Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information

Extended Topological Line Defects in Graphene for Individual Identification of DNA Nucleobases

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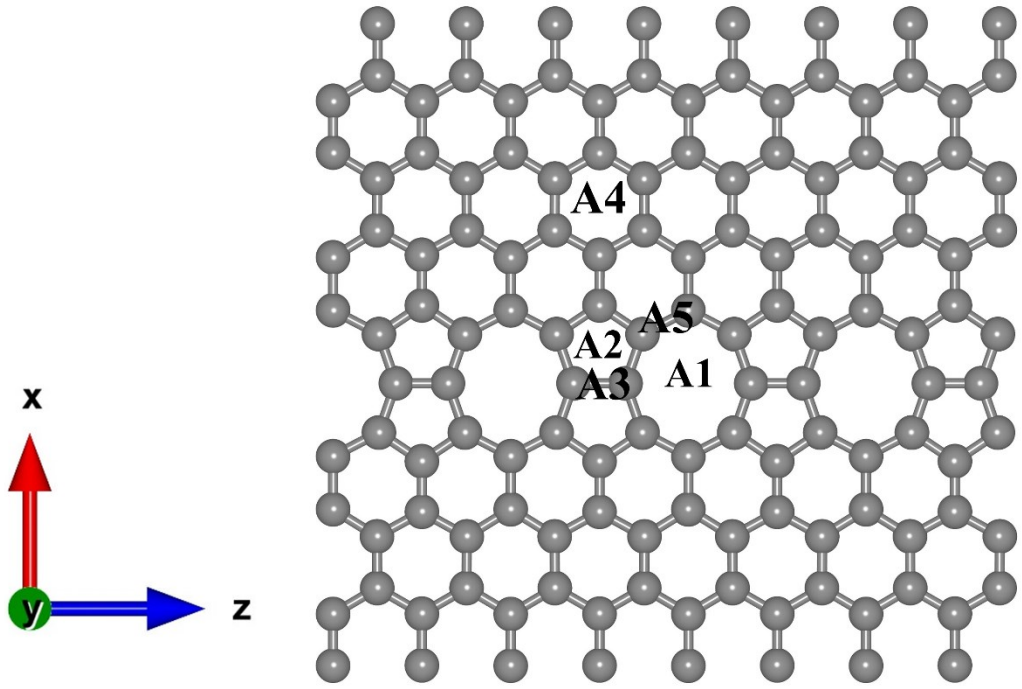

Figure S1. Showing possible adsorption sites of the ELDs graphene (A1-A5).

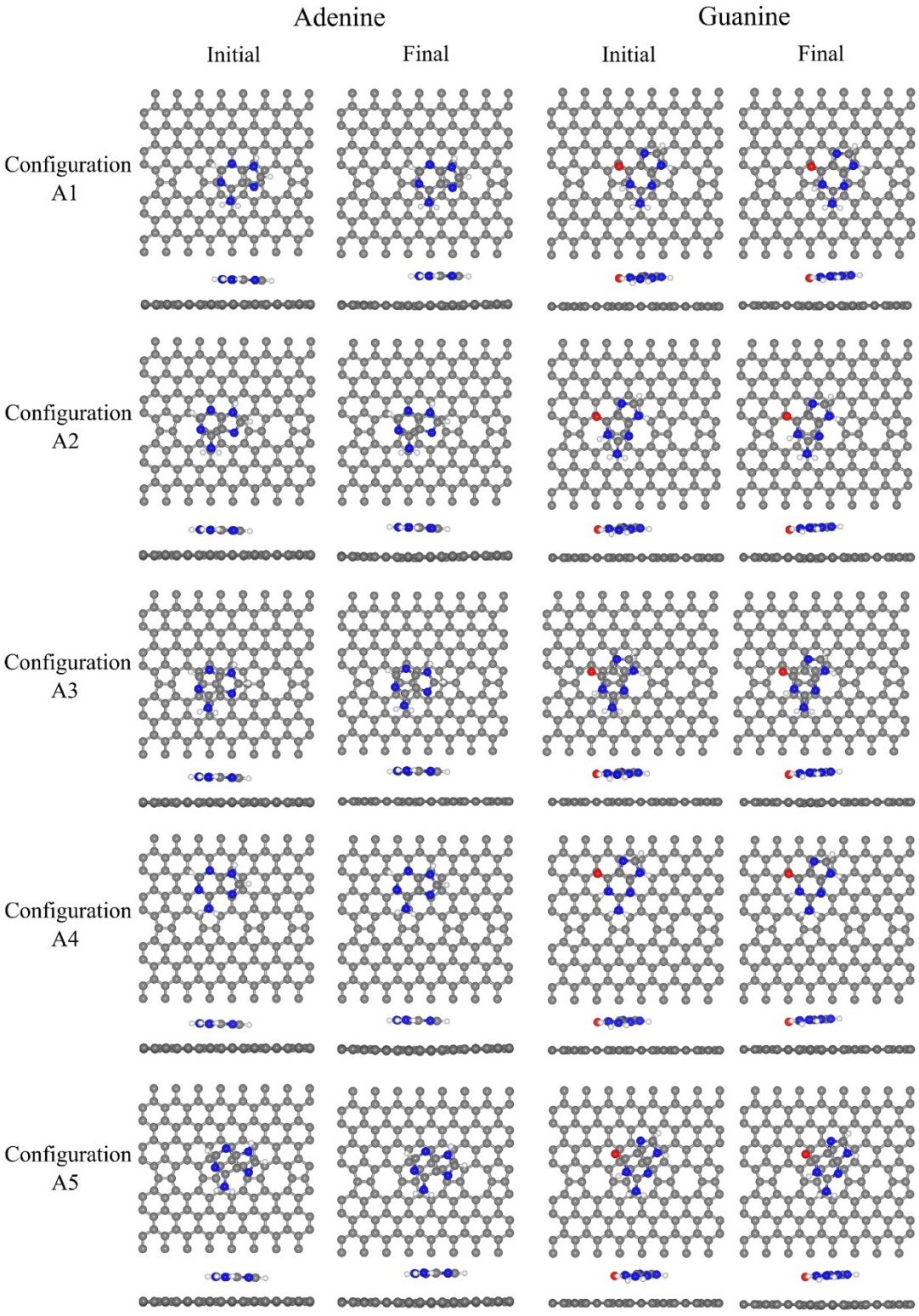

Figure S2. Initial and final configurations (A1-A5) of the ELDs graphene+nucleobase (A and G) systems.

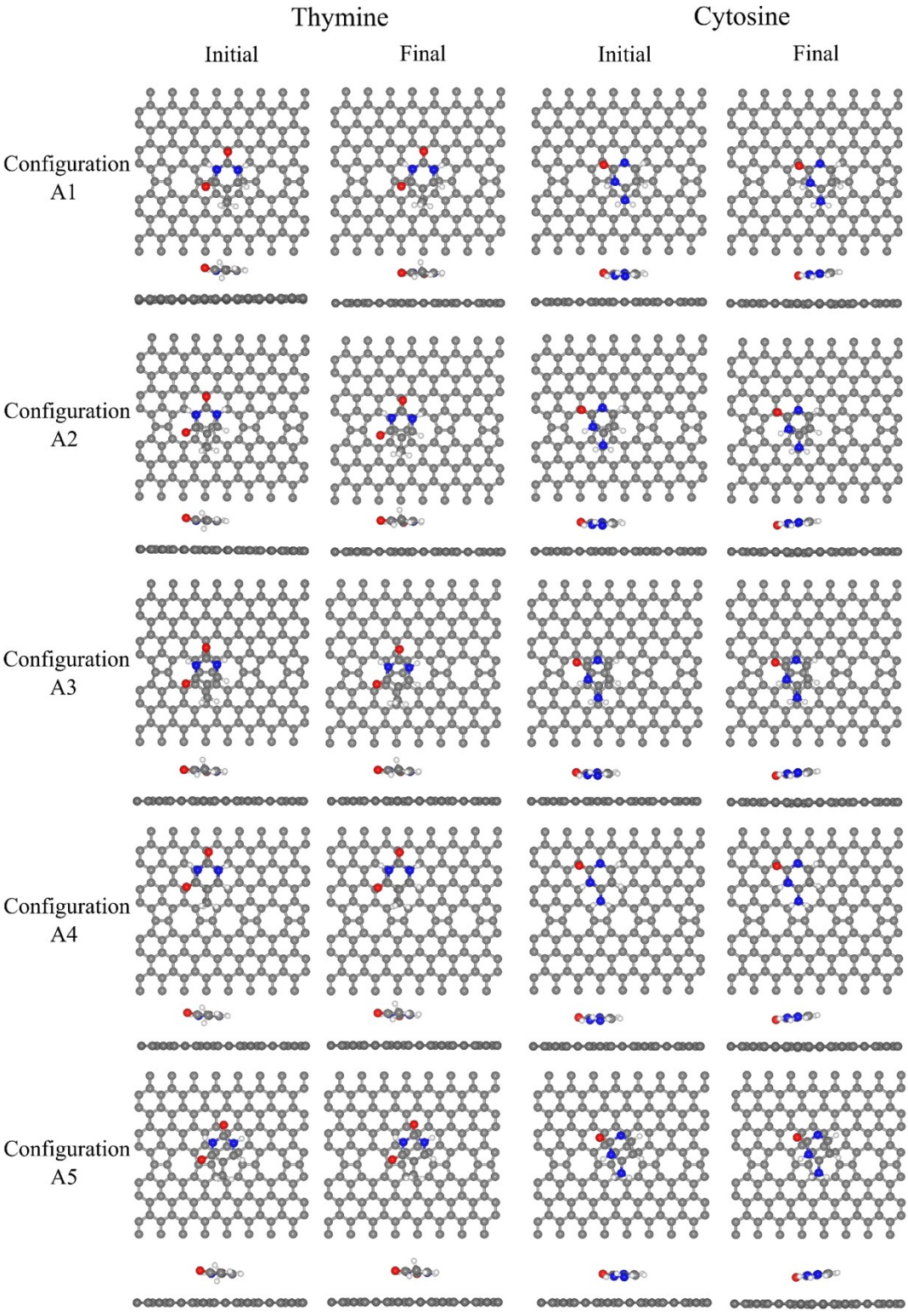

Figure S3. Initial and final configurations (A1-A5) of the ELDs graphene+nucleobases (T and C) systems.

Table S1. Relative energy values (in eV) of the ELDs graphene+nucleobase (A, G, T, and C) systems when nucleobases are adsorbed at different adsorption sites (A1-A5).

Nucleobase	A1	A2	A3	A4	A5
Adenine	0.006	0.001	**0.000**	0.007	0.003
Guanine	0.043	0.054	0.024	0.031	**0.000**
Thymine	0.005	0.024	0.021	0.038	**0.000**
Cytosine	0.055	0.052	0.049	0.031	**0.000**

Comparative Discussion of GGA-PBE and vdW-DF-cx Results:

The energetically most stable configuration of adsorbed A, G, T, and C on the ELDs graphene sheet obtained using the GGA+PBE and vdW-DF-cx level of theories. **Table S2** shows the adsorption height (*h,* in Å) between the nucleobase and the ELDs graphene sheet, obtained by using the GGA+PBE and vdW-DF-cx level of theory. The '*h'* is the vertical shortest distance between the substrate and molecule. Herein, in the case of ELDs graphene+A, the adsorption height is the shortest distance between C (of ELDs graphene) and H atoms (of A nucleobase), as shown in **Figure 3**. The GGA+PBE (vdW-DF-cx) calculated adsorption height values are 3.257 (2.981), 2.806 (2.711), 2.901 (2.721), and 2.944 (2.651) for A, G, T, and C respectively. Thus, the vdW-DF-cx calculated adsorption height values are less compared to the GGA-PBE calculated values. This is because vdW-DF-cx includes the nonlocal corrections and describes accurately the important π-π interaction between the target molecules and the ELDs graphene sheet. Also, the calculated adsorption energies (E_{ads}, in eV) for all the four ELDs graphene+nucleobase systems using the GGA+PBE and vdW-DF-cx are tabulated in **Table S2**. We find that GGA+PBE (vdW-DF-cx) calculate E_{ads} values are -0.535 (-1.554), -0.718 (-1.717), -0.547 (-1.395), and -0.630 (-1.501) eV for adsorbed A, G, T, and C, respectively. Hence, the E_{ads} order of all the four nucleobases is G > C > T > A for GGA+PBE and G > A > C > T for vdW-DF-cx. However, there is not much difference in the calculated adsorption energy values of A, C, and T. It is found that

the vdW-DF-cx E_{ads} values are larger than the GGA+PBE. This is because the vdW-DF-cx includes the nonlocal corrections from first-principles DFT calculations. Therefore, the computed E_{ads} values using the vdW-DF-cx level indicate that there is a strong non-covalent interaction between the device and the nucleobases.

Table S2. Computed adsorption energy values (E_{ads}, in eV), and adsorption heights (h, in Å) of the ELDs graphene+nucleobase systems.

Nucleobase	E_{ads} **(eV)**		***h*** **(Å)**	
	GGA-PBE	**vdW-DF-cx**	**GGA-PBE**	**vdW-DF-cx**
Adenine	-0.53	-1.55	3.26	2.98
Guanine	-0.71	-1.72	2.81	2.71
Thymine	-0.54	-1.39	2.90	2.72
Cytosine	-0.63	-1.50	2.94	2.65

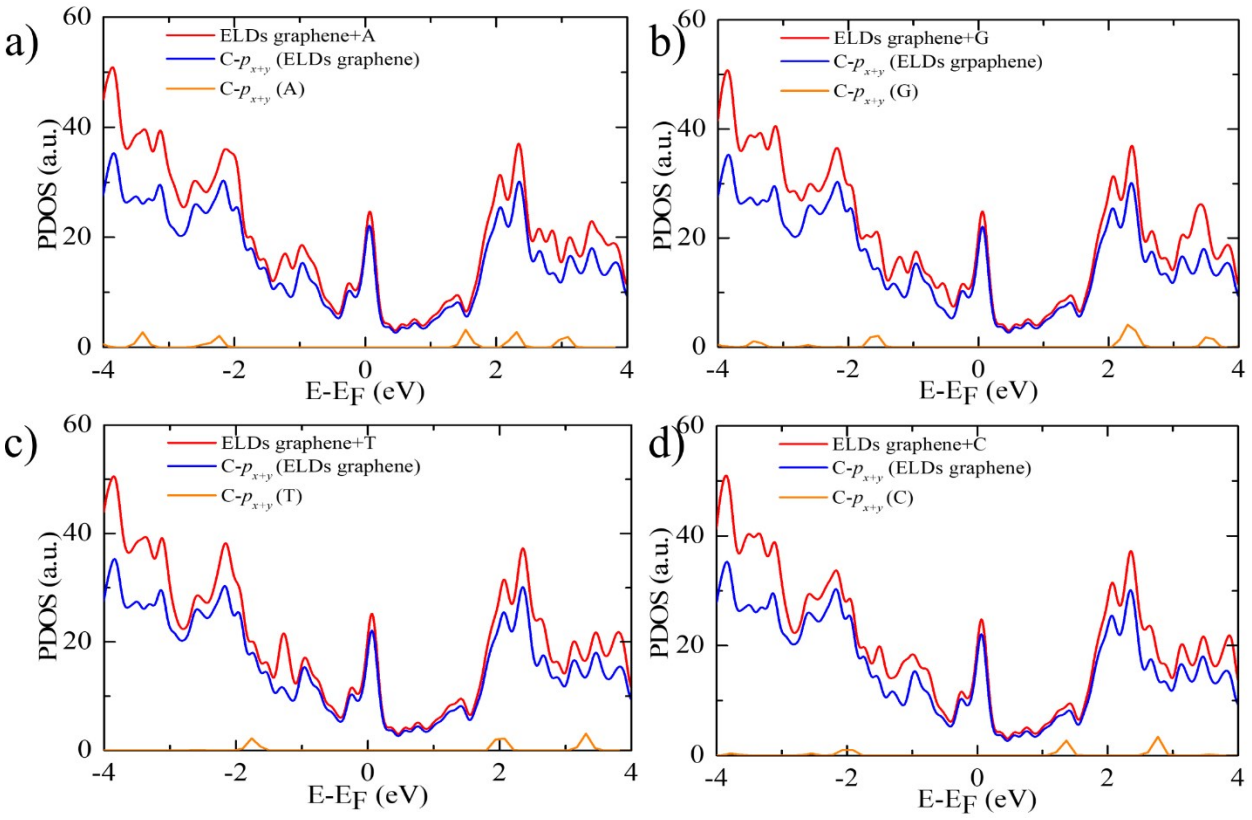

Figure S4. (a-d) Electronic DOS of the ELDs graphene and ELDs graphene+nucleobase systems and the PDOS of C-p_{x+y} for ELDs graphene+nucleobases. The Fermi level (E-E$_F$) is set to zero.

Scheme. Adsorption Heights and Rotation of DNA Nucleobases on the ELDs graphene surface:

We have increased adsorption heights of all the four nucleobases on the ELDs graphene surface to see the changes in the transmission function. For this, the target nucleobase is rotated along the y-axis in the xz-plane from 0.2 to 0.6 Å, as shown in **Figure S5**. The changes in transmission function with respect to varying adsorption heights are presented in **Figure S6**. Further, we have considered the rotations of all the four nucleobases on the ELDs graphene surface around the y-axis in the xz-plane from 0° to 180° in the steps of 30° as shown in **Figure S6** and the transmission function results are presented in **Figure S7**.

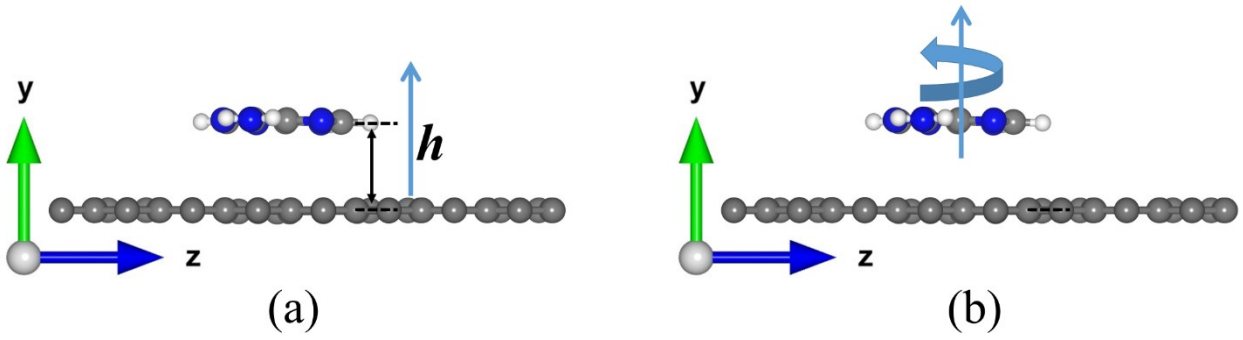

Figure S5. Illustrates the (a) adsorption heights (*h*) and (b) rotation of the four nucleobase molecules on the ELDs graphene sheet.

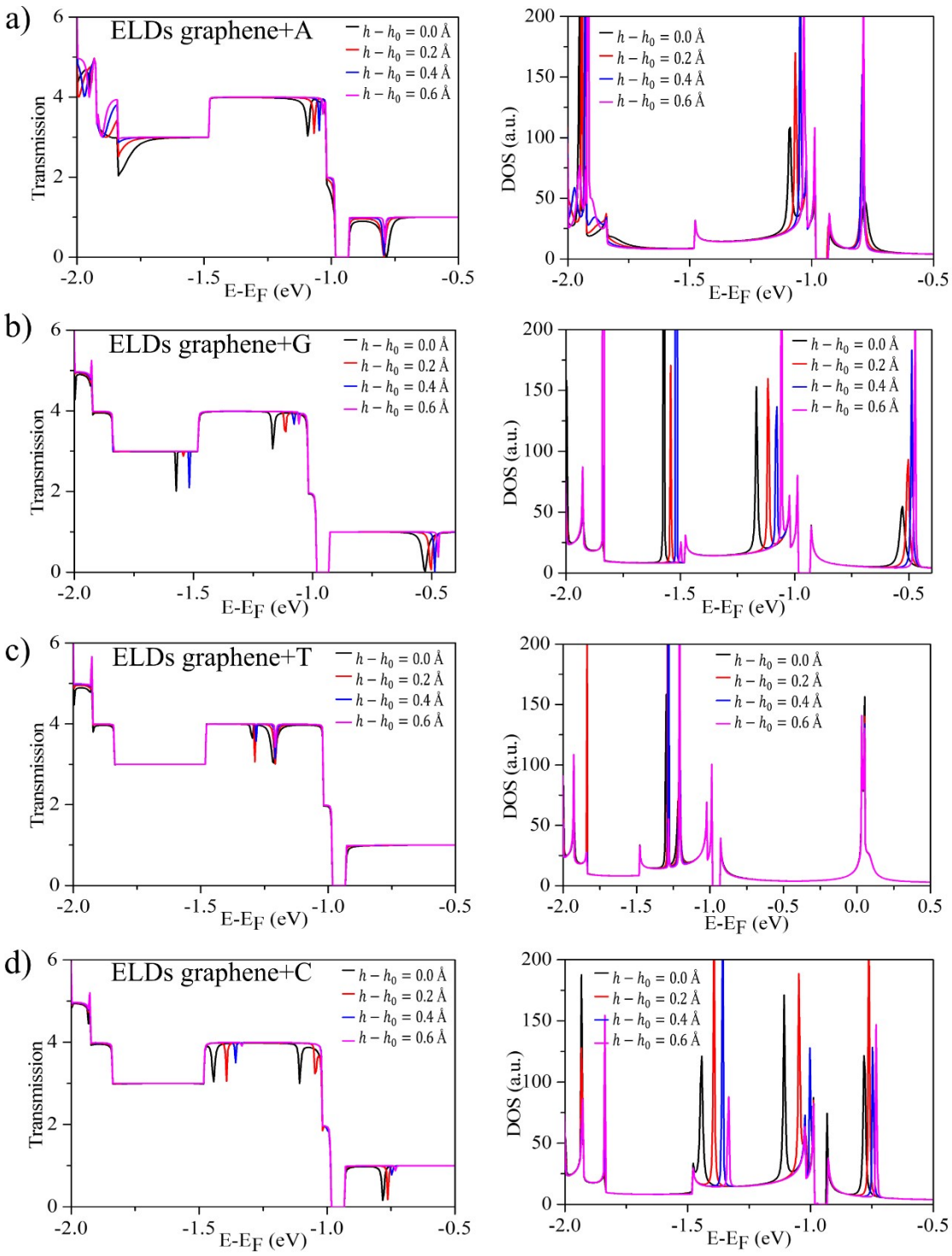

Figure S6. (a-d) Change in transmission function and density of states of the ELDs graphene+nucleobase systems due to change in adsorption height of the nucleobase. Here h and h_0 denote the initial and translated distances, respectively.

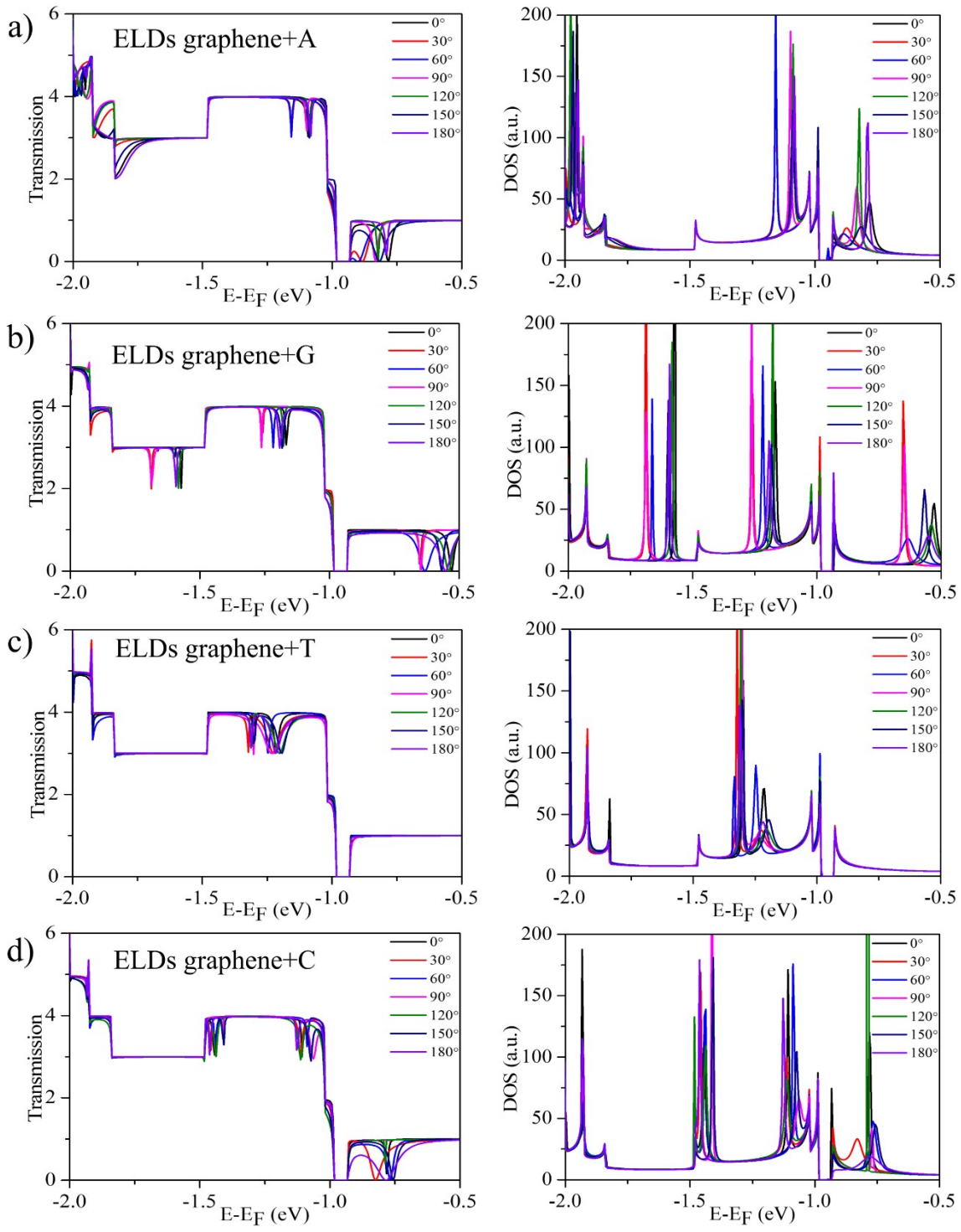

Figure S7. (a-d) Change in transmission function and density of states of the ELDs graphene+nucleobase (A, G, T, and C) systems due to the rotation of the nucleobase.

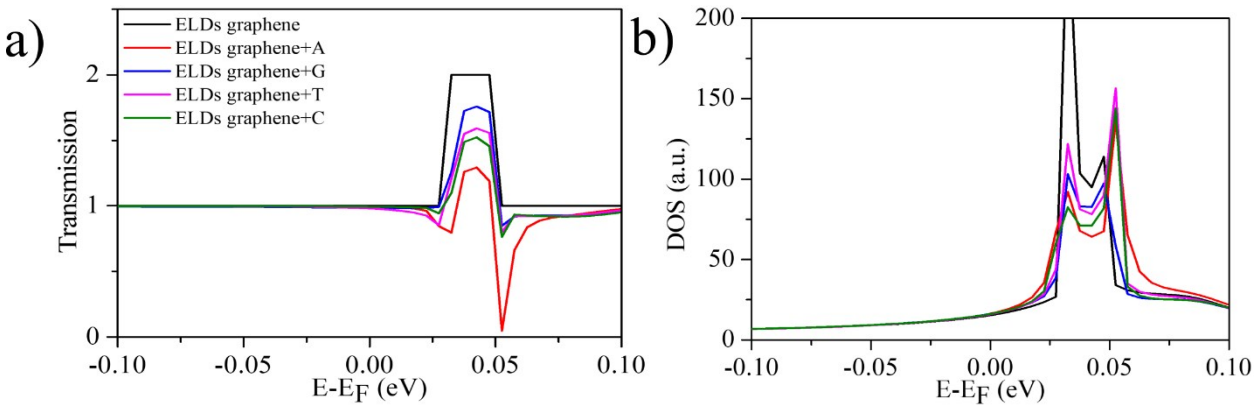

Figure S8. (a) The zero-bias transmission functions of the ELDs graphene and ELDs graphene+nucleobase systems. (b) Electronic density of states.