Electronic Supplementary Information

Ultrahigh energy storage and ultrafast ion diffusion in borophene-based anodes for rechargeable metal ion batteries†

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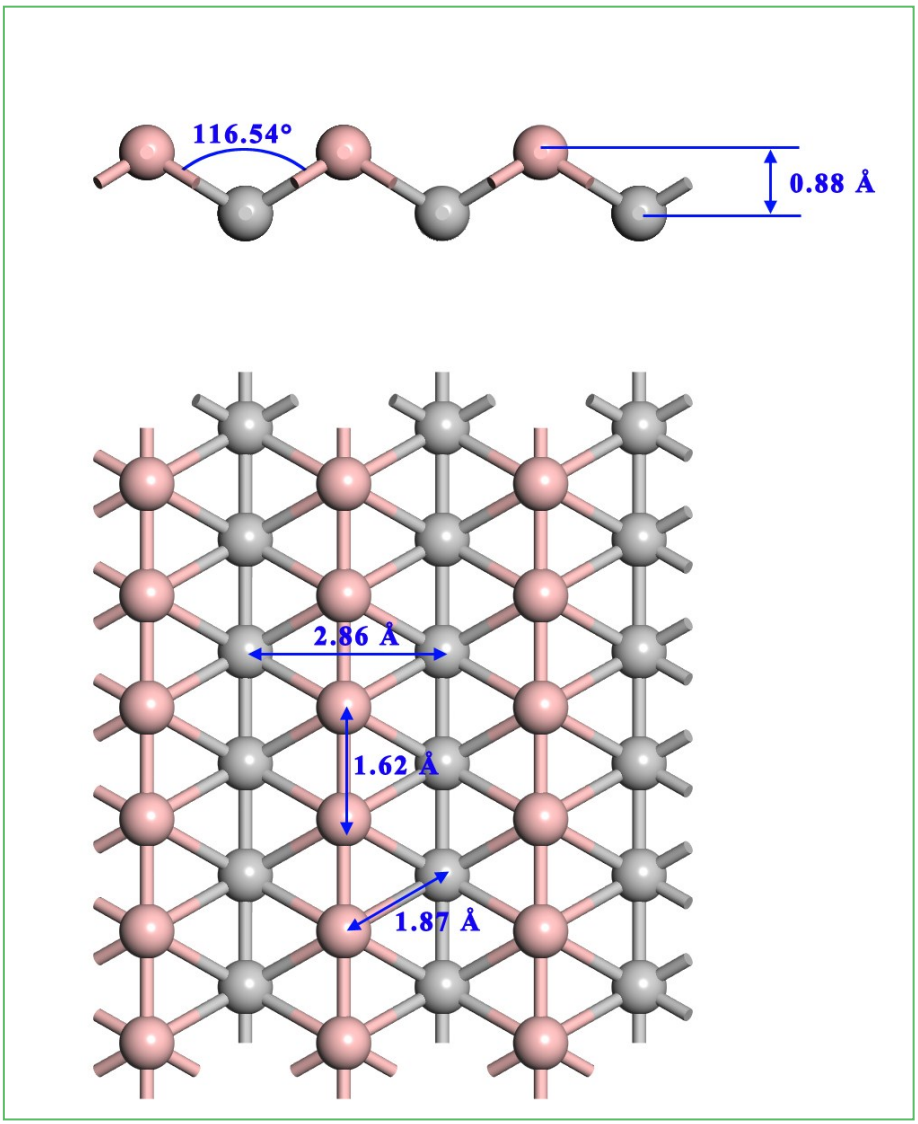

Fig. S1 DFT-optimized supercell of borophene (B_{36}).

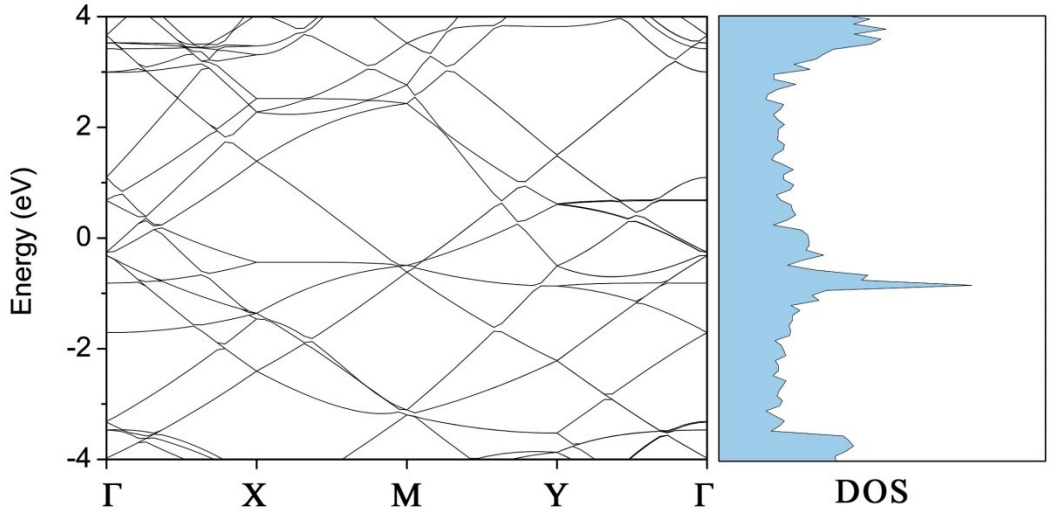

Fig. S2 Band structure and DOS of borophene.

Table S1 The shortest distance between metal and B atom on borophene (unit: Å).

Metal	B at groove	B at bulge	atomic radii[1]
Al	2.79	2.42	1.43
Li	2.75	2.37	1.52
Mg	2.80	2.39	1.60
Na	3.12	2.58	1.86
Ca	3.04	2.54	1.97
K	3.54	2.94	2.27

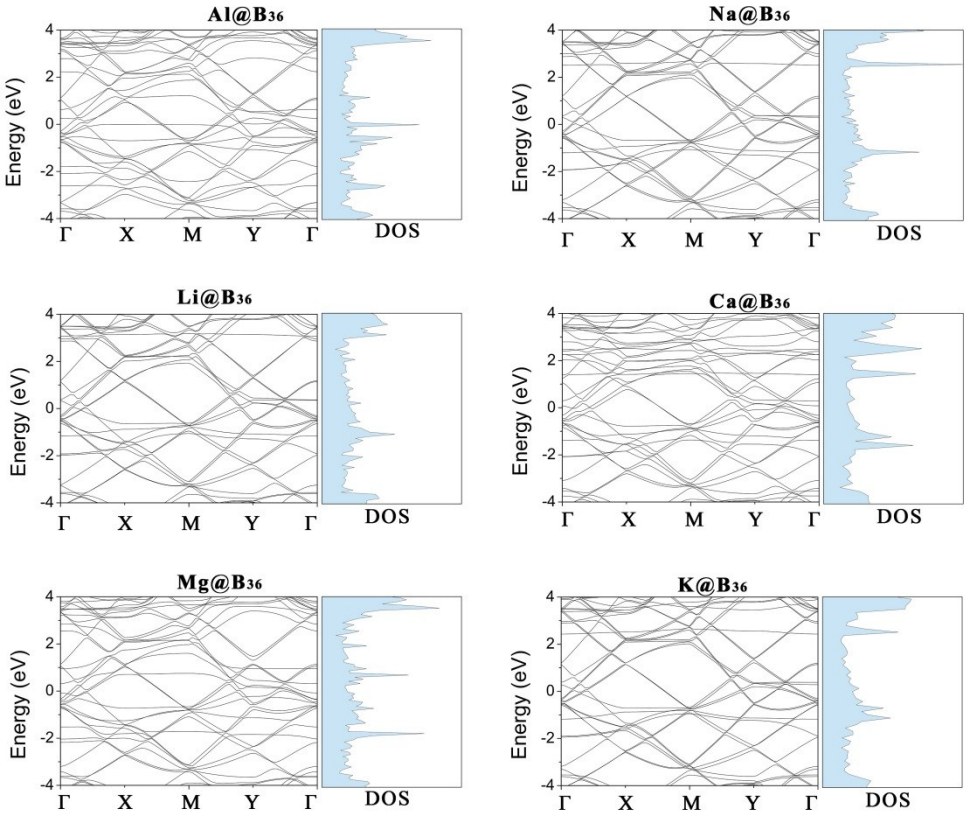

Fig. S3 Band structures and DOSs of metals on borophene (B_{36}).

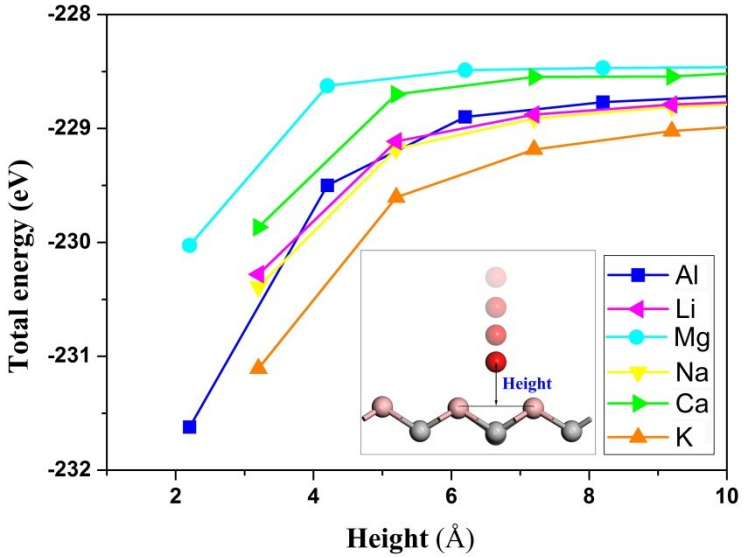

Fig. S4 Total energy of metals on borophene as a function of the height from metal to borophene surface.

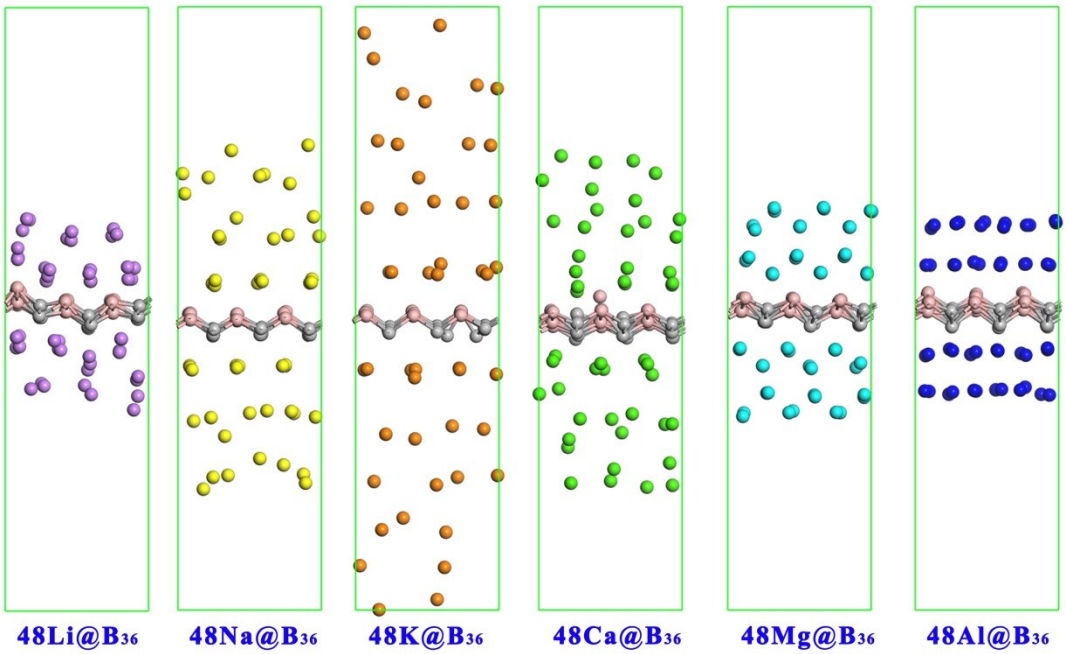

Fig. S5 Thermostable structures of 48 metal atoms adsorbed on B_{36} at 300 K after 5 ps (for 48Li@B_{36}, a much longer 15 ps simulation was performed).

Table S2 Average binding energies of metals on borophene and their cohesive energies (unit: eV).

	Al	**Li**	**Mg**	**Na**	**K**
One atom	3.18	3.50	1.95	3.00	3.09
Multiple atoms	3.96	2.37	1.82	1.81	1.60
First-layer atoms	4.00	2.77	1.89	2.11	1.90
Second-layer atoms	3.93	1.97	1.74	1.47	1.15
Cohesive energy[1]	3.39	1.63	1.51	1.113	0.934

Table S3 Diffusion barriers of metals on B_{36} along selected paths.

	P1 (in meV)	P2 (in eV)	P3 (in eV)
Li	10.53	0.456	0.417
Na	2.55	0.300	0.300
K	7.61	0.223	0.213
Mg	11.76	0.476	0.475
Al	39.24	0.196	0.172

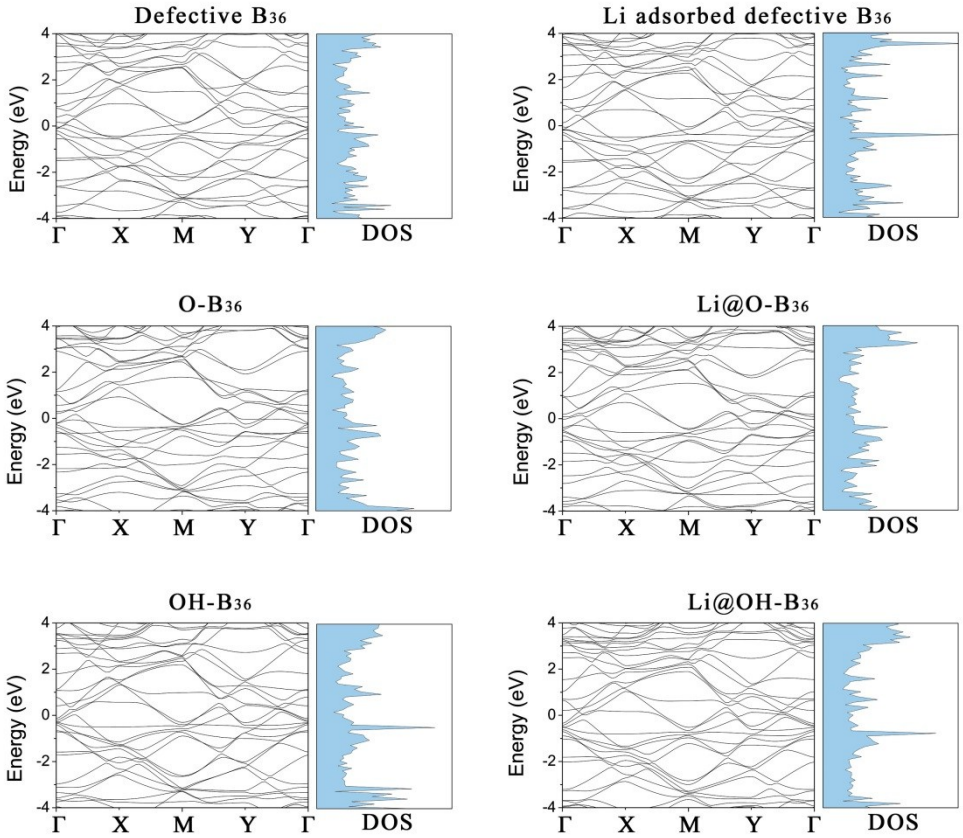

Fig. S6 Band structure and DOS of non-ideal borophene sheets (defective borophene, O- and OH-terminated borophene) and Li-adsorbed samples.

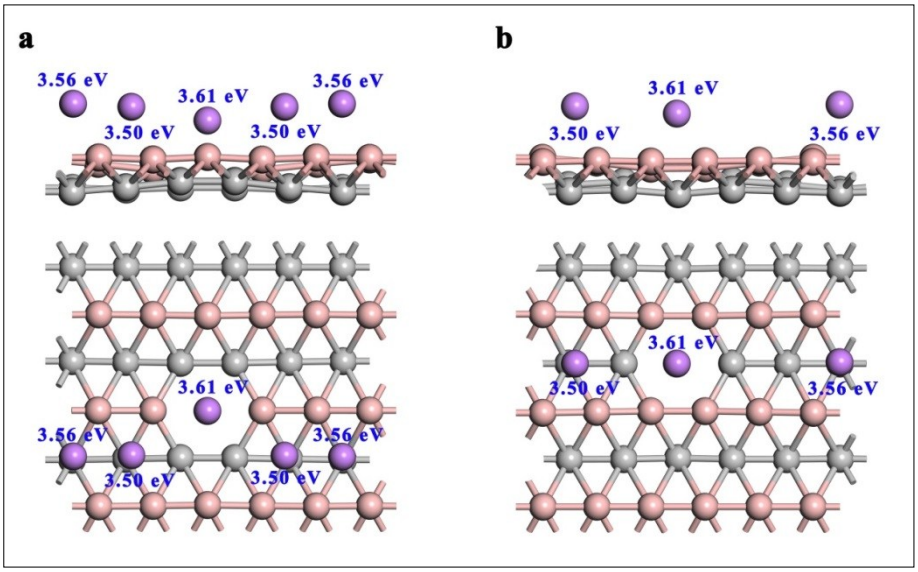

Fig. S7 Optimized adsorptive sites of Li on defective borophene and corresponding binding energies. Purple balls are Li, and pink and grey balls are B.

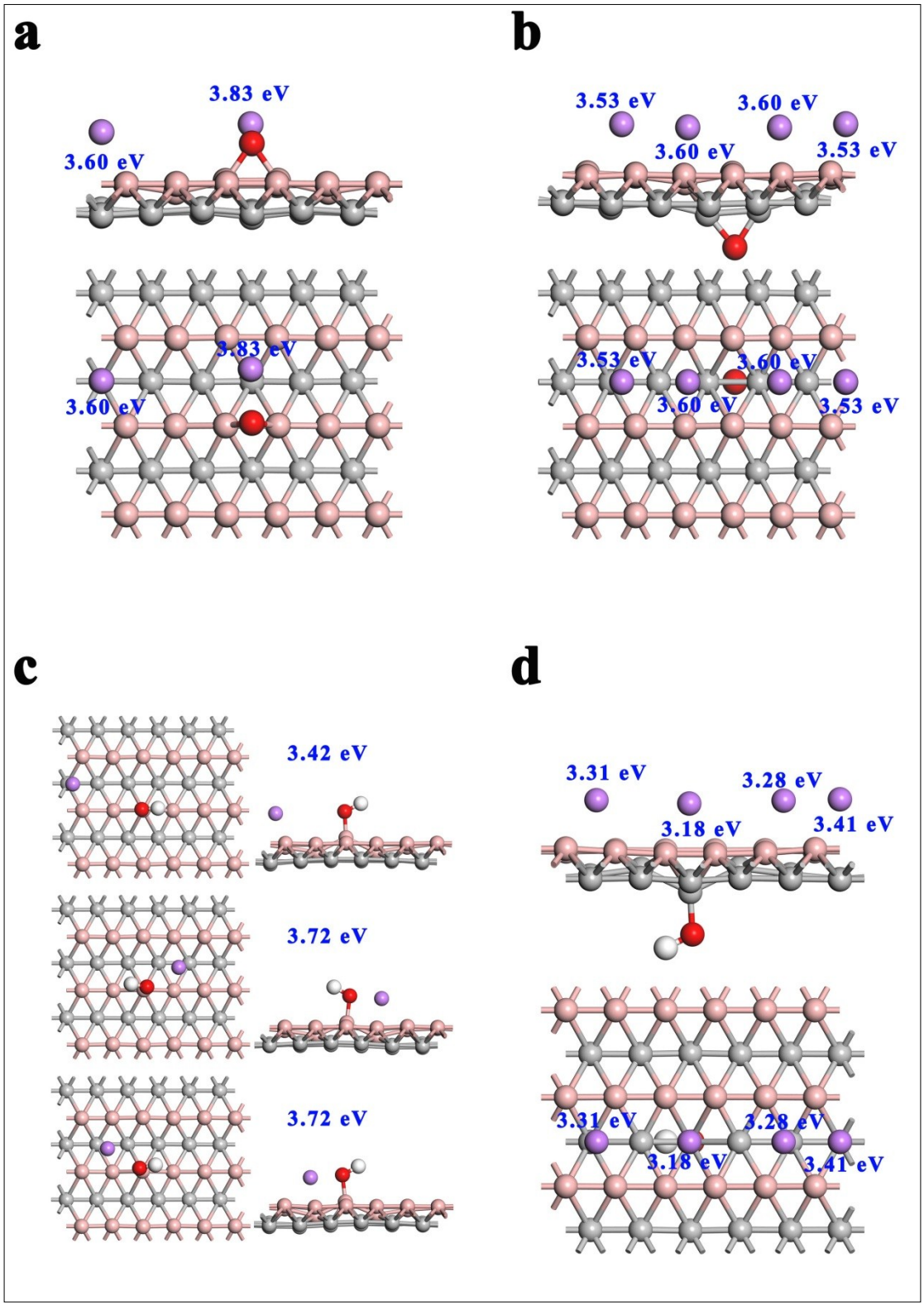

Fig. S8 Optimized adsorptive sites and corresponding binding energies. For Li on (a) nearest groove of O-B_{36}, and (b) the groove opposite to the O-attached side of O-B_{36}, (c) nearest groove of OH-B_{36} and (d) the groove opposite to the O-attached side of OH-B_{36}. Purple balls are Li, and pink and gray balls are B, red balls are O and white balls are H.

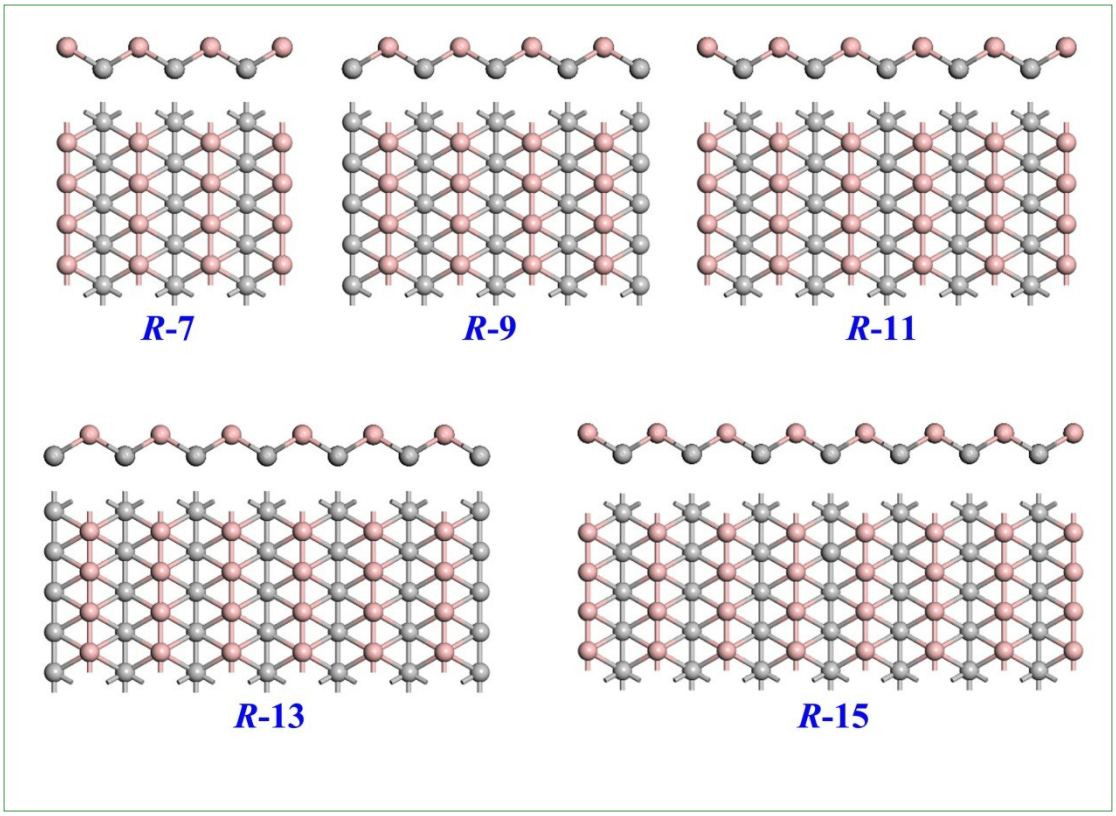

Fig. S9 Models of selected borophene ribbons.

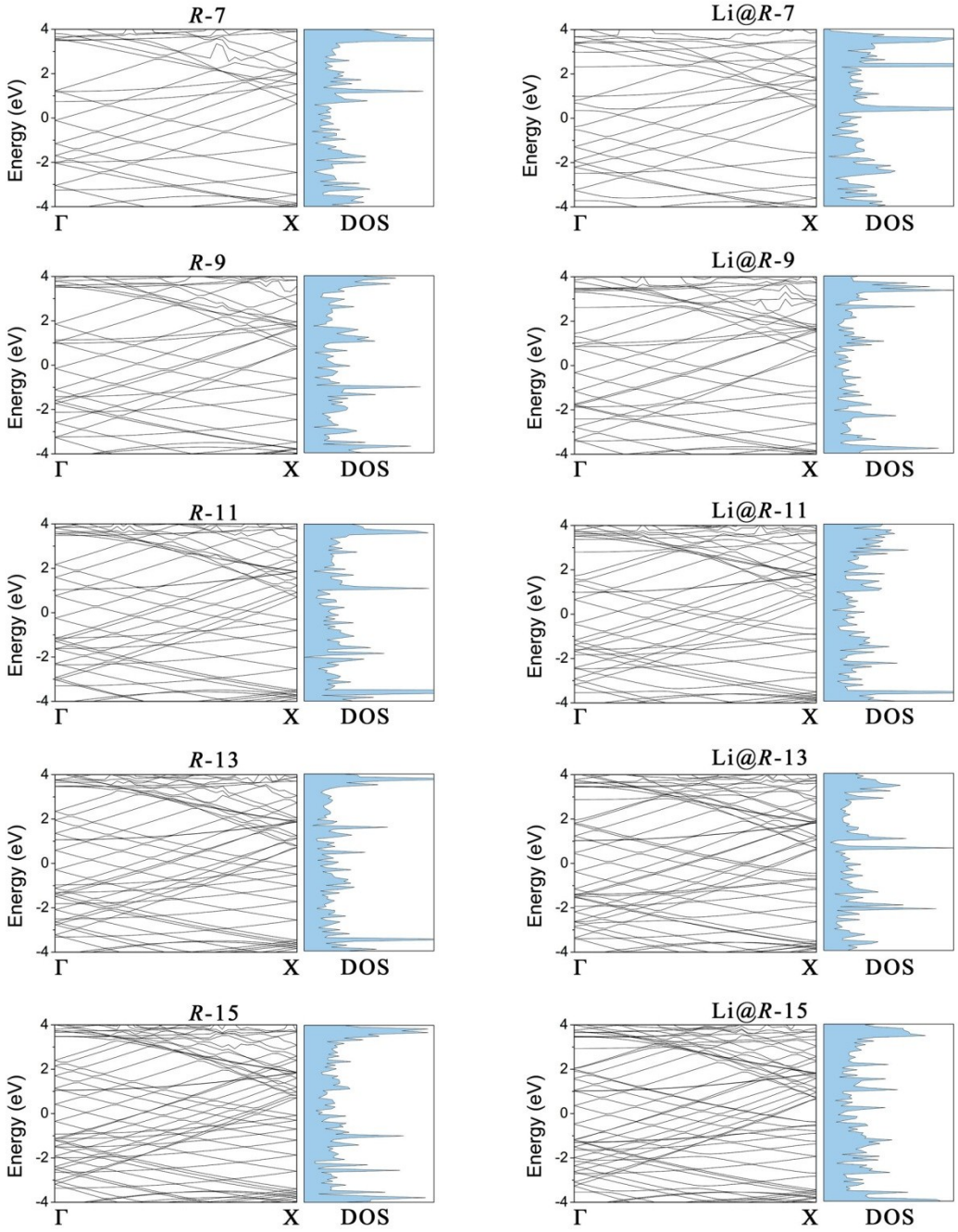

Fig. S10 Band structures and DOSs of ribbons and their Li-adsorbed samples.

Reference

1 Kittle, C. *Introduction to Solid State Physics*. **2005**, *8th Edition*, John Wiely & Sons, Inc.