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


**Supporting information**

**for**

# Computational studies on the interactions of glycine amino acid with graphene, h-BN and h-SiC monolayers

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

[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)

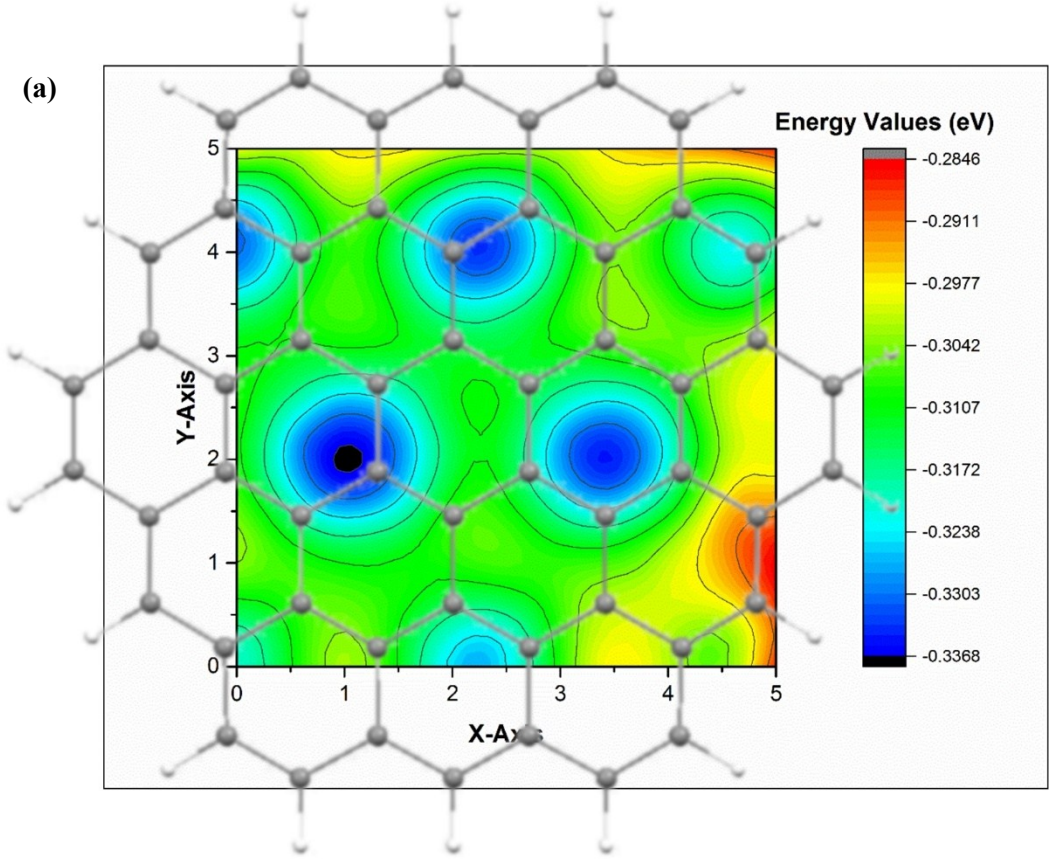
[c] Department of Electrical Engineering, Faculty of Engineering, University of Guilan, Rasht, Guilan, Iran

* Corresponding Authors: *E-mail address: ganji_md@yahoo.com (M.D. Ganji).

**Table S1. Binding energy value obtained from initial relaxation step for the glycine/h-BN system.**

| Configuration | Degree | Binding Energy (eV) |
|---|---|---|
| 1 | 0 | -0.15933 |
| 2 | 30 | -0.29867 |
| 3 | 60 | -0.29815 |
| 4 | 90 | -0.29683 |
| 5 | 120 | -0.29559 |
| 6 | 150 | -0.16123 |
| 7 | 180 | -0.16463 |
| 8 | 210 | -0.29698 |
| 9 | 240 | -0.29702 |
| 10 | 270 | -0.29924 |
| 11 | 300 | -0.29807 |
| 12 | 330 | -0.29248 |
| $NH_2$ | --- | -0.07969 |
| OH | --- | -0.08572 |

**Figure S1. (a) and (b) PES plots with overlapped graphene and h-BN lattices, respectively.**



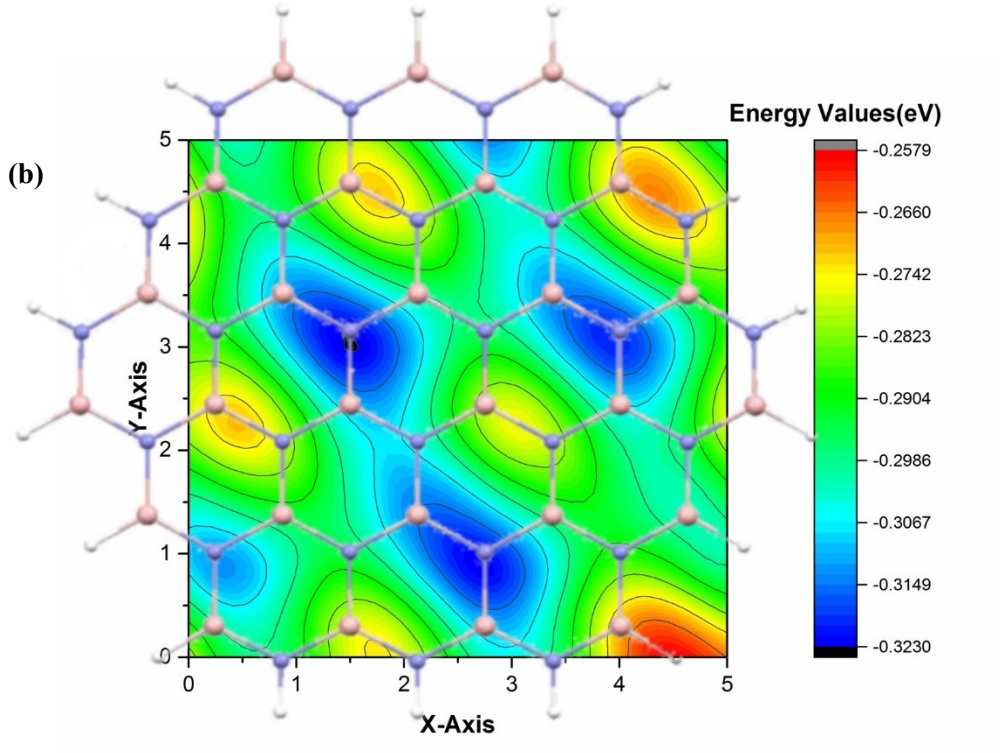



**Figure S2. Optimized geometry of glycine/graphene complex at the B3LYP-D3 Level**

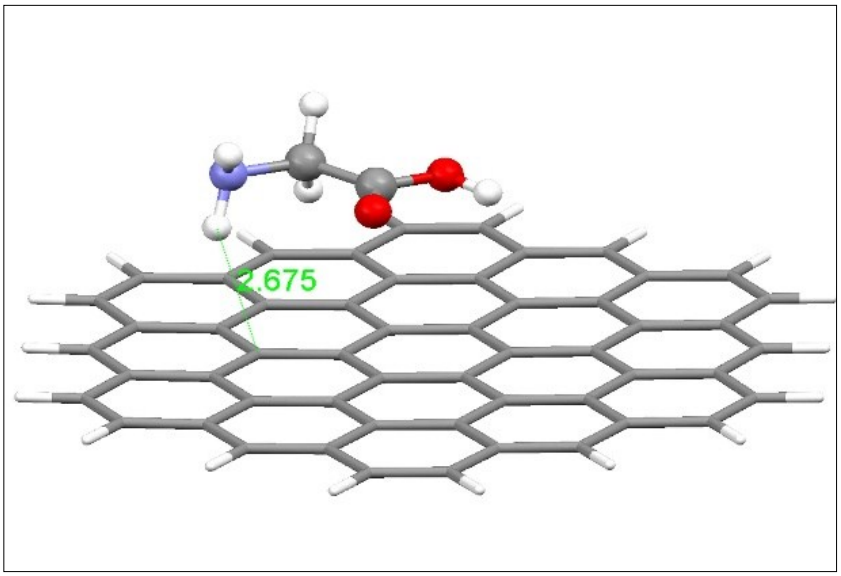


**Figure S3. PDOS plot for the glycine/h-BN system in wider energy range. The dashed vertical line corresponds to the HOMO level.**

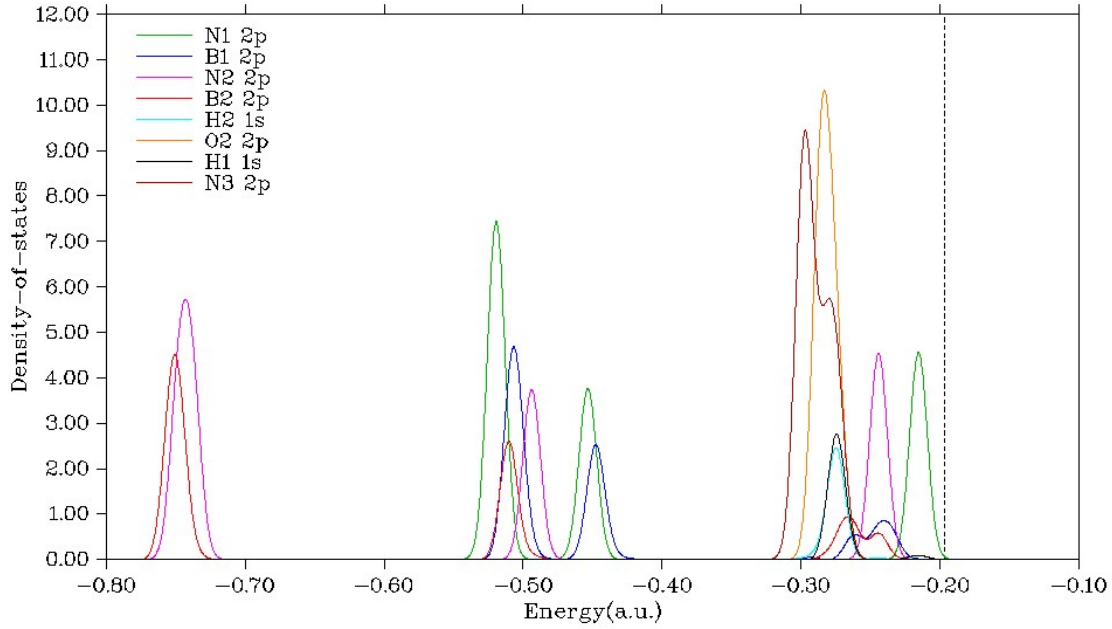


**Figure S4. Visualization of (a) HOMO and (b) LUMO of the hexagonal SiC**

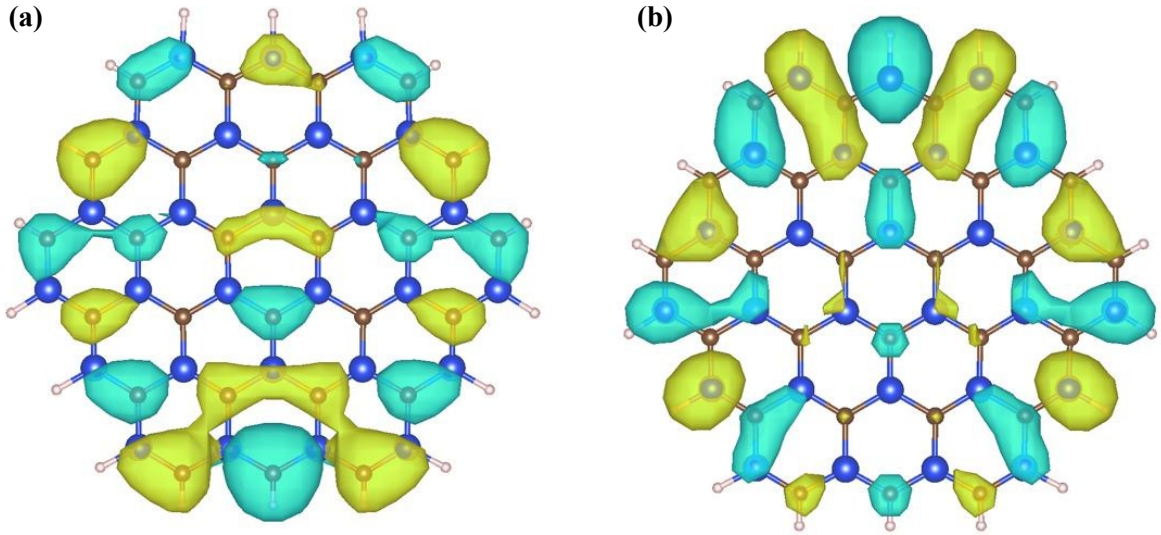


**Figure S5. Optimized structure of the glycine/h-SiC system with constrained edge atoms.**

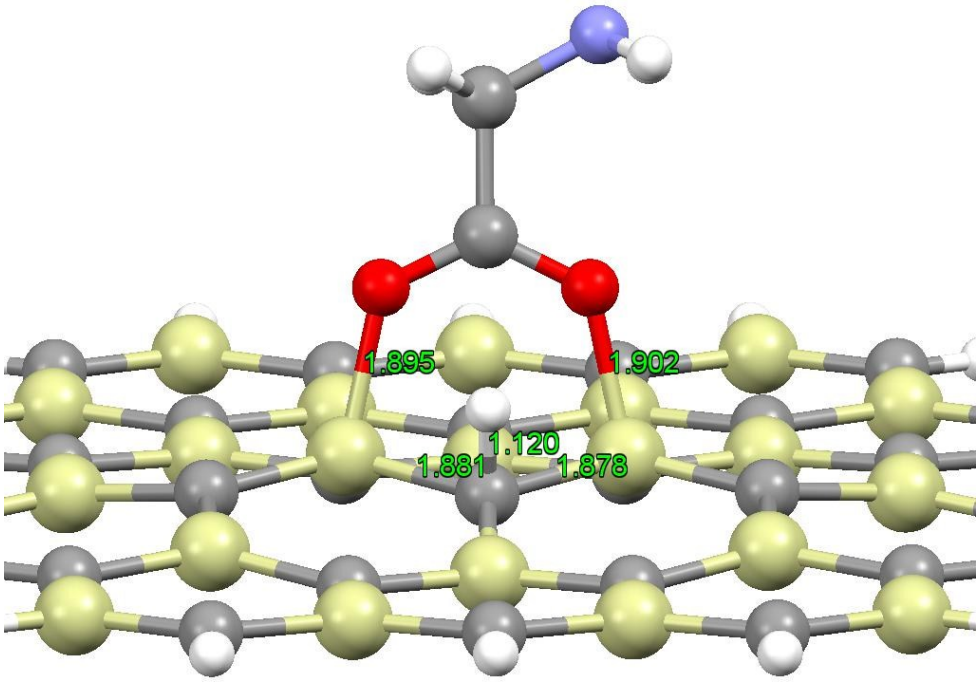


**Figure S6. PDOS plot for the glycine/h-SiC system in wider energy range. The dashed vertical line corresponds to the HOMO level.**

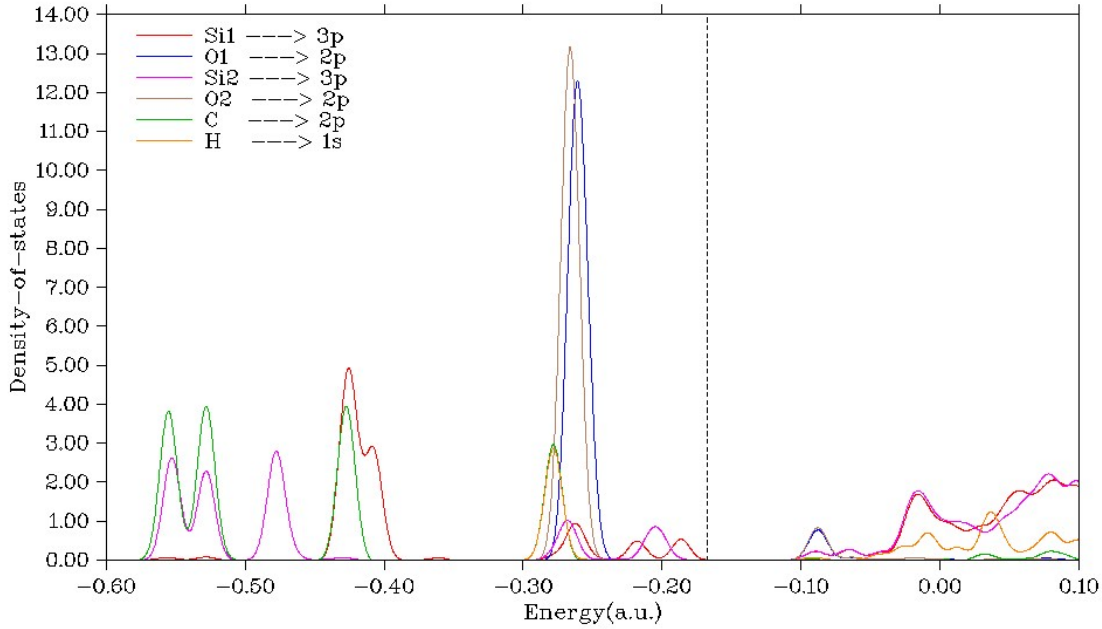


**Figure S7. (a)-(c) Optimized structures of glycine/graphene, glycine/h-BN and glycine/h-SiC systems in solvent phase, respectively. (d)-(f) Optimized structures of zwitter/graphene, zwitter/h-BN and zwitter/h-SiC systems, respectively.**

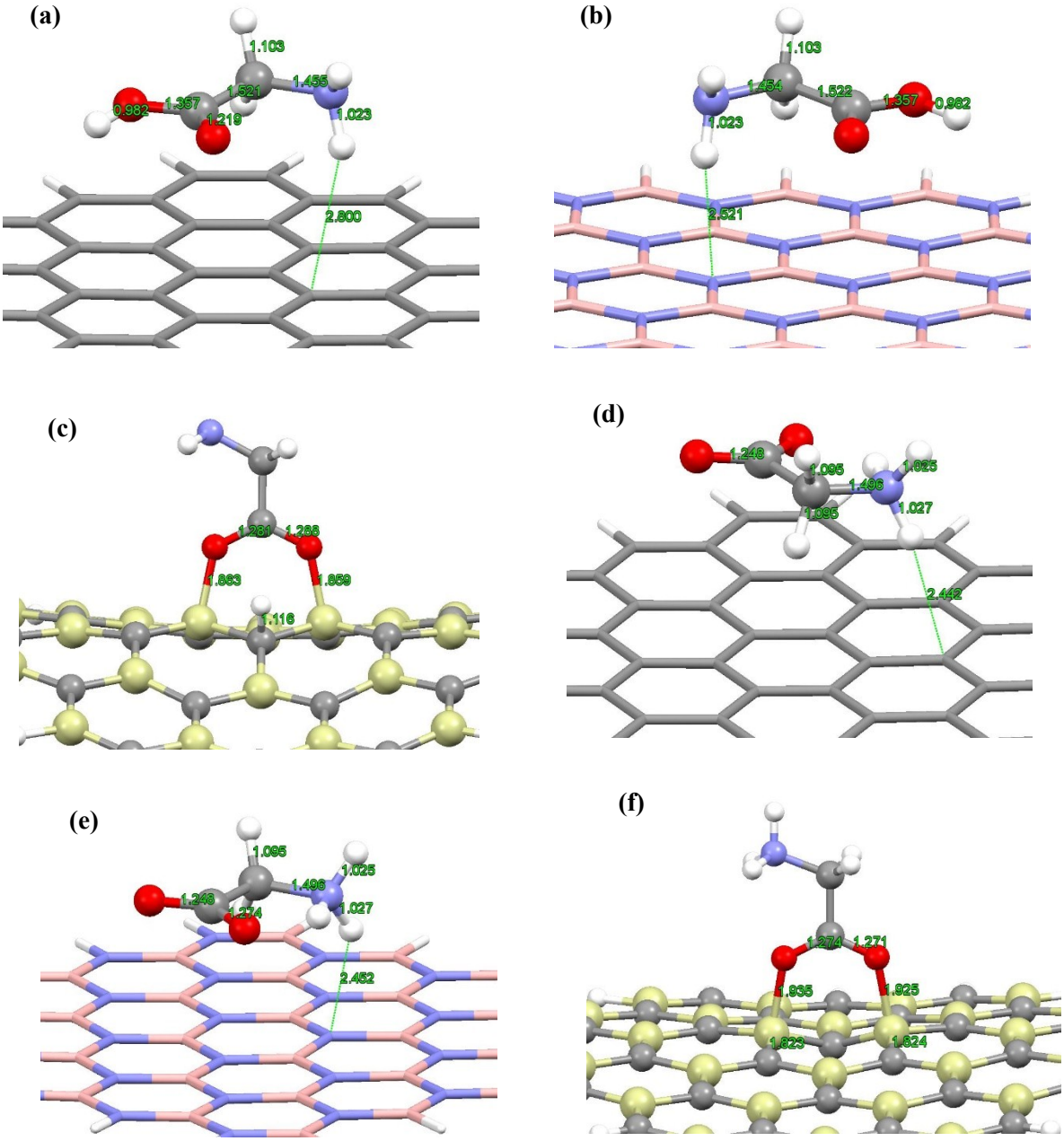


**Figure S8. Optimized structures of the miniaturized system of (a) glycine/graphene, (b) zwitter/graphene, (c) glycine/h-SiC and (d) zwitter/h-SiC at the PBE-D3 Level.**

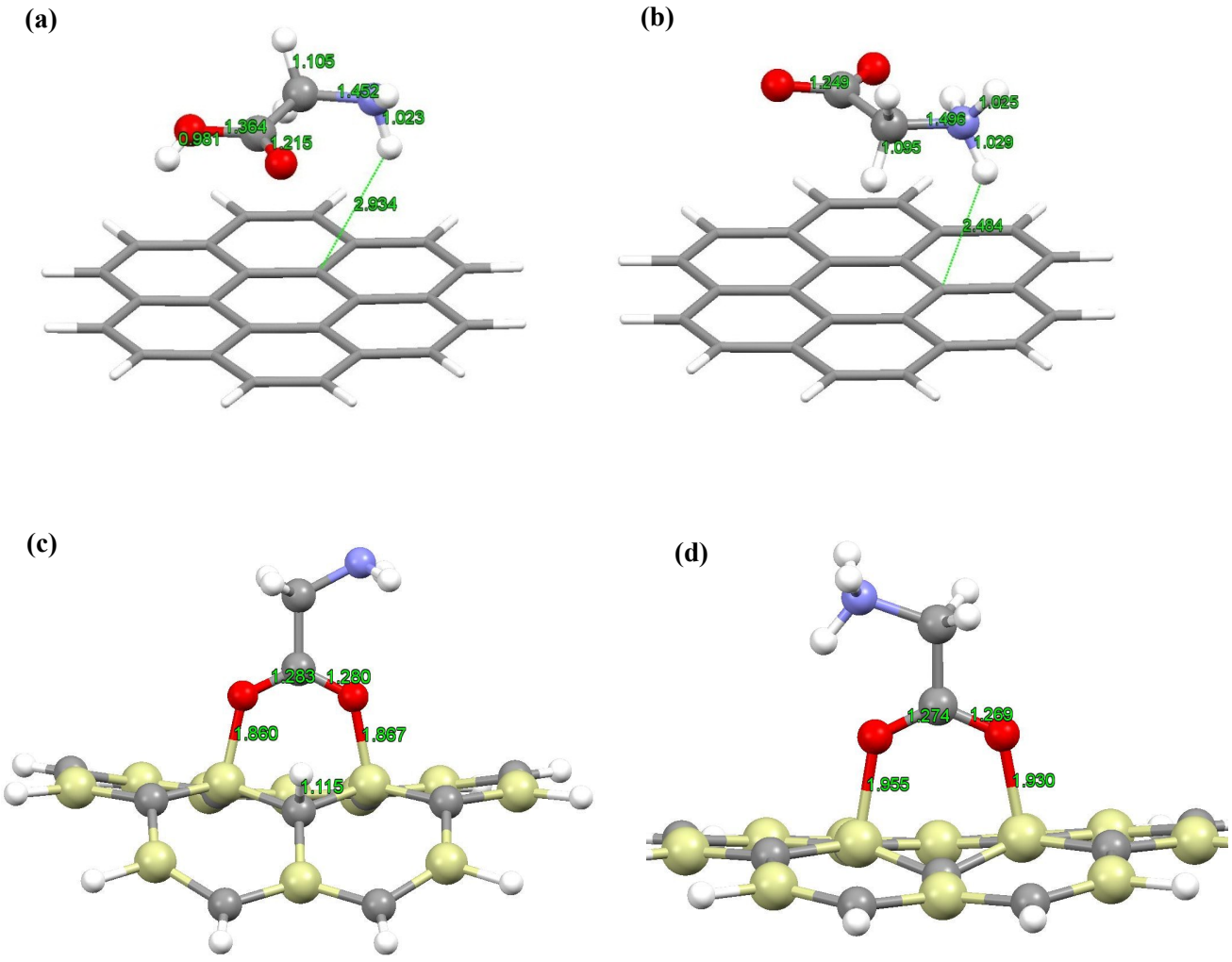


**Figure S9. Optimized structures of the miniaturized system of (a) glycine/graphene, (b) zwitter/graphene, (c) glycine/h-SiC and (d) zwitter/h-SiC at the PW6B95-D3 Level.**