Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supplementary Information

Tuning the Binding Behaviors of Protein YAP65WW Domain on Graphenic Nano-Sheets with Boron or Nitrogen Atom Doping

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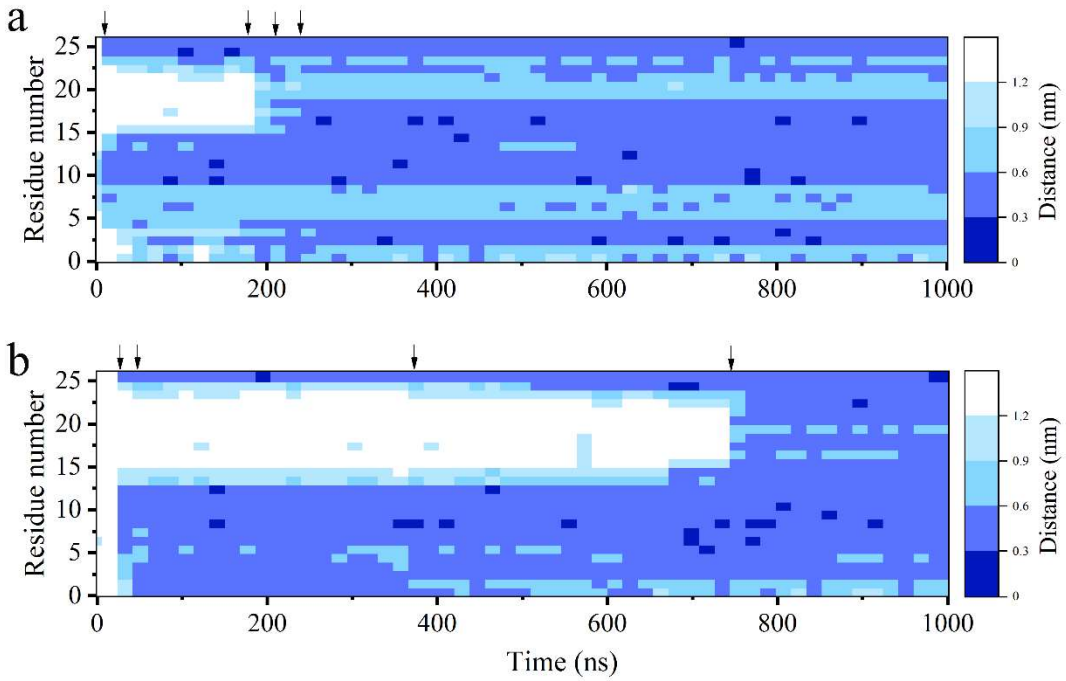

Figure S1. The evolutions of the contact state of protein residues with (a) BC_3 and (b) C_3N. Deep blue indicates formation of intimate contacts.

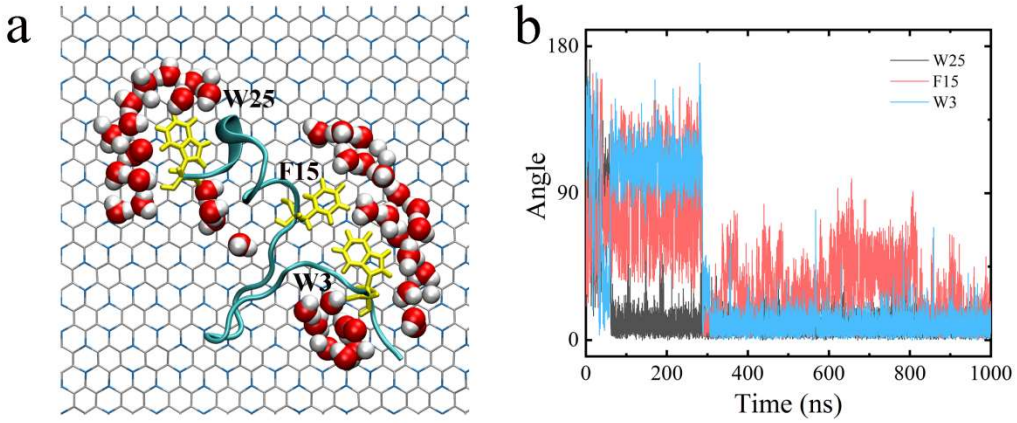

Figure S2. (a) The top view of YAP65WW on BC_3 at 1000ns. The water molecules within 0.6nm to both BC_3 and contacting residues (W3, F15 and W25) are shown as spheres. (b) Time evolutions of the stacking angle between contacting aromatic residues (W3, F15 and W25) and the BC_3 sheet. Angles are defined by the normal directions of the aromatic rings and the z-axis (normal direction of BC_3 sheet). Thus, a value of 0 degree represents face-to-face stacking.

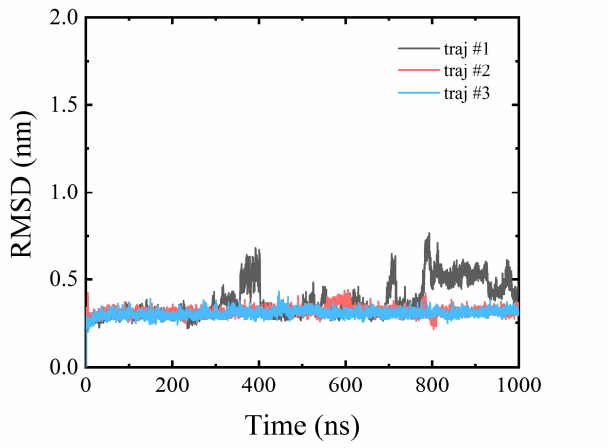

Figure S3. Time evolutions of the root-mean-squared deviation (RMSD) of the YAP65WW heavy atoms in water with respect to the crystal structure in three trajectories.

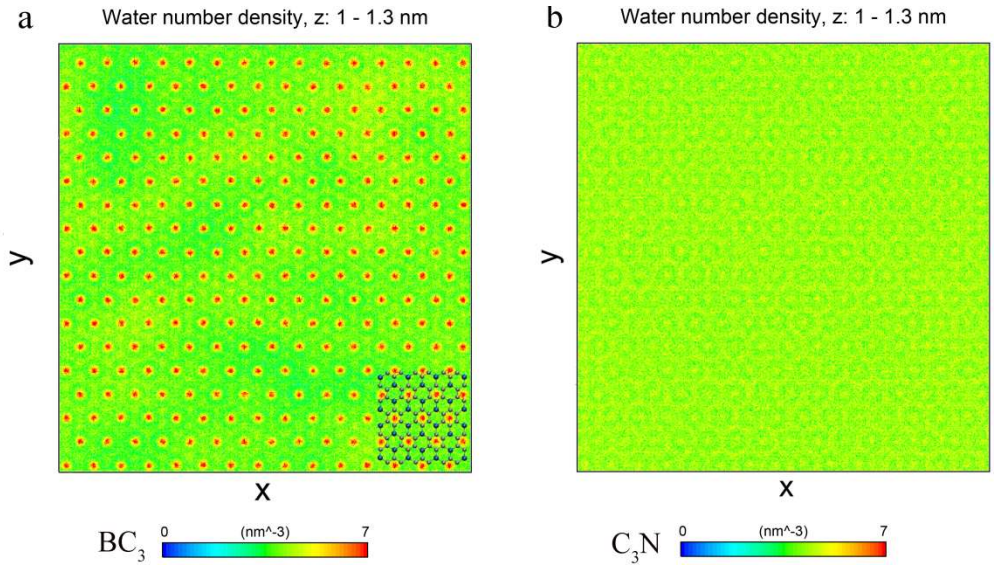

Figure S4. Two dimensional density contour map of the solvation water shell of (a) BC_3 and (b) C_3N.

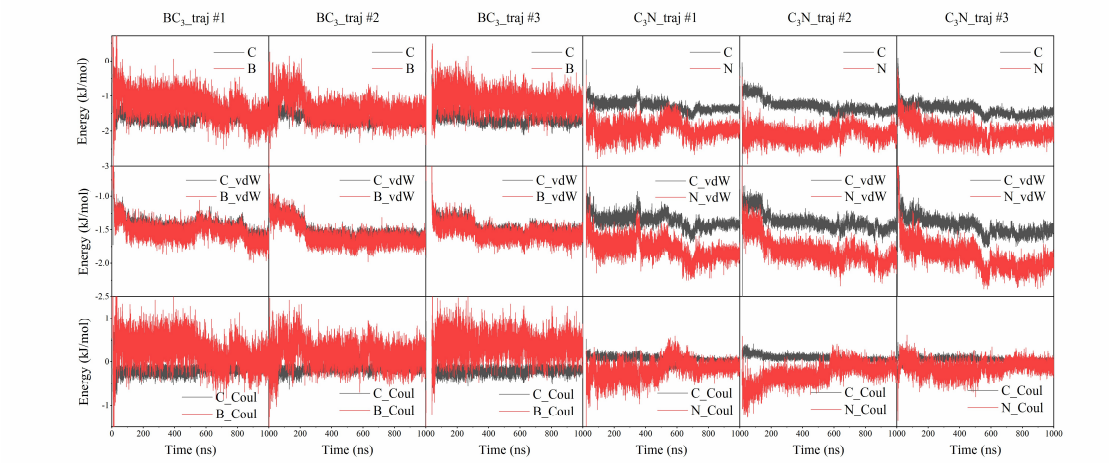

Figure S5. The time evolutions of total interaction energy, van der Waals (vdW) and Coulomb (Coul) contributions between protein and atoms in BC_3/C_3N.