The B/N modified GDY as a rare bases 2D sensor: A first-principles study

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Fig. S1 Optimized configurations and cohesion energy of (a) B atoms (b) N atoms at positions C1, C2 and C3 with

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doping concentrations of 1.4%, 2.8%, 4.2%, and 5.6%, respectively.

Fig. S2 (a) Optimized geometries, distances and the adsorption energy for complexes of rare bases (5mC, 5hmC, 5fC, 5caC) with B-GDY nanosheet. The complexes are shown from both top and side perspectives. Band structure of the complexes of rare bases (b) 5mC, (c) 5hmC, (d) 5fC, (e) 5caC with B-GDY.

Fig. S3 PDOS plot of the of rare bases (a) 5mC, (b) 5hmC, (c) 5fC, (d) 5caC

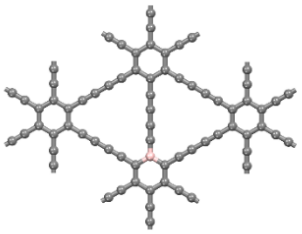
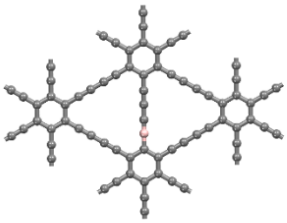
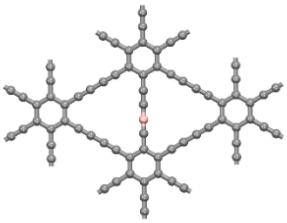
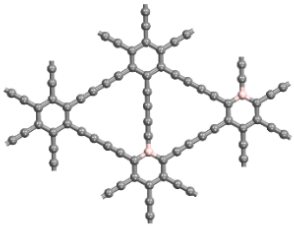
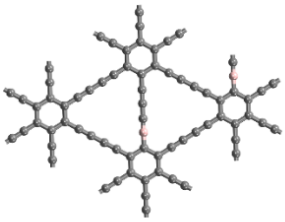
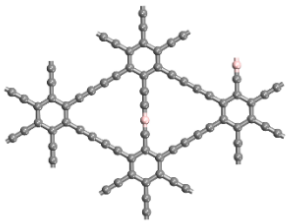
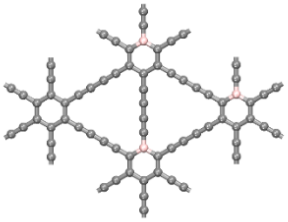
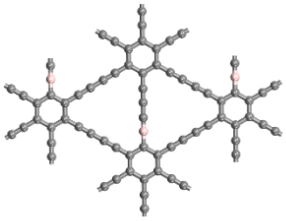
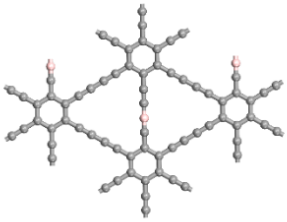
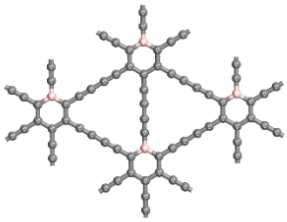
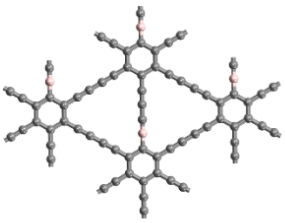
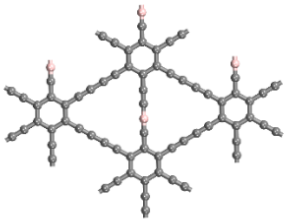
Fig. S4 The DOS plot, CDD (isosurface value is 0.0002 e $Å^{-1}$) and PDOS plot of (a) 5mC-B-GDY, (b) 5hmC-B-GDY, (c) 5caC-B-GDY and (d) 5fC-B-GDY. The yellow and blue are the charge accumulation and depletion, respectively.

Fig. S5 (a) Optimized geometries, distances and the adsorption energy for complexes of rare bases (5mC, 5hmC, 5fC, 5caC) with N-GDY nanosheet. The complexes are shown from both top and side perspectives. Band structure of the complexes of rare bases (b) 5mC, (c) 5hmC, (d) 5fC, (e) 5caC with N-GDY.

Fig. S6 The DOS plot, CDD (isosurface value is 0.0002 e $Å^{-1}$) and PDOS plot of (a) 5mC-N-GDY, (b) 5hmC-N-GDY, (c) 5caC-N-GDY and (d) 5fC-N-GDY. The yellow and blue are the charge accumulation and depletion, respectively.

Table S1 Adsorption energy (Eads/eV) and Translocation time (τ/s) of other molecules adsorbed on GDY and R-GDY (R = B/N) surfaces

(a)

System	C1	C2	C3
1.4%			
	E_{coh} = -7.09 eV	E_{coh} = -7.08 eV	E_{coh} = -7.08 eV
2.8%			
	E_{coh} = -7.08 eV	E_{coh} = -7.05 eV	E_{coh} = -7.05 eV
4.2%			
	E_{coh} = -7.06 eV	E_{coh} = -7.03 eV	E_{coh} = -7.02 eV
5.6%			
	E_{coh} = -7.04 eV	E_{coh} = -7.00 eV	E_{coh} = -6.99 eV

(b)

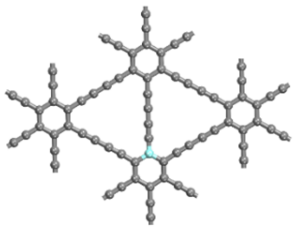
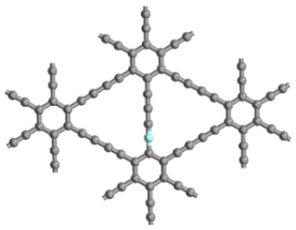
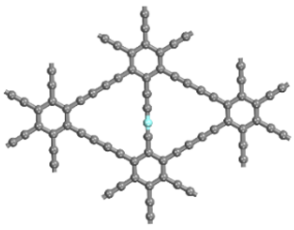
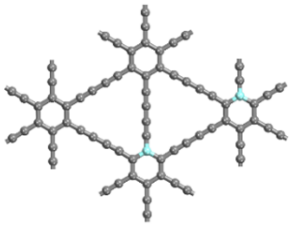
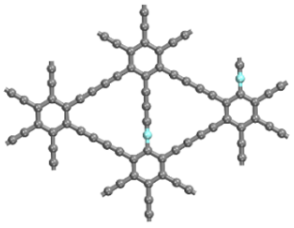
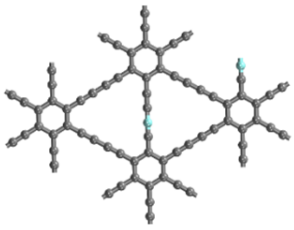
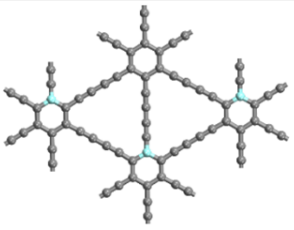
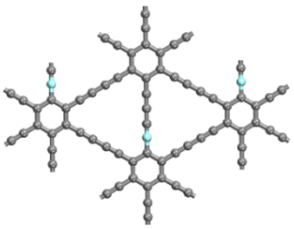
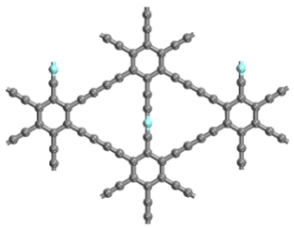
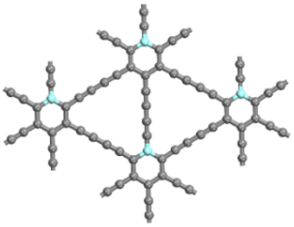
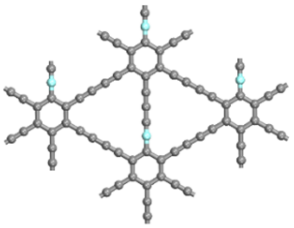
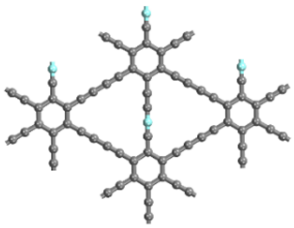
System	C1	C2	C3
1.4%			
	E_{coh} = -7.04 eV	E_{coh} = -7.06 eV	E_{coh} = -7.05 eV
2.8%			
	E_{coh} = -7.00 eV	E_{coh} = -7.03 eV	E_{coh} = -7.02 eV
4.2%			
	E_{coh} = -6.95 eV	E_{coh} = -6.99 eV	E_{coh} = -6.99 eV
5.6%			
	E_{coh} = -6.91 eV	E_{coh} = -6.97 eV	E_{coh} = -6.95 eV

Fig. S1 Optimized configurations and cohesion energy of (a) B atoms (b) N atoms at positions C1, C2 and C3 with doping concentrations of 1.4%, 2.8%, 4.2%, and 5.6%, respectively.

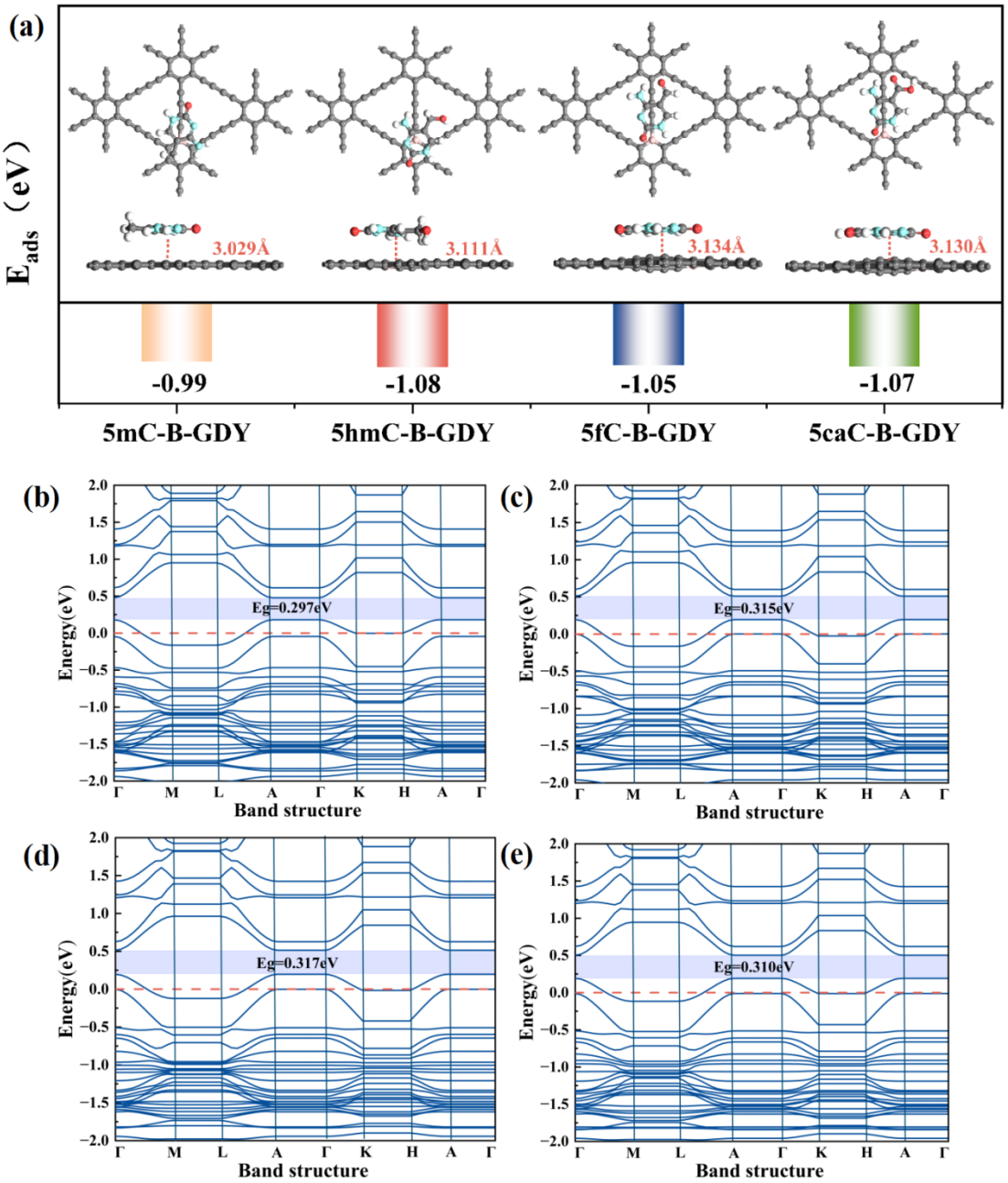


Fig. S2 (a) Optimized geometries, distances and the adsorption energy for complexes of rare bases (5mC, 5hmC, 5fC, 5caC) with B-GDY nanosheet. The complexes are shown from both top and side perspectives. Band structure of the complexes of rare bases (b) 5mC, (c) 5hmC, (d) 5fC, (e) 5caC with B-GDY.

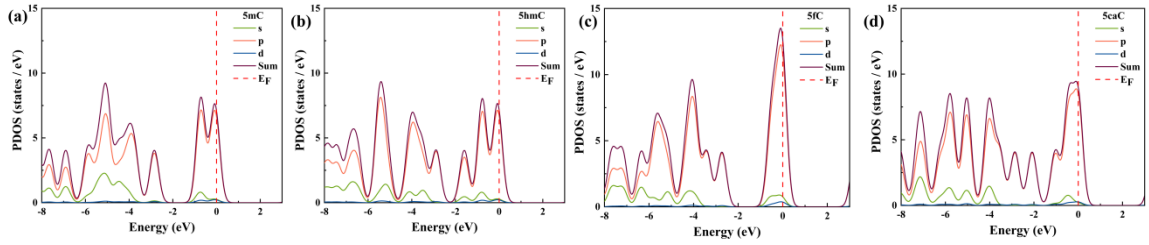


Fig. S3 PDOS plot of the of rare bases (a) 5mC, (b) 5hmC, (c) 5fC, (d) 5caC

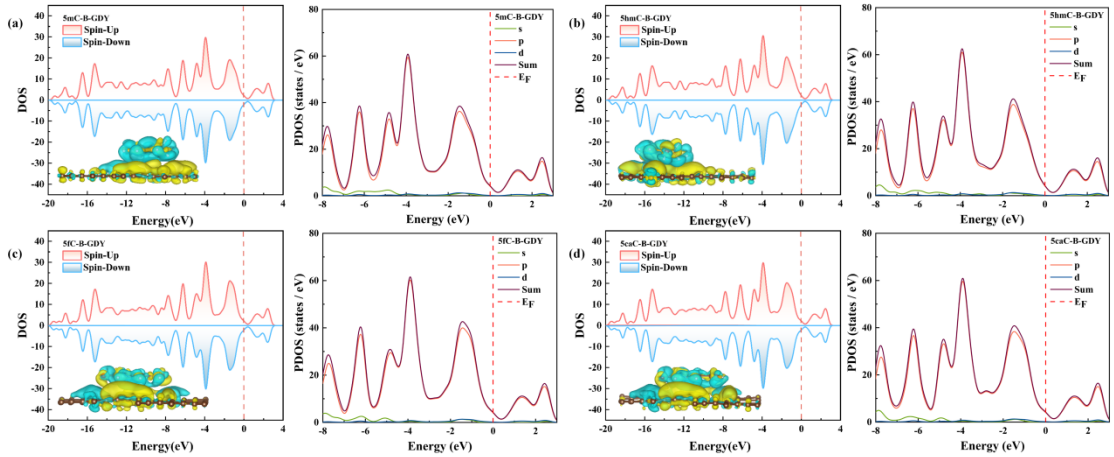


Fig. S4 The DOS plot, CDD (isosurface value is 0.0002 e Å^{-1}) and PDOS plot of (a) 5mC-B-GDY, (b) 5hmC-B-GDY, (c) 5caC-B-GDY and (d) 5fC-B-GDY. The yellow and blue are the charge accumulation and depletion, respectively.

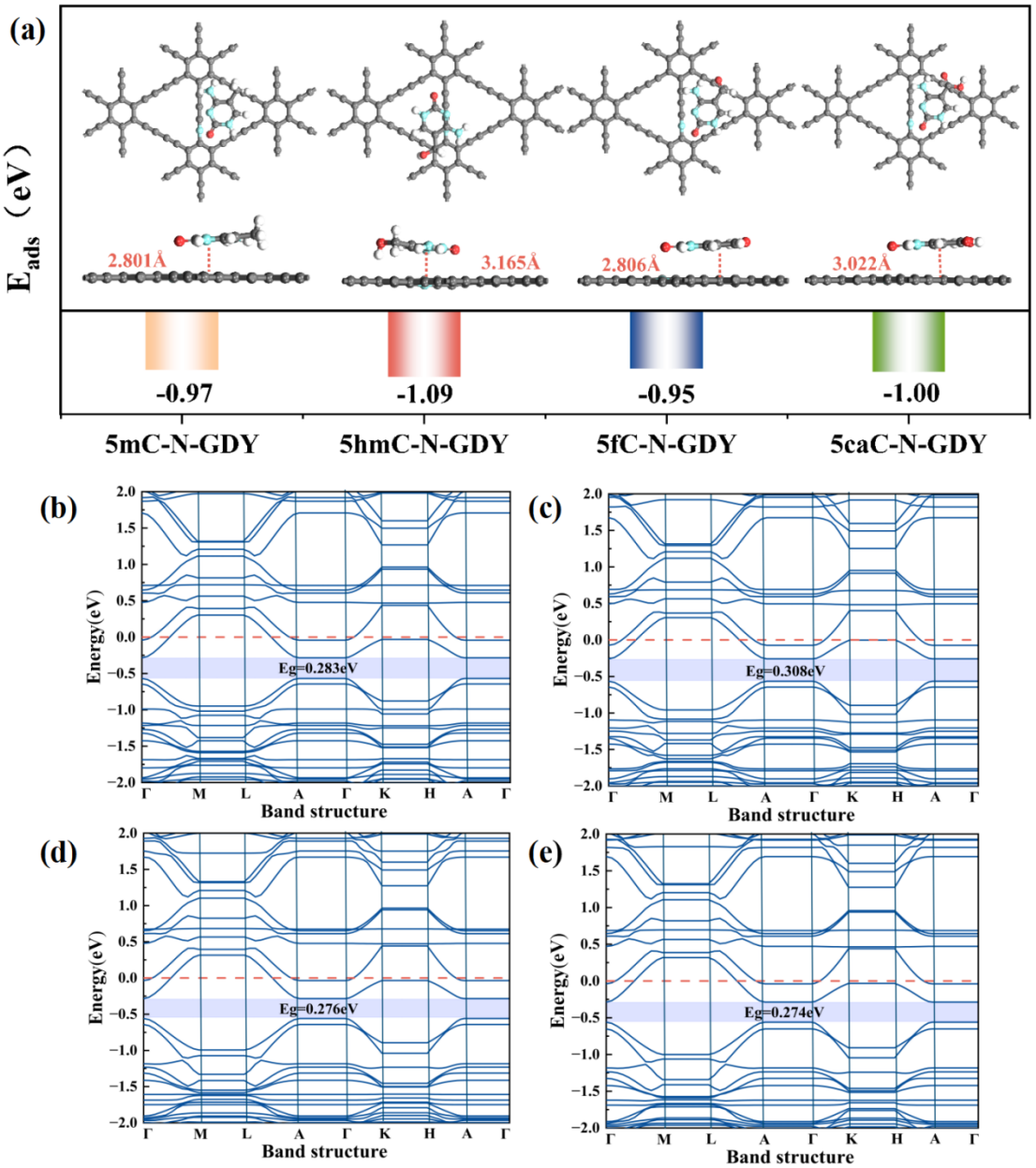


Fig. S5 (a) Optimized geometries, distances and the adsorption energy for complexes of rare bases (5mC, 5hmC, 5fC, 5caC) with N-GDY nanosheet. The complexes are shown from both top and side perspectives. Band structure of the complexes of rare bases (b) 5mC, (c) 5hmC, (d) 5fC, (e) 5caC with N-GDY.

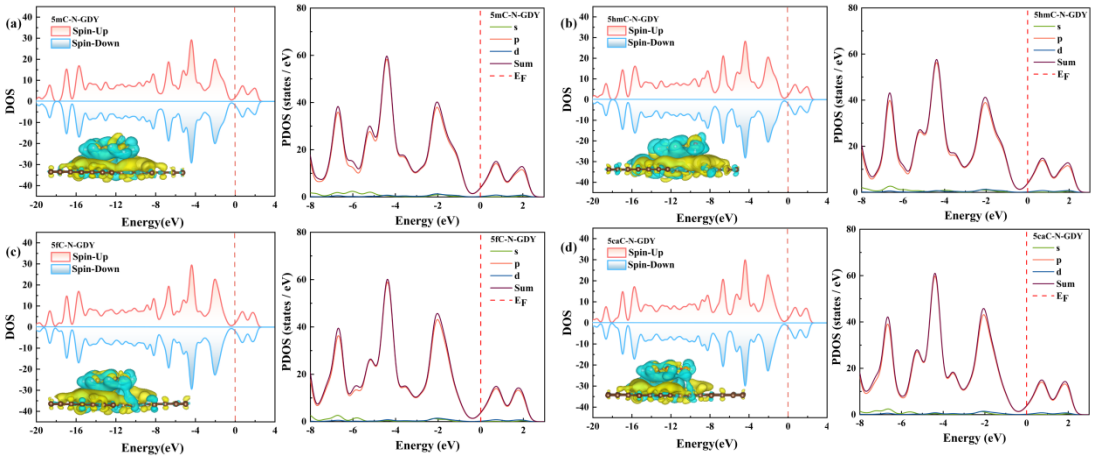


Fig. S6 The DOS plot, CDD (isosurface value is 0.0002 e Å^{-1}) and PDOS plot of (a) 5mC-N-GDY, (b) 5hmC-N-GDY, (c) 5caC-N-GDY and (d) 5fC-N-GDY. The yellow and blue are the charge accumulation and depletion, respectively.

Table S1 Adsorption energy (Eads/eV) and Translocation time (τ/s) of other molecules adsorbed on GDY and R-GDY (R = B/N) surfaces

System		E_{ads}	τ
GDY	O_2	0.428	-
	H_2O	-0.327	3.12×10^{-11}
	NO	-0.097	4.26×10^{-15}
	NH_3	-0.022	2.34×10^{-16}
B-GDY	O_2	-0.098	4.36×10^{-15}
	H_2O	-0.320	2.32×10^{-11}
	NO	-0.458	4.95×10^{-9}
	NH_3	-0.591	8.49×10^{-7}
N-GDY	O_2	0.313	-
	H_2O	-0.358	1.04×10^{-10}
	NO	-0.125	1.26×10^{-14}
	NH_3	-0.038	4.35×10^{-16}