Supporting Information for "**Enhancement of multilayer lithium storage in a β₁₂-borophene/graphene heterostructure with built-in dipoles**"

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Table S1. The mismatch degree and binding energy of selected 6 structures.

borophene	δ_3	χ_3	β_{12}	χ_6	α-sheet	α_8
mismatch	4.77%	2.55%	2.55% 3.06%	0.295%	2.64% 2.67%	0.30%
binding energy (eV/atom)	-0.0949	-0.0919	-0.0948	-0.0423	-0.0608	-0.0422

Table S2. Adsorption energy of Li on the surface of borophene.

	Adsorption site	E_{ad}/eV
Li/B/G	H1	-1.50
	H2	-1.50
	T1	-0.75
	T2	-0.74
	B1	-0.77
	B2	-0.77
	B3	-1.00

Table S3. Adsorption energy of Li on the interlayer of B/G heterostructure.

	Adsorption site	E_{ad}/eV
B/Li/G	H1	-1.62
	H2	-1.54
	H3	-0.86
	T1	-0.99
	B1	-1.02
	B2	-1.27

Table S4. Adsorption energy of Li on the surface of graphene.

	Adsorption site	E_{ad}/eV
B/G/Li	H1	-0.03
	H2	-0.04
	H3	-0.04
	H4	-0.03
	H5	-0.03
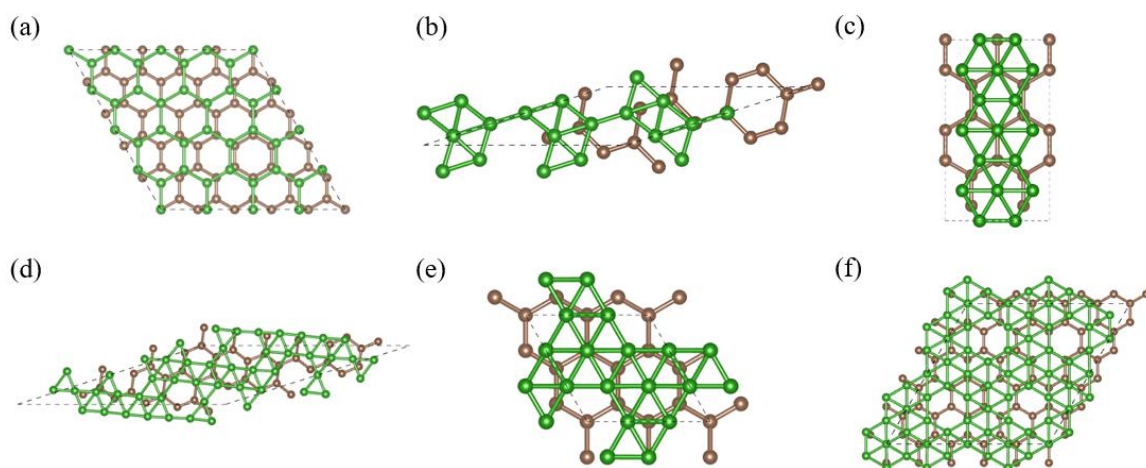
Fig. S1 The atomic configurations of (a) δ_3-B/G, (b) χ_3-B/G, (c) β_{12}-B/G, (d) χ_6-B/G, (e) α-sheet-B/G, and (f) α_8-B/G heterostructure.
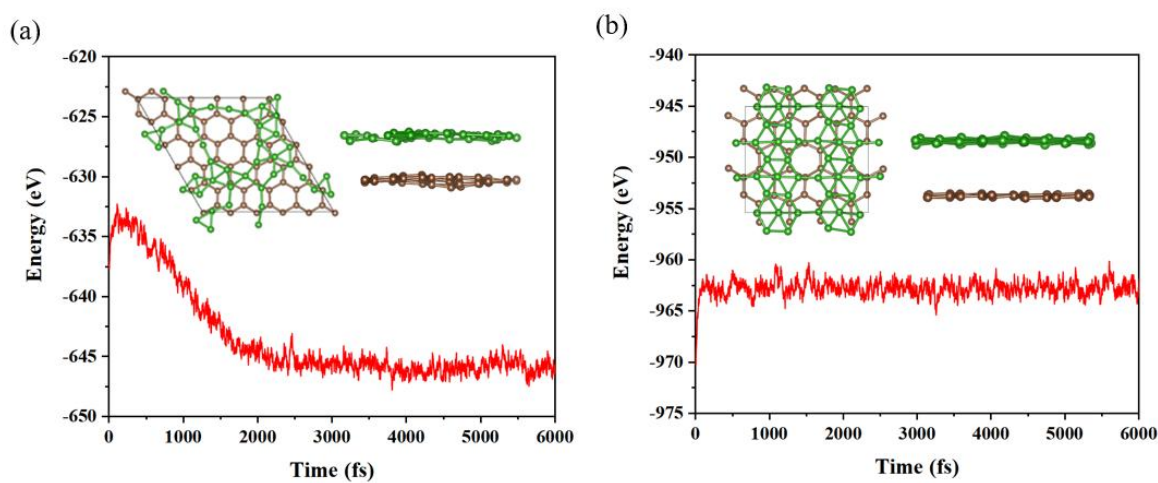

Fig. S2 The free energy of (a) δ_3-B/G and (b) β_{12}-B/G heterostructure by ab initio molecular dynamics (AIMD) at 300 K. Each inset is the final snap shot of AIMD simulation.
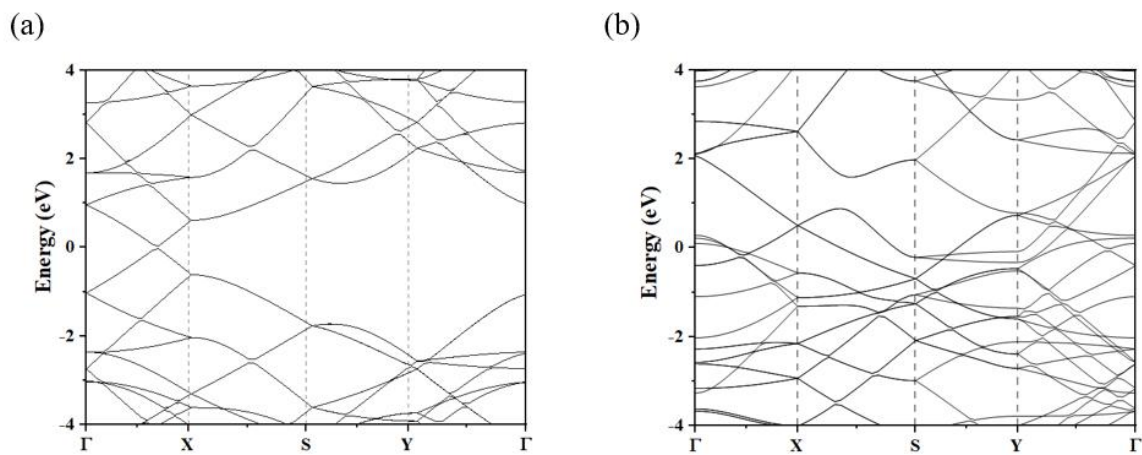
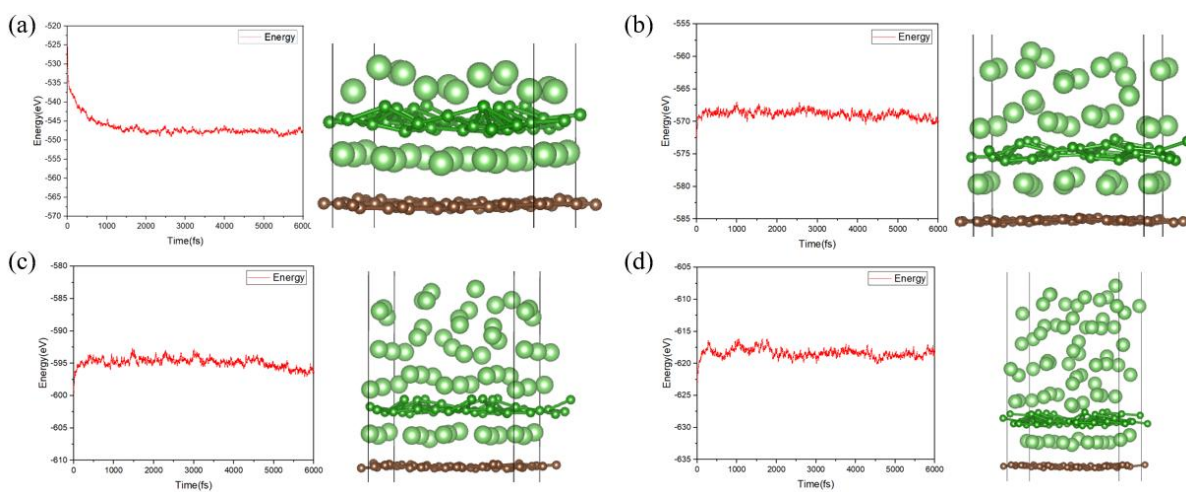Fig. S3 The band structures of (a) monolayer borophene and (b) monolayer graphene.

Fig. S4 The free energy of B/G heterostructure with (a) 3-layers, (b) 5-layers, (c) 7-layers, and (d) 9-layers lithium adsorption by AIMD simulation at 300 K.