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ARTICLE

Supporting Information

Density functional study on noncovalent functionalization of pyrazinamide chemotherapeutic with graphene and its prototypes

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Table S1. The adsorption energy (E_{ads}, eV), HOMO–LUMO energy gap (eV) and dipole moment (Debye) values for graphene sheet and its prototypes including SW defect graphene and BN sheets.

System	E_{ads}	HOMO – LUMO gap	Dipole moment
Pyrazinamide	–	0.330	3.923
6×6 graphene	–	0.041	0.000
PZA/6×6 graphene (top)	1.943	0.043	2.518
PZA/6×6 graphene (bridge)	1.874	0.043	2.554
PZA/6×6 graphene (hollow)	1.807	0.043	2.722
6×6 BN nanosheet	–	0.361	8.632
PZA/6×6 BN nanosheet (N top)	2.301	0.306	8.937
PZA/6×6 BN nanosheet (B top)	1.816	0.304	8.710
PZA/6×6 BN nanosheet (bridge)	2.088	0.304	9.009
PZA/6×6 BN nanosheet (hollow)	1.960	0.305	8.950
6×6 C-doped BN nanosheet	–	0.197	15.302
PZA/6×6 C-doped BN nanosheet (top)	1.786	0.2009	13.875
PZA/6×6 C-doped BN nanosheet (bridge)	1.769	0.2008	13.932
PZA/6×6 C-doped BN nanosheet (hollow)	1.678	0.2007	13.914
6×6 BN doped graphene	–	0.080	10.862
PZA/6×6 BN doped graphene (N top)	2.601	0.071	14.533
PZA/6×6 BN doped graphene (B top)	2.189	0.077	12.079
PZA/6×6 BN doped graphene (hollow)	2.499	0.071	14.880
PZA/6×6 BN doped graphene (bridge)	2.542	0.071	14.646
SW_graphene	–	0.0440	0.095
SW_graphene/PZA over 5ring	0.551	0.0441	6.388
SW_graphene/PZA over 7ring	0.640	0.044	6.725
SW_BN sheet	–	0.335	10.516
SW_BN sheet/PZA over 5ring	0.714	0.289	10.321
SW_BN sheet/PZA over 7ring	0.755	0.290	13.347

Table S2. The noncorrected adsorption energy (E_{ads}, eV) and BSSE corrected adsorption energy values of PZA/nanosheets calculated using the hybrid B3LYP functional and 6-31G(d,p) basis set of G09 program. All parameters are in units of eV.

System	E_{ads} (B3LYP/6-316 (d,p)	BSSE corrected E_{ads} energy (B3LYP/6-316 (d,p)	BSSE correction
PZA/6×6 graphene (Top site)	0.775	0.636	0.1385
PZA/6×6 BN sheet (N top site)	0.956	0.792	0.164
PZA/6×6 BN doped graphene (N top site)	1.203	0.960	0.243
PZA/6×6 C–doped BN sheet (top site)	0.858	0.719	0.1382

Table S3. Best docking poses of PZA and PZA/nanosheets onto the binding site of pncA protein using MVD, based on MolDock and re–rank score. The parameters are in arbitrary units.

Molecule	MolDock Score	Re-rank score
PZA	-54.644	-46.609
PZA/graphene	-135.694 (sheet)	-40.401 (sheet)
	-56.054 (PZA)	-47.553 (PZA)
PZA/BN nanosheet	-141.116 (sheet)	-119.941(sheet)
	-53.987 (PZA)	-45.734 (PZA)
PZA/C doped BN nanosheet	-149.580 (sheet)	-59.196 (sheet)
	-52.008 (PZA)	-44.155 (PZA)
PZA/BN doped graphene	-166.440 (sheet)	-111.381(sheet)
	-53.705 (PZA)	-44.417 (PZA)

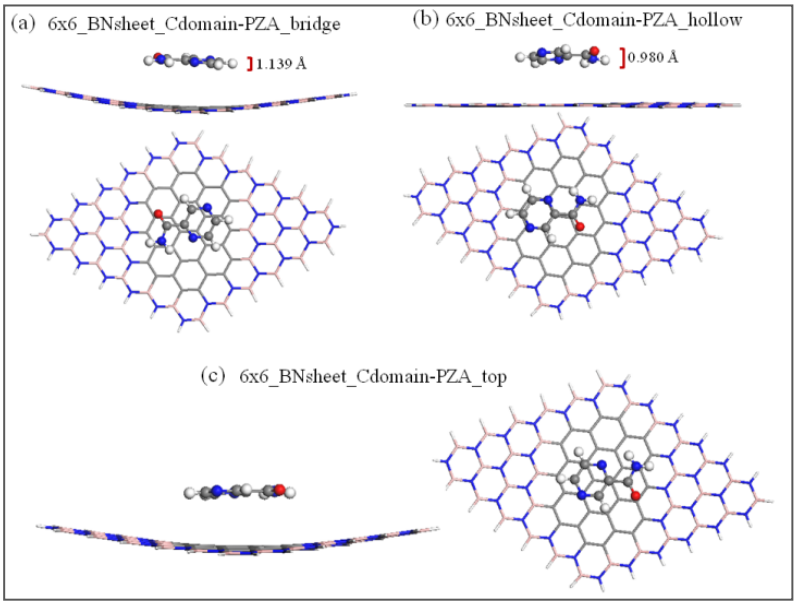

Fig. S1 The side and front view of PZA adsorbed onto C doped 6×6 BN sheet at (a) bridge, (b) hollow, and (c) top sites. The values in square bracket denote the degree of slanting of PZA molecule upon adsorption onto C doped BN surface.

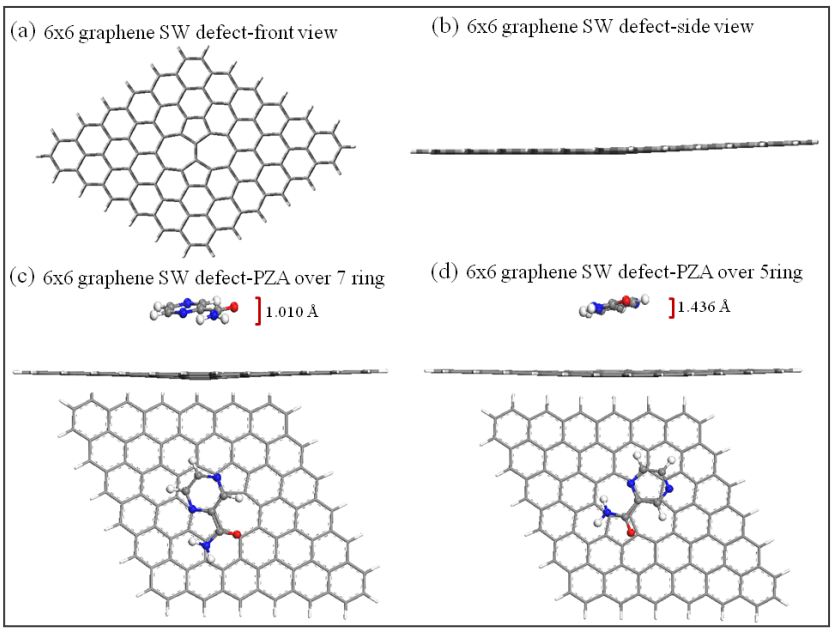

Fig. S2 The optimized geometries of SW-defect incorporated 6×6 graphene sheet for (a) front view, (b) corresponding side view, (c) front and side view depiction of PZA adsorbed onto SW-defect modified 6×6 graphene sheet over the heptagon ring, (d) front and side view depiction of PZA adsorbed onto SW-defect modified 6×6 graphene sheet with the pyrazine ring of PZA over the pentagon.

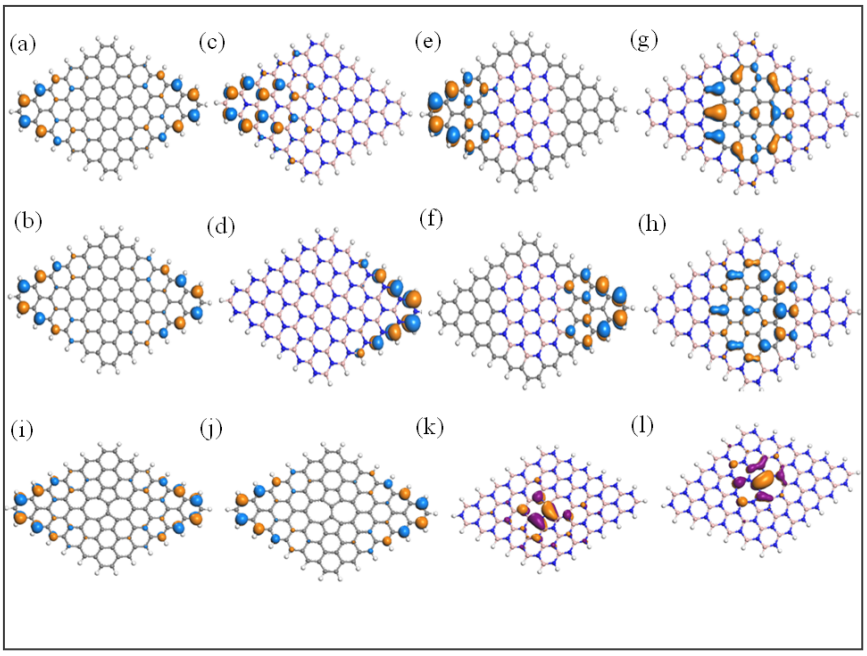

Fig. S3 (a) HOMO isosurface of 6×6 graphene sheet, (b) LUMO plot of 6×6 graphene sheet, (c) HOMO plot of 6×6 BN sheet, (d) corresponding LUMO plot, (e) HOMO plot of BxNy co-doped 6×6 graphene sheet, (f) LUMO plot of BxNy co-doped 6×6 graphene sheet, (g) HOMO plot of C doped 6×6 BN sheet, (h) corresponding LUMO plot, (i) HOMO plot of SW-defect modified 6×6 graphene sheet, (j) corresponding LUMO of SW-defect modified 6×6 graphene sheet, (k) HOMO plot of SW-defect modified 6×6 BN sheet, (l) corresponding LUMO of SW-defect modified 6×6 BN sheet.

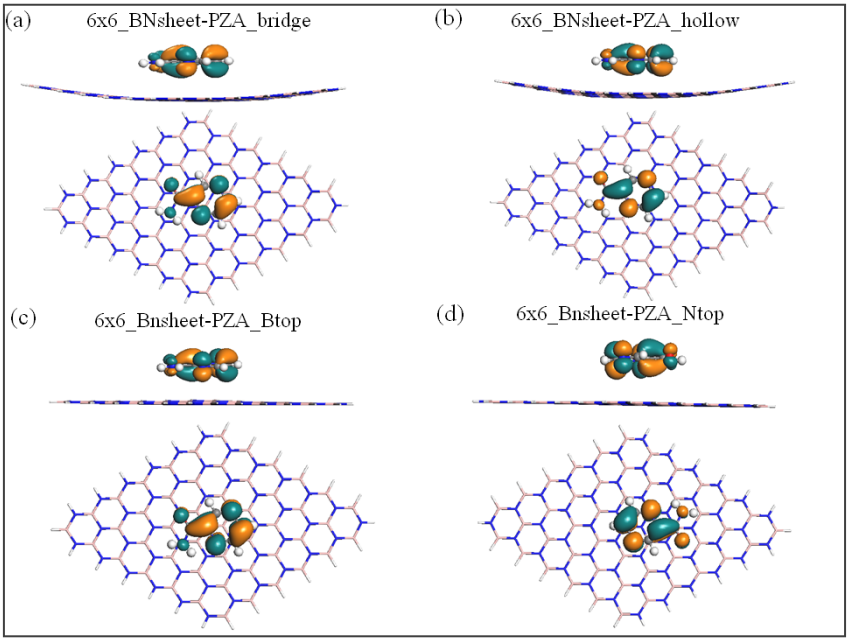

Fig. S4 The LUMO isosurface of 6×6 BN sheet with PZA drug adsorbed at (a) bridge, (b) hollow, (c) B top and (d) N top sites.

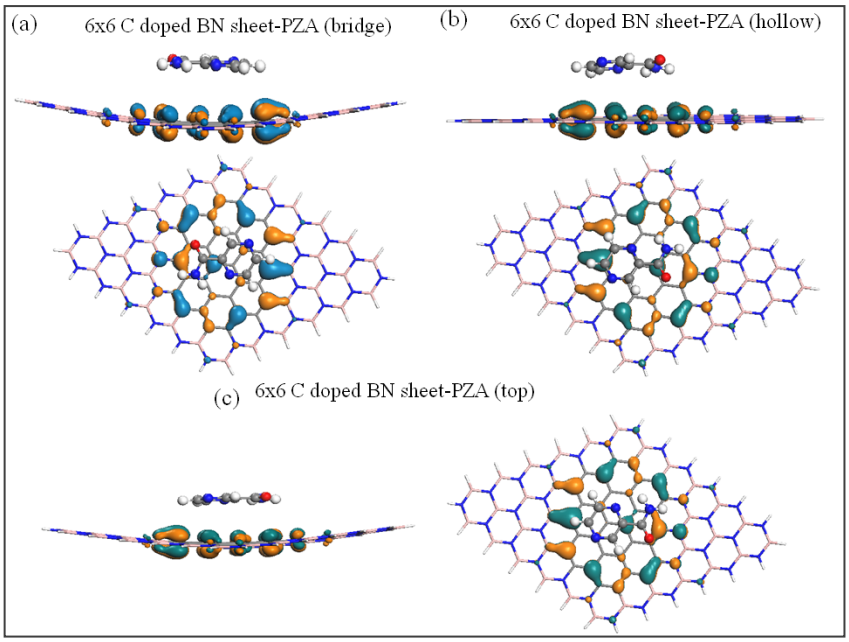

Fig. S5 The HOMO isosurface of C doped 6×6 BN sheet with PZA drug adsorbed at (a) bridge, (b) hollow, and (c) top sites.

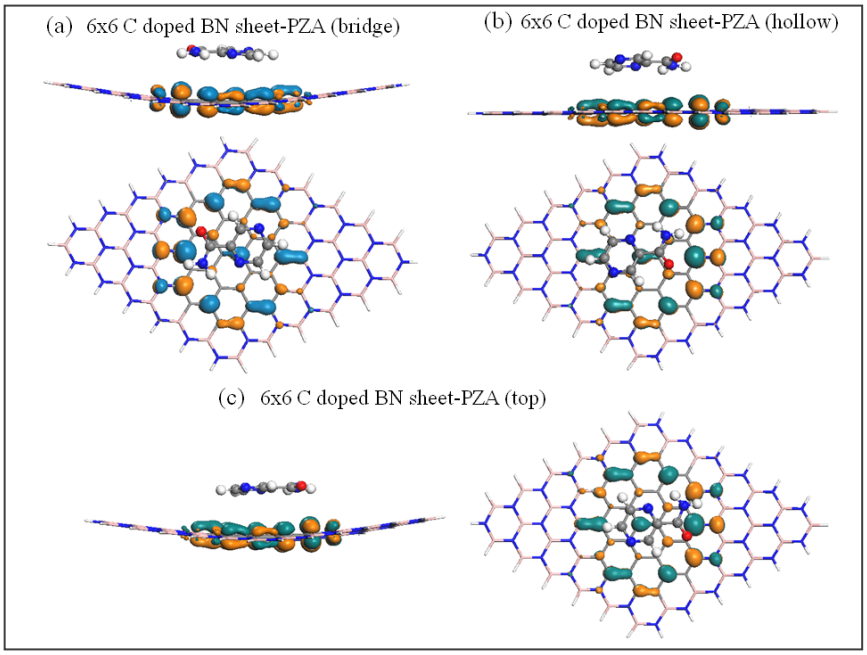

Fig. S6 The LUMO isosurface of C doped 6×6 BN sheet with PZA drug adsorbed at (a) bridge, (b) hollow, and (c) top sites.

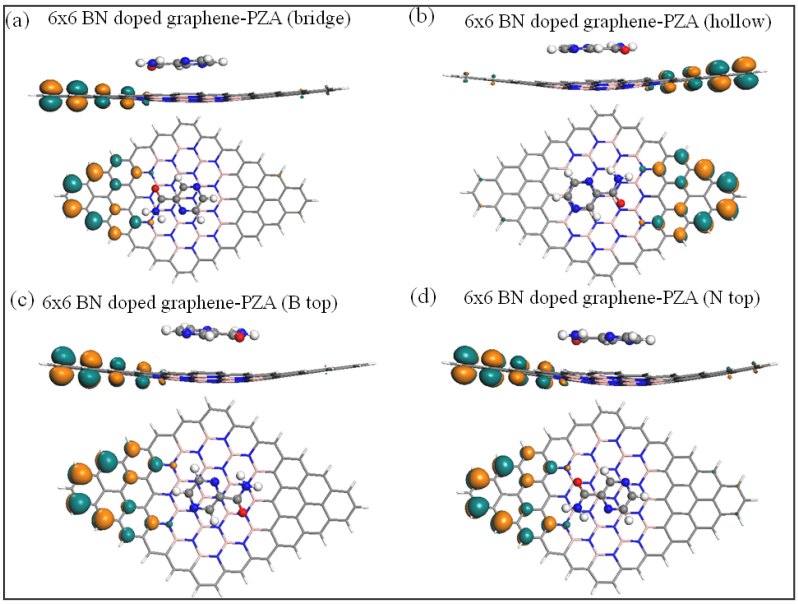

Fig. S7 The HOMO isosurface of BxNy doped 6×6 graphene sheet with PZA drug adsorbed at (a) bridge, (b) hollow, (c) B top and (d) N top sites.

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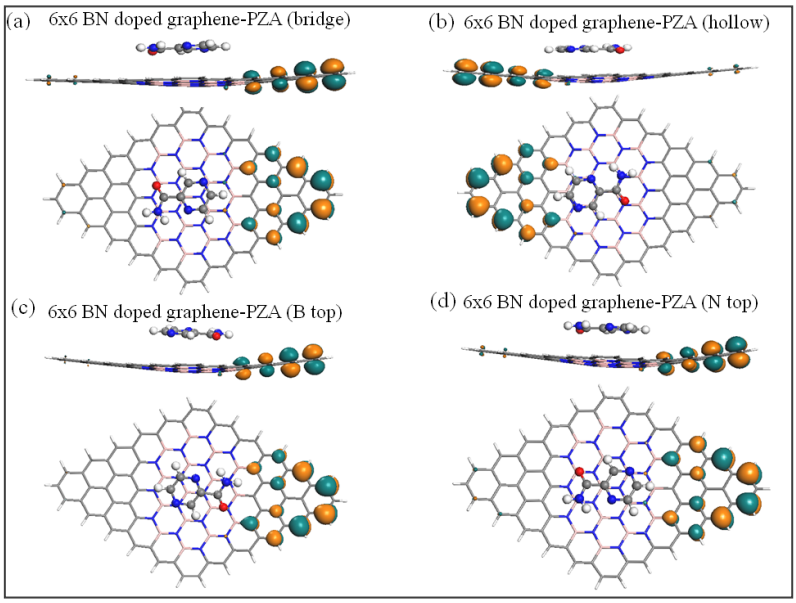

Fig. S8 The LUMO isosurface of BxNy doped 6×6 graphene sheet with PZA drug adsorbed at (a) bridge, (b) hollow, (c) B top and (d) N top sites.

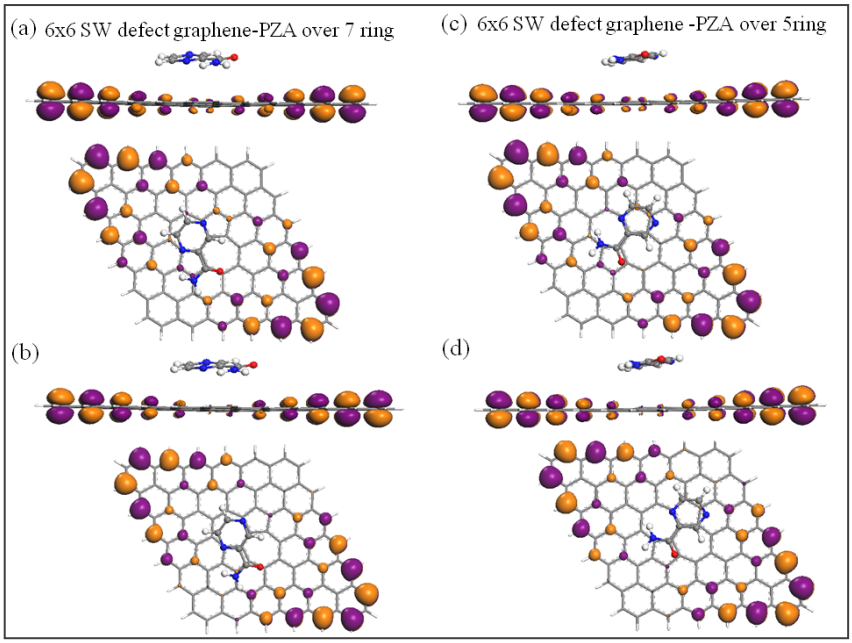

Fig. S9 (a) The HOMO of PZA/SW-defect 6×6 BN sheet with the pyrazine ring of PZA over heptagon ring, (b) HOMO of PZA/SW-defect modified 6×6 BN sheet with the pyrazine ring of PZA over the pentagon ring, (c) LUMO of PZA/SW-defect modified 6×6 BN sheet with the pyrazine ring of PZA over heptagon ring, (b) LUMO of PZA/SW-defect modified 6×6 BN sheet with the pyrazine ring of PZA over pentagon ring.

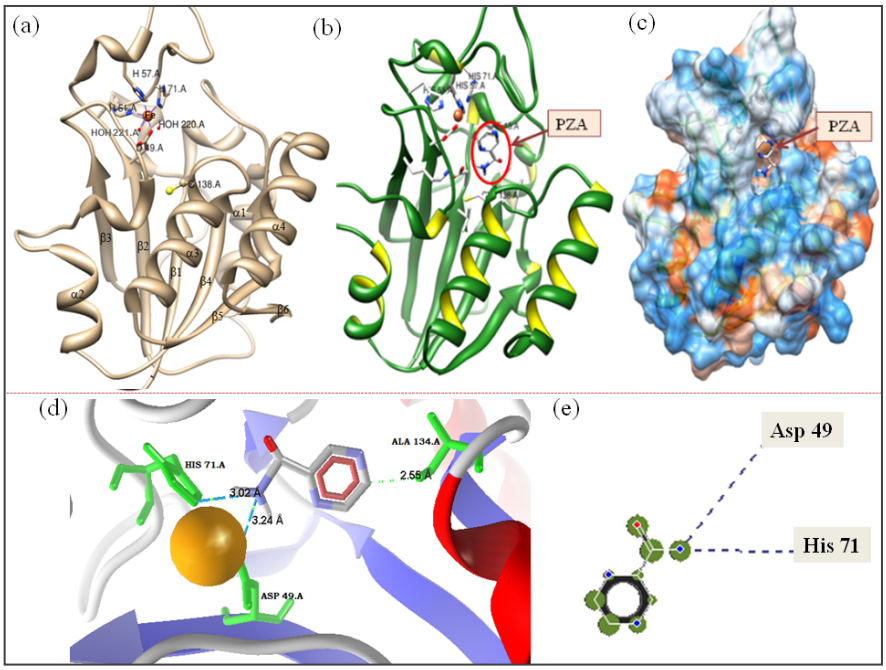

Fig. S10 (a)The optimized structure of pncA protein depicting the active binding residues and the Fe^{2+} cofactor, (b) docked conformation of PZA within the active binding site of pncA protein (PZA drug is denoted within the red circle), and (c) the hydrophobic surface of PZA drug docked within pncA protein, (d) Hydrogen bond interaction between PZA and His71 and Asp49 (lines shown in blue) and non-bonded interaction between PZA and Ala134 (lines shown in green) of the protein pncA. The Fe^{+2} co-factor is depicted in orange circle. The Figure is adapted from Ref[64].