Supporting Information

Theoretical study of protein adsorption on graphene/h-BN heterostructures

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Note 1. Force field parameters of GRA and h-BN

C atoms in GRA and B and N atoms in h-BN are all constructed as Lennard-Jones particles. Lennard-Jones parameters of C, B and N atoms are taken from previous groups[1-3]: $\sigma_{C\text{-}C}$=0.3580 nm, $\varepsilon_{C\text{-}C}$=0.277399 kJ/mol, $\sigma_{B\text{-}B}$=0.3453 nm, $\varepsilon_{B\text{-}B}$=0.397133 kJ/mol, $\sigma_{N\text{-}N}$=0.3365 nm, $\varepsilon_{N\text{-}N}$=0.606024 kJ/mol.

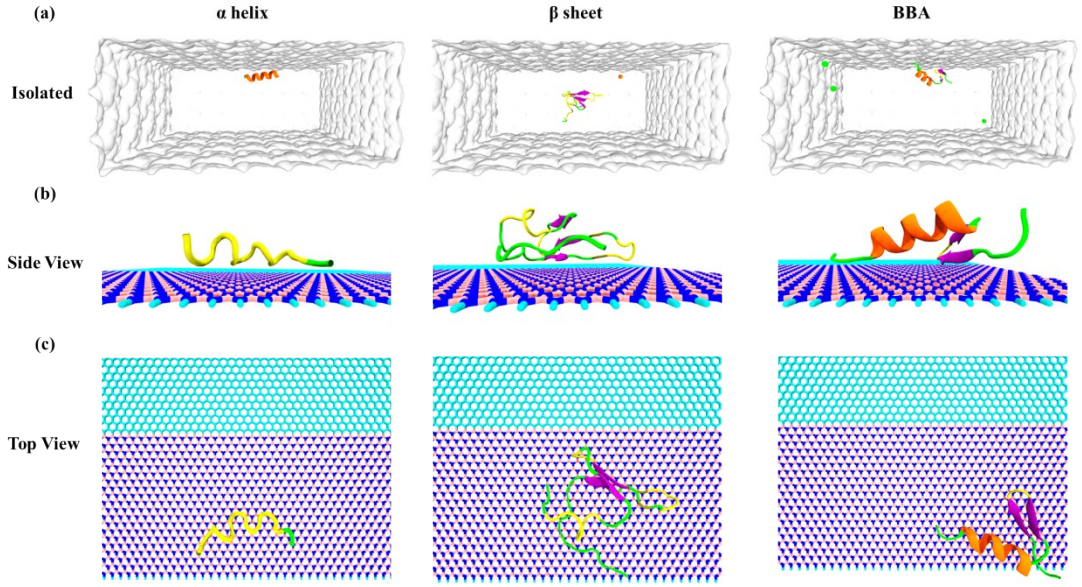

Figure S1. The initial simulated conformations of three protein in separated aqueous solutions: (a) isolated. The final conformation of orientation 1 of each protein after 200 ns MD simulation: (b) side view. (c) top view. The water molecules are implicitly expressed as gray surfaces. The protein molecules were setained according to the secondary structure, with the α-helix in orange, β-sheet in purple, β-bridge in tan, coil in green, turn in yellow, and ions (represented by balls) stained according to the element type (Na^+: orange, CL^-: green). Herein, the α helix in the first column represents λ_{2-16} protein, the β sheet in the second column represents WW domain protein, and the last column represents BBA protein. For the clarity, no water molecule was shown (b) and (c).

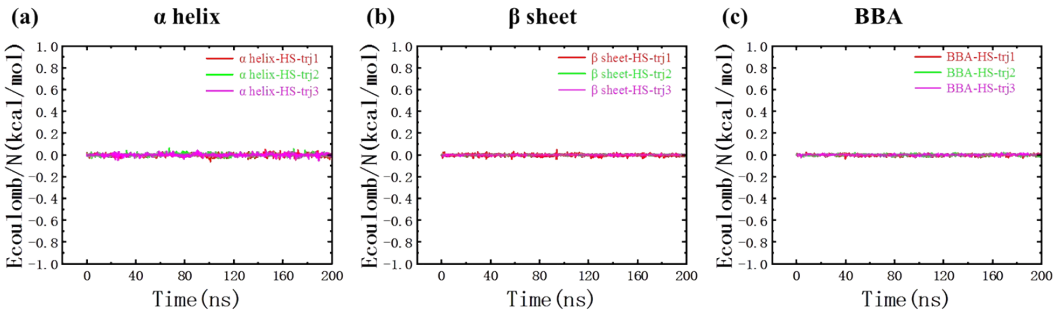

Figure S2. Coulomb interaction between three protein and GRA/h-BN heterojunction (average to per contact residue): (a) λ_{2-16} protein. (b) WW domain protein. (c) BBA protein.

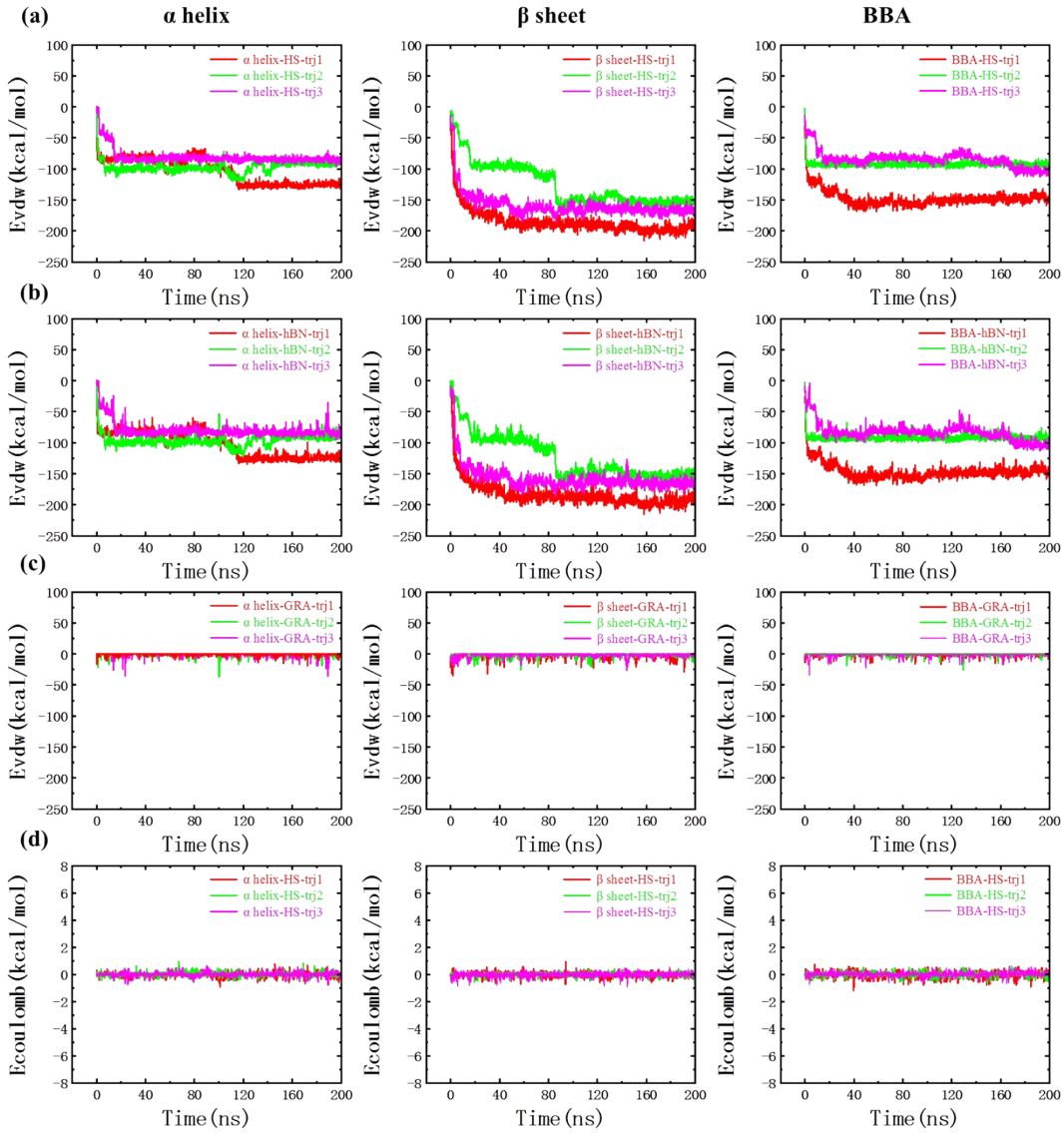

Figure S3. The total vdW and Coulomb interaction energies of all residues of three protein species with GRA/h-BN: (a) the vdW interaction between protein and the

whole heterojunction plane (HS stands for the whole heterojunction plane). (b) the vdW interaction between protein and hBN region of heterojunction. (c) the vdW interaction between protein and GRA region of heterojunction. (d) the Coulomb interaction between protein and the whole heterojunction plane. Herein, the α helix in the first column represents λ2–16 protein, the β sheet in the second column represents WW domain protein, and the last column represents BBA protein.

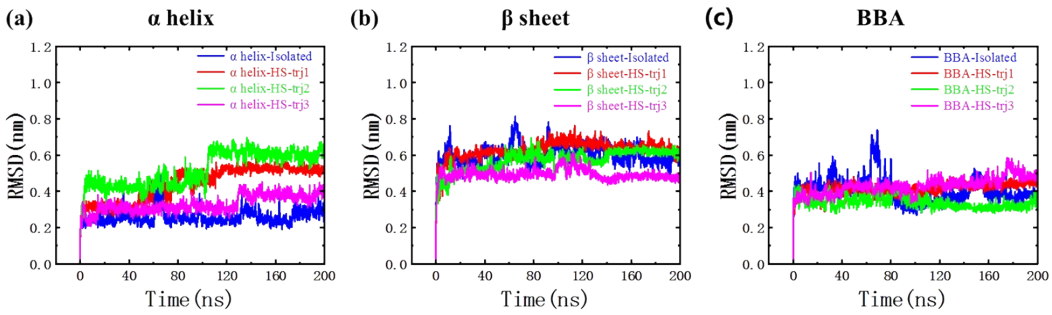

Figure S4. The evolution of three protein root mean square deviation (RMSD) with time in the simulation process: (a) λ_{2-16} protein. (b) WW domain protein. (c) BBA protein.

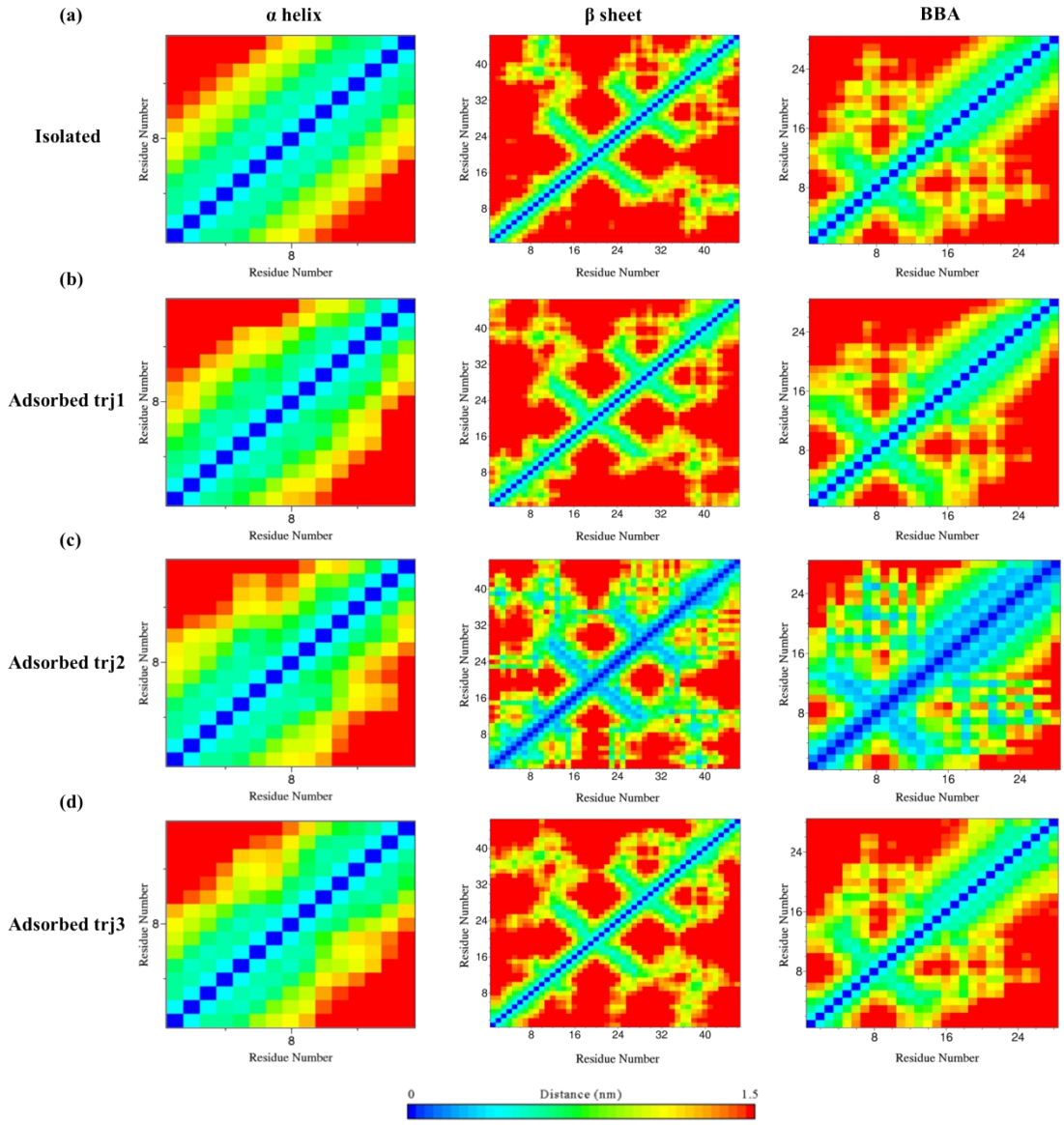

Figure S5. The average distance of Cα (c-alpha) atoms of three kinds of protein residues :(a) isolated. (b) orientation 1. (c) orientation 2. (d) orientation 3. Herein, the α helix in the first column represents λ_{2-16} protein, the β sheet in the second column represents WW domain protein, and the last column represents BBA protein.

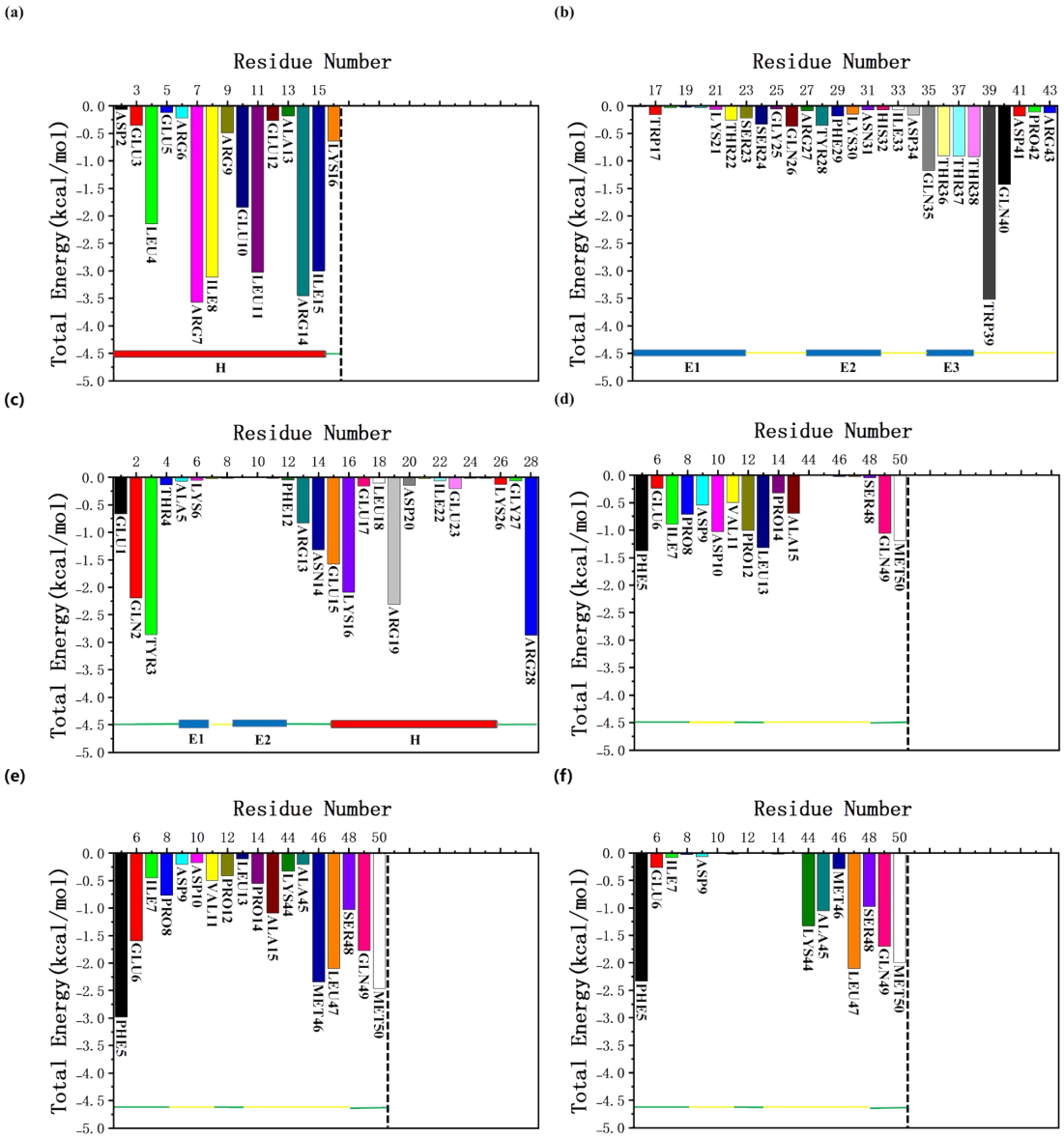

Figure S6. Energy contribution of protein residues to binding free energy in the third initial orientation: (a) λ_{2-16} protein. (b) WW domain protein. (c) BBA protein. Energy contribution of bend and coil region residues in the head and tail of WW domain protein (Non-core β-sheet structure region) to binding free energy: (d) orientation 1 of WW domain protein. (e) orientation 2 of WW domain protein. (f) orientation 3 of WW domain protein.

References

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