Supporting Information

Identification of DNA Nucleotides by Conductance and Tunnelling Current Variation through Borophene Nanogap

Milan Kumar Jena, Biswarup Pathak*

Department of Chemistry, Indian Institute of Technology Indore, Indore, Madhya Pradesh, 453552, India

*E-mail: biswarup@iiti.ac.in

Contents:

1. **Schematic representation of fully optimized structures of all the four nucleotides (dAMP, dTMP, dGMP, and dCMP) at different orientations (0º to 180º in the step of 30º) in yz plane along the x-axis.**

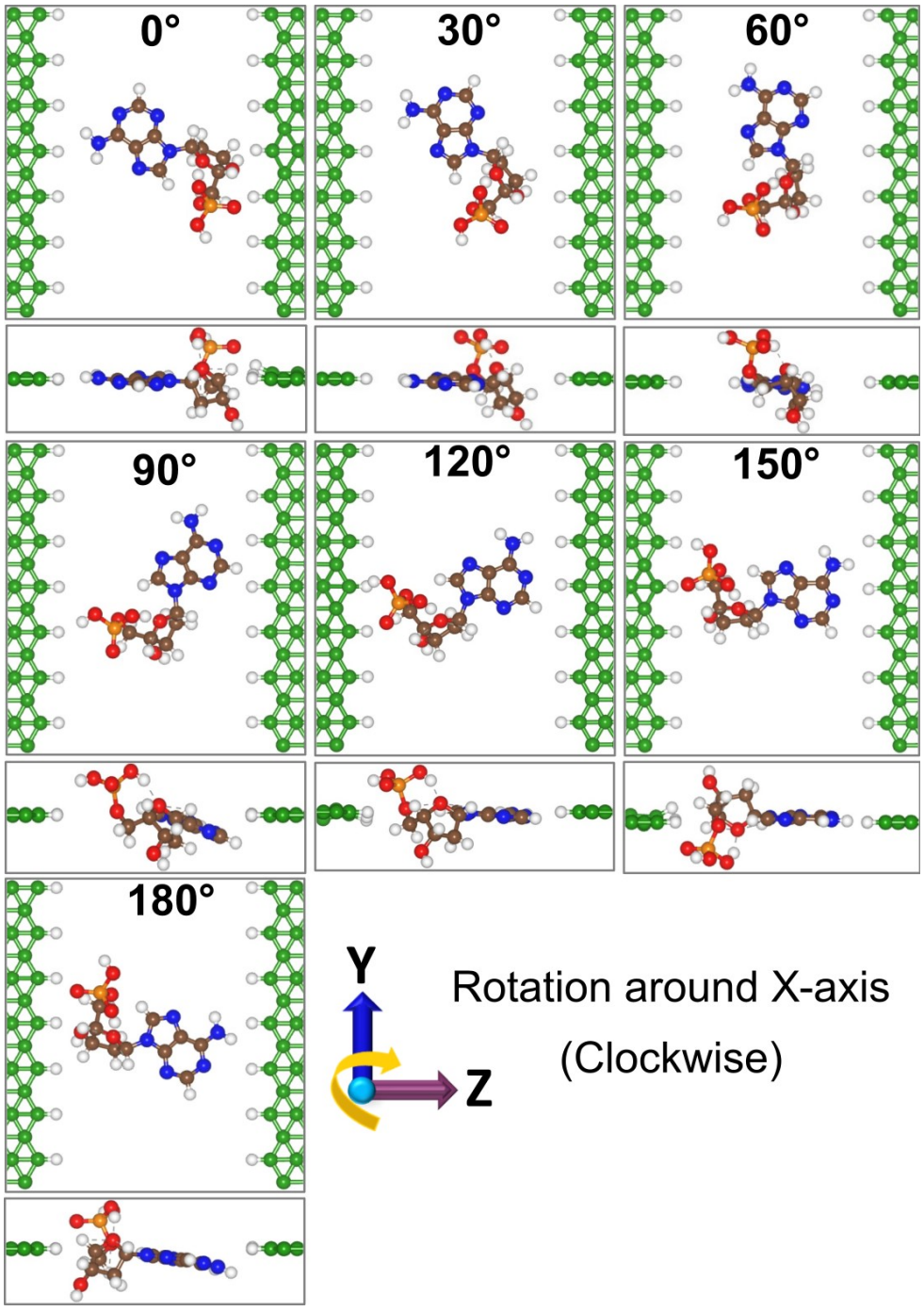

Figure S1. The schematic representations (top and side views) of fully relaxed structures of dAMP at 0°, 30°, 60°, 90°, 120°, 150°, and 180°.

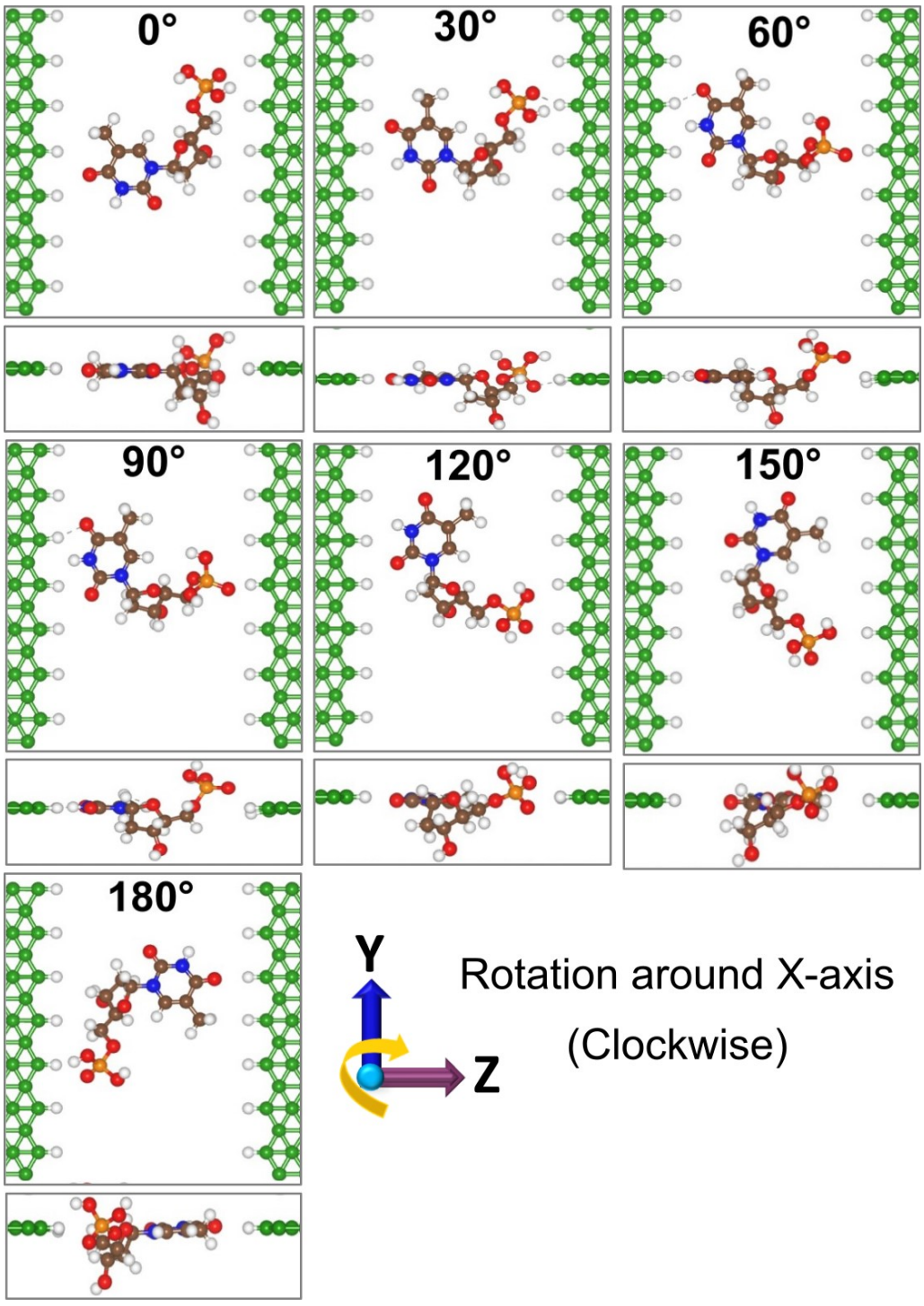

Figure S2. The schematic representations (top and side views) of fully relaxed structures of dTMP at 0°, 30°, 60°, 90°, 120°, 150°, and 180°.

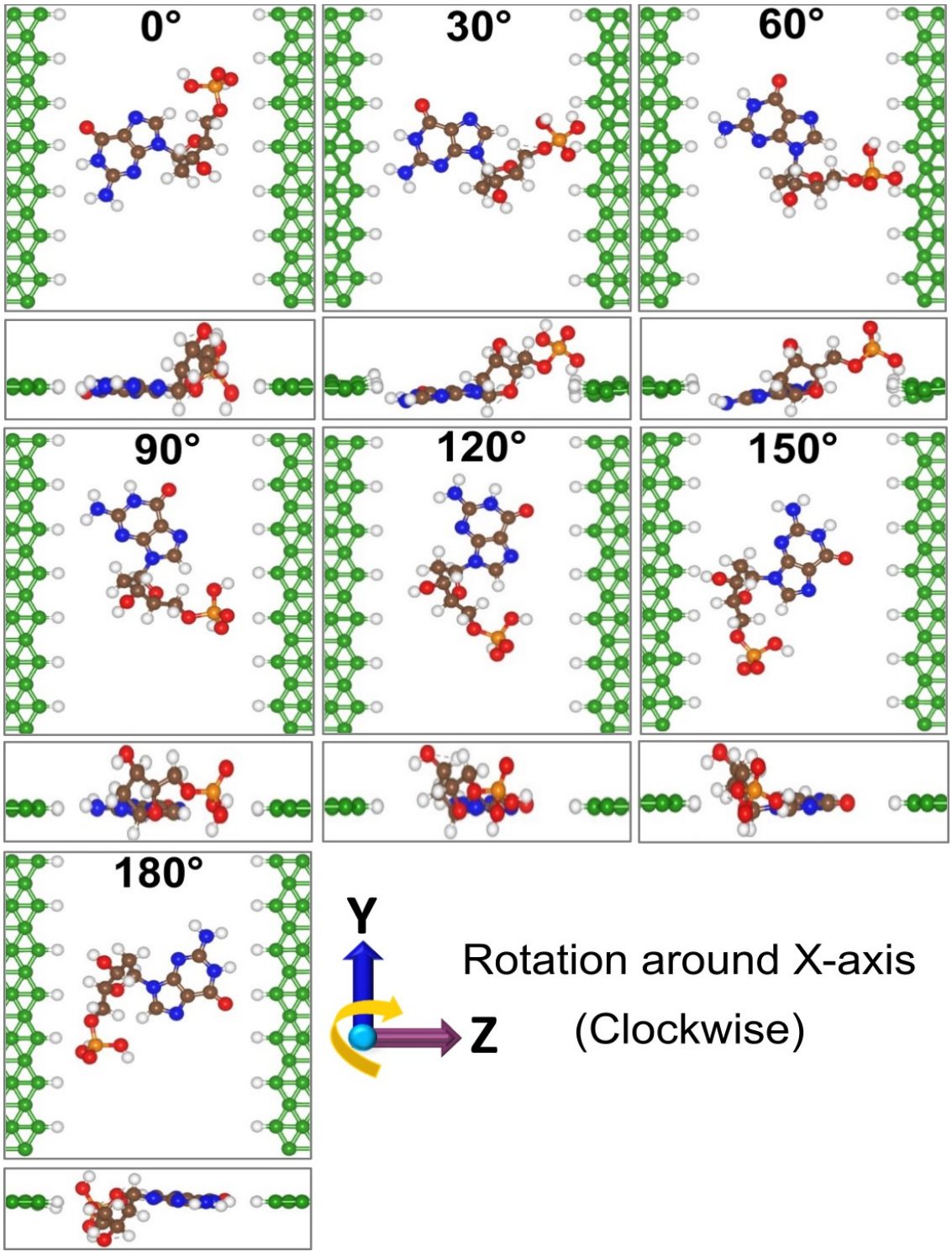

Figure S3. The schematic representations (top and side views) of fully relaxed structures of dGMP at 0°, 30°, 60°, 90°, 120°, 150°, and 180°.

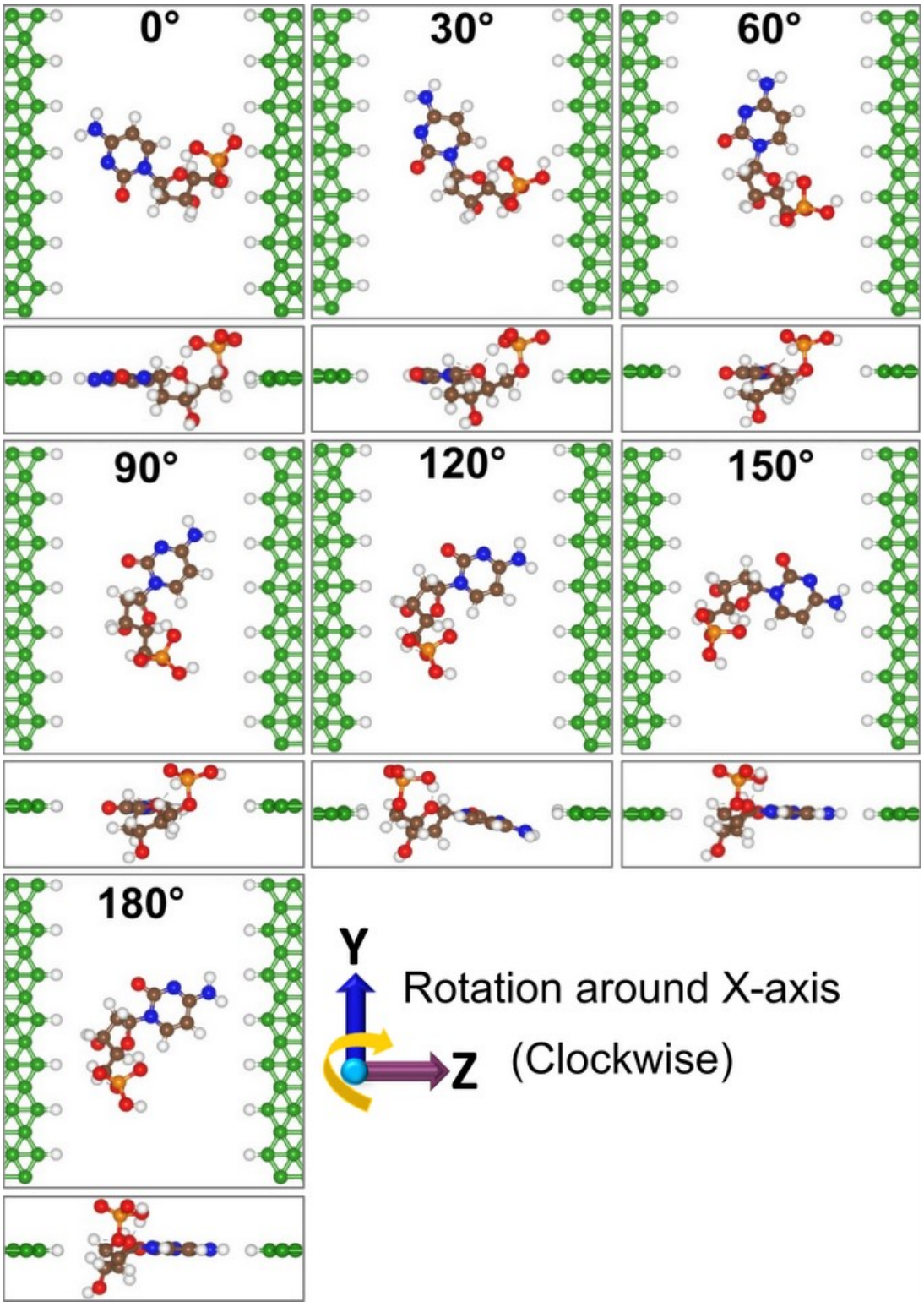

Figure S4. The schematic representations (top and side views) of fully relaxed structures of dCMP at 0°, 30°, 60°, 90°, 120°, 150°, and 180°.

2. **Relative energy (in eV) table of the rotated configurations of all the four nucleotides in the borophene nanogap around x-axis in yz-plane in the steps of 30º.**

Systems/ Rotations (°)	0°	30°	60°	90°	120°	150°	180°
dAMP	0.20	0.08	0.16	0.56	**0**	0.02	0.40
dTMP	**0**	0.14	0.13	0.13	0.56	0.18	0.13
dGMP	0.14	**0**	0.23	0.47	0.65	0.51	0.09
dCMP	**0**	0.02	0.32	0.36	0.17	0.14	0.15

Table S1. The calculated relative energy (in eV) of all the four nucleotides with respect to the in-plane rotated configuration.

3. **To check the nanogap width effect on the transmission function, the gap size from increased 12.6 Å to 14.7 Å (H to H distance) for all the four DNA nucleotides.**

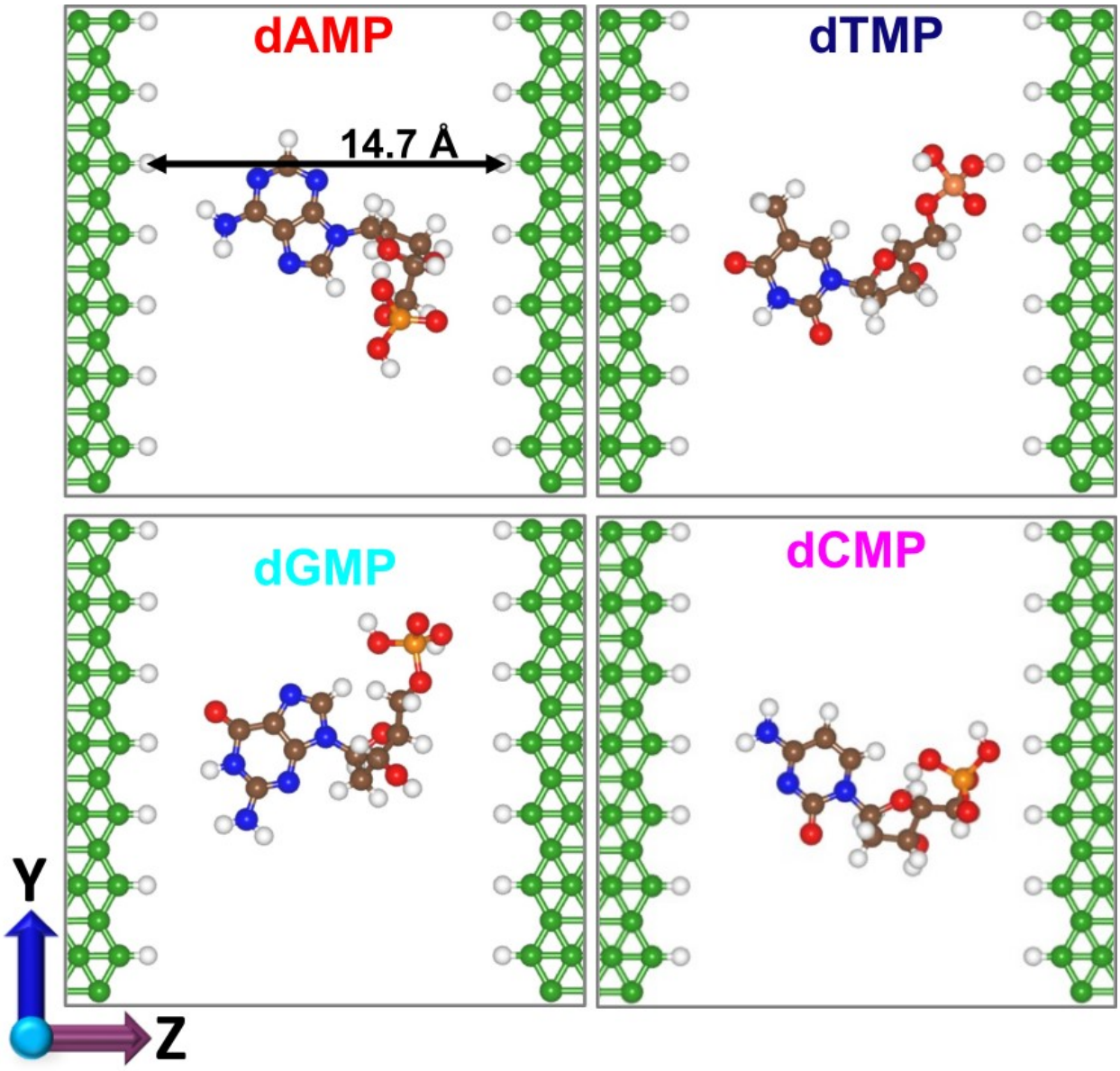

Figure S5. The schematic representations of the fully relaxed structure of all the four nucleotides when the nanogap width increased from 12.6 Å to 14.6 Å.

4. **Scheme of dAMP nucleotide translated in-plane along the z-axis in positive and negative directions by ± 0.5 Å both inside the borophene nanogap.**

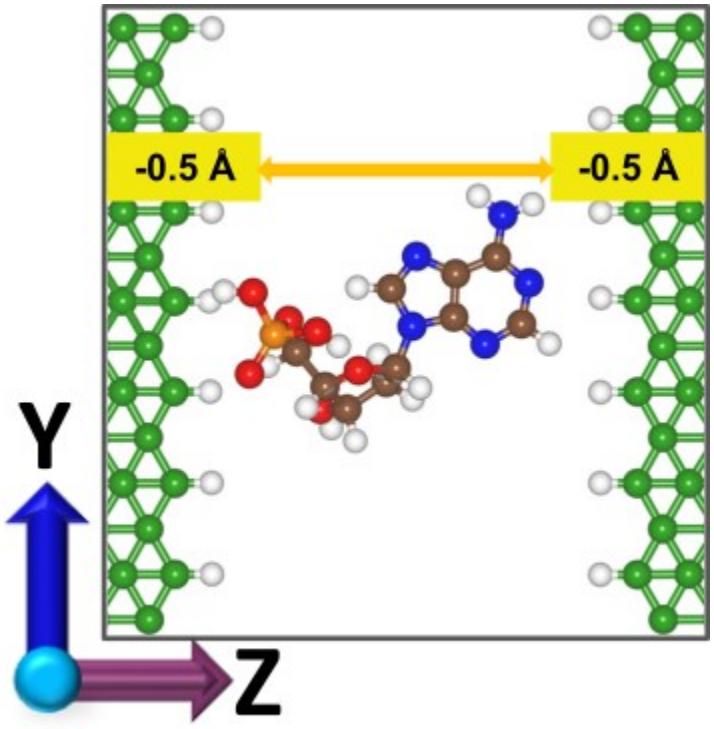

Figure S6. The schematic representations of dAMP nucleotide translated in-plane along the z-axis in positive and negative directions by ± 0.5 Å.

5. Scheme of dAMP nucleotide translated out-of-plane along the x-axis in positive and negative directions by ± 1.0 Å for borophene nanogap.

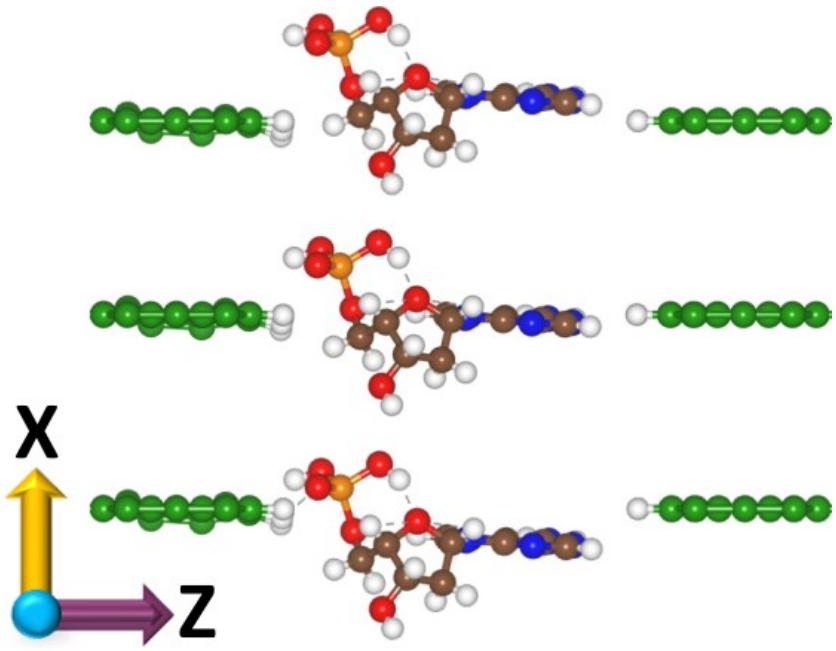

Figure S7. The schematic representations of dAMP nucleotide translated out-of-plane along the x-axis in positive and negative directions by ± 1.0 Å.

6. Zero-bias transmission function for all four nucleotides (dAMP, dTMP, dGMP, and dCMP) inside the borophene nanogap.

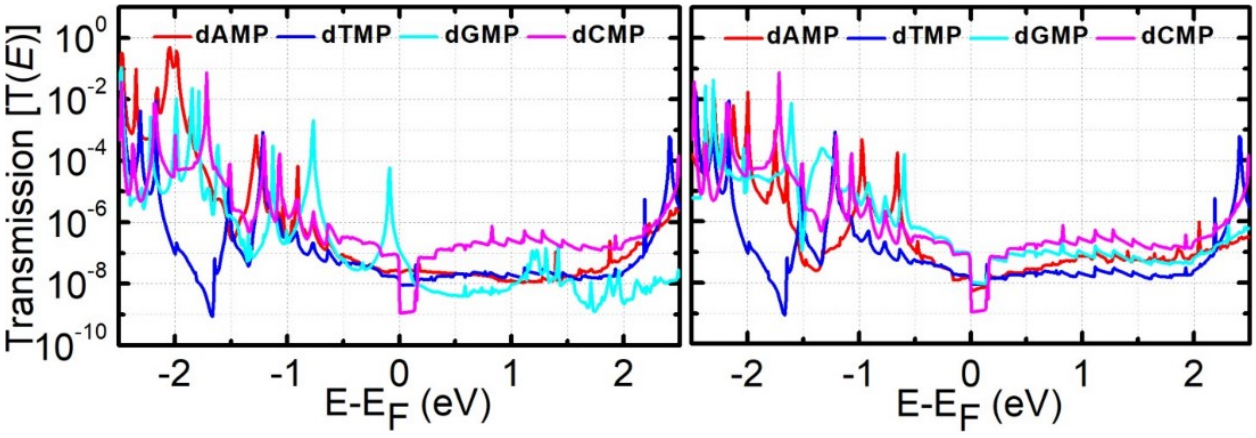

Figure S8. Zero-bias transmission function for all four nucleotides (dAMP, dTMP, dGMP, and dCMP) inside the borophene nanogap at their most stable and 0° orientation.

7. **Eigenchannel wavefunctions for all the four borophene nanogap+nucleotides at a specific energy value of -1.750 eV.**

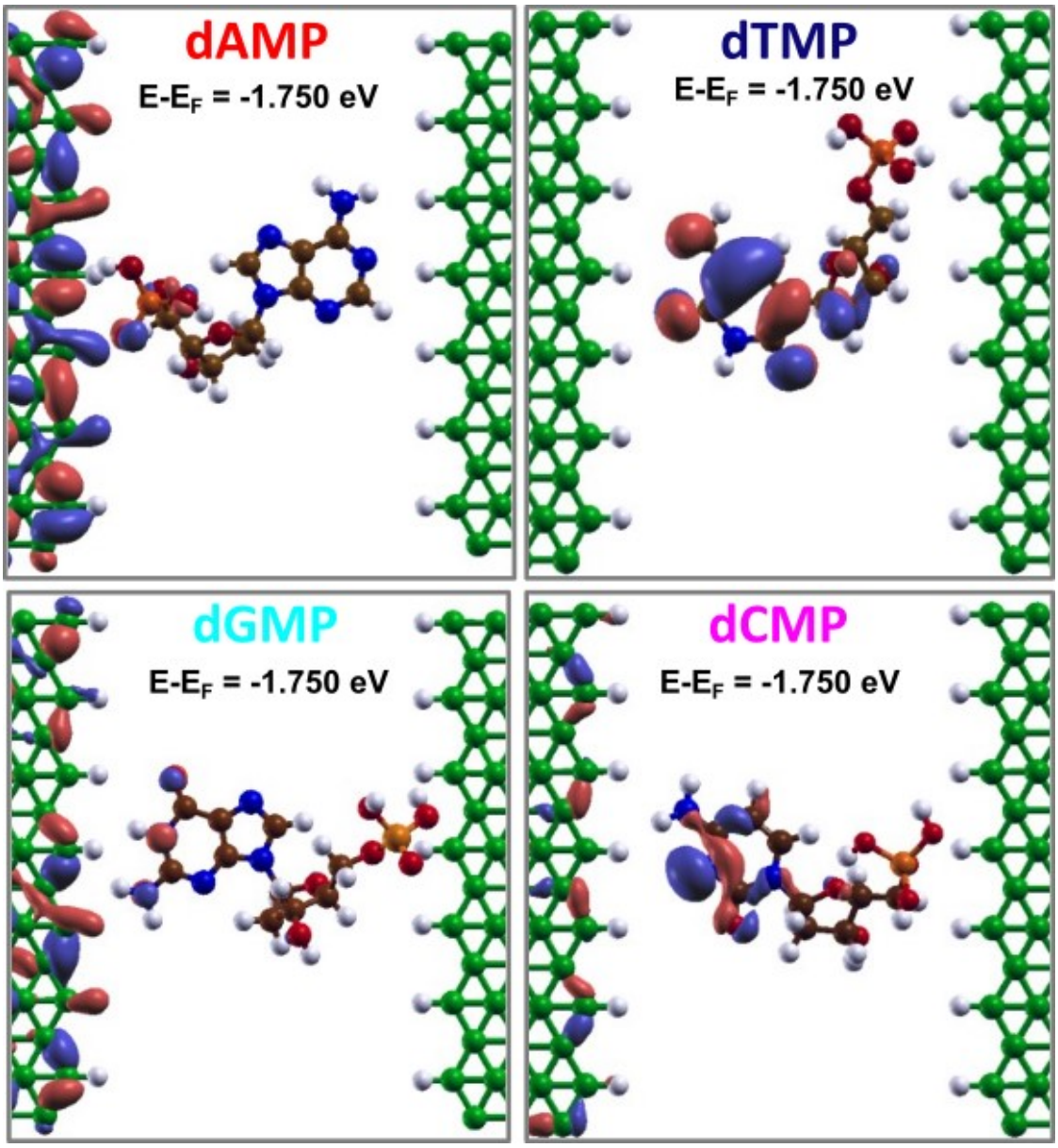

Figure S9. Eigenchannel wavefunctions for all the four borophene nanogap+nucleotides at a specific energy value of -1.750 eV below the Fermi level (isosurface value is 0.09 e/Å^3). The negative lobes are in blue and the positive in red colors, respectively.