Supporting Information

# Conductance and Tunnelling Current Characteristics for Individual Identification of Synthetic Nucleic Acids with Graphene Device

Rameshwar L. Kumawat*[1,2] and Biswarup Pathak*[1]

[1]Department of Chemistry, Indian Institute of Technology (IIT) Indore, Indore, Madhya Pradesh, 453552, India
[2]Center for Computational Molecular Science and Technology, School of Chemistry and Biochemistry, and School of Computational Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332-0400, USA

*E-mail: rameshwarlal1122@gmail.com; biswarup@iiti.ac.in
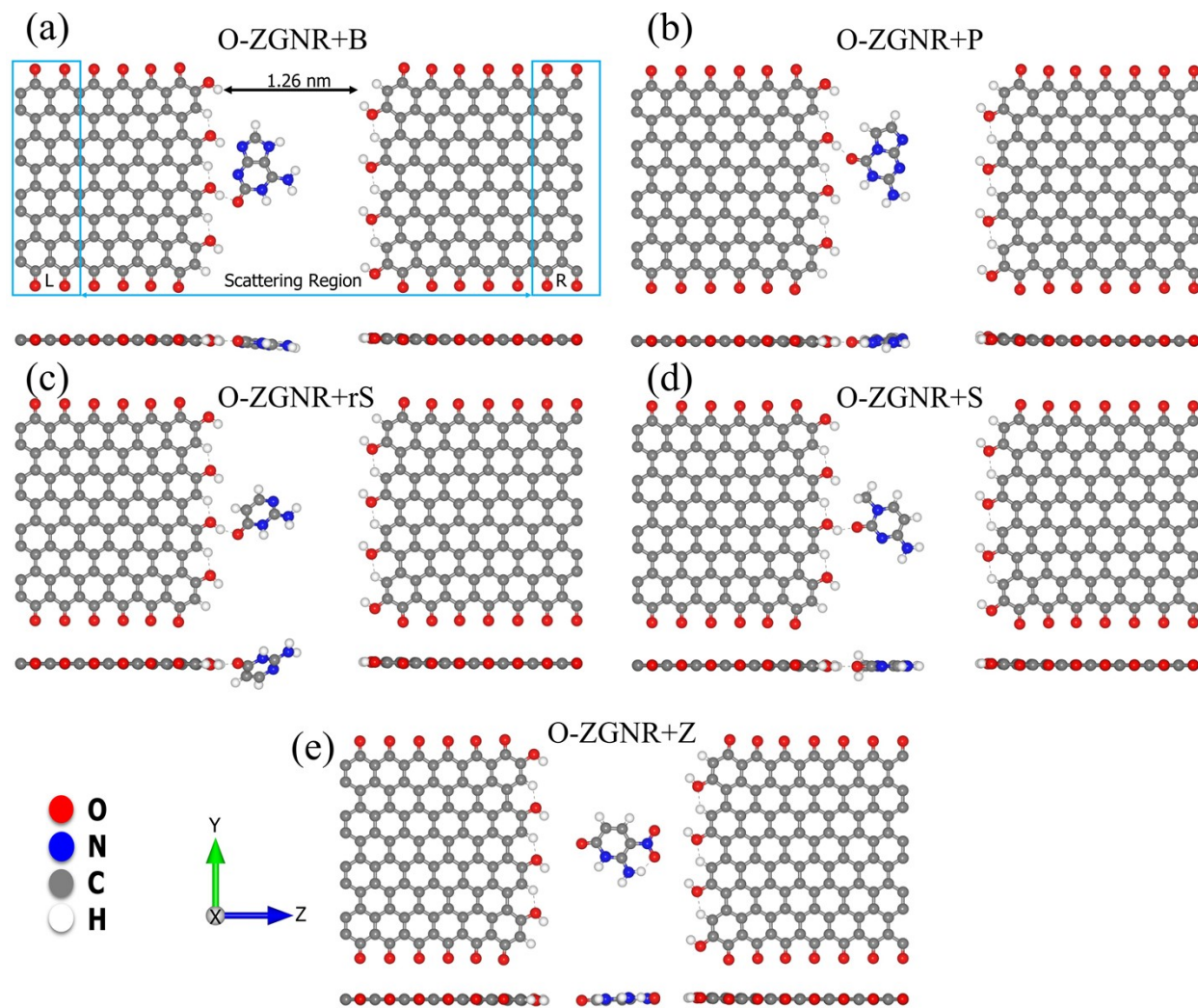
Figure S1. (a-e) Fully optimized atomic structures of O-ZGNR+Hachimoji nucleobases (B, P, rS, S, and Z) showing both nanoelectrodes (L and R) and a scattering (device) region. Here, Z-axis refers the transport direction.
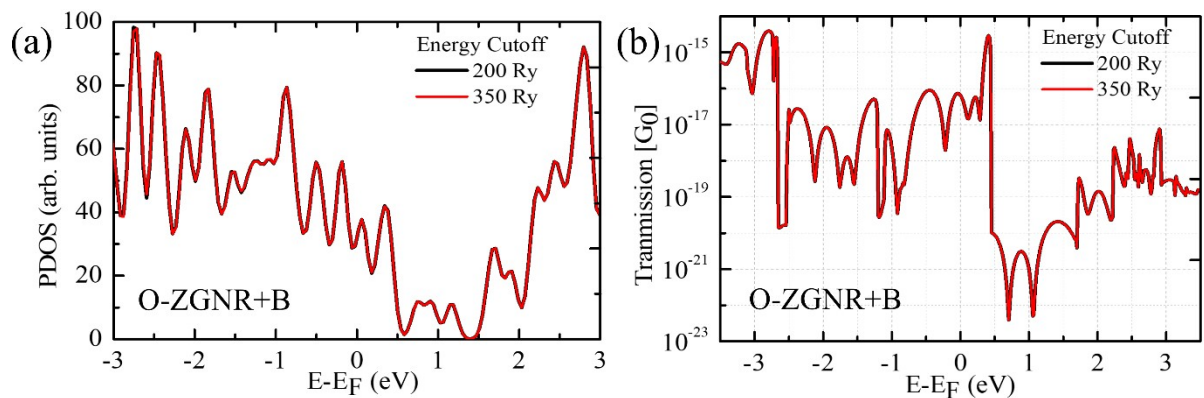
Figure S2. The density of States and Transmission function are computed at different energy cutoffs for the O-ZGNR+B system.
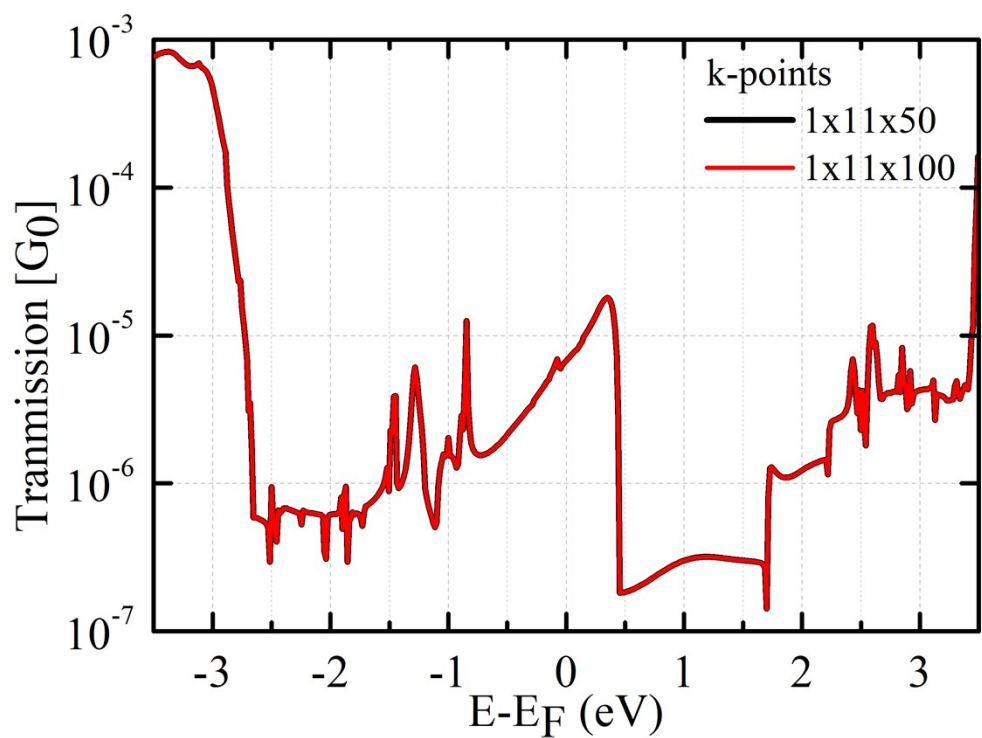

Figure S3. The transmission function for the O-ZGNR device calculated at different k-points.

Scheme 1. Rotation of DNA Nuclobases inside the Nanogap:

We have considered the rotations of all the five DNA nucleobases around x-axis in the yz-plane from 0° to 180° in the steps of 30° as shown in **Figure S4-S8**. The relative energy values are tabulated in **Table S1**.

Table S1. Relative energies (in eV) of the O-ZGNR+nucleobase (nucleobase = B, P, rS, S, Z) system when nucleobases are rotated inside the nanogap at different angles from 0° to 180° in steps of 30˚.

| Nucleobases	0°	30°	60°	90°	120°	150°	180°
B	0.0	5.39	3.41	6.31	2.19	2.42	2.39
P	0.0	0.21	1.02	1.59	3.55	1.91	0.15
rS	0.0	2.26	0.39	0.54	0.89	1.01	1.10
S	0.0	0.13	0.16	1.98	4.61	1.22	1.08
Z	0.0	0.20	0.44	0.54	0.46	0.08	0.07
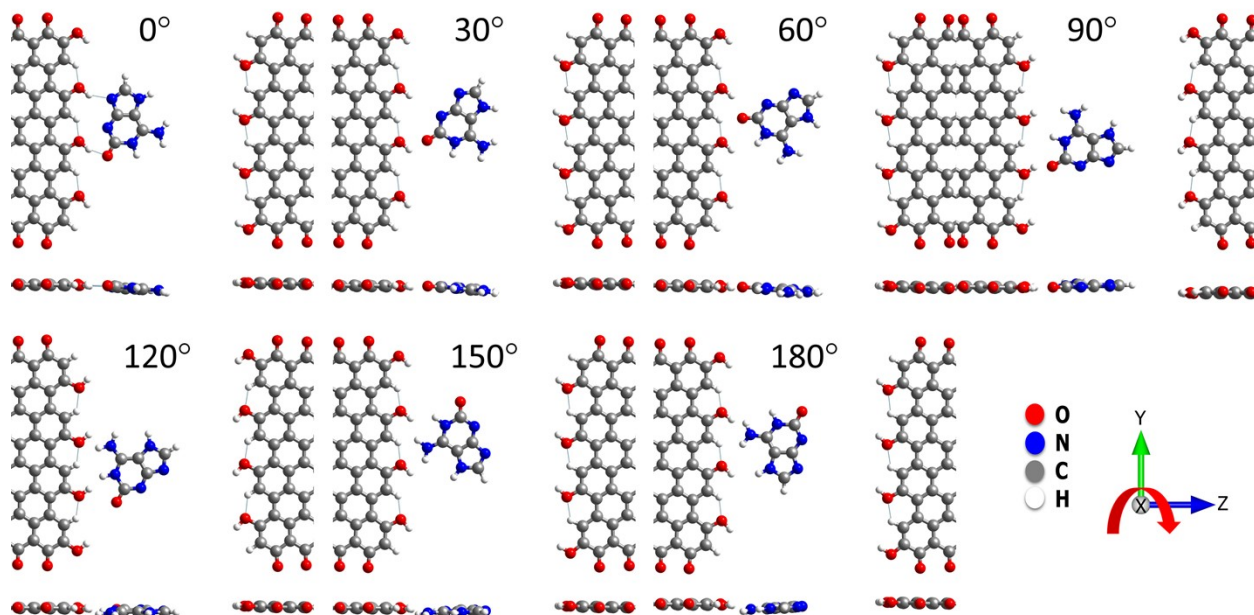
Figure S4. The representative orientations of fully optimized B nucleobase corresponding to rotations (from 0° to 180° in the steps of 30°) are illustrated.
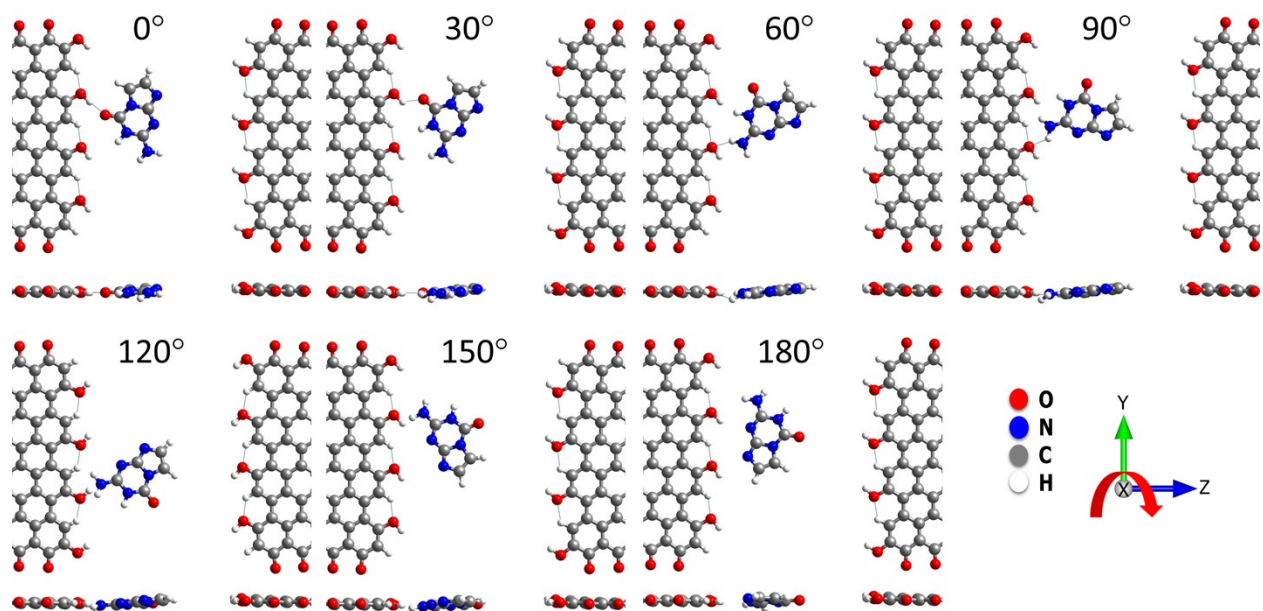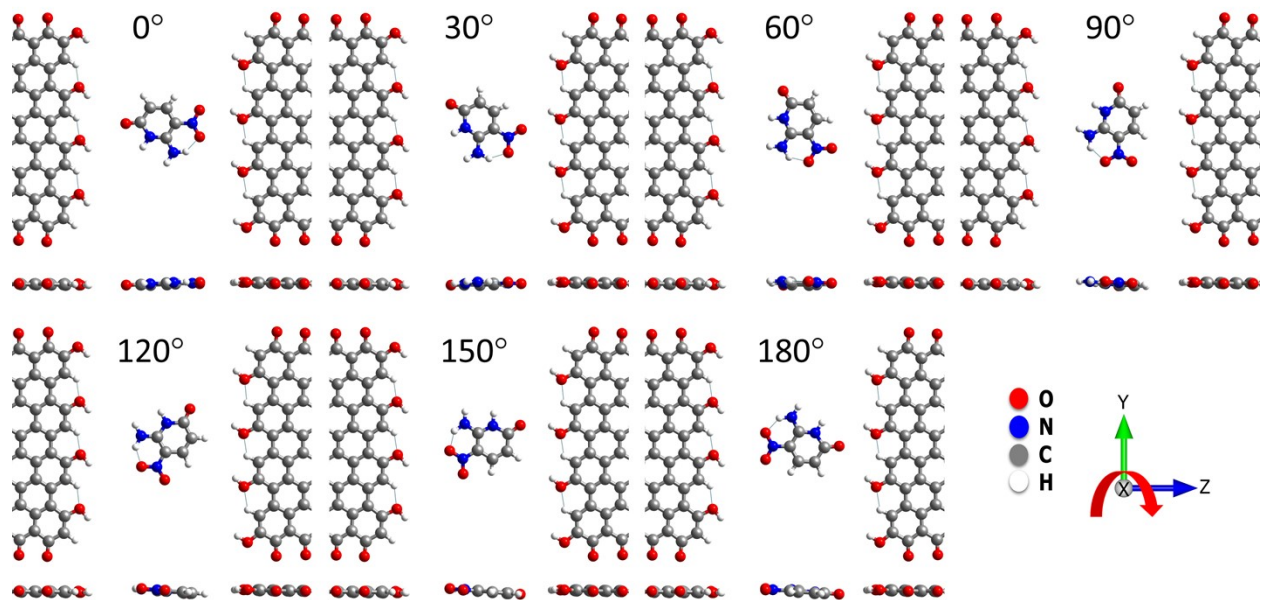
Figure S5. The representative orientations of fully optimized P nucleobase corresponding to rotations (from 0° to 180° in the steps of 30°) are illustrated.
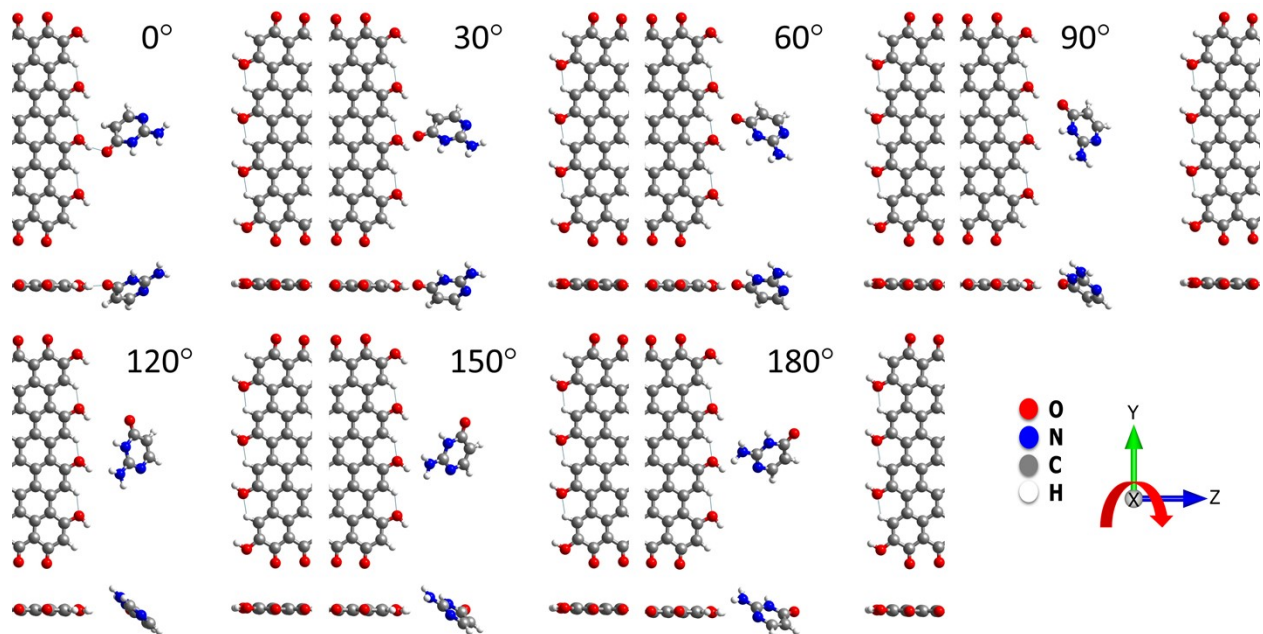
Figure S6. The representative orientations of fully optimized rS nucleobase corresponding to rotations (from 0° to 180° in the steps of 30°) are illustrated.
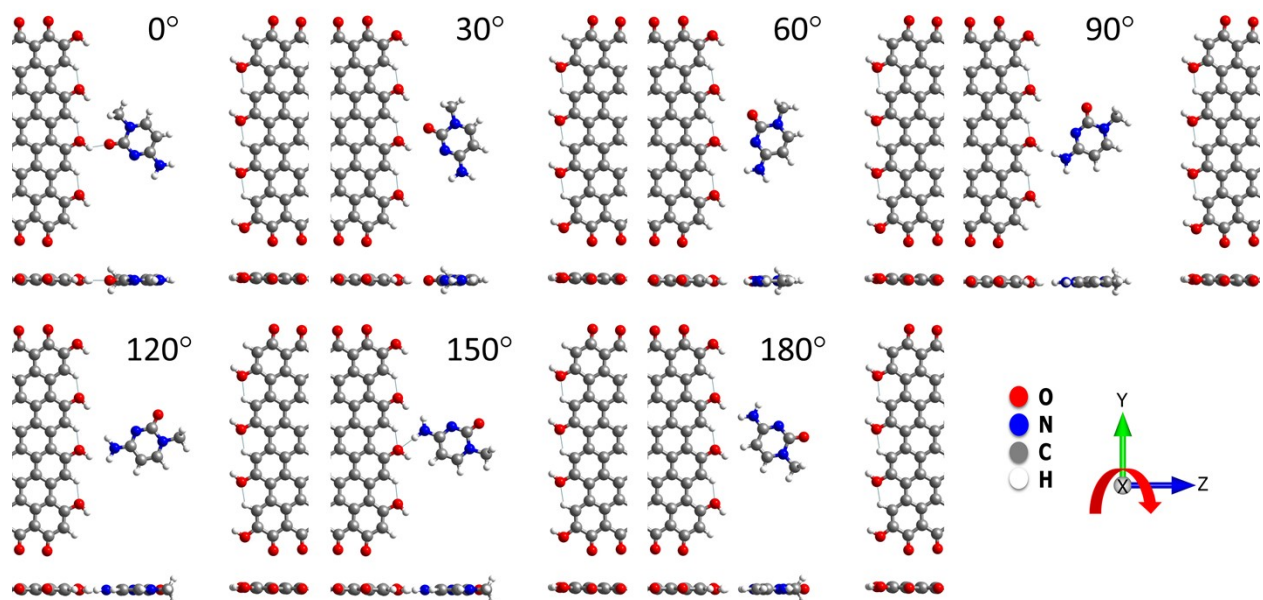
Figure S7. The representative orientations of fully optimized S nucleobase corresponding to rotations (from 0° to 180° in the steps of 30°) are illustrated.
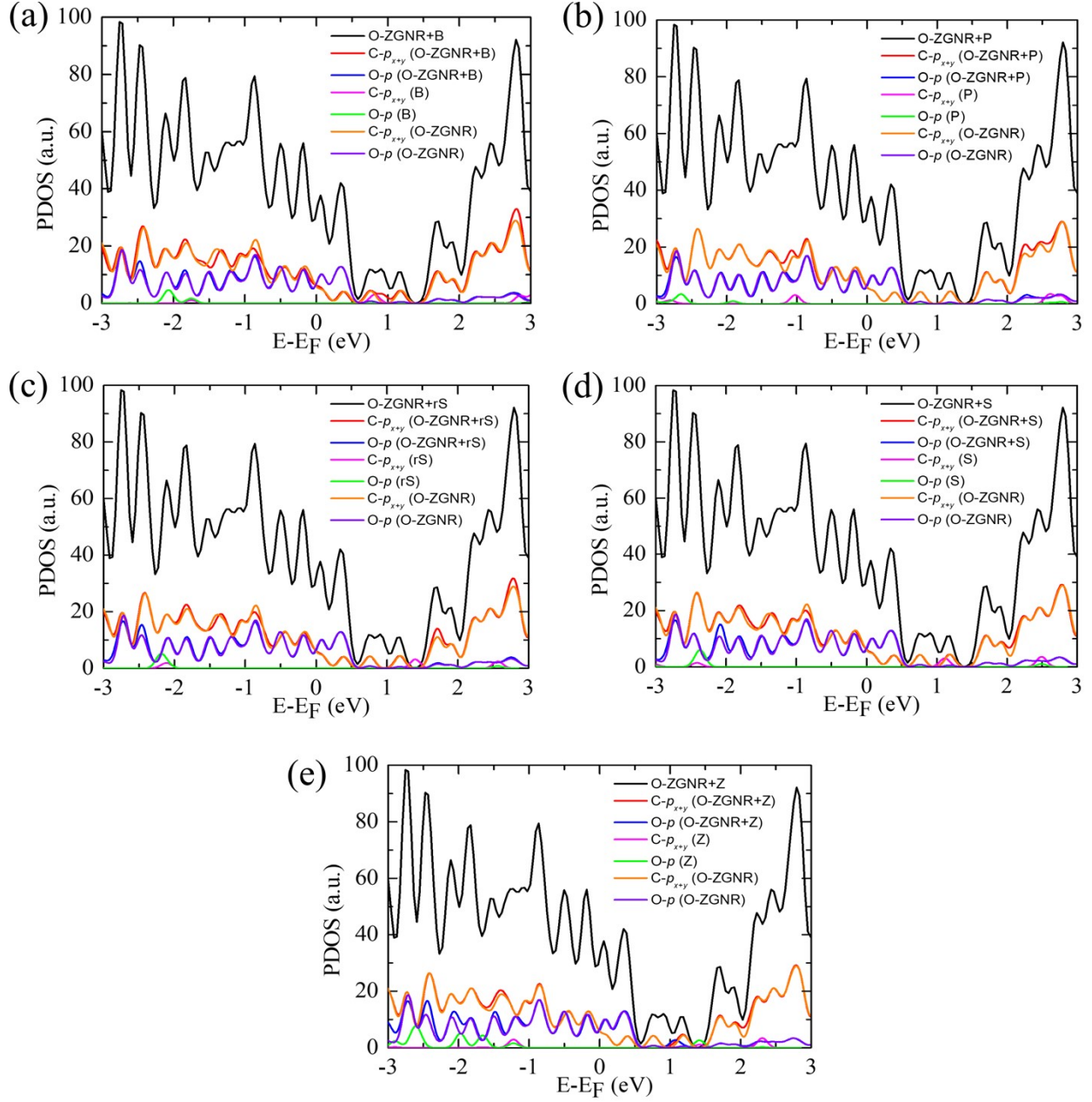

Figure S8. The representative orientations of fully optimized Z nucleobase corresponding to rotations (from 0° to 180° in the steps of 30°) are illustrated.

Figure S9. (**a-e**) Electronic DOS of the O-ZGNR+nucleobase (nucleobase: B, P, rS, S, and Z) and the PDOS of C-p_{x+y} and O-p of O-ZGNR, O-ZGNR+nucleobase and nucleobases. The Fermi level (E-E_F) is set to zero.