

Supplementary Information

Two-Dimensional AlB_4 and Al_2B_2 : High-Performance Dirac Anodes for Sodium-Ion Batteries

Ru-Feng Zou,^a Xiao-Juan Ye,^{b,*} Xiao-Hong Zheng,^c Ran Jia,^d Chun-Sheng Liu^{a,*}

^a*College of Electronic and Optical Engineering, Nanjing University of Posts and Telecommunications, Nanjing 210023, China*

^b*College of Integrated Circuit Science and Engineering, Nanjing University of Posts and Telecommunications, Nanjing 210023, China*

^c*College of Information Science and Technology, Nanjing Forestry University, Nanjing 210037, China*

^d*Institute of Theoretical Chemistry, College of Chemistry, Jilin University, Changchun 130023, China*

*Email: yexj@njupt.edu.cn (X.-J.Y.).

*Email: cslu@njupt.edu.cn (C.-S.L.).

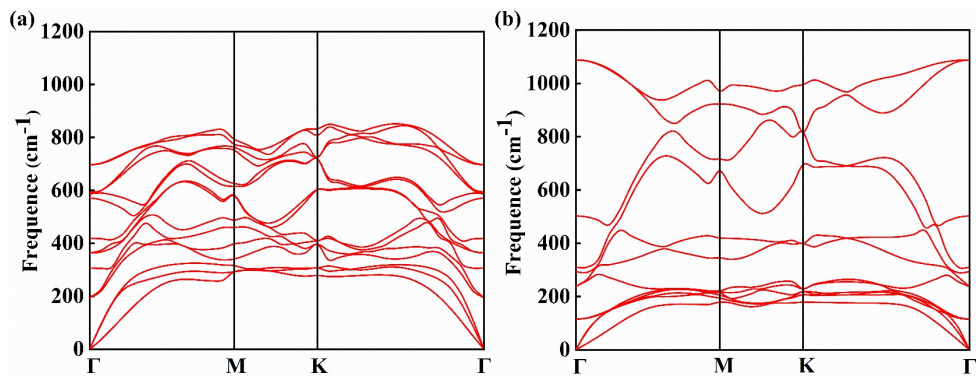


Fig. S1 Phonon spectra of (a) monolayer AlB_4 and (b) Al_2B_2 .

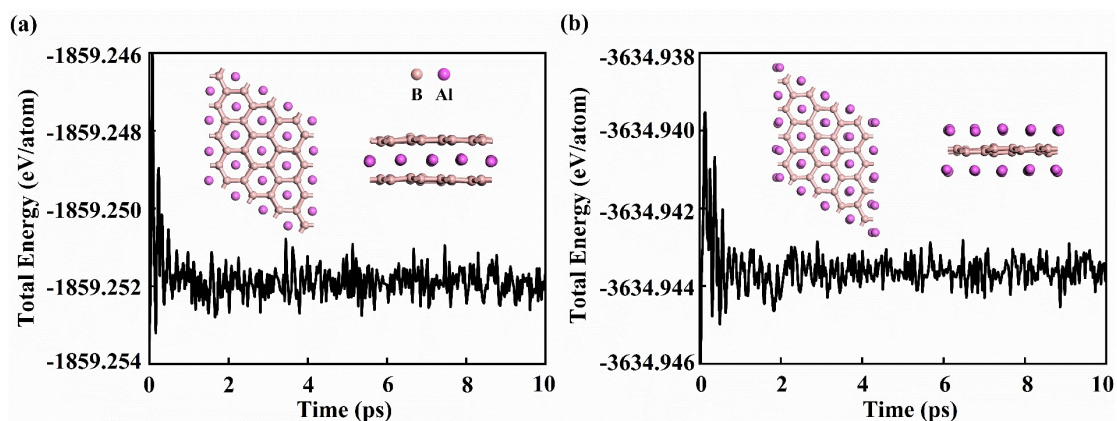


Fig. S2 AIMD simulations at 400 K of (a) monolayer AlB_4 and (b) Al_2B_2 . The insets represent top and side views of the final snapshots.

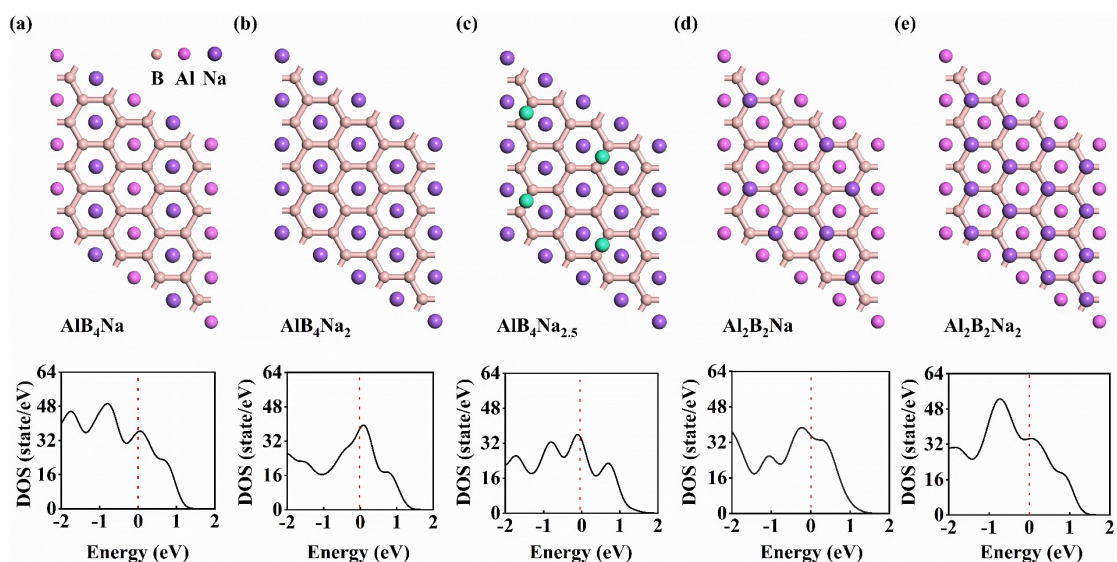


Fig. S3 Top views and DOS of (a) AlB_4Na , (b) AlB_4Na_2 , (c) $\text{AlB}_4\text{Na}_{2.5}$, (d) $\text{Al}_2\text{B}_2\text{Na}$, and (e) $\text{Al}_2\text{B}_2\text{Na}_2$. The green and cyan balls represent Na atoms adsorbed on the first layer and the second

layer, respectively.

Table S1 The calculated differential adsorption energies of Na atoms adsorbed on AlB₄ and Al₂B₂ monolayers.

Number of Na atoms	$E_{\text{diff-ads}}$ (eV) of AlB ₄	$E_{\text{diff-ads}}$ (eV) of Al ₂ B ₂
1	3.55	2.03
2	3.38	1.95
3	3.15	1.87
4	3.12	1.75
5	2.91	1.62
6	2.82	1.51
7	2.57	1.48
8	2.55	1.42
9	3.15	1.81
10	3.01	1.77
11	2.81	1.63
12	2.70	1.55
13	2.54	1.43
14	2.44	1.30
15	2.20	1.28
16	2.13	1.20
17	2.60	1.77
18	2.46	1.59
19	2.33	1.49
20	2.26	1.40
21	2.19	1.33
22	2.10	1.27
23	2.00	1.22
24	1.91	1.19
25	2.37	1.58

26	2.25	1.53
27	2.13	1.46
28	2.11	1.37
29	1.98	1.32
30	1.83	1.27
31	1.67	1.25
32	1.57	1.18
33	1.81	1.09
34	1.75	—
35	1.56	—
36	1.43	—
37	1.37	—
38	1.31	—
39	1.22	—
40	1.17	—
41	1.05	—
