Supporting Information For

BC_2N/graphene heterostructures as anode materials with improved performance for lithium-ion battery

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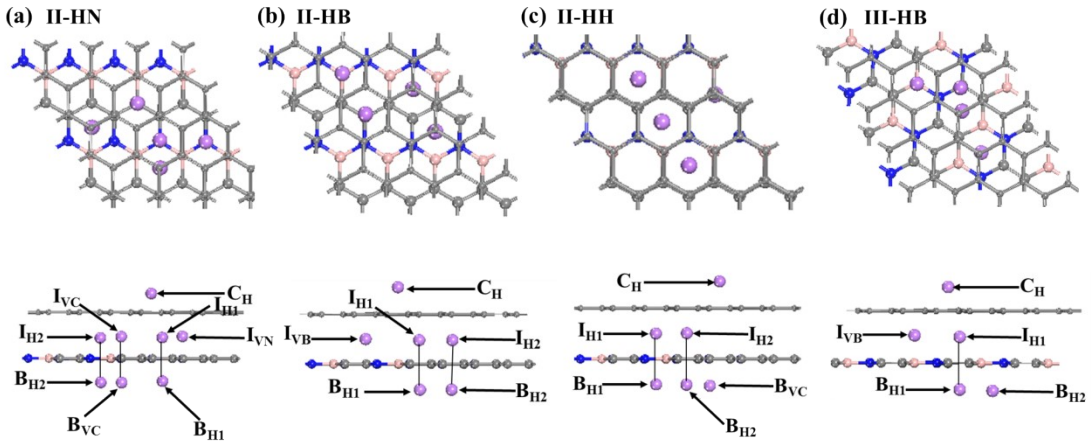

Fig. S1 Top and side views of stable adsorption sites for Li-ion adsorption in Li/G/BC_2N, G/Li/BC_2N, and G/BC_2N/Li of II-HN, II-HB, II-HH, and III-HB.

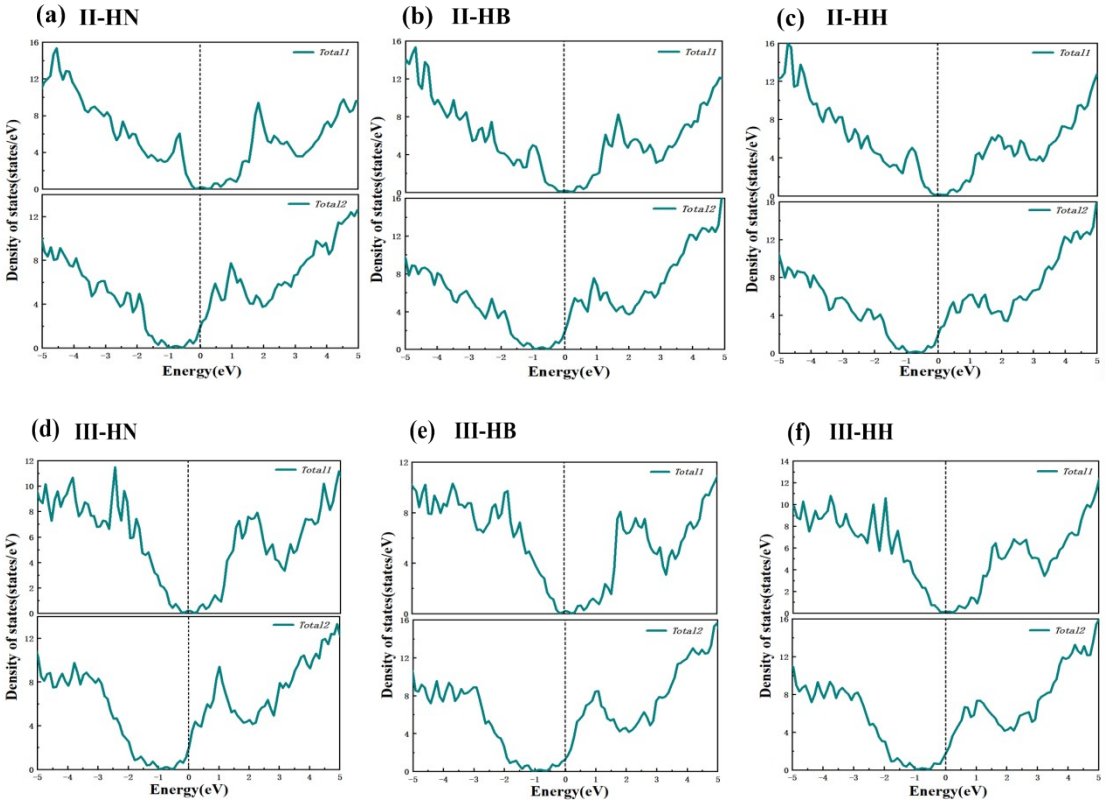

Fig. S2 Total densities of states of II-HN, II-HB, II-HH, III-HN, III-HB, and III-HH heterostructures before and after Li adsorption.

Table S1 Calculated the formation energies (E_{stack}), as well as the total energy of the BC_2N/graphene heterostructures ($E_{BC_2N/G}$), graphene (E_G), and BC_2N monolayer(E_{BC_2N}).

system	E_{stack}(eV)/C atom	E_{stack}(eV)	$E_{BC_2N/G}$(eV)	E_G(eV)	E_{BC_2N}(eV)
II-HN	-0.023	-0.736	-580.067	-296.717	-282.614
II-HB	-0.045	-1.44	-580.771	-296.717	-282.614
II-HH	-0.04	-1.28	-580.583	-296.717	-282.614
III-HN	-0.05	-1.6	-571.384	-296.717	-273.067
III-HB	-0.02	-0.64	-571.206	-296.717	-273.067
III-HH	-0.04	-1.28	-570.777	-296.717	-273.067

Table S2 Calculated adsorption energies (E_{ad}), bader charge transfer (q), and the height between Li atom and monolayer at the more stable adsorption sites, for Li adsorbed on II-HN, II-HB, II-HH, and III-HB heterostructures.

system	Li site	E_{ad} (eV)	q ($\|e\|$)	Height (Å)
II-HN (BC_2N/Li/G)	I_{H1}	-0.59	0.84	1.41
	I_{H2}	-0.39	0.85	1.53
	I_{VN}	-0.48	0.85	1.62
	I_{VC}	-0.57	0.84	1.63
II-HN (Li/BC_2N/G)	B_{H1}	-0.12	0.88	1.67
	B_{H2}	-0.08	0.90	1.66
	B_{VC}	-0.10	0.90	1.77
II-HN (BC_2N/G/Li)	C_H	-0.06	0.89	4.94
II-HB (BC_2N/Li/G)	I_{H1}	-0.69	0.85	1.64
	I_{H2}	-0.52	0.85	1.57
	I_{VB}	-0.58	0.85	1.57
II-HB (Li/BC_2N/G)	B_{H1}	-0.10	0.88	1.67
	B_{H2}	-0.15	0.90	1.68
II-HB (BC_2N/G/Li)	C_H	-0.04	0.89	5.04
II-HH (BC_2N/Li/G)	I_{H1}	-1.05	0.85	1.68
	I_{H2}	-0.89	0.85	1.70
II-HH (Li/BC_2N/G)	B_{H1}	-0.12	0.88	1.68
	B_{H2}	-0.10	0.90	1.69
	B_{VC}	-0.07	0.90	1.75

II-HH (BC_2N/G/Li)	C_H	-0.06	0.89	5.13
III-HB	I_{H1}	-0.71	0.85	1.73
(BC_2N/Li/G)	I_{VB}	-0.81	0.85	1.83
III-HB	B_{H1}	-0.21	0.88	1.7
(Li/BC_2N/G)	B_{H2}	-0.11	0.89	1.77
III-HB (BC_2N/G/Li)	C_H	-0.09	0.89	4.87