Supplementary Information

Computational Seeking of Two-dimensional Borides with Planar Octacoordinated Main Group Elements

Jiashu Yang[1,2], Linke Yu,[1] Fengyu Li[1,*]

[1] *School of Physical Science and Technology, Inner Mongolia University, Hohhot, 010021, China*

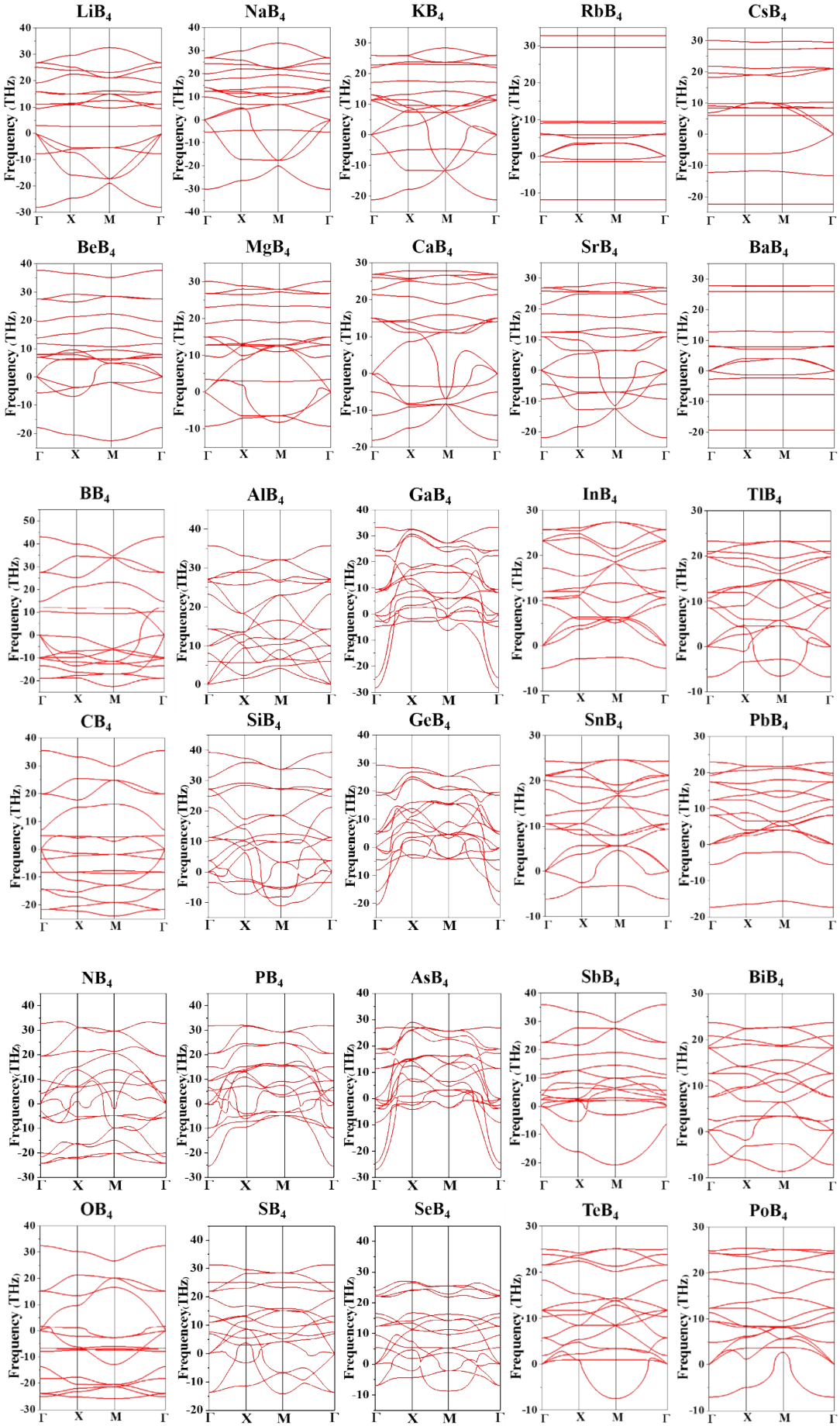
[2] *Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Dalian University of Technology), Ministry of Education, School of Physics, Dalian 116024, China*

* Corresponding Author: fengyuli@imu.edu.cn (FL)

Table S1 The calculated geometry parameters of XB_4 monolayers including the lattice constants ($a = b$), the distance of X−B (d_1), the B−B bond lengths of B squares (d_2) and the shared B−B edges between adjacent X©B_8 wheels (d_3).

	LiB_4	BeB_4	BB_4	CB_4	NB_4	OB_4	FB_4	NeB_4
***a* (Å)**	4.13	3.97	3.84	4.02	4.02	4.09	4.19	4.34
d_1 (Å)	2.25	2.14	2.07	2.17	2.17	2.21	2.26	2.37
d_2 (Å)	1.68	1.66	1.62	1.69	1.68	1.71	1.71	1.73
d_3 (Å)	1.76	1.62	1.54	1.63	1.65	1.67	1.72	1.90
	NaB_4	**MgB_4**	**AlB_4**	**SiB_4**	**PB_4**	**SB_4**	**ClB_4**	**KrB_4**
***a* (Å)**	4.35	4.18	4.04	4.05	4.11	4.13	4.31	4.70
d_1 (Å)	2.39	2.27	2.18	2.18	2.22	2.24	2.34	2.60
d_2 (Å)	1.69	1.71	1.70	1.71	1.72	1.71	1.77	1.76
d_3 (Å)	1.96	1.76	1.64	1.63	1.69	1.72	1.82	2.21
	KB_4	**CaB_4**	**GaB_4**	**GeB_4**	**AsB_4**	**SeB_4**	**BrB_4**	**ArB_4**
***a* (Å)**	4.72	4.51	4.11	4.21	4.25	4.24	4.29	4.51
d_1 (Å)	2.63	2.48	2.22	2.27	2.30	2.30	2.34	2.45

d_2 (Å)	1.68	1.72	1.72	1.76	1.75	1.73	1.73	1.82
d_3 (Å)	2.34	2.07	1.68	1.71	1.78	1.80	1.85	1.94
	RbB_4	**SrB_4**	**InB_4**	**SnB_4**	**SbB_4**	**TeB_4**	**IB_4**	**XeB_4**
a (Å)	5.46	4.75	4.31	4.30	4.42	4.37	4.13	**NeB_4**
d_1 (Å)	3.17	2.65	2.34	2.33	2.41	2.39	2.24	4.24
d_2 (Å)	1.59	1.69	1.76	1.77	1.77	1.75	1.71	2.30
d_3 (Å)	3.21	2.35	1.83	1.79	1.91	1.90	1.72	1.73
	CsB_4	**BaB_4**	**TlB_4**	**PbB_4**	**BiB_4**	**PoB_4**	**AtB_4**	**RnB_4**
a (Å)	4.80	5.18	4.44	4.51	4.54	4.51	4.48	6.40
d_1 (Å)	2.71	2.96	2.42	2.46	2.49	2.48	2.45	3.84
d_2 (Å)	1.63	1.63	1.78	1.80	1.76	1.73	1.75	1.53
d_3 (Å)	2.50	2.87	1.92	1.96	2.04	2.06	2.01	4.25


LiB4
NaB4
KB4
RbB4
CsB4
BeB4
MgB4
CaB4
SrB4
BaB4
BB4
AlB4
GaB4
InB4
TlB4
CB4
SiB4
GeB4
SnB4
PbB4
NB4
PB4
AsB4
SbB4
BiB4
OB4
SB4
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PoB4
Frequency (THz)
Frequencey (THz)
Γ X M Γ

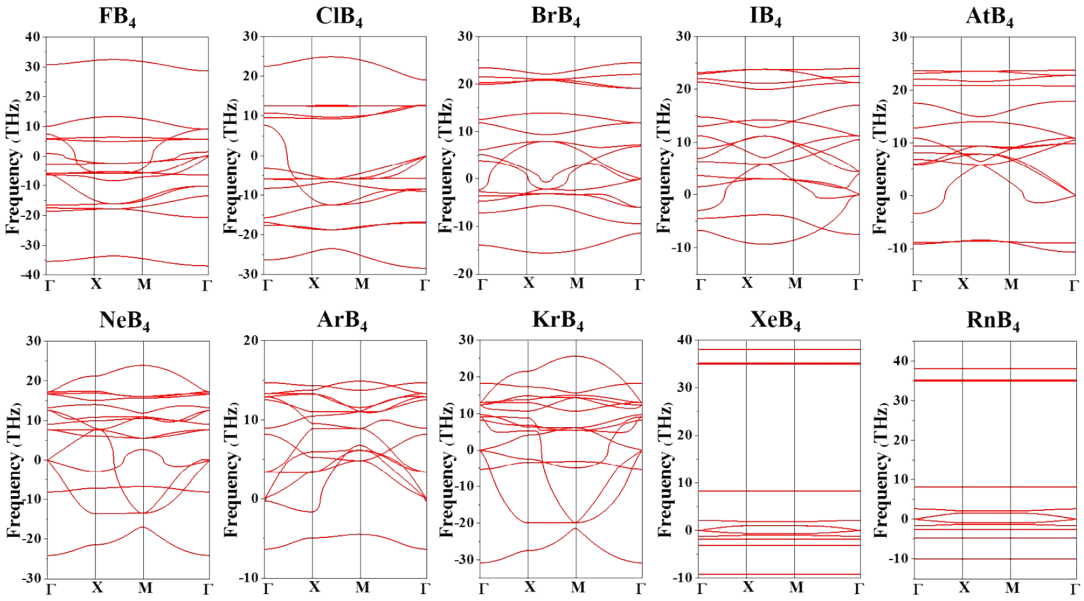

Fig. S1 Phonon dispersion of the 40 planar XB_4 monolayer (X = As, Ga, Ge, N, P, S, Se, Si). Γ (0, 0, 0), X (0.0 0.5 0.0), and M (0.5 0.5 0.0) refer to special *k*-points in the first Brillouin zone in the reciprocal space.

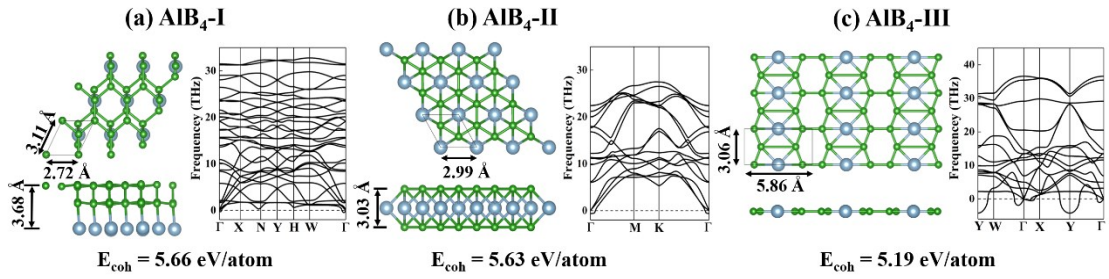

Fig. S2 Two views and phonon dispersions of the AlB_4 sheets obtained by PSO search: AlB_4-I (a), AlB_4-II (b) and AlB_4-III (c). Al and B atoms are denoted by blue and green spheres, respectively. The unit cell is marked by a black parallelogram. The tinny U-shape of negative frequencies near Γ point in the phonons of AlB_4-I and AlB_4-II does not indicate the dynamical instability of the two sheets, it is a common phenomenon in the calculated phonon spectra of 2D structures [V. Zolyomi, N. D. Drummond and V. I. Fal'ko, *Phys. Rev. B*, 2014, **89**, 205416; H. Yin, G. Zheng, Y. Wang and B. Yao, *Phys. Chem. Chem. Phys.*, 2018, **20**, 19177.].

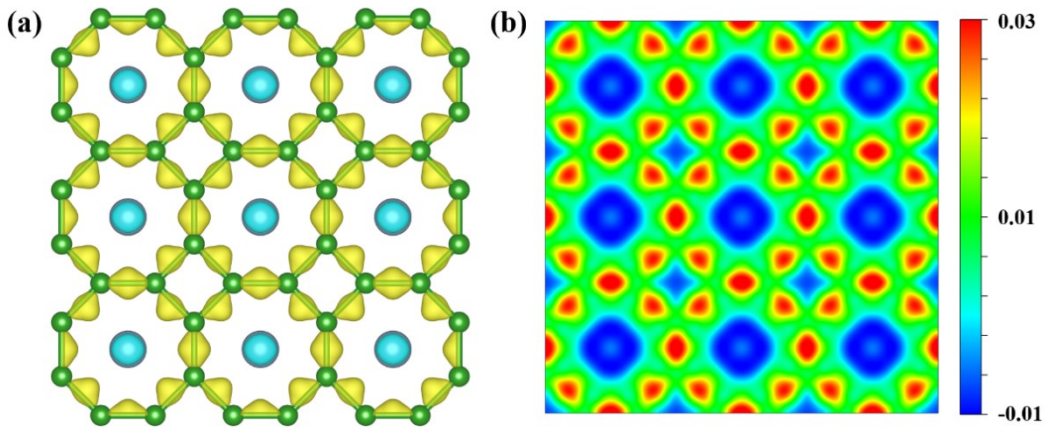

Fig. S3 The 3D (a) and 2D (b) differential charge density map of the AlB_4 monolayer.