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

Supplementary Information

1. Different other orientations of amino acid adsorbed complexes.

In order to scrutinize the most stable and favourable orientation of amino acid adsorbed nanomaterials, different orientations of all the amino acids with respect to the structure of nanomaterials have been optimized in the present study (shown in Fig S1).

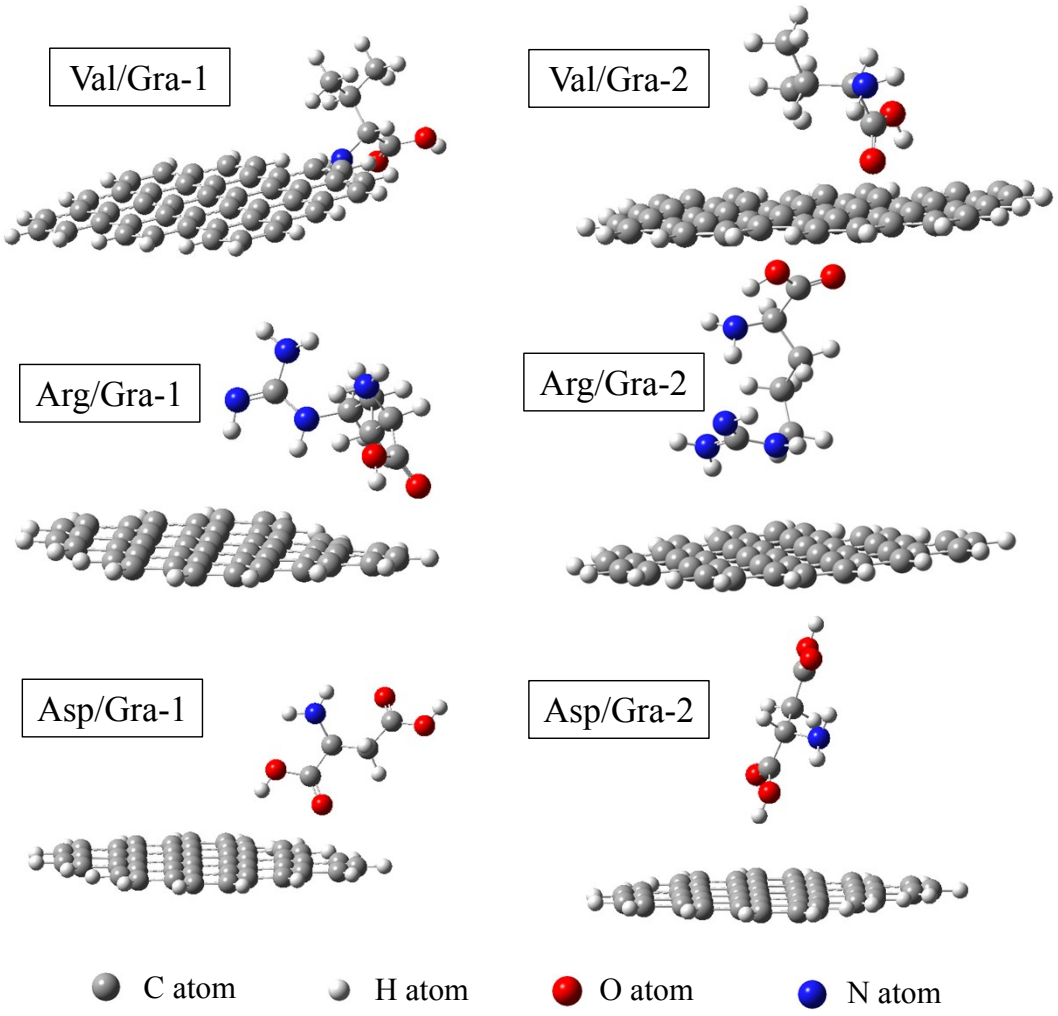

Fig S1: Optimized geometry of amino acid adsorbed graphene complexes in different orientations.

2. Implementation of dispersion correction upon freezing the nanomaterial

The coordinates of optimized BN nanosheet were fixed and then upon applying the dispersion correction on the optimized arginine adsorbed BN nanosheet complex, amino acid orient itself in such a way that the adsorption energy of the complex became -175.91 kcal/mol. The optimized geometry of arginine adsorbed BN nanosheet is shown in Fig S2.

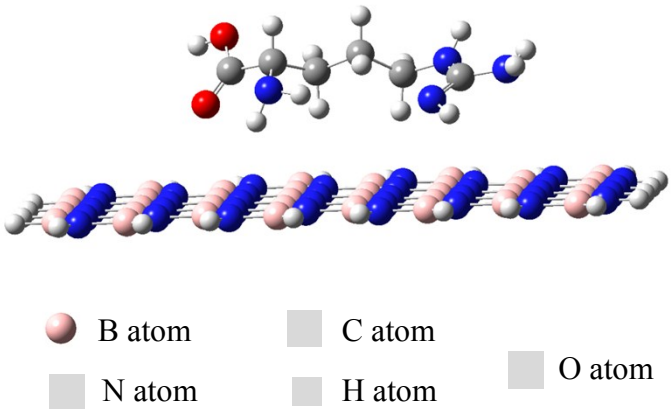

Fig S2: Optimized geometry of arginine adsorbed BN nanosheet by fixing the BN nanosheet coordinates.

3. Density of State (DOS) plot of pristine and amino acid adsorbed nanostructures.

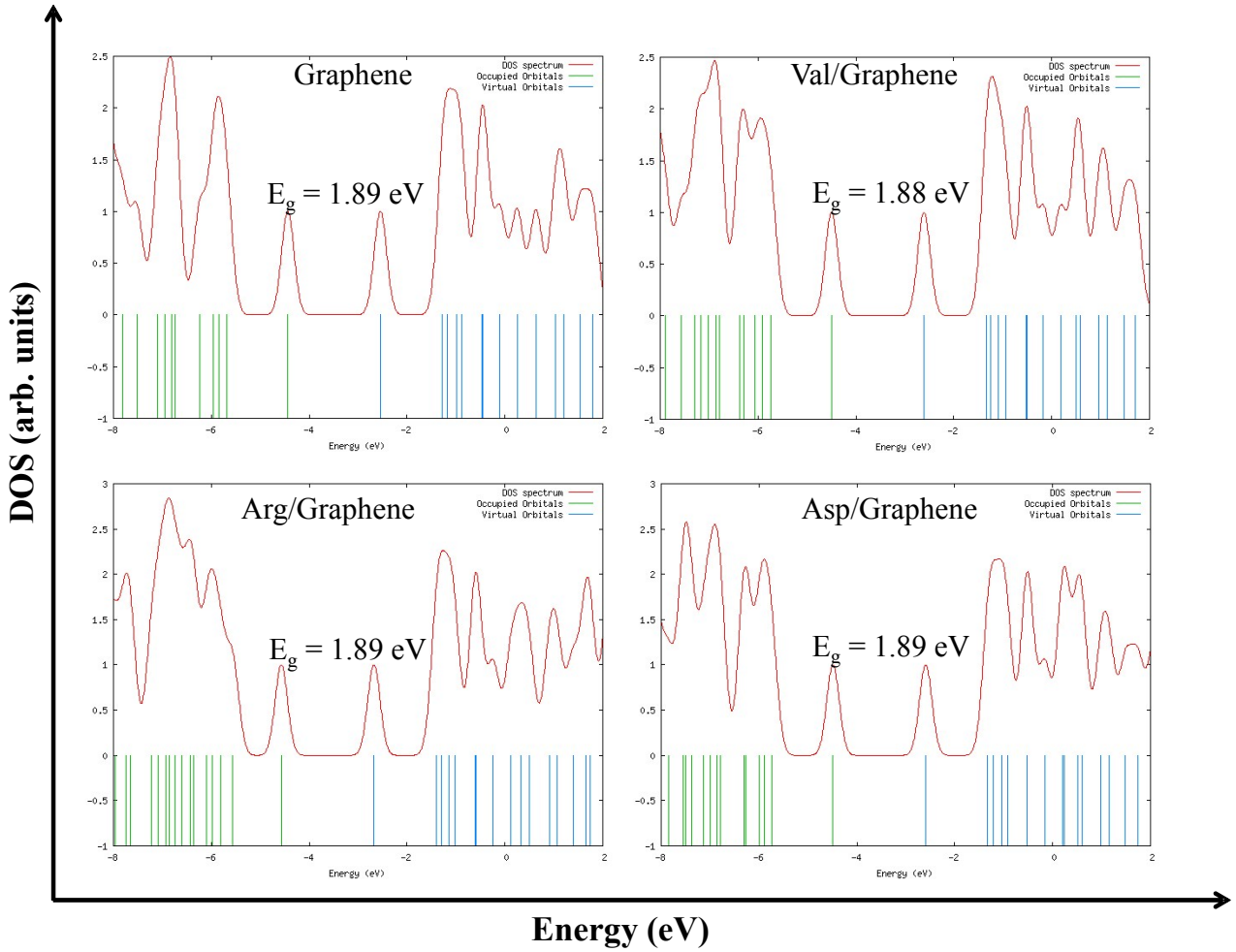

Fig S3. DOS plot of graphene and amino acids adsorbed graphene.

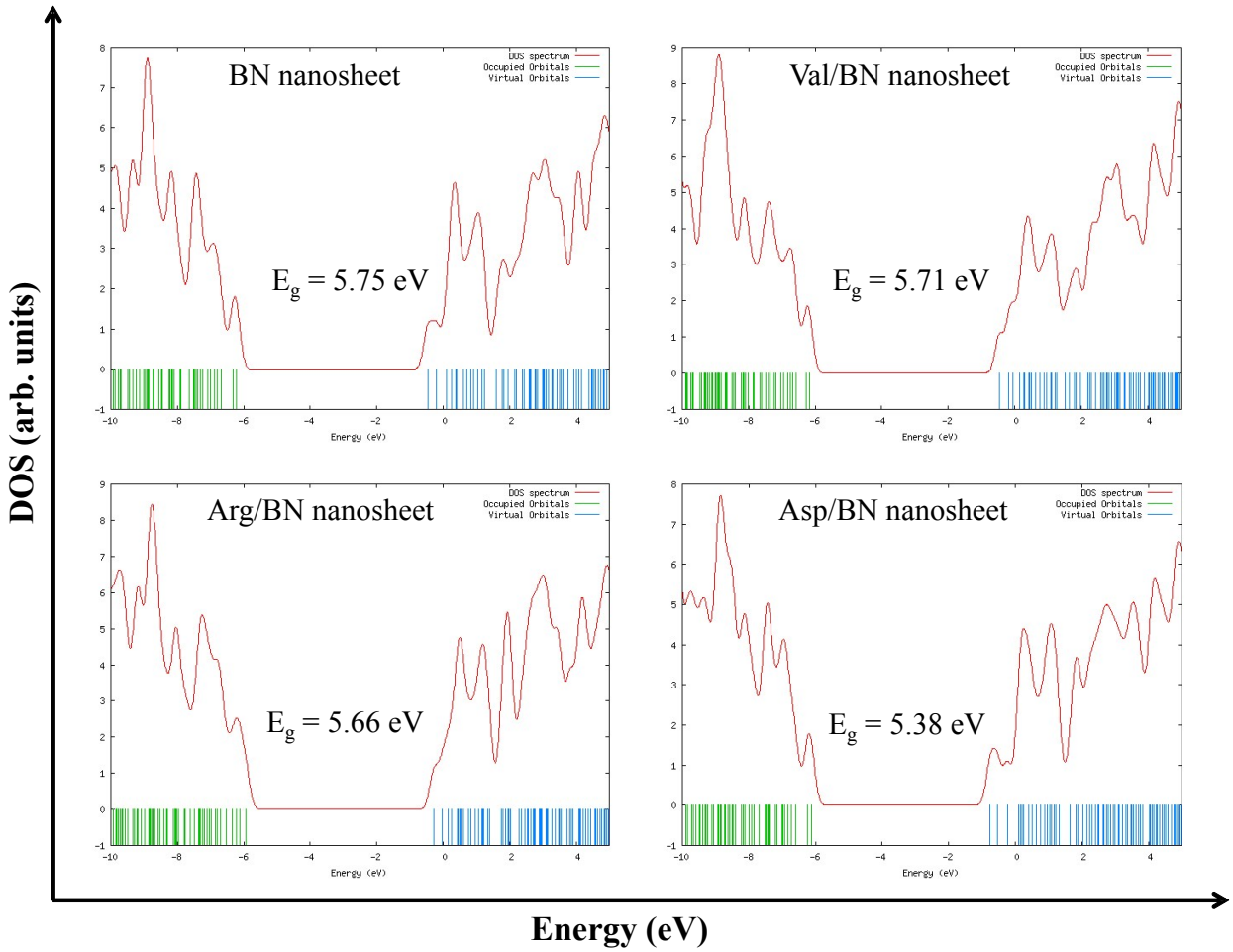

Fig S4: DOS plots of BN nanosheet and amino acids adsorbed BN nanosheet.

4. HOMO-LUMO energy gap and work function

Table S1: Values of HOMO-LUMO energy gap and work function of pristine and amino acid adsorbed nanosheet complexes.

System	HOMO-LUMO energy gap (eV)	Work function (eV)
Graphene	1.893	0.128
Val/Gra	1.888	0.130
Arg/Gra	1.892	0.134
Asp/Gra	1.894	0.132
BN nanosheet	5.750	0.122

Val/BN	5.710	0.121
Arg/BN	5.665	0.113
Asp/BN	5.379	0.127