Supporting information

Metallic borophene polytypes as lightweight anode materials for non-lithium-ion batteries

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Table S1. The calculated E_{ad} values for all considered adsorption configurations. The arrows indicate that metal ions diffuse to their most energetic sites spontaneously after full geometry optimization. Green marked areas represent the most energetic configurations and the corresponding E_{ad}.

□	□	Al	Ca	K	Na	Mg
	B	→H				
	1	1	→H1	→H1	→H1	→H1
	B	1.25	-	-	-	
	2	7	0.155	1.155	0.479	1.305
	B	→B				
	3	3	→H1	→H1	→B3	→H1
	T	1.25	-	-	-	-
S	1	2	0.183	1.124	0.458	0.326
1	T	→H				
	2	1	→H1	→H1	→H1	→H1
	T	→H				
	3	1	→H1	→H1	→H1	→H1
	H	0.14	-	-	-	-
	1	2	1.165	1.445	1.009	0.326
	H	→H				
	2	1	→H1	→H1	→H1	→H1
	B	1.30		-	-	
	1	1	→H1	1.221	0.640	0.902
	B	→H		-	-	
	2	1	→H1	1.294	0.641	→H1
	B	→H				
	3	1	→H1	→H1	→H1	→H1
	B	→H				
	4	1	→H1	→H1	→H1	→H1
	T	→H				
	1	1	→H1	→H1	→H1	→H1
S	T	→H				
2	2	1	→H1	→H1	→H1	→H1
	T	→H				
	3	1	→H1	→H1	→H1	→H1
	H	0.68	-	-	-	
	1	8	0.901	1.426	0.872	0.099
	H	→H				
	2	1	→H1	→H1	→H1	→H1
	H	→T				
	3	2	→H1	→H1	→H1	→H1
	H	→H				
	4	1	→H1	→H1	→H1	→H1
S	B	1.11	→B2	-	-	0.457

	1	9		1.698	1.058	
	B	0.91	-	-	-	-
	2	8	1.599	1.882	1.268	0.114
	T	1.12		-	-	
	1	4	→B2	1.699	1.060	→B2
3	T	0.88	-	-	-	-
	2	9	1.527	1.879	1.270	0.099
	H	→B				
	1	2	→B2	→B2	→B2	→B2
	H	→T				
	2	2	→T2	→T2	→T2	→T2

Table S2. E_{ad} values for metal ions multilayer adsorption on borophene.

		1Layer	2Layer	3Layer	4Layer	5Layer
S1	Ca	-0.475	-0.216	0.048	-	-
	K	-0.373	-0.027	0.017	-	-
	Na	-0.322	0.055	-	-	-
S2	Ca	-0.522	0.097	-	-	-
	K	-0.206	0.045	-	-	-
	Na	-0.151	-0.071	-0.037	-0.005	0.006
S3	Ca	-0.269	0.085	-	-	-
	Na	-0.191	0.020	-	-	-

Figure S1

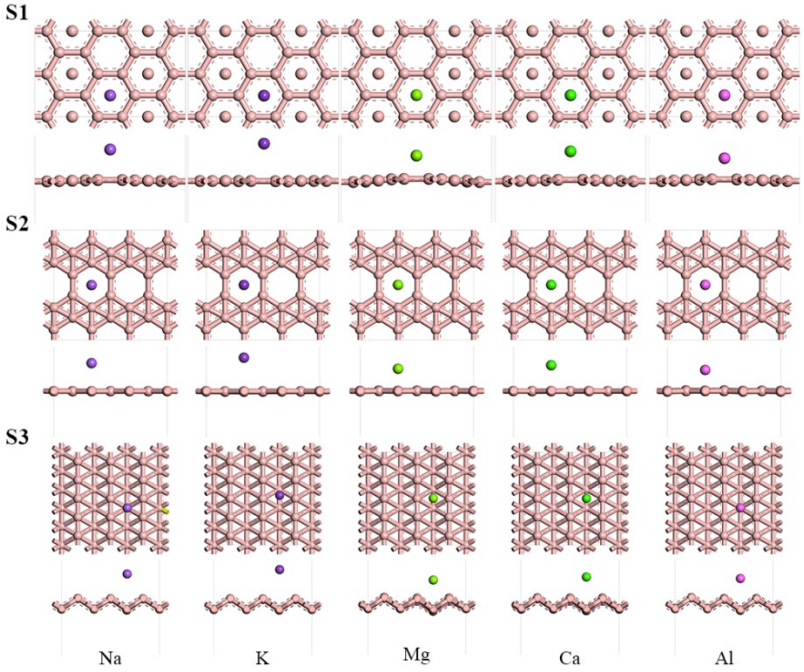

Figure S1. Top and side view of the most energy favorable adsorption configurations of Na, K, Mg, Ca and Al on S1, S2 and S3, respectively.

Figure S2

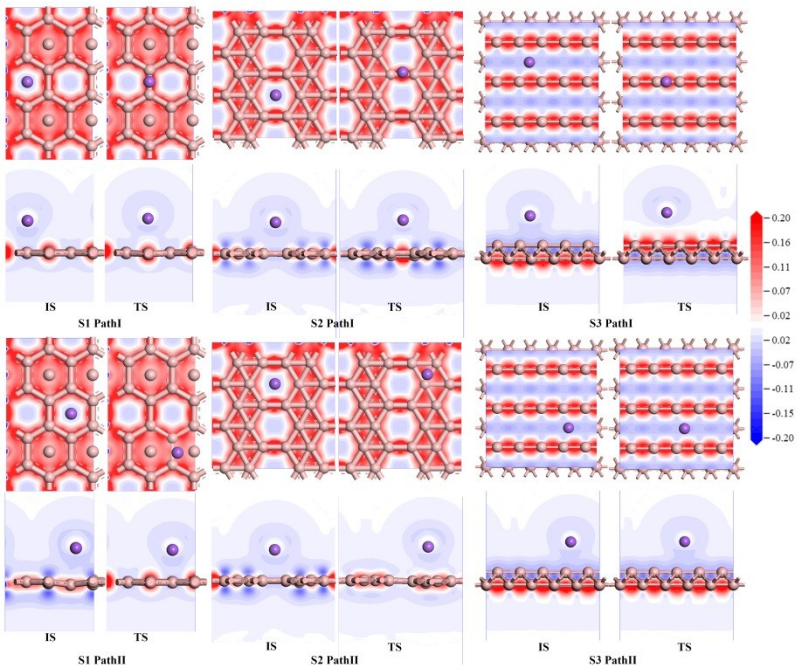

Figure S2. Slice of the charge density difference for Na diffusing on three types of borophene. The results of both Path I and Path II are presented, where IS and TS represent the initial states and transition states, respectively. Red and blue areas represent the accumulation and depletion of electrons.

Figure S3

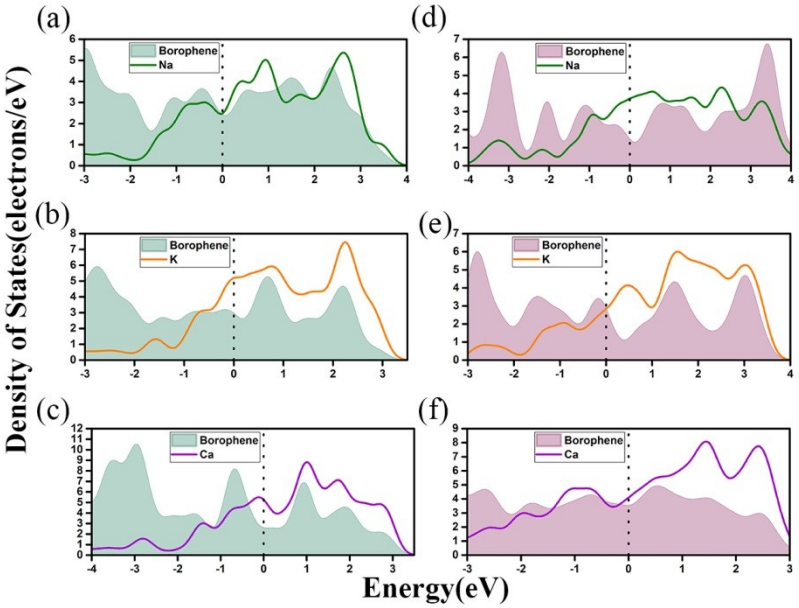

Figure S3. Partial density of states (PDOS) of S2 (a-c) and S3 (d-e) with single layer of Na, K and Ca ions adsorbed. The Fermi levels are set to zero and are indicated by the dashed lines.

Figure S4

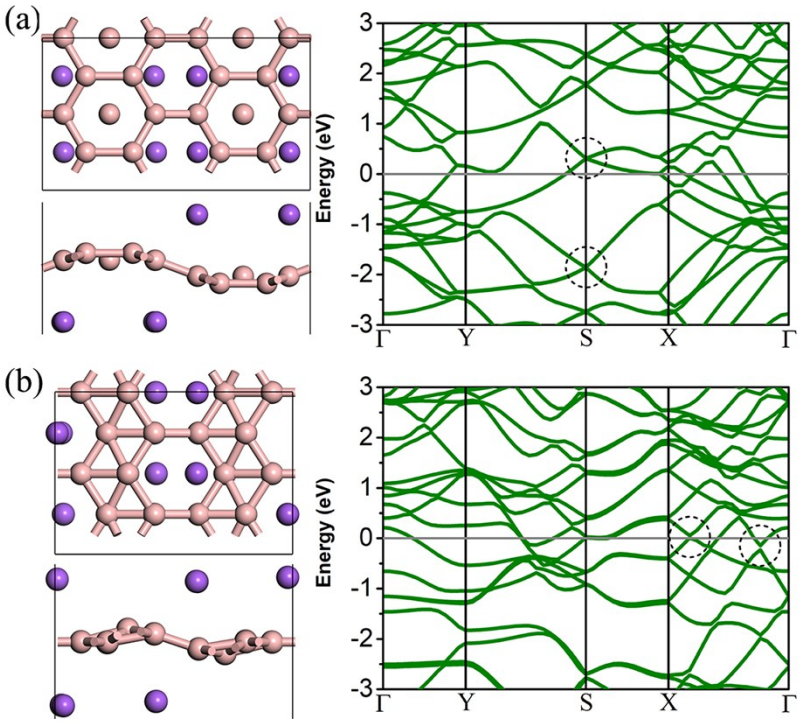

Figure S4. Top and side views of the optimized structures and band structures of Na-metalized S1(2×2) (a) and S2 (1×2) (b). The Dirac cones are highlighted by dashed circles.