664744	0.601914797	0.104798913
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Au	0.102800199	0.603295831	0.156716085
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Au	-0.000233684	0.797910543	-0.000458090
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Au	0.100592883	0.799397347	0.051286344
Au	0.000488997	0.899943308	0.050752836
Au	0.001677513	0.801359156	0.104314009
Au	0.101728597	0.901480065	0.104371468
Au	0.102779642	0.803018013	0.156281662
Au	0.002778653	0.903071144	0.155787547
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Au	0.299539989	0.099534977	0.000545704
Au	0.300227125	0.000472075	0.051933105
Au	0.200307100	0.100615772	0.051558386
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Au	0.302826844	0.002967539	0.156419045
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Au	0.302909147	0.302625851	0.106407100
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Au	0.202688623	0.302053922	0.157142405
Au	0.200002323	0.398537287	0.000578467
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Au	0.300938446	0.403360919	0.158597004
Au	0.202410146	0.504065649	0.156977780
Au	0.199745473	0.597298949	0.000318251
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Au	0.300777479	0.599098725	0.052398662
Au	0.200083774	0.699547123	0.051468028
Au	0.201545655	0.601685949	0.105008721
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Au	0.202655941	0.702876269	0.156784320
Au	0.199260461	0.798126353	-0.000275761
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Au	0.299840130	0.799614399	0.051810345
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Au	0.498282250	0.098893256	0.000545440
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Au	0.501802606	0.101381805	0.105417455
Au	0.503597808	0.002606633	0.156727625
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Au	0.507024647	0.402892852	0.157773871
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Au	0.501952246	0.701435301	0.104940748
Au	0.504333451	0.603803997	0.157045734
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Au	0.701660020	0.101487984	0.104658108
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Au	0.603659661	0.102759826	0.156659183
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Au	0.599870474	0.500285535	0.051778609
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Au	0.698379646	0.898604866	-0.000451539
Au	0.699957831	0.799460756	0.051268895
Au	0.600252330	0.899802755	0.051527726
Au	0.602118834	0.800904496	0.104836829
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Au	0.798235604	-0.000872723	-0.000515167
Au	0.898820235	0.099317891	-0.000467169
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Au	0.802332038	0.001068661	0.103823484
Au	0.901950052	0.101528233	0.104097328
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 Au    0.802852028       0.503120937       0.156520959
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 Au    0.902763744       0.603291561       0.156383896
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 Au    0.901840693       0.901518787       0.103766872
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K_POINTS {automatic}
1 1 1 0 0 0
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References

1. Bag, S., et al., *Dramatic changes in DNA conductance with stretching: structural polymorphism at a critical extension.* Nanoscale, 2016. **8**(35): p. 16044-16052.
2. Livshits, G.I., et al., *Long-range charge transport in single G-quadruplex DNA molecules.* Nature nanotechnology, 2014. **9**(12): p. 1040.