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

Electronic Supplementary Information

Implications of boron doping on electrocatalytic activities of graphyne and graphdiyne family: A first principles study

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Table S1: properties of optimized structures, B doping percentage and references of prior works of αGy, βGy, γGy, δGy, 6,6,12Gy, RGy and Gdy.

Structure	Lattice parameters		Space Group	No. of atoms in 2x2 cell	Doping percentage	References of prior works
	a (A^0)	b (A^0)				
α-Gy	6.96	6.96	P6/mmm(191)	32	3.1%	1, 2, 3, 4
β-Gy	9.5	9.5	P6/mmm(191)	72	1.4%	1, 3, 5
γ-Gy	6.83	6.83	P6/mmm(191)	48	2.1%	1, 3, 4, 6
δ-Gy	9.44	10.67	Pm(6)	80	1.3%	7
Gdy	9.46	9.46	P6/mmm(191)	72	1.4%	4, 8, 9
6,6,12-Gy	10.16	6.89	Pmmm(47)	72	1.4%	1, 10
R-Gy	6.02	6.02	P4/mmm(123)	32	3.1%	11

Table S2: Parameters of single B doping in pristine Gy/ Gdy systems for all other considered systems; E_{for} is the formation energy of the B doped configurations, Q_B is the Bader charge transfer from dopant B atom.

B doped configuration	E_{for} (eV)	Q_B (e)
Ch_{sp}-αGy	1.874	1.74
Ch_{sp}-βGy	1.466	1.76
Ch_{sp}-γGy	1.766	1.79
H_{sp2}-δGy	1.155	1.87
Ch_{sp}-δGy	1.915	1.76
Ch^{n}_{sp}-Gdy	1.446	1.77
Ch^{f}_{sp}-Gdy	1.508	1.81
H_{sp2}-6,6,12Gy	0.367	1.92
H^{x}_{sp2}-6,6,12Gy	0.615	1.89
Ch^{x}_{sp}-6,6,12Gy	1.490	1.77
Ch_{sp}-6,6,12Gy	1.486	1.74
Ch_{sp}-RGy	1.717	1.78

Table S3: Parameters for O_2 adsorption on B doped Gy/ Gdy hosts for all other considered structures; E^{do}_{ads} is the O_2 adsorption energy, $d_{O\text{-}O}$ is the bond length of O_2 in adsorbed state, $\Delta d_{O\text{-}O}$ is the amount of stretching occurred after adsorption, $d_{O(B)\text{-}Gy/\ Gdy}$ is the distance of the O atom adsorbed on B from the Gy/ Gdy plane, $d_{O(C)\text{-}Gy/\ Gdy}$ is the distance of O atom adsorbed on C from the Gy/ Gdy plane, Q_O is the bader charge transferred to the O_2 molecule during adsorption.

Configuration	O_2 adsorption site	Adsorption energy (eV)	Stretched bond length (A^0)	Bond stretching (%)	$d_{O(B)\text{-}Gy/\ Gdy}$ (A^0)	$d_{O(C)\text{-}Gy/\ Gdy}$ (A^0)	Total charge transfer to O_2 molecule (e)
H_{sp2}-βGy	B-C_{sp2} bridge	-0.03	1.448	16.59	1.544	1.507	0.53
H_{sp2}-γGy	B-C_{sp} bridge	0.161	1.308	5.31	1.622	-	0.93
H_{sp2}-Gdy	B-C_{sp2} bridge	-0.037	1.455	17.15	1.540	1.502	0.96
Ch_{sp2}-6,6,12Gy	B-C_{sp2} bridge	0.429	1.315	5.88	1.607	2.601	0.57
R_{sp2}-RGy	B-C_{sp2} bridge	-0.098	1.469	18.28	1.522	1.482	1.00

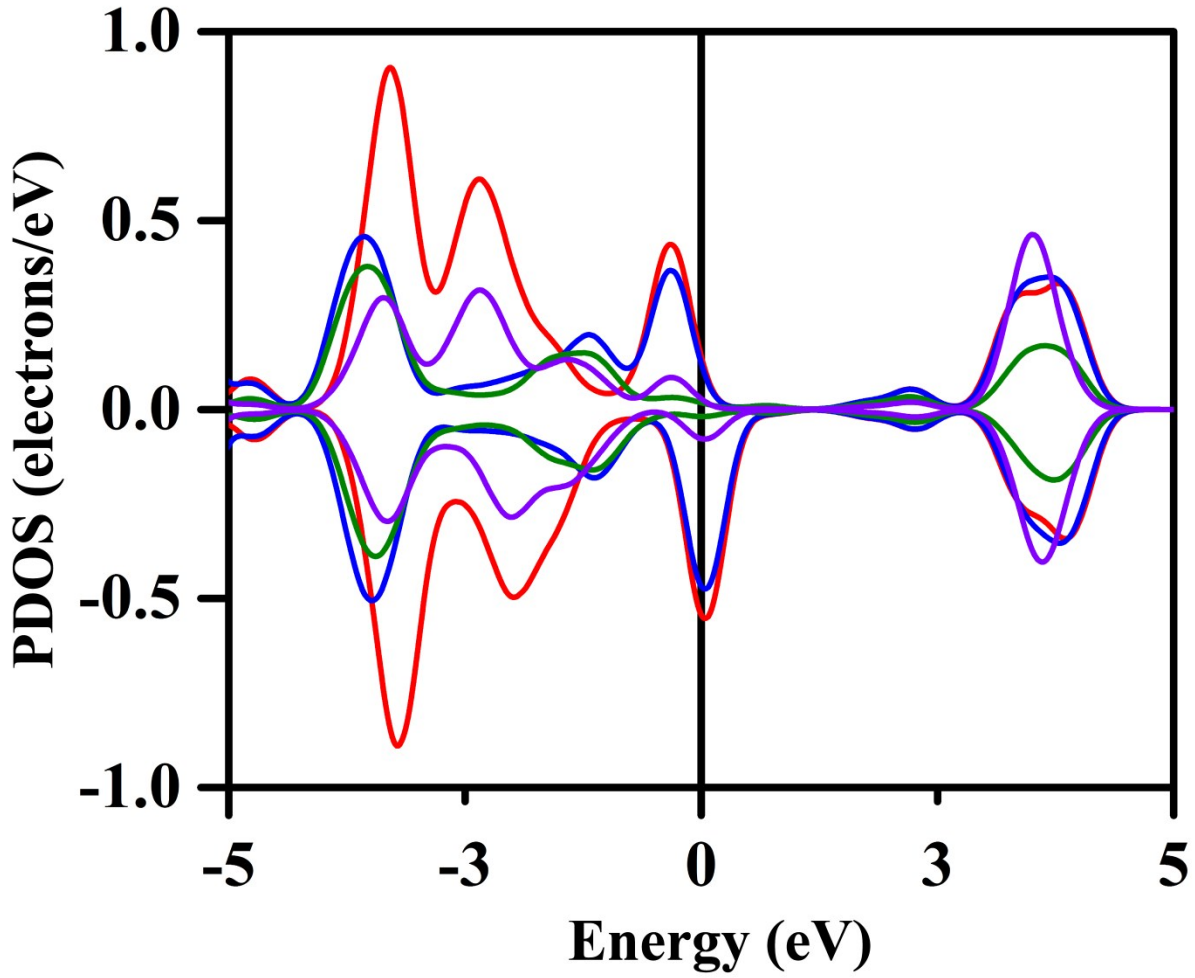

Figure S1. PDOS of dioxygen adsorbed on B-C_{sp} bridge of B doped R-S_{sp2}Gy configuration. Red and blue lines represent the PDOS of O_B and O_C p states respectively. Green and violet lines represent the B and C p states respectively.

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