Supplementary information

for

Trends on the amino acids adsorption onto the graphene and graphene oxide surface: A dispersion corrected DFT study

H. Tavassoli Larijani [a], **M. Darvish Ganji** [b, *], **and M. Jahanshahi** [a, *]

[a] Nanotechnology Research Institute, School of Chemical Engineering, Babol University of Technology, Babol, Iran

[b] Department of Nanochemistry, Faculty of Pharmaceutical Chemistry, Pharmaceutical Sciences Branch, Islamic Azad University, Tehran - Iran (IAUPS)

Corresponding Authors: *E-mail address: ganji_md@yahoo.com (M.D. Ganji). Tel.: +98 911 113 7150.

Configurations	E_b (eV)	Distance (Å)	Configurations	E_b (eV)	Distance (Å)
Histidine			**Glycine**		
D1: CH_3+5	-0.25	2.98	D18: NH_2+7	-0.23	3.197
D2: CH_3+6	-0.26	3.002	D19: OH+5	-0.16	3.004
D3: CH_3+7	-0.24	3.008	D20: OH+6	-0.18	3.05
D4: N+5	-0.30	3.324	D21: OH+7	-0.18	3.203
D5: N+6	-0.29	3.394	D22: Parallel	-0.40 (-0.48)	2.437
D6: N+7	-0.28	3.463	**Phenylalanine**		
D7: Ring+5	-0.57	3.376	D23: CH_2+RH+5	-0.52	2.974
D8: Ring+6	-0.60 (-0.63)	3.132	D24: CH_2+RH+6	-0.53	2.886
D9: Ring+7	-0.56	3.417	D25: CH_2+RH+7	-0.52	2.872
Glycine			D26: CH+RH_2+5	-0.54	2.923
D10: CH_2+5	-0.30	2.768	D27: CH+RH_2+6	-0.55	2.88
D11: CH_2+6	-0.29	2.598	D28: CH+RH_2+7	-0.53	2.957
D12: CH_2+7	-0.31	2.719	D29: Ring+5	-0.57	3.161
D13: Co+5	-0.22	3.059	D30: Ring+6	-0.60 (-0.76)	3.369
D14: Co+6	-0.20	3.168	D31: Ring+7	-0.58	3.356
D15: Co+7	-0.20	3.014			
D16: NH_2+5	-0.20	3.146			
D17: NH_2+6	-0.22	3.267			

Table S1. Binding energies and equilibrium distances resulted in SPE calculations for Defect/A.A complexes. The value in parentheses denote the binding energy of the most stable configurations after full structural optimization but without BSSE corrections. The numbers 5, 6 and 7 in the configurations column denote to the pentagon, hexagon and heptagon site of the defected graphene, respectively.

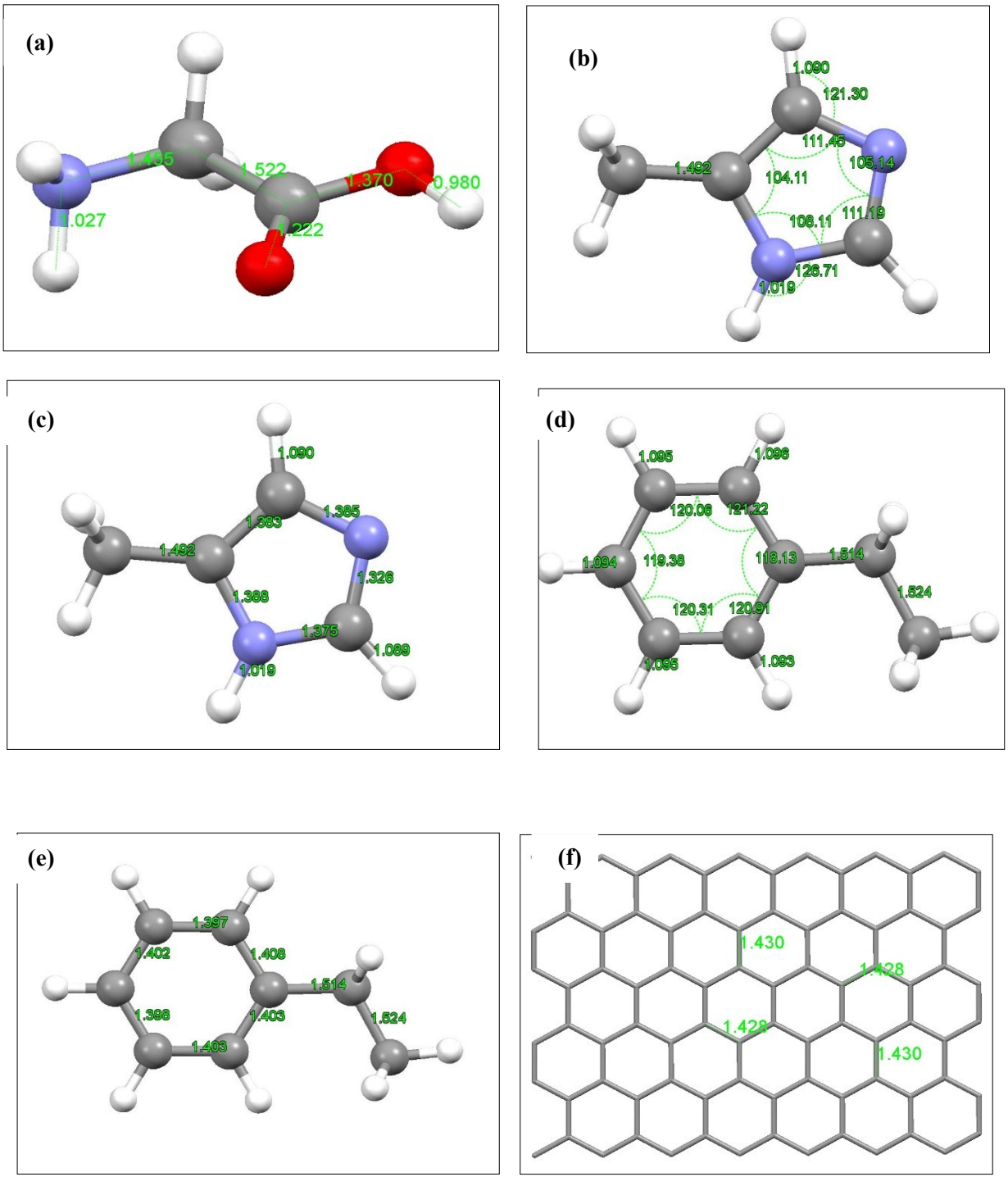

Figure S1. Optimized structures and geometrical parameters of: (a) glycine (b),(c) histidine, (d),(e) phenylalanine and (f) graphene sheet. (Red: O, Blue: N, Gray: C and White: H).

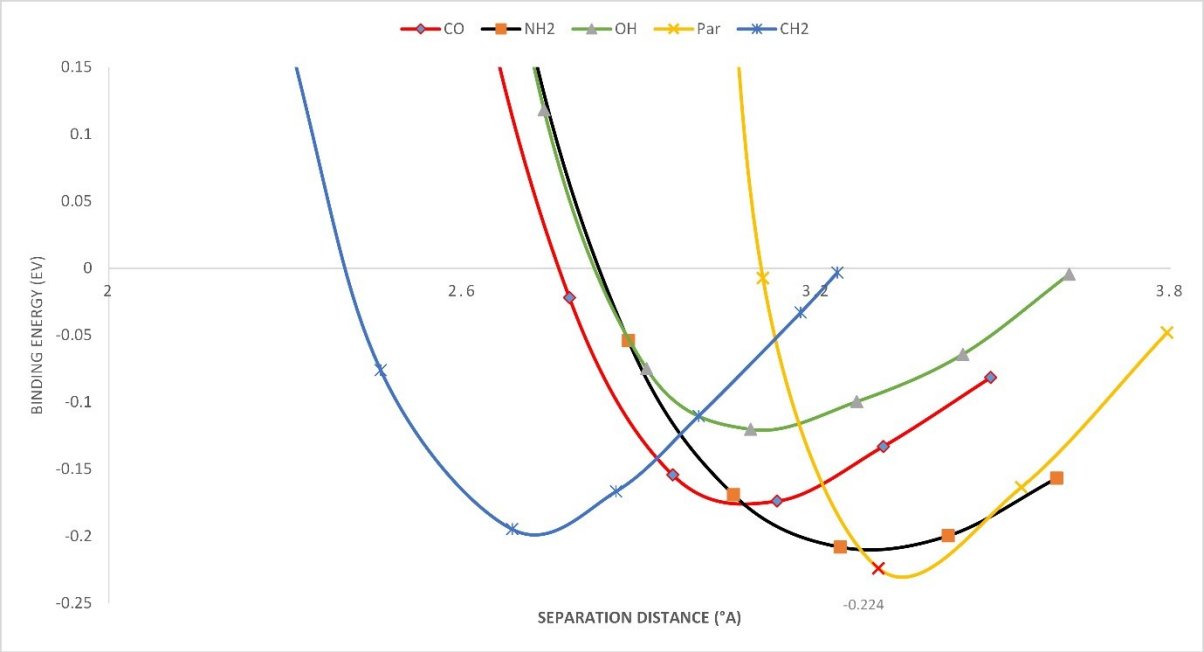

Figure S2. Single point energy plot as a function of distance between the glycine molecule and graphene monolayer for all configurations. The red multiplication sign on the plot corresponding to the parallel configuration represents the approximate most favorable orientation.

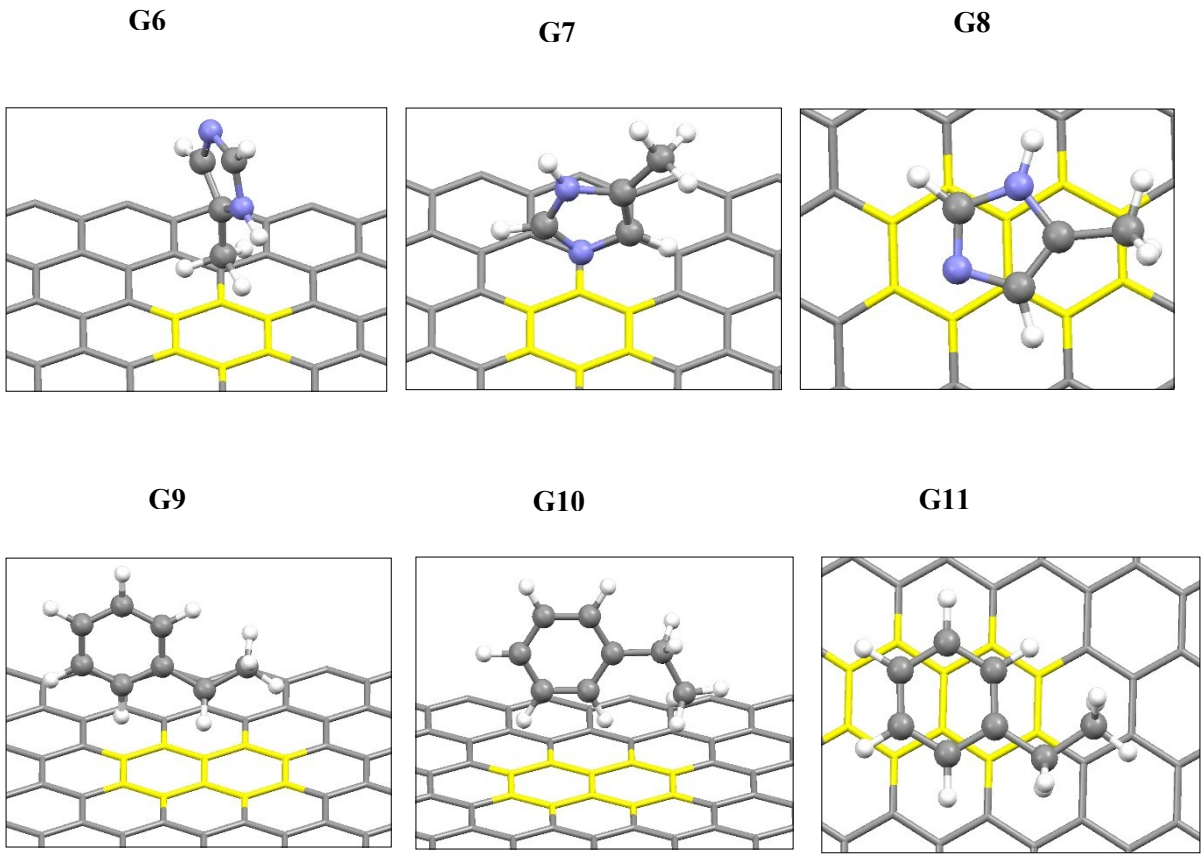

Figure S3. Orientation schemes for the Histidine and phenylalanine molecules approaching the hexagonal network of the graphene sheet with their respective active sites. (Blue: N, Gray: C and White: H).

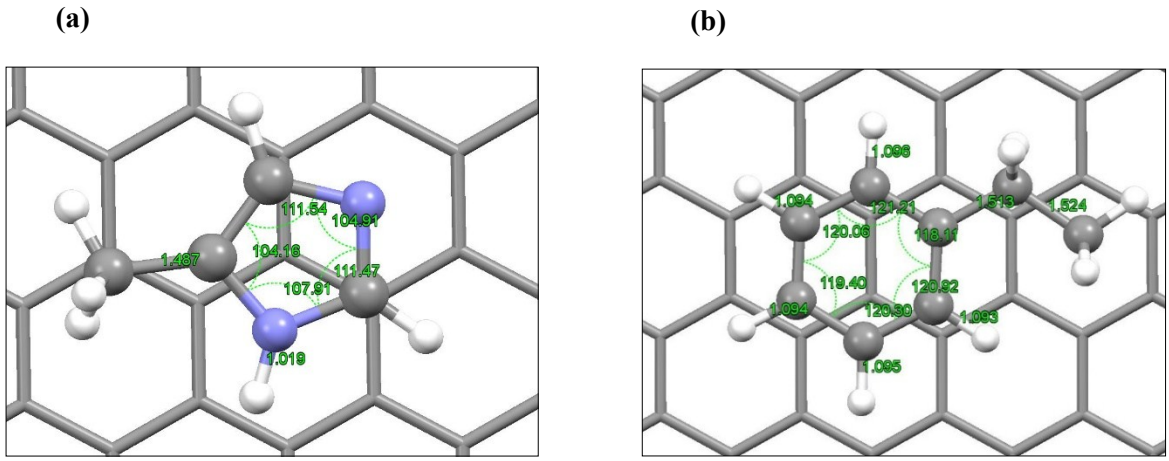

Figure S4. Optimized structures and geometrical parameters of: (a) graphene/Histidine and (b) graphene/phenylalanine complexes. (Blue: N, Gray: C and White: H).

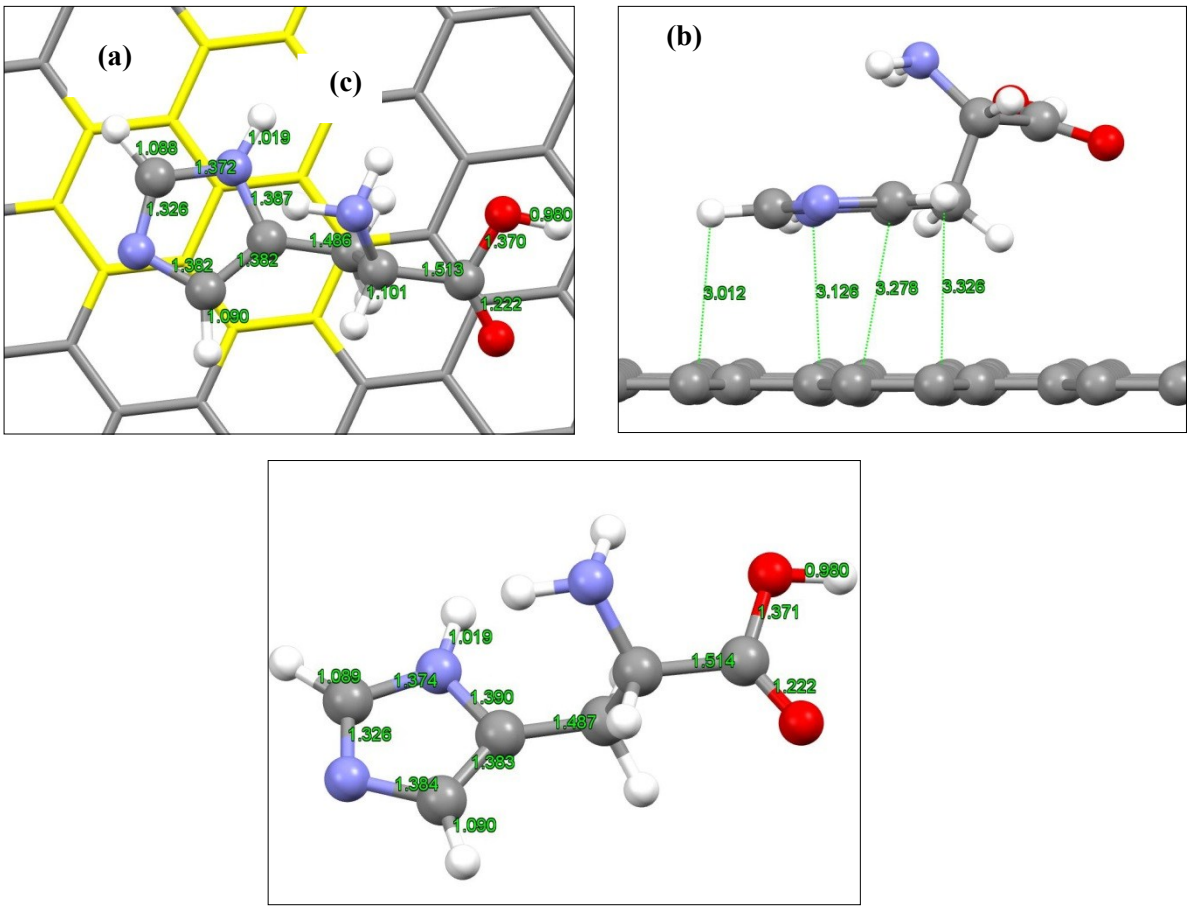

Figure S5. Optimized structures and geometrical parameters of: (a) top view of L-histidine/graphene complex, (b) side view of the complex and (c) L-histidine molecule.

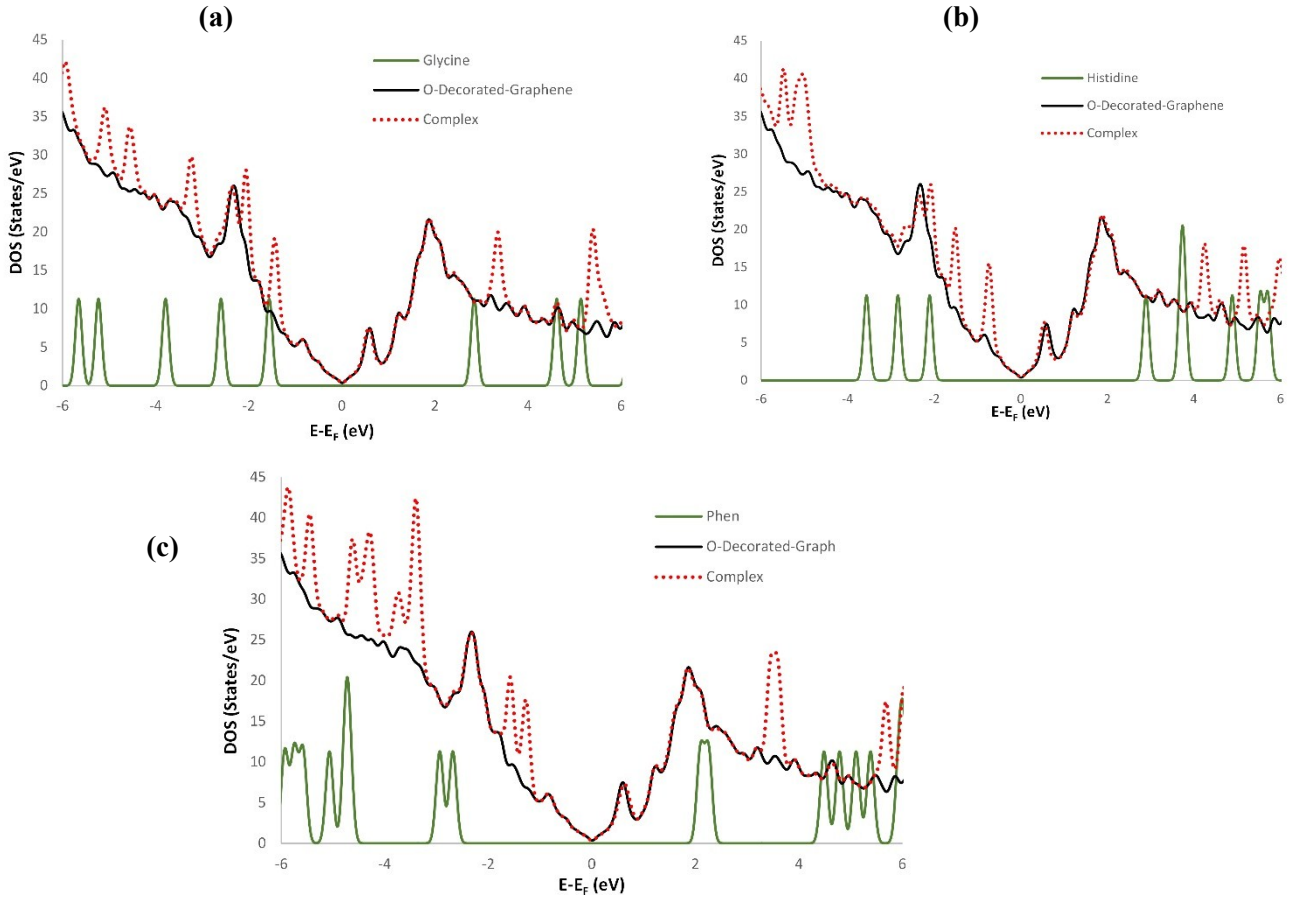

Figure S6. Total density of states of: (a) GO/glycine, (b) GO/histidine and (c) GO/phenylalanine complexes.

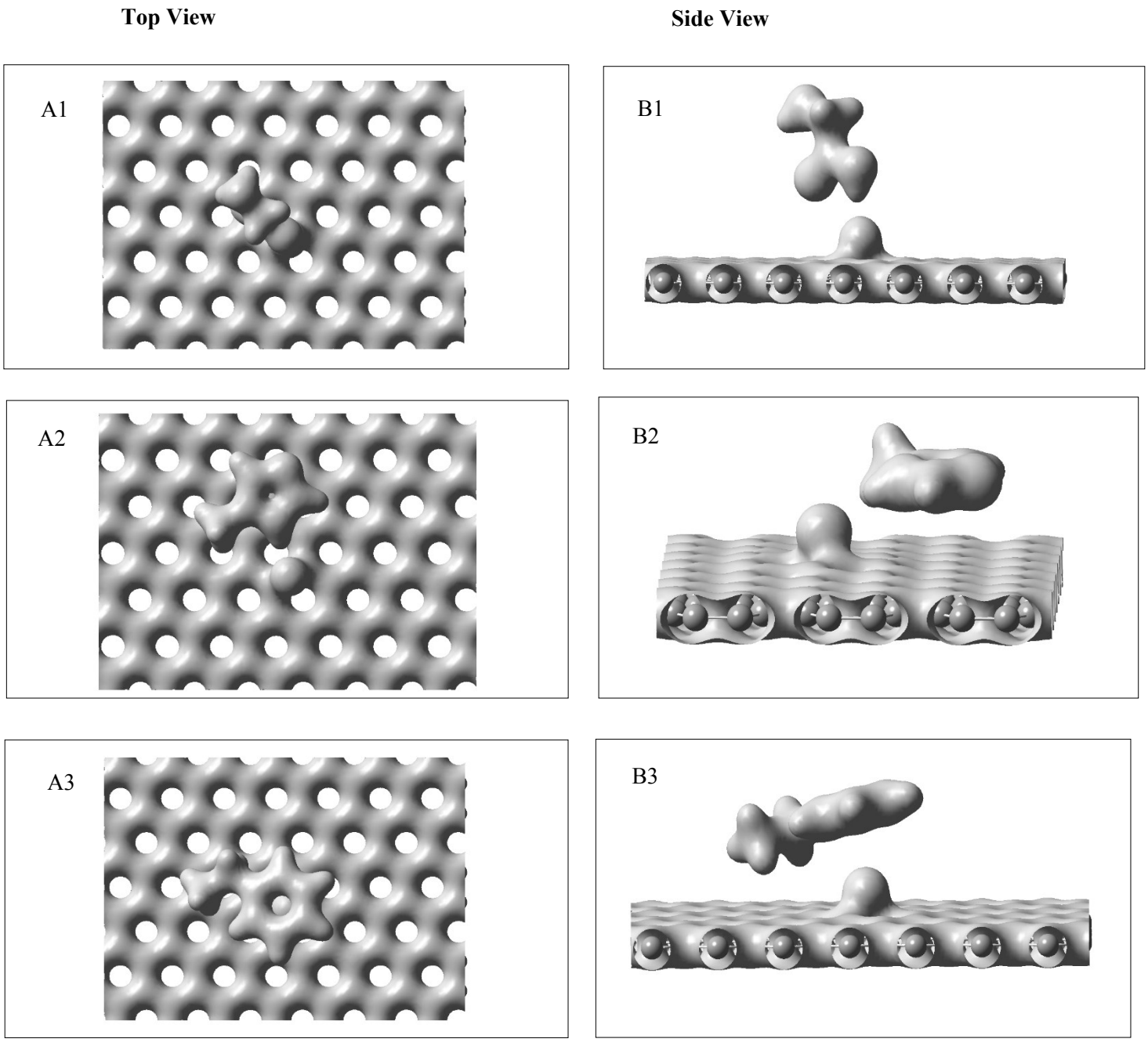

Figure S7. Isosurface maps of the total charge density for the GO/A.A complexes with isosurface value of 0.07 a.u. ((A1-A3), top views of total electron densities for the GO/glycine, GO/histidine and GO/phenylalanine complexes, respectively. (B1-B3), side

views of total electron densities for the GO/glycine, GO/histidine and GO/phenylalanine complexes, respectively)

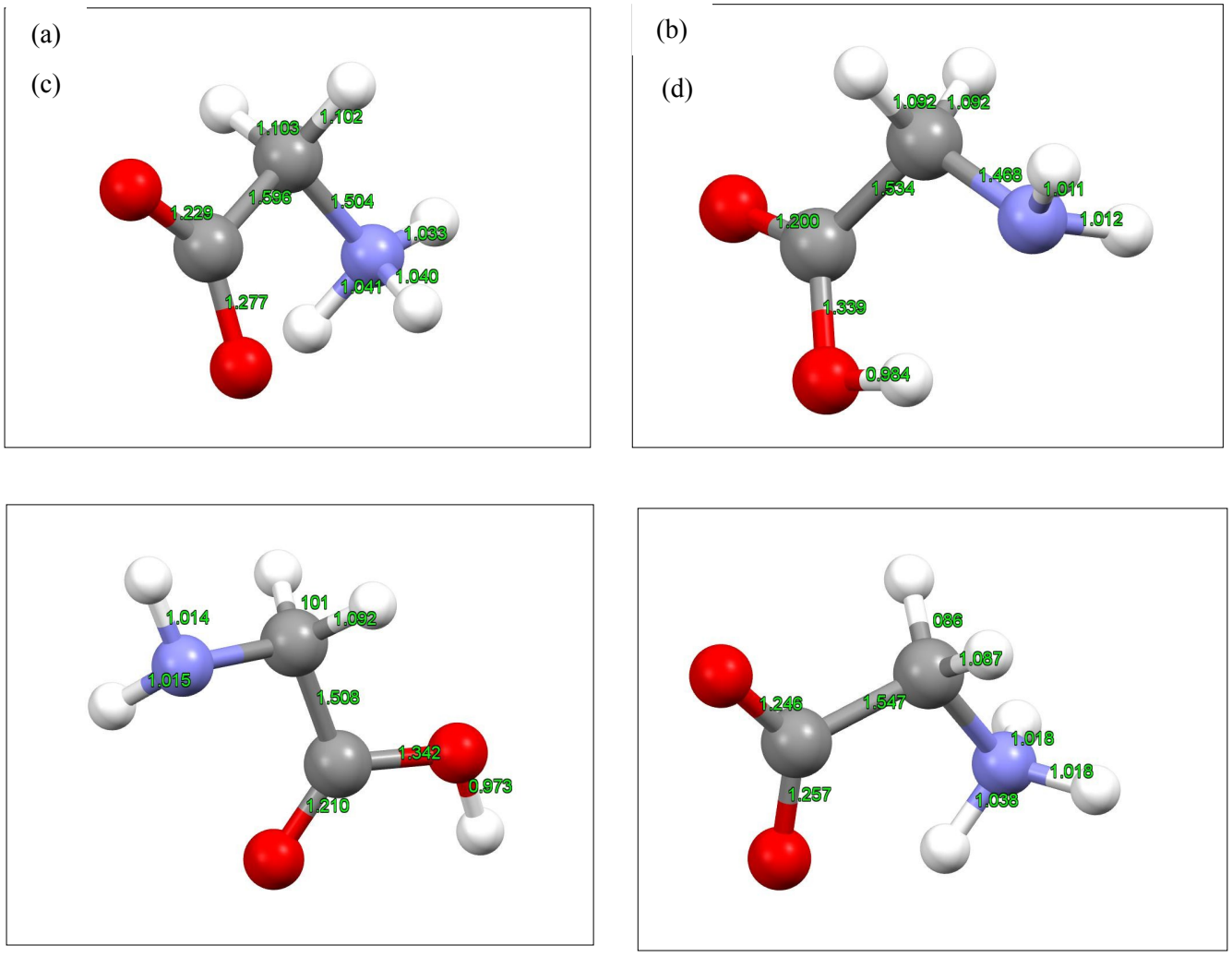

Figure S8. Schematic representations of: (a) zwitter ionic conformer before optimization, (b) optimized zwitter ionic conformer in gas phase, (c) optimized neutral conformer in water and (d) optimized zwitter ionic glycine in water. (Red: O, Blue: N, Gray: C and White: H)