Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

New Refractory MAB Phases and Their 2D Analogous: Insight into the Effects of Valence Electron Concentration and Chemical Compositions

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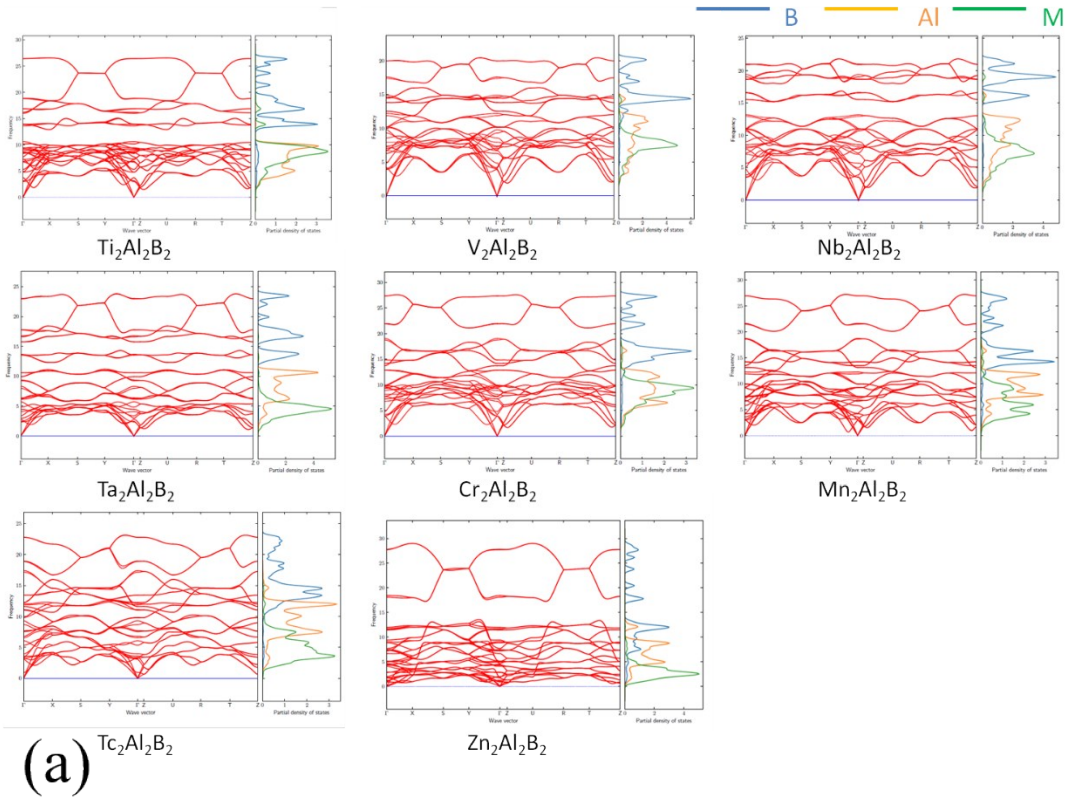


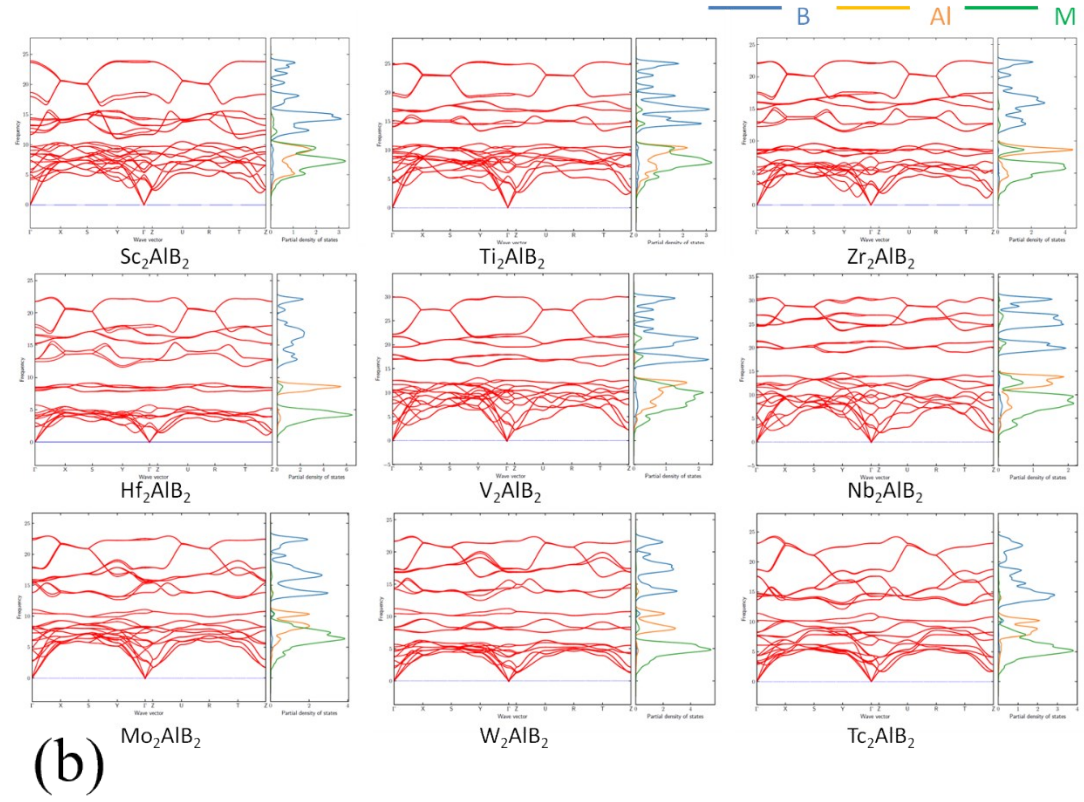


Figure S1. The phonon band structure and phonon partial density of state for (a) 222-MAB phases and (b) 212-MAB phases, respectively.

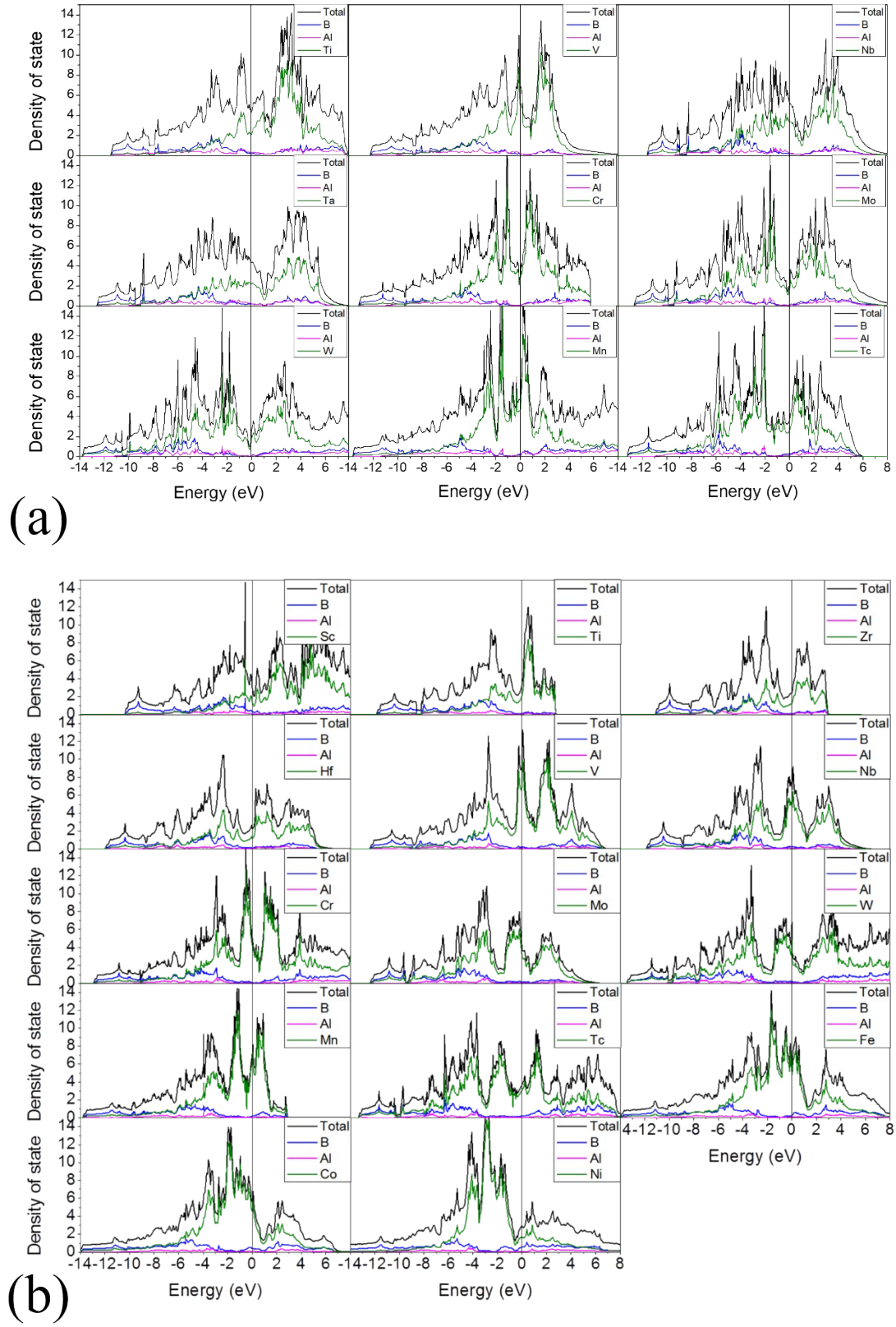


Figure S2. Total and partial density of states for the (a) 222-MAB phases and (b) 212-MAB phases, respectivly.

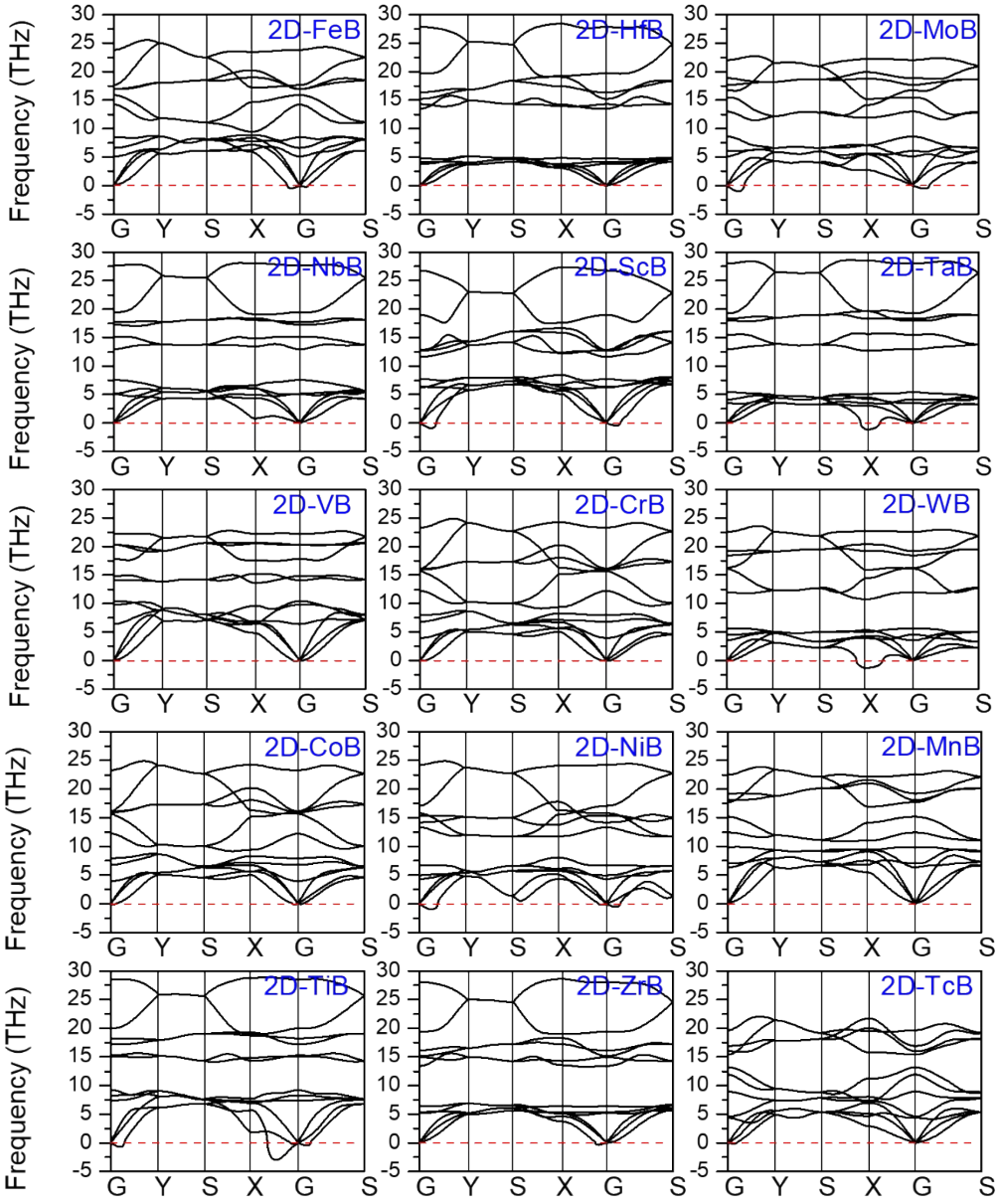


Figure S3. The phonon band structure for monolayer MABene phases.

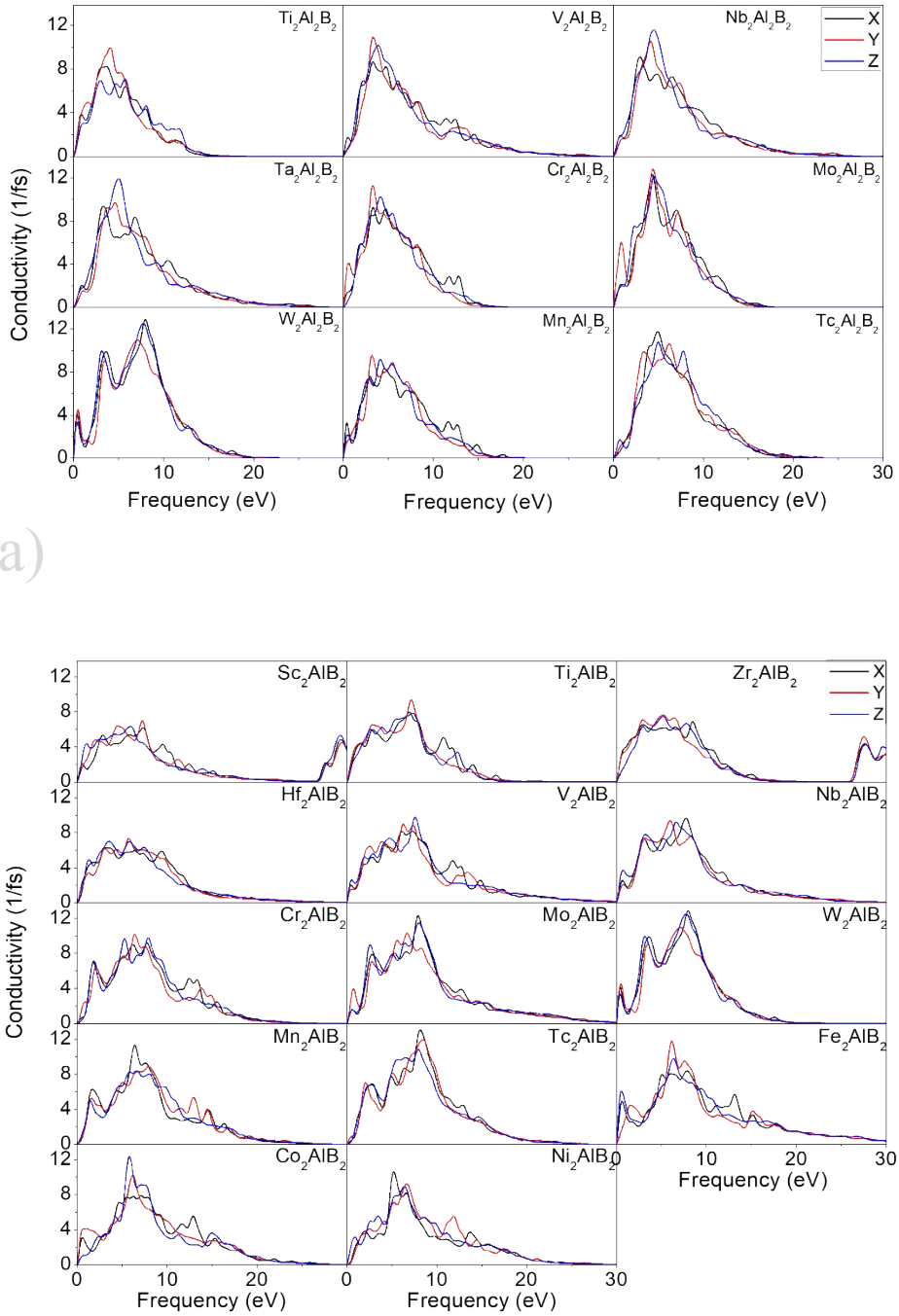


Figure S4. Optical conductivities of the (a) 222-MAB phases and (b) 212-MAB phases, respectivly.

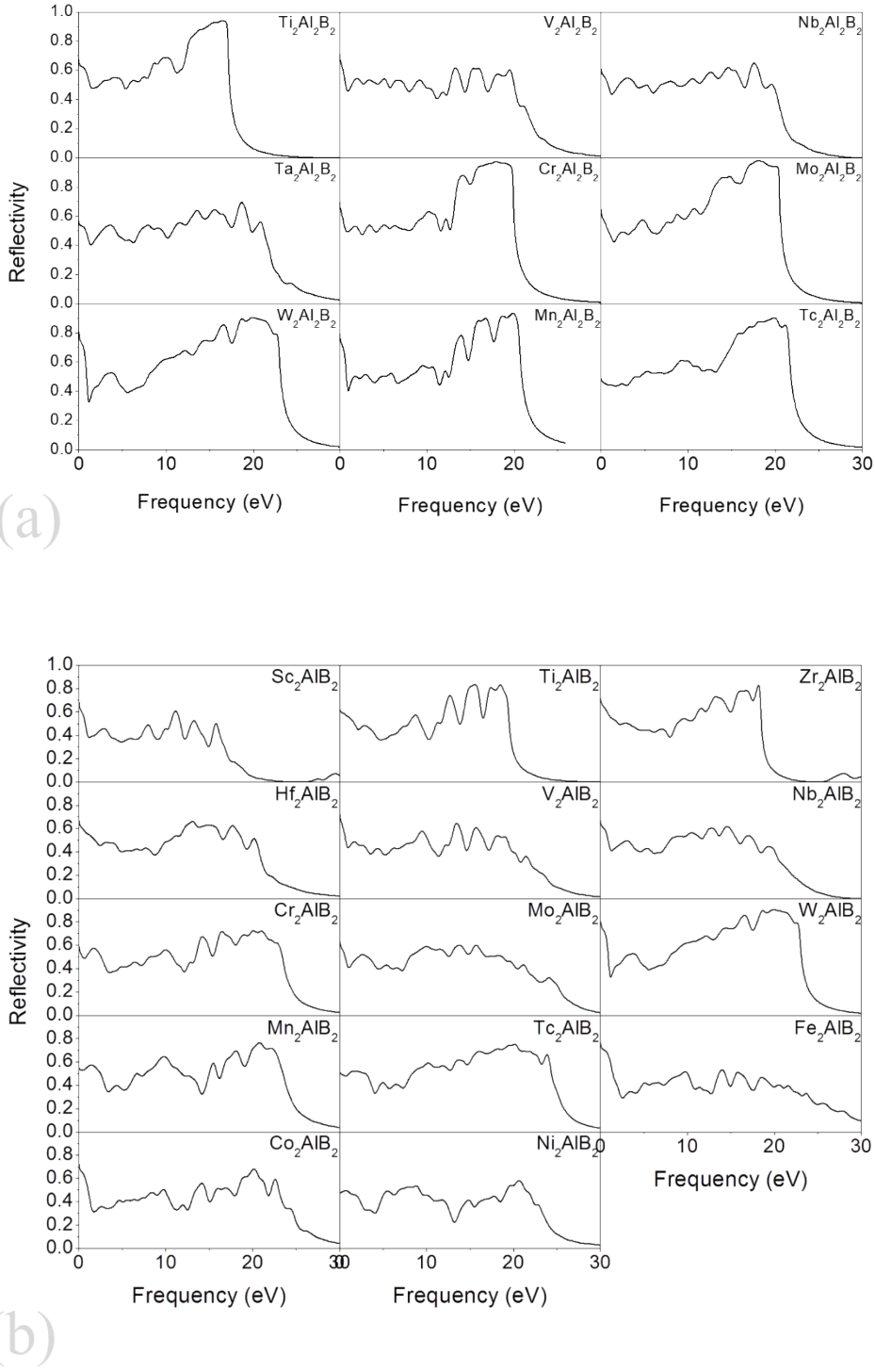
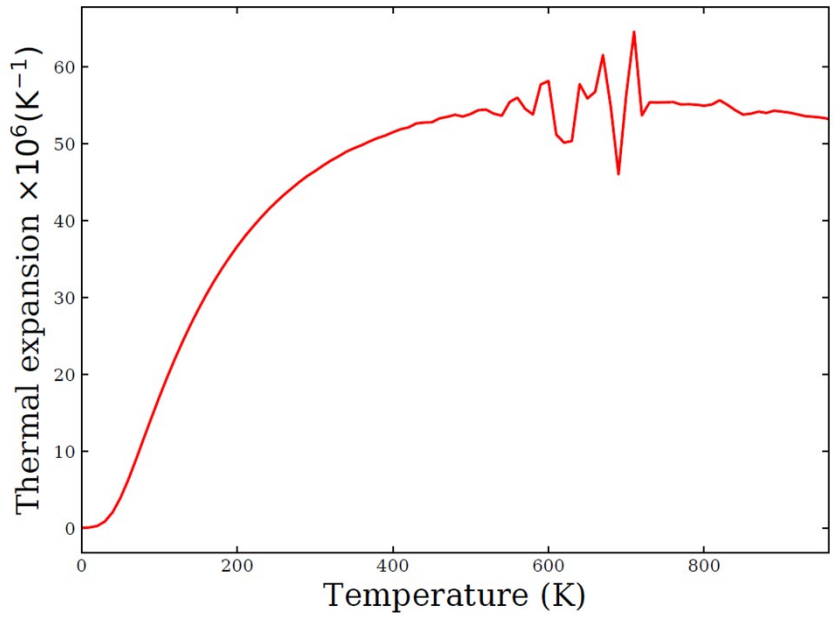
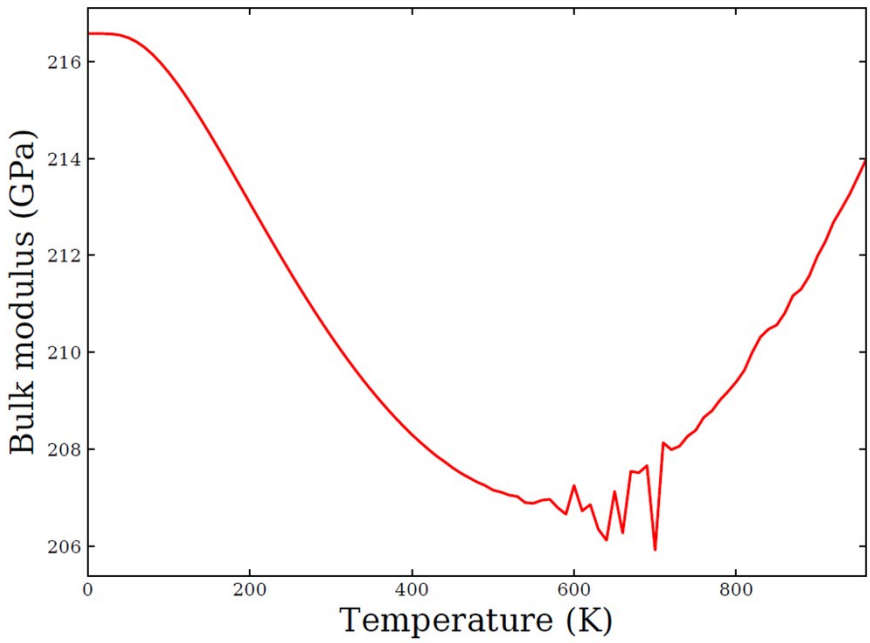


Figure S5. Optical reflectivity of the (a) 222-MAB phases and (b) 212-MAB phases, respectivly.



(a)



(b)

Figure S6. (a) Thermal expansion and (b) bulk modulus versus temperature by QHA method for $Mo_2Al_2B_2$ for comparing.

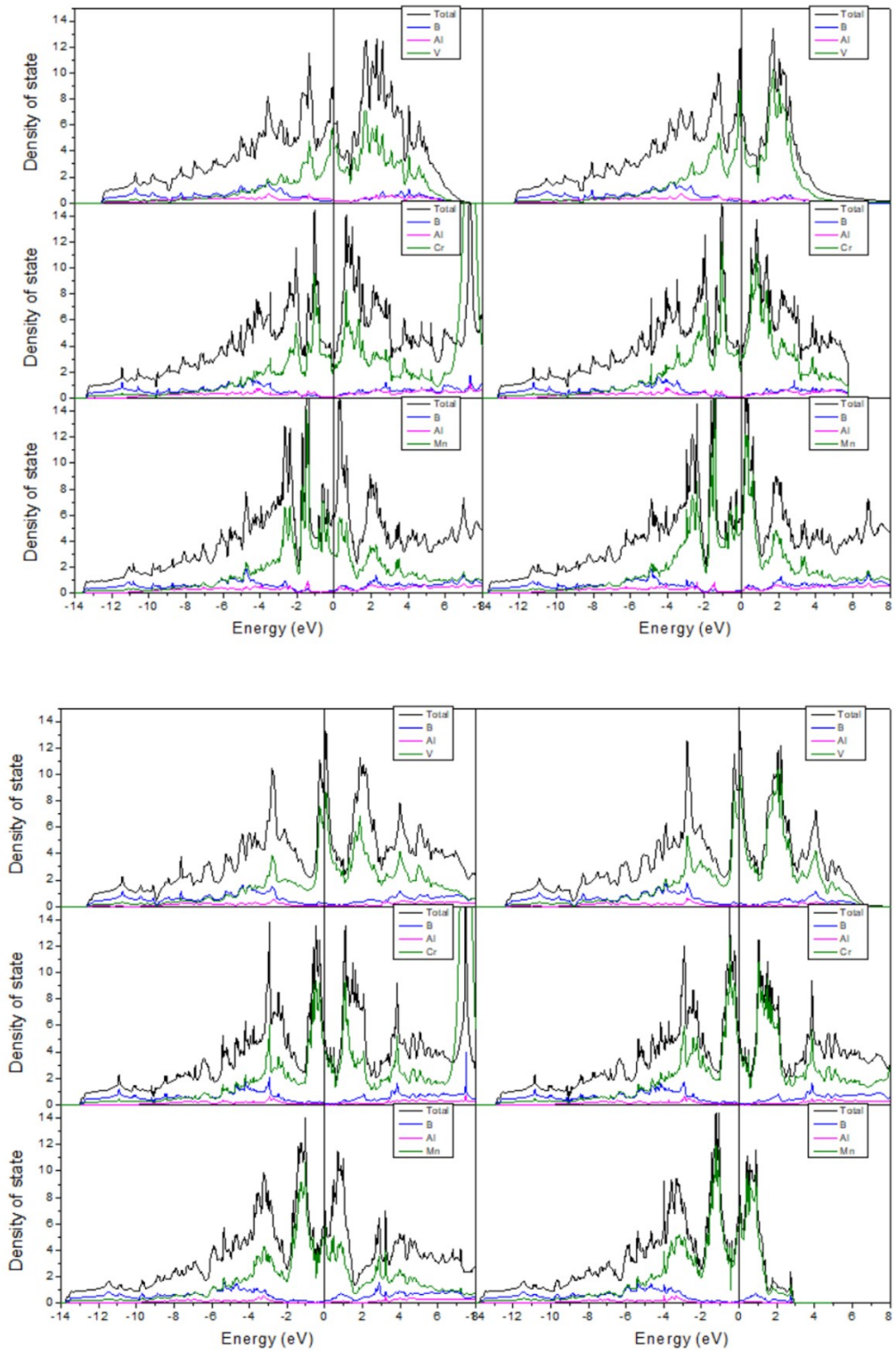


Figure S7. Total and partial density of states with DFT+U correction (left) and without correction (right) for the 222-MAB phases (upper) and 212-MAB phases (lower), respectivly. The value for the Hubbard-U parameter are 3.35 eV, 2.65 eV and 3.9eV for V, Cr and Mn element, respectively.

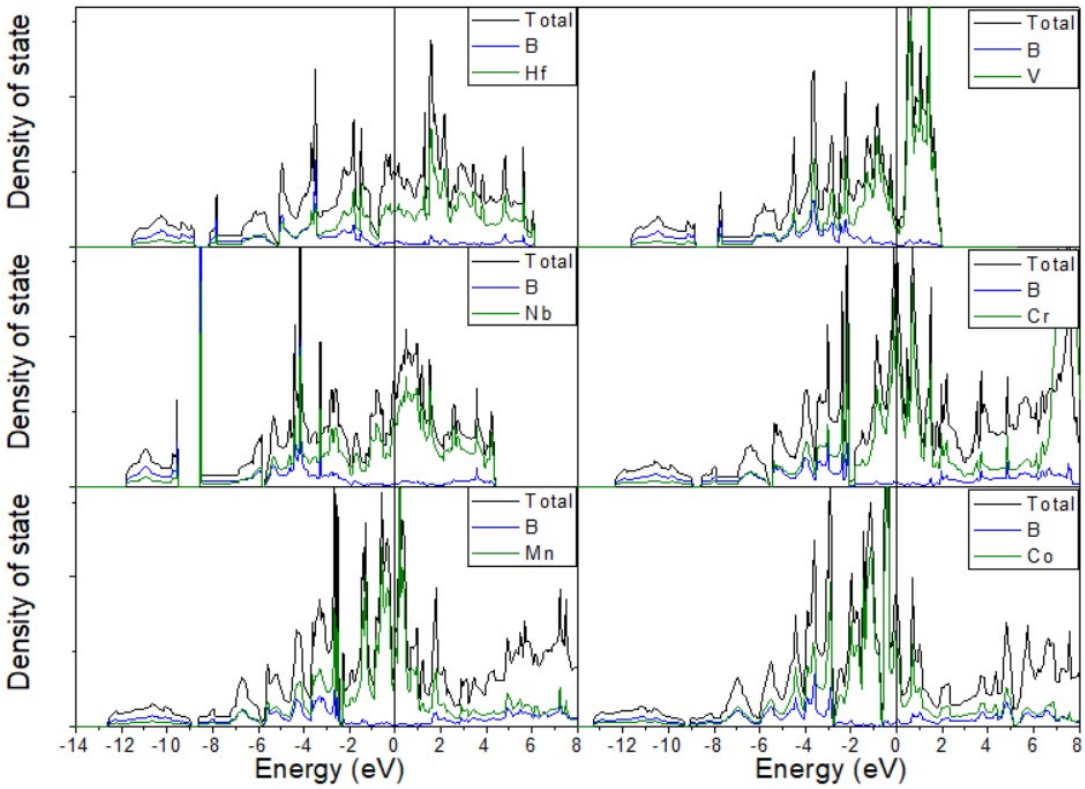


Figure S8 Total and partial density of states for six MBenes

Table S1. Cauchy pressure P (in GPa), anisotropy index Au (in %), theoretical hardness Hv (from the empirical formula developed by ourselves) and experimental hardness of studied 9 222-MAB typed MAB phases.

	P_a	P_b	P_c	A_u	H_V	*H (expt.)*
$Ti_2Al_2B_2$	−29	−48	−84	0.48	17	—
$V_2Al_2B_2$	−71	−27	−77	0.58	19	—
$Nb_2Al_2B_2$	−51	−48	−40	0.46	19	—
$Ta_2Al_2B_2$	−49	−47	−50	0.57	20	—
$Cr_2Al_2B_2$	−42	−73	−48	0.54	21	—
$Mo_2Al_2B_2$	−26	−62	−16	0.33	21	13.6
$W_2Al_2B_2$	−23	−52	18	0.45	22	21.7
$Mn_2Al_2B_2$	−21	−15	−24	1.67	15	—
$Tc_2Al_2B_2$	−7	61	10	0.51	17	—

Table S2. Cauchy pressure P (in GPa), anisotropy index Au (in %), theoretical hardness Hv (from the empirical formula developed by ourselves) and experimental hardness of studied 14 212-MAB typed MAB phases.

	P_a	P_b	P_c	A_u	H_V	*H (expt.)*
Sc_2AlB_2	17	4	−21	0.13	21	—
Ti_2AlB_2	−68	−85	−113	0.45	22	—
Zr_2AlB_2	−20	−50	−79	1.24	16	—
Hf_2AlB_2	−47	−53	−81	0.53	19	—
V_2AlB_2	13	6	−98	0.34	19	—
Nb_2AlB_2	14	20	−9	0.47	17	—
Cr_2AlB_2	−52	−53	−97	0.08	26	7
Mo_2AlB_2	17	4	−21	0.13	21	—
W_2AlB_2	31	38	24	0.16	21	—
Mn_2AlB_2	−40	−1	−97	0.17	25	9.6
Tc_2AlB_2	57	73	−29	0.39	20	—
Fe_2AlB_2	−2	16	−52	0.13	20	14.7
Co_2AlB_2	54	98	16	0.66	14	—
Ni_2AlB_2	54	26	47	0.56	14	—

Table SIII The calculated atomic distance (bond length, Å), bond stiffness (GPa) and the ratio of the bond stiffness A/B of studied 9 222-MAB typed MAB phases.

	B-B	M-B1	M-B2	Al-B	M-Al	Al-Al	A/B
$Ti_2Al_2B_2$	1437	820	1135	621	746	498	0.35
$V_2Al_2B_2$	1171	699	1053	521	595	385	0.33
$Nb_2Al_2B_2$	1586	641	1056	485	595	469	0.30
$Ta_2Al_2B_2$	1464	694	1033	562	641	500	0.34
$Cr_2Al_2B_2$	1111	787	1128	633	658	403	0.36
$Mo_2Al_2B_2$	1197	781	1195	746	730	515	0.43
$W_2Al_2B_2$	1217	885	1229	862	826	562	0.46
$Mn_2Al_2B_2$	1377	-	1299	391	476	234	0.17
$Tc_2Al_2B_2$	1730	1588	1834	1082	1202	704	0.41

Table SIV The calculated atomic distance (bond length, Å), bond stiffness (GPa) and the ratio of the bond stiffness A/B of studied 14 212-MAB typed MAB phases.

	B-B	M-B1	M-B2	Al-B	M-Al	A/B
Sc_2AlB_2	885	435	562	251	358	0. 28
Ti_2AlB_2	1306	926	1221	592	694	0.45
Zr_2AlB_2	1867	893	1270	369	602	0.20
Hf_2AlB_2	1002	645	885	332	474	0.33
V_2AlB_2	962	806	1338	513	488	0.33
Nb_2AlB_2	1765	826	1265	356	524	0.20
Cr_2AlB_2	1145	862	1223	592	637	0.48
Mo_2AlB_2	1150	971	1281	568	654	0.44
W_2AlB_2	1092	1156	1418	625	704	0.44
Mn_2AlB_2	1185	1023	1453	568	610	0.39
Tc_2AlB_2	1851	1804	1894	901	1124	0.48
Fe_2AlB_2	1336	1230	1374	478	521	0.35
Co_2AlB_2	1531	962	1657	671	529	0.36
Ni_2AlB_2	1743	709	1202	621	565	0.32

Table SV lattice parameter (Å) of six MBenes

	a	**b**	**c**	**α=β=γ**
Hf2B2	3.06758	3.23409	20	90°
V2B2	2.91722	3.23181	20	90°
Nb2B2	2.99991	3.20713	20	90°
Cr2B2	2.9019	2.85258	20	90°
Mn2B2	2.86687	2.79973	20	90°
Co2B2	2.80382	2.79853	20	90°