Supporting Information

Prospects of Graphene-hBN Heterostructure Nanogap for DNA Sequencing

Vivekanand Shukla,[a] Naresh K. Jena, [a,*] Anton Grigoriev, [a] Rajeev Ahuja [a,b*]

[a]Condensed Matter Theory, Materials Theory Division, Department of Physics and Astronomy, Uppsala University, Box 516, SE-751 20, Uppsala, Sweden
[b]Applied Materials Physics, Department of Materials and Engineering, Royal Institute of Technology (KTH), SE-100 44, Stockholm, Sweden
*Corresponding author email: NKJ(Naresh.Jena@physics.uu.se; jenanaresh@gmail.com);
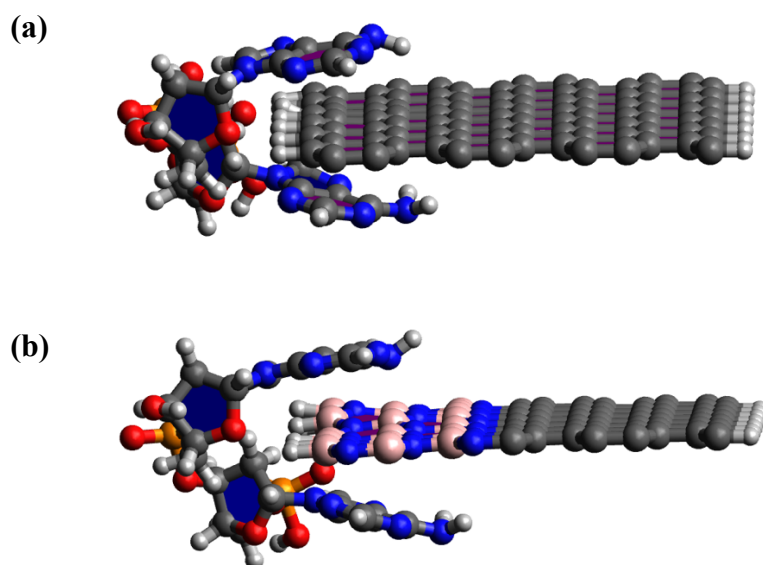RA(Rajeev.Ahuja@physics.uu.se)

(a)

(b)

Figure S1: Optimized structures displaying the interaction of poly-adenine (two-mer) with graphene (a) and graphene-hBN heterostructure (b) edges. In a nanogap consisting of these electrodes (graphene vs graphene-hBN heterostructure) the strength of interaction of incoming DNA with the electrodes determines the speed of DNA sequencing. Our calculations reveal that pristine graphene edge is more reactive towards the base compared to a graphene-hBN heterostructure edge.

Effect of Rotation of Nucleobases on Transmission

We have considered the rotations of all four nucleobases around x-axis in the yz plane with an interval of 60^0. The corresponding transmission functions are presented in figure S2. The relative energy of these rotated configurations with respect to the original (zero degree) orientation is also reported in Table S1. It is noted that the zero-degree orientation is the ground state configuration whereas all other rotated geometries have energies higher than the former. Further, comparing these results against the case of pristine graphene edges (Ref. 29 in the manuscript), we find lesser variation in the transmission functions. Moreover, for a given nucleobase the largest deviation in the transmission functions corresponds to the orientation which have the highest energy (120^0) and hence least probable.

Table S1: Relative energies of the rotated configurations of nucleobases in the nanogap

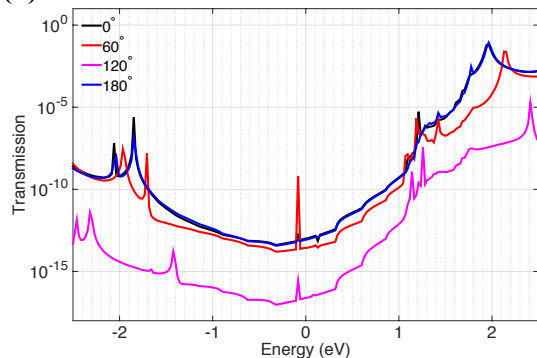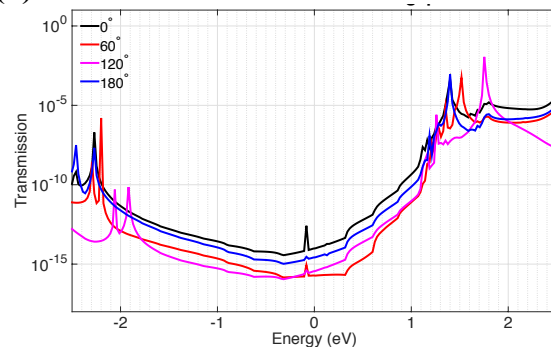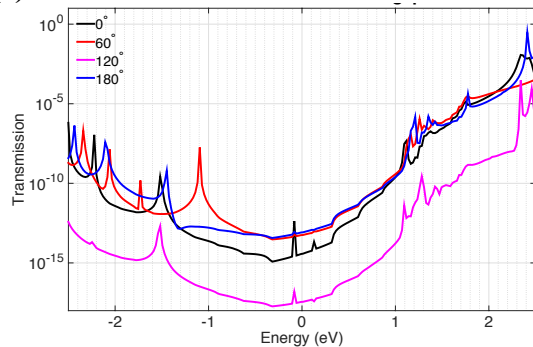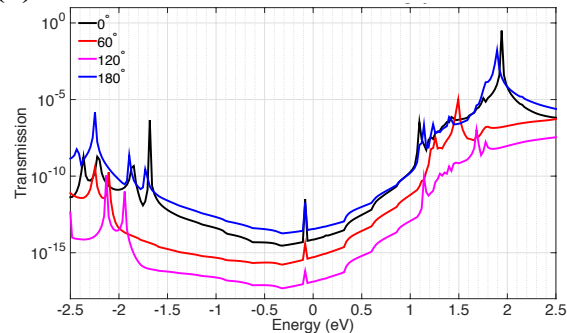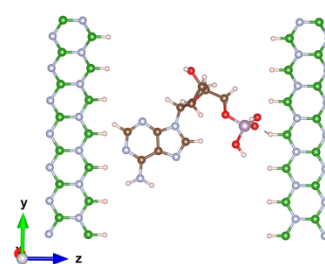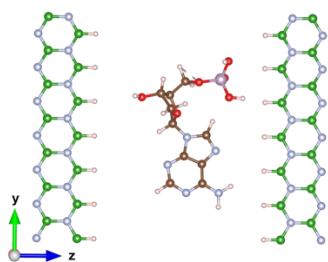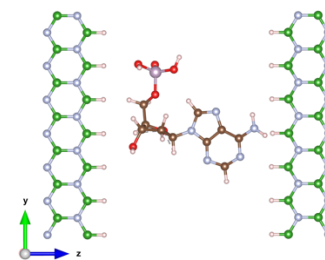| Rotation (Deg.)	dAMP ($\triangle$eV)	dTMP ($\triangle$eV)	dGMP ($\triangle$eV)	dCMP ($\triangle$eV)
0^0	0	0	0	0
60^0	0.41	0.38	0.43	0.02
120^0	0.42	0.74	0.41	0.23
180^0	0.31	0.31	0.27	0.23

(a) dAMP

(b) dTMP

(c) dGMP

(d) dCMP

(e)
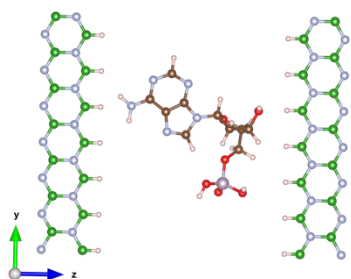
(f)

(g)

(h)

Figure S2: Zero-bias transmission functions of the nucleobases ((a) dAMP, (b) dTMP, (c) dGMP, (d) dCMP) considering in plane (yz) rotation around x-axis with respect to their original positions. The representative orientations of one nucleobase (dAMP) corresponding to rotations of 0^0, 60^0, 120^0, 180^0 have been illustrated in panels (e)-(h) respectively.

Effect of Nanogap Width and Lateral Translation of Nucleobases on Transmission

We have considered the effect of variation of width of nanogap from our original value of 12.6 Å to 14.7 Å as discussed in Ref. 29 (*Nano Letters* **2011,** *11* (5), 1941-1945) in our manuscript. Two representative nucleobases one from purine (dGMP) and other from pyrimidine (dCMP) class, have been considered. Further, in the wider gap of 14.7 Å, we have also laterally displaced the nucleobase to left (-0.5 Å) and right (+0.5 Å) from their mean positions (0.0 Å) and investigated the zero-bias transmission functions. All these results have been summarized figure S3. With variation of the width of nanogap, the intensities of the transmission functions are diminished whereas the key features of the curve remain almost similar, in agreement with the results reported in Ref. 29 for pristine graphene electrodes. Furthermore, with lateral displacements of bases, the qualitative features of the transmission functions also remain largely unchanged.
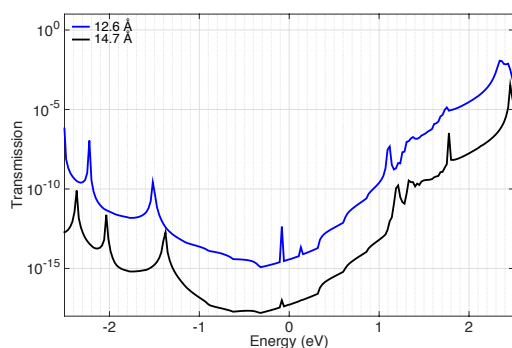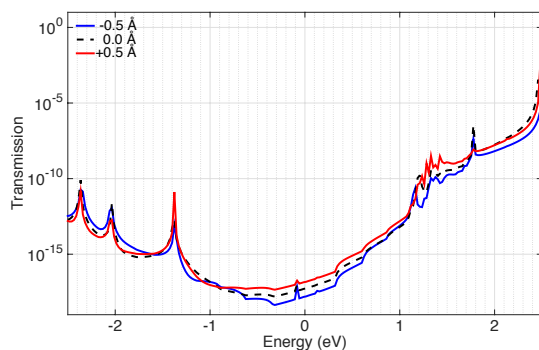
(a) dGMP　　　　　　　　　　　　　**(b) dCMP**
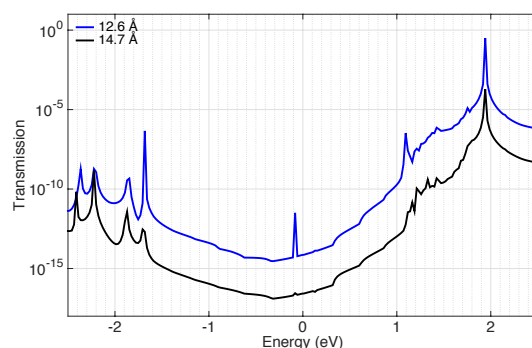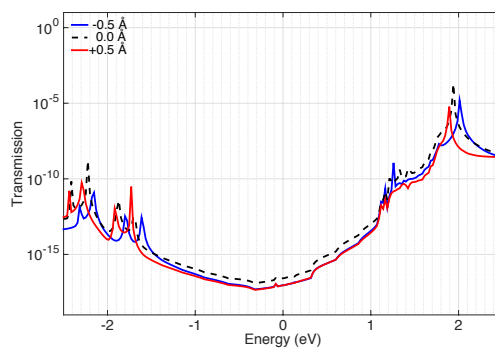

(c) dGMP　　　　　　　　　　　　　**(d) dCMP**

Figure S3: Zero-bias transmission functions of the nucleobases with respect to width variation of nanogap from 12.6 Å to 14.7 Å ((a) dGMP, (b) dCMP) and lateral displacements of the bases ((c) dGMP, (d) dCMP) in the wider nanogap (14.7 Å).