Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary material

The influence of the nucleotide on the transmission spectrum of various nanopores is plotted in Fig. S1, and the sensitivities are calculated based on the relative changes in the transmission probability at -0.5 eV.

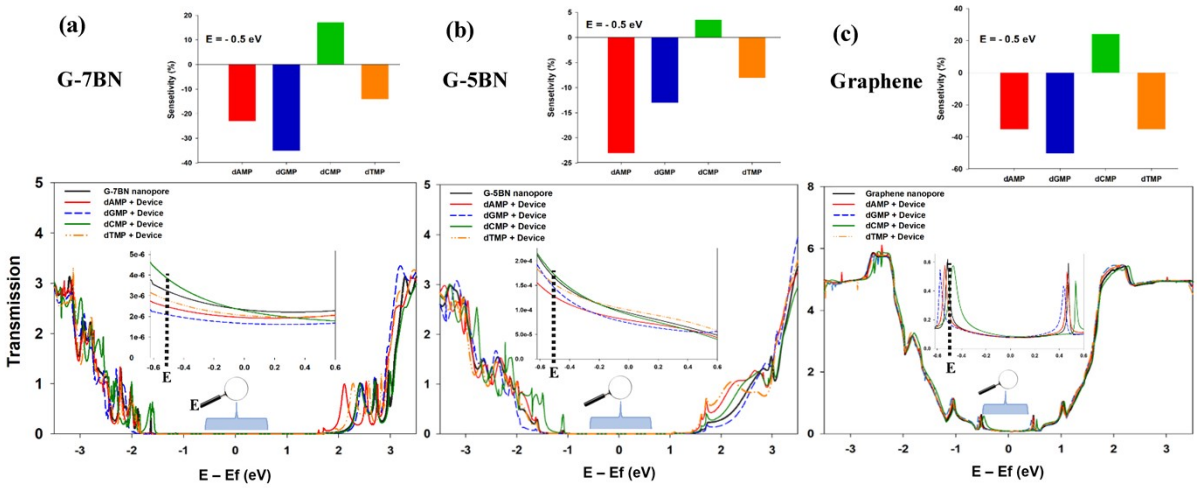

Figure S1: Transmission spectrum and sensitivity at $E = -0.5\ eV$. (a) G-7BN, (b) G-5BN and (c) Graphene nanopores.

The current in nanopores on the opposite voltage polarity, in which the nucleotide's backbone is adjacent to the negative pole, is illustrated in table SI. Also, the corresponding sensitivity is shown in Fig. S2.

Table SI: Electronic current for opposite polarity at V_{ds} = - 0.5V

Nucleotide	Empty	dAMP	dGMP	dCMP	dTMP
Graphene (µA)	1.40	1.55	1.59	1.62	1.53
G-5BN (nA)	1.86	1.60	1.52	1.84	1.79
G-7BN (pA)	45.56	37.69	33.37	44.1	41.6

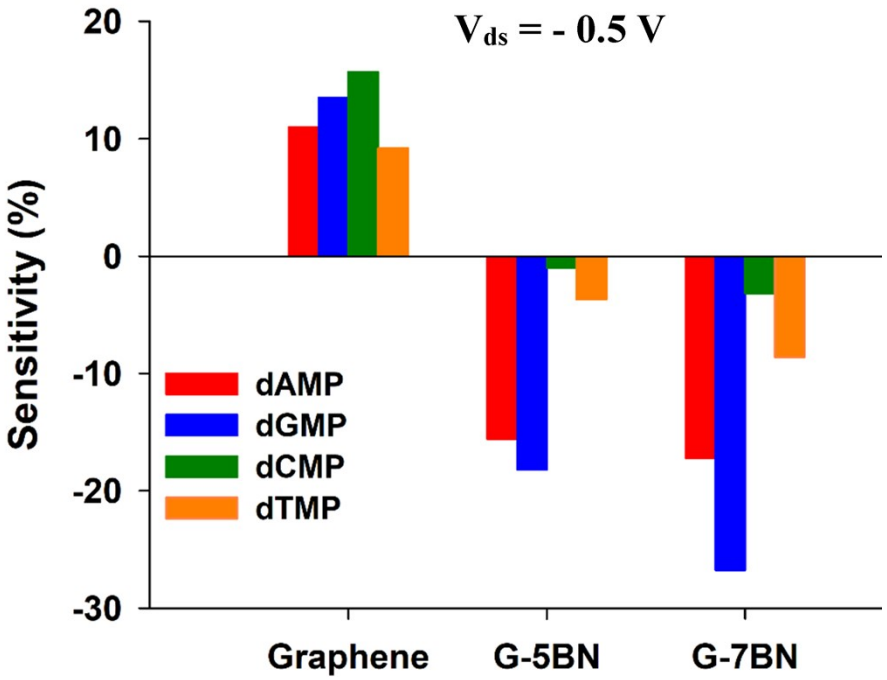

Figure S2: Sensitivity of graphene, G-5BN and G-7BN nanopores towards different nucleotides at reverse polarity ($V_{ds} = -0.5V$).

For comprehending the impact of the interaction with the nucleotide on the structural deformation of nanopores, lateral currents are calculated for the empty but deformed membrane/nanopore structures. The results for the graphene, G-5BN, and G-7BN nanopores are depicted in Tables. SII. Also, the structural deformation impact on the G7BN orbital current contours due to its interaction with dCMP and dGMP is depicted in Fig. S3.

Table SII: The influence of nucleotide on the current flow in the graphene, G-5BN, and G-

7BN nanopore at $V_{ds} = 0.5\ V$.

Nanopore	Empty	dAMP	dGMP	dCMP	dTMP
G-0BN (Nucleotides removed) (µA)	1.40	1.46	1.46	1.47	1.45
G-5BN (Nucleotides removed) (nA)	1.86	1.46	1.52	1.48	1.45
G-7BN (Nucleotides removed) (pA)	45.56	36.05	35.41	37.34	40.61

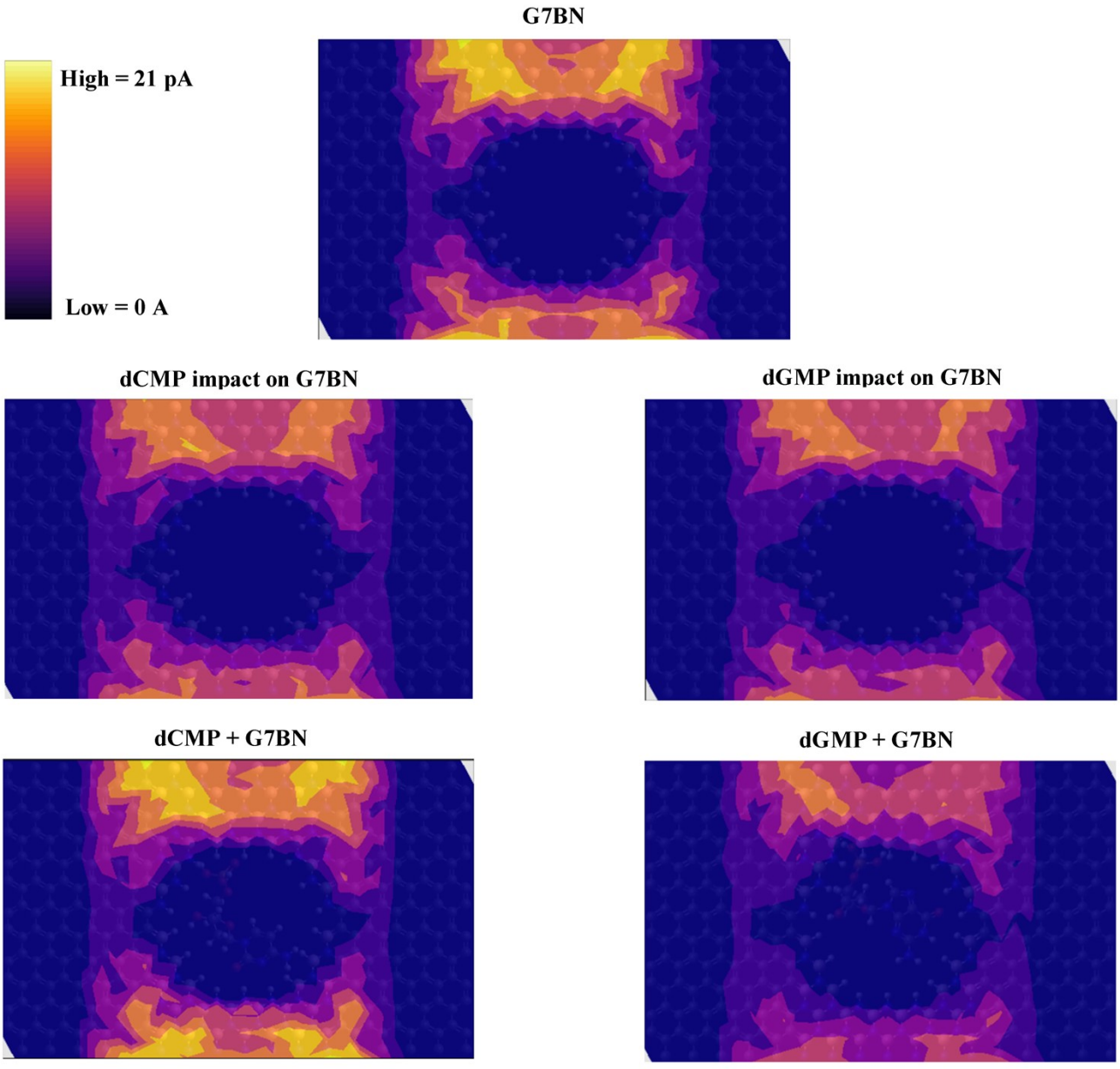

Figure S3: Atomic orbital current of empty G7BN and deformed G7BN, after interacting with dCMP and dGMP, at V_{ds} = 0.5V.

In order to test the effect of electrostatic interaction on the current modulation in the proposed nanopore structures a hydrogen fluoride (HF) molecule is placed in the G-5BN nanopore as it is illustrated in Fig. S4. HF placement near the right-side electrode is shown in Fig. S4 (a), and Fig. S4 (b) depicts its placement near the lower edge of the nanoribbon.

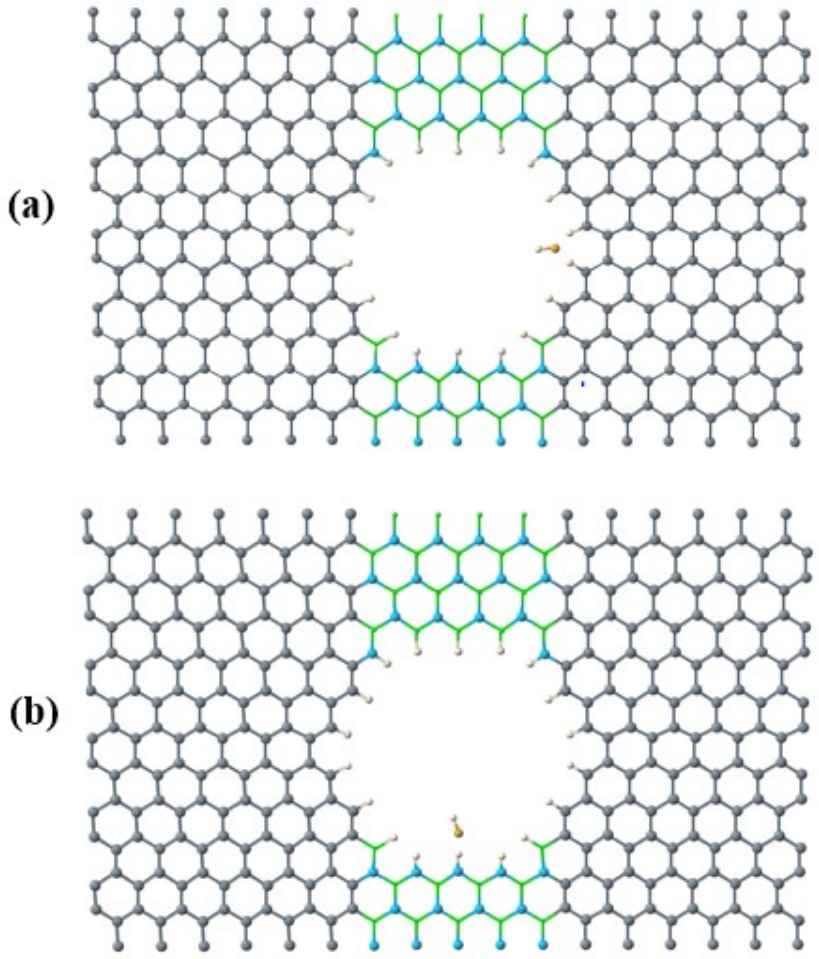

Figure S4: G5BN nanopore with a HF molecule. (a) HF is placed near the right side electrode. (b) HF is placed near the lower edge of the nanoribbon.

For investigating the influence of initial structure on the relaxed geometry of the system, we conducted a test in which nucleotides have rotated for 5 degrees in G-5BN nanopore compared to the initial placement. As can be seen in Fig. S5, the relaxed geometry of the structure after 5 degrees rotation is fairly similar to the results obtained from the initial one. Also, Table SII illustrates the in-plane current for V_{ds} = 0.5 V, and the corresponded sensitivity is plotted in Fig. S6. The results indicate that the in-plane current and sensitivity are correlated to the initial placement. Therefore, a slight deviation in the initial placement of nucleotide won't impact the results.

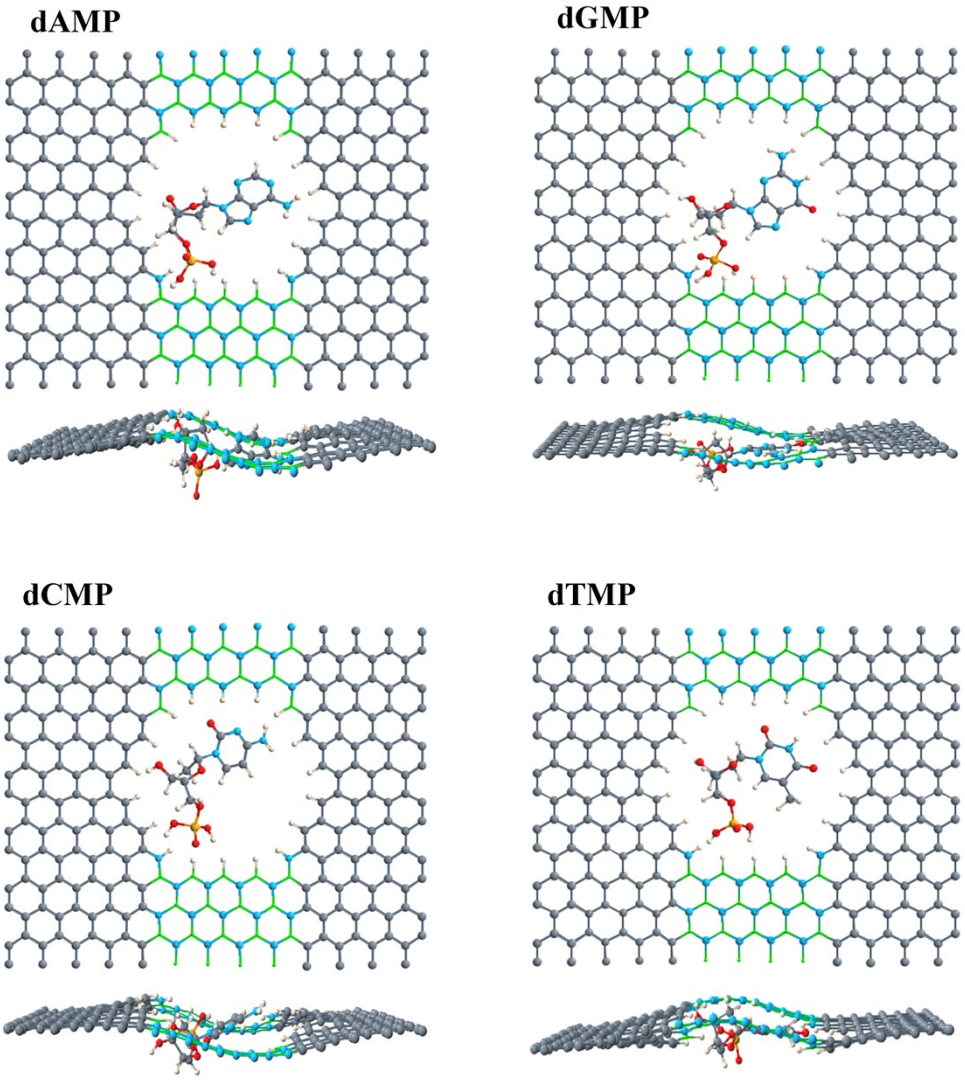

Figure S5: Relaxed geometries of dAMP, dGMP, dCMP, and dTMP in G-5BN heterostructure after 5 degrees in-pane rotation.

Table SII: G-5BN nanopore current at $V_{ds} = 0.5\ V$ after 5 degrees in-plane rotation of nucleotides.

heterostructure/nanopore	Empty	dAMP	dGMP	dCMP	dTMP
G-5BN (nA)	1.86	1.56	1.47	1.84	1.64

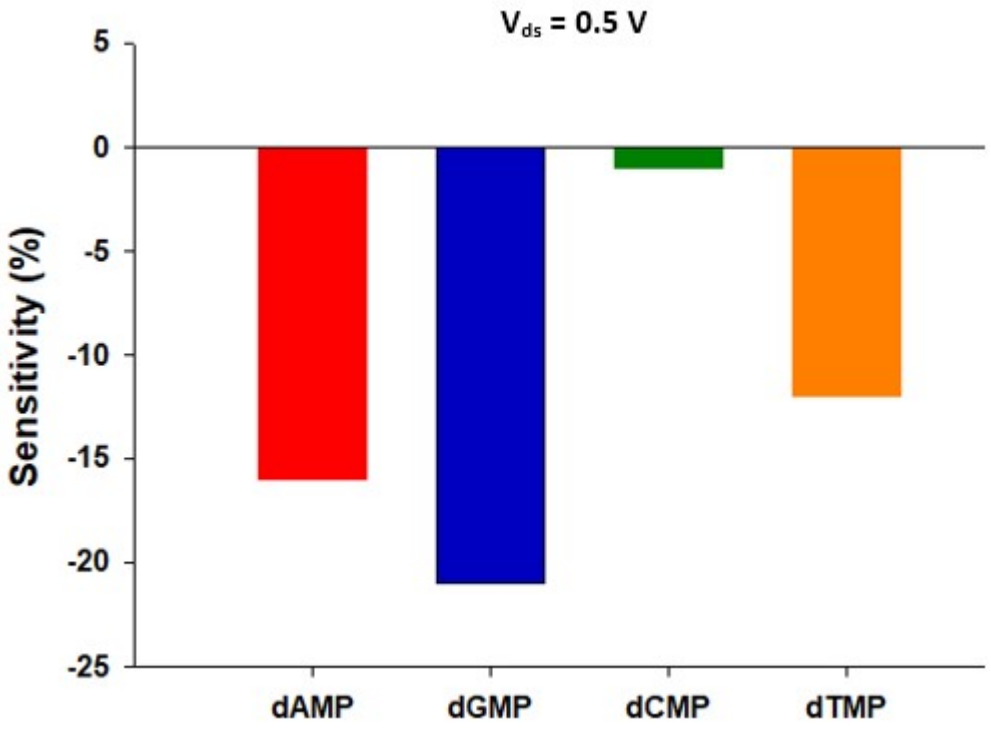

Figure S6: Sensitivity of G-5BN nanopore towards different nucleotides with 5 degrees rotation at Vds = 0.5.