

Supporting Information

for

**Adsorption of Nucleobases on Transition-metal Dichalcogenides
and Graphene Sheet: A First Principles Density Functional
Theory Study.**

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Table S1. Total energies of nucleobases adsorbed on different sites of MoS₂, WS₂ and GRA using vdW-DF method.

| System | Total energy (in kJ/mol) | System | Total energy (in kJ/mol) | System | Total energy (in kJ/mol) |
|---------------------|-----------------------------|--------------------|-----------------------------|--------|-----------------------------|
| MoS ₂ -G | | WS ₂ -G | | G-G | |
| A | -59633.5 | A | -66534.8 | A | -61907.6 |
| B | -59633.4 | B | -66536.4 | B | -61915.6 |
| C | -59633.9 | C | -66538.8 | C | -61909.6 |
| MoS ₂ -A | | WS ₂ -A | | G-A | |
| A | -59161.7 | A | -66063.4 | A | -61434.1 |
| B | -59160.9 | B | -66064.3 | B | -61437.5 |
| C | -59162.4 | C | -66064.5 | C | -61436.6 |
| MoS ₂ -T | | WS ₂ -T | | G-T | |
| A | -58668.8 | A | -65570.4 | A | -60943.6 |
| B | -58667.7 | B | -65569.1 | B | -60950.5 |
| C | -58671.1 | C | -65573.3 | C | -60944.6 |
| MoS ₂ -C | | WS ₂ -C | | G-C | |
| A | -57716.3 | A | -64617.8 | A | -59987.0 |
| B | -57714.9 | B | -64617.4 | B | -59987.9 |
| C | -57711.6 | C | -64615.1 | C | -59994.4 |
| MoS ₂ -U | | WS ₂ -U | | G-U | |
| A | -57220.4 | A | -64122.0 | A | -59494.5 |
| B | -57220.0 | B | -64121.7 | B | -59501.4 |
| C | -57219.3 | C | -64122.3 | C | -59495.2 |

Table S2. Calculated vertical distances between nucleobases and substrates using PBE and DFT-D2 methods.

| | | Vertical distance (in Å) | | | | | |
|---|--|--------------------------|--------|-----------------|--------|------|--------|
| | | MoS ₂ | | WS ₂ | | GRA | |
| | | PBE | DFT-D2 | PBE | DFT-D2 | PBE | DFT-D2 |
| G | | 3.73 | 3.36 | 3.80 | 3.26 | 3.93 | 3.22 |
| A | | 3.78 | 3.41 | 3.88 | 3.27 | 3.96 | 3.26 |
| T | | 3.89 | 3.33 | 3.85 | 3.28 | 3.96 | 3.29 |
| C | | 3.73 | 3.33 | 3.79 | 3.28 | 3.97 | 3.24 |
| U | | 3.77 | 3.38 | 3.93 | 3.23 | 3.85 | 3.23 |

Table S3. Calculated binding energies of MoS₂, WS₂ and GRA-nucleobase complexes using PBE and DFT-D2 methods.

| | Binding energy (kJ/mol) | | | | | |
|---|-------------------------|--------|-----------------|--------|------|--------|
| | MoS ₂ | | WS ₂ | | GRA | |
| | PBE | DFT-D2 | PBE | DFT-D2 | PBE | DFT-D2 |
| A | 5.40 | 60.40 | 5.45 | 77.43 | 5.04 | 69.83 |
| C | 8.06 | 55.76 | 7.92 | 69.16 | 6.93 | 62.01 |
| G | 9.53 | 65.99 | 10.58 | 92.93 | 9.57 | 81.52 |
| T | 4.94 | 55.81 | 5.10 | 71.47 | 5.04 | 65.20 |
| U | 3.98 | 46.57 | 4.57 | 59.07 | 3.93 | 57.40 |

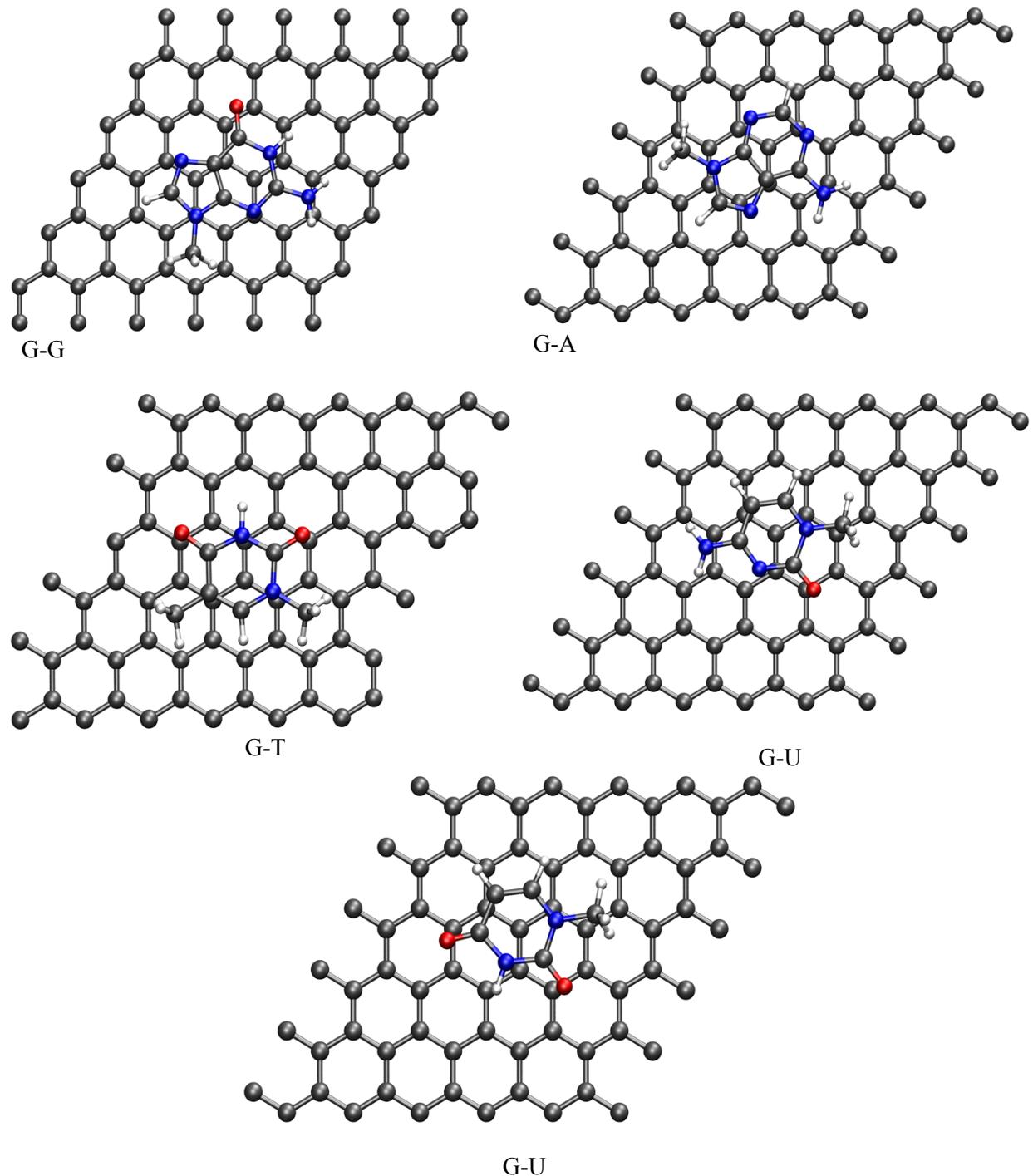


Figure S1. Optimized structures of nucleobases adsorbed on monolayer GRA (Red: O, Blue: N, Gray: C and White: H).

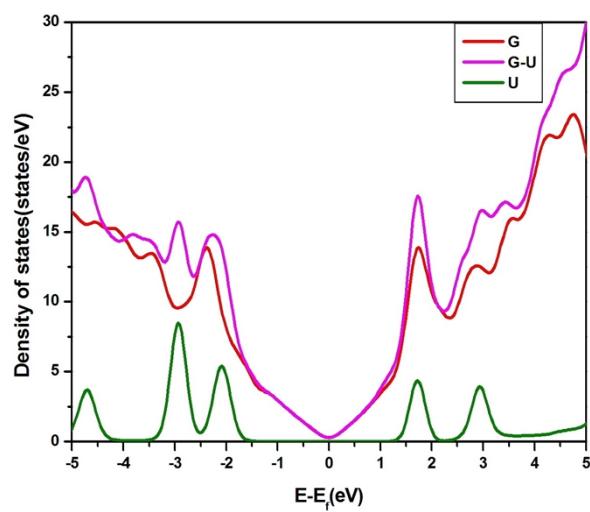
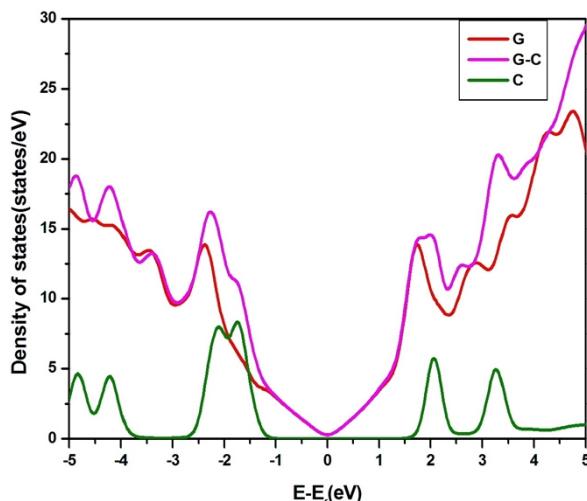
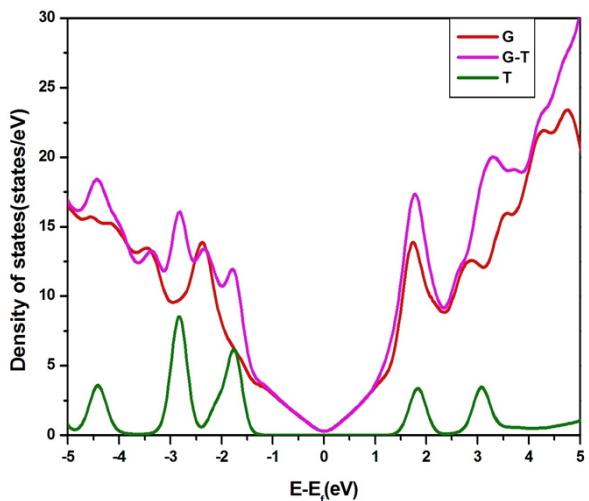
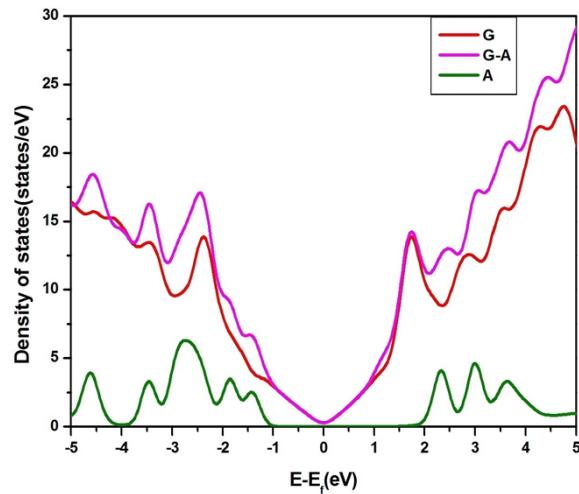
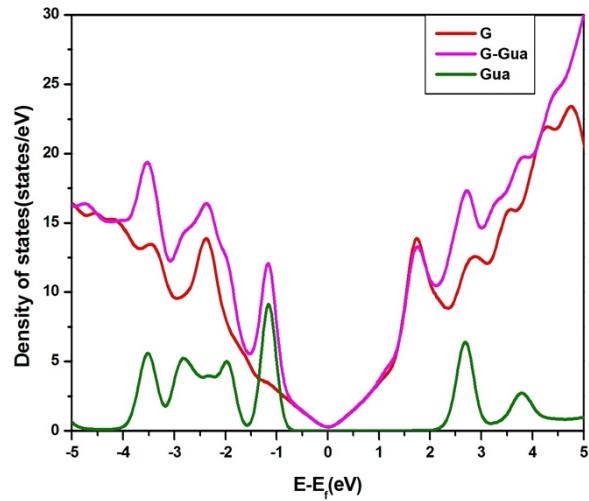


Figure S2. Total densities of states of pristine GRA, GRA-nucleobase complexes and nucleobases.

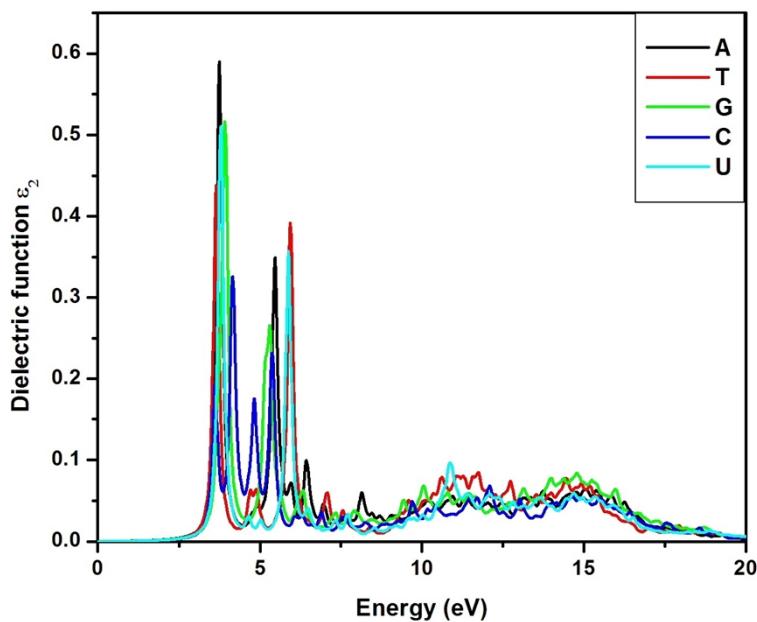
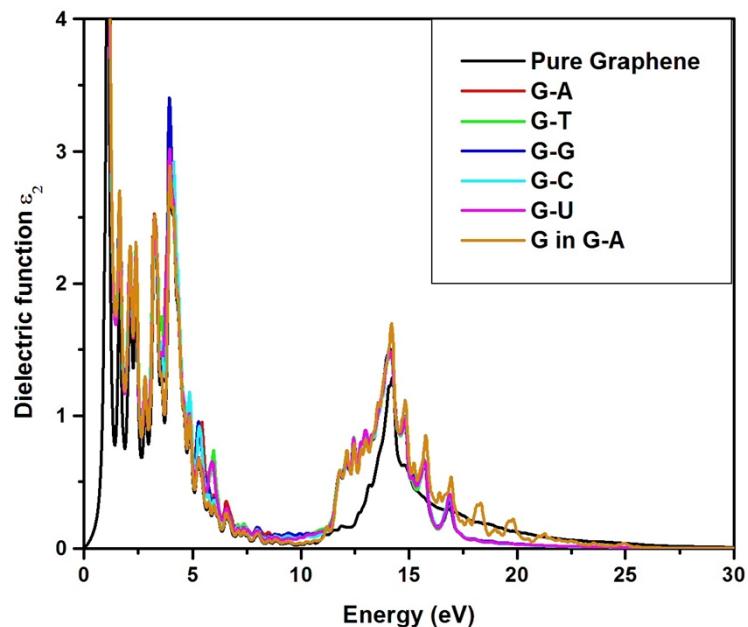


Figure S3. Imaginary part of the dielectric functions of pristine GRA, complexes with nucleobases and free nucleobases.