Supporting Information

Designing Ultrastrong 5d Transition Metal Diborides with Excellent Stability for Harsh Service Environments

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Table S1. Inorganic Crystal Structure Database (ICSD) prototype library for screening the thermodynamically feasible structure of 5d transition metal diborides at 0 and 100GPa.

No.	Prototype	Pearson symbol	Space group	Lattice parameters (Å)						SG number	Ref.
				a	*b*	*c*	*α*	*β*	*γ*		
1	NbO_2	tI96	$I4_1/a$	13.696		5.981				88	1
2	Te_2Br	oP24	Pnma	14.921	12.843	4.005				62	2
3	SiO_2	mS144	Cc	18.494	4.991	25.832		117.7		9	3
4	VO_2	mS24	C2/m	12.030	3.693	6.420		106.1		12	4
5	SnF_2	mS48	C2/c	13.353	4.909	13.787		109.1		15	5
6	FeS_2	cP12	Pa-3	5.428						205	6
7	$AlPt_2$	oP24	Pmma	16.297	3.921	5.439				51	7
8	SrS_2	tI12	I4/mcm	6.095		7.616				140	8
9	$CaSb_2$	mP6	$P2_1/m$	4.746	4.177	9.084		106.3		11	9
10	$TiSi_2$	oF24	Fddd	8.267	4.800	8.550				70	10
11	$BaSi_2$	hP3	P-3m1	4.047		5.330				164	11
12	LaS_2	oP24	Pnma	8.131	16.340	4.142				62	12
13	SiO_2	aP240	F1	9.932	17.216	81.864				1	13
14	VO_2	aP12	P-1	9.065	5.749	4.521	90.0	91.1	89.8	2	14
15	$NdAs_2$	mP12	$P2_1/c$	4.108	6.820	10.443		106.7		14	15
16	GeS_2	mP48	$P2_1/c$	6.875	22.550	6.809		120.4		14	16
17	Fe_2Tb	hR6	R-3m	5.207		5.207				166	17
18	$ZnCl_2$	oP12	$Pna2_1$	6.443	7.693	6.125				33	18
19	CrP_2	mS12	C2/m	8.213	3.034	7.098		119.5		12	19
20	$SrSi_2$	cP12	$P4_332$	6.515						212	20
21	CuF_2	mP6	$P2_1/c$	3.307	4.546	4.599		96.6		14	21
22	$YbCl_2$	oP24	Pbca	13.15	6.942	6.693				61	22
23	CdI_2	hP18	P3m1	4.240		41.010				156	23
24	AgF_2	oP12	Pbca	5.529	5.813	5.073				61	24
25	V_2N	hP9	P-31m	4.917		4.568				162	25
26	CdI_2	hP21	P3m1	4.240		41.010				156	26
27	CdI_2	hP12	P3m1	4.240		27.34				156	27
28	CdI_2	hP24	P3m1	4.240		54.68				156	27
29	CdI_2	hP30	P3m1	4.240		68.35				156	27
30	CdI_2	hR18	R3m	4.240		123.03				160	28
31	TiO_2	tI12	$I4_1/amd$	3.785		9.514				141	29
32	FeS_2	aP12	P1	5.417	5.417	5.417	90.0	90.0	90.0	1	30
33	F_2Sn	oP12	$P2_12_12_1$	5.073	5.073	8.491				19	31
34	Cl_4Ga_2	oP24	Pnna	7.240	7.240	9.500				52	32
35	Te_2W	oP12	$Pmn2_1$	6.282	3.496	14.070				31	33

36	$MoTe_2$	mP12	$P2_1/m$	6.330	3.469	13.860	93.9	11	33
37	$NbTe_2$	mS18	C2/m	19.390	3.642	9.375	134.6	12	34
38	$BaSi_2$	oP24	Pnma	8.920	6.750	11.570		62	35
39	B_8S_{16}	mP48	$P2_1/c$	12.091	4.063	21.870	107.6	14	36
40	STi_2	oP36	Pnnm	11.350	14.060	3.320		58	37
41	O_2Si	oS24	$C222_1$	8.740	5.050	8.240		20	38
42	CdI_2	hP27	P3m1	4.240		61.515		156	39
43	$CaSi_2$	hR3	R-3m	3.820		15.980		166	40
44	Cl_2Pb	oP12	Pnma	7.620	9.050	4.535		62	41
45	H_2O	hR36	R-3	12.983		6.253		148	42
46	Cl_2Zn	mP36	$P2_1/c$	6.540	11.310	13.957	117.9	14	43
47	As_2Cd	tI12	$I4_122$	7.956		4.674		98	44
48	O_2Ti	tP6	$P4_2/mnm$	4.594	4.594	2.959		136	45
49	PdS_2	oP12	Pbca	5.460	5.541	7.531		61	46
50	$CrSi_2$	hP9	$P6_222$	4.431		6.364		180	47
51	S_2Si	tI12	I-42d	5.420		8.718		122	48
52	Se_2Ta	hP12	$P6_3/mmc$	3.460		25.180		194	49
53	P_2Zn	tP24	$P4_12_12$	5.080		18.590		92	50
54	As_2Nb	mS12	C121	9.357	3.382	7.792	119.5	5	51
55	O_2Zr_1	mP12	$P2_1/c$	5.145	5.207	5.311	99.2	14	52
56	MnO_2	tI24	I4/m	9.815		2.847		87	53
57	As_2Zr	oP12	Pnma	6.801	3.689	9.027		62	54
58	O_2Pb	oP12	Pbcn	4.948	5.951	5.497		60	55
59	As_2Ti	oP24	Pnnm	8.915	13.230	3.479		58	56
60	CdI_2	hP9	P-3m1	4.240		20.500		164	57
61	HgI_2	oS12	$Cmc2_1$	4.702	7.432	13.872		36	58
62	O_2V	oP12	Pbnm	9.390	2.930	4.890		62	59
63	CO_2	cP12	Pa-3	5.630				205	60
64	HgI_2	tP6	$P4_2/nmc$	4.357		12.360		137	61
65	Cl_2Hg	oP12	Pnma	12.776	5.986	4.333		62	62
66	$FeSi_2$	oS48	Cmca	9.863	7.791	7.833		64	53
67	F_2Kr	tP6	$P4_2/mnm$	4.585		5.827		136	63
68	Cu_2S	mP144	$P2_1/c$	15.246	11.884	13.494	116.3	14	64
69	B_2W	hP12	$P6_3/mmc$	2.983		13.879		194	65
70	B_2Re	hP6	$P6_3/mmc$	2.900		7.478		194	66
71	As_2Ge	oP24	Pbam	14.760	10.160	3.728		55	67
72	MoS_2	hP6	$P6_3/mmc$	3.150		12.300		194	68
73	O_2Se	tP24	$P4_2/mbc$	5.061		8.370		135	69
74	Li_2Si	mS12	C2/m	7.700	4.410	6.560	113.4	12	70
75	As_2Ni	oP24	Pbca	5.770	5.838	11.419		61	71
76	O_4Sb_2	cF96	Fd-3m	10.240				227	72

77	I_2Pb	hP9	P3m1	4.557		20.937		156	73
78	Ag_2Te	mP12	$P2_1/c$	8.090	4.480	8.960	123.3	14	74
79	MoO_2	mP12	$P2_1/c$	5.539	4.856	5.628	119.7	14	75
80	$FeSi_2$	tP3	P4/mmm	2.684		5.128		123	76
81	Ga_2I_4	hR36	R3c	25.215		7.839		161	77
82	Br_2Sr	tP30	P4/n	11.630		7.146		85	78
83	Nb_2Se	mS24	C2/m	13.992	3.422	9.283	91.7	12	79
84	STa_2	oP36	Pbcm	7.379	5.574	15.190		57	80
85	CdP_2	oP12	$Pna2_1$	9.900	5.408	5.171		33	81
86	$HoSb_2$	oS6	C222	3.343	5.790	7.84		21	82
87	Se_2Ta	hP12	$P6_3mc$	3.436		25.532		186	83
88	$AsPd_2$	oS24	$Cmc2_1$	3.245	16.844	6.576		36	84
89	Te_2U	oI12	Immm	4.162	6.127	13.965		71	85
90	N_2S_4	tP24	$P4_2nm$	11.146		3.773		102	86
91	C_2Th	mS12	C2/c	6.530	4.240	6.560	104.0	15	87
92	F_2Xe	tI6	I4/mmm	4.315		6.99		139	88
93	Cl_2Cu	mS6	C2/m	6.850	3.300	6.674	120.6	12	89
94	TeO_2	oP24	Pbca	5.464	5.607	12.035		61	90
95	$MoSi_2$	tI6	I4/mmm	3.200		7.861		139	91
96	$CeSe_2$	mP12	$P2_1/c$	8.420	4.210	8.420	90.0	14	92
97	D_2S	tP12	$P4_2/mnm$	6.735		4.101		136	93
98	S_2Si	oI12	Ibam	5.564	9.545	5.552		72	94
99	O_2Si	hP9	$P3_121$	4.965		5.424		152	95
100	Ag_2F	hP3	P-3m1	2.996		5.691		164	96
101	CdI_2	hP39	P3m1	4.240		88.800		156	97
102	Cl_2Pd	oP6	Pnnm	3.820	11.020	3.350		58	98
103	$PdSn_2$	tI48	$I4_1/acd$	6.490		24.378		142	99
104	BFe_2	tI12	I-42m	5.109		4.249		121	100
105	Mo_2N	tI12	$I4_1/amd$	4.200		4.981		141	101
106	Mg_2Ni	hP18	$P6_222$	5.205		13.236		180	102
107	Br_2Zn	tI96	$I4_1/acd$	11.389		21.773		142	103
108	$C_{12}N_6$	cP72	Pa-3	10.781				205	104
109	GeS_2	oF72	Fdd2	11.680	22.380	6.870		43	105
110	B_2Ru	oP6	Pmmn	2.867	4.644	4.045		59	106
111	CS_2	oS12	Cmca	6.086	5.286	9.462		64	107
112	O_2V	oF96	F222	5.795	12.597	13.015		22	108
113	H_2O	tP36	$P4_12_12$	6.730		6.830		92	109
114	O_2Si	tP36	$P4_32_12$	7.456		8.604		96	110
115	$I_{12}Zr_6$	hR18	R-3	14.502		9.996		148	111
116	CuP_2	mP12	$P2_1/c$	12.658	7.256	14.630	107.5	14	112
117	CdI_2	hP45	P3m1	4.240		102.540		156	113

118	CdI_2	hP48	P3m1	4.240		109.380				156	113
119	Cs_2Te	oP12	Pnma	9.109	5.871	11.494				62	114
120	CdI_2	hP24	$P6_3mc$	4.240		54.680				186	115
121	CdI_2	hR12	R-3m	4.240		82.000				166	115
122	CdI_2	hP6	$P6_3mc$	4.240		13.700				186	116
123	KO_2	tI6	F4/mmm	5.704		6.699				139	117
124	$ReSi_2$	oI6	Immm	3.128	3.144	7.677				71	118
125	MoS_2	hR3	R3m	3.166		18.410				160	119
126	O_2Si	aP9	P1	4.350	4.180	4.620	83.8	101.6	119.0	1	120
127	O_2Si	tI288	I-4m2	20.067		13.411				119	121
128	O_2Si	mS168	C2/c	24.863	5.012	24.372		107.7		15	122
129	PZr_2	oS108	Cmmm	19.063	29.509	3.607				65	123
130	O_2Si	hP12	$P6_3/mmc$	5.052		8.270				194	124
131	BaS_2	mS12	C2/c	9.347	4.761	9.050		118.4		15	125
132	CdI_2	hP60	P3m1	4.240		136.700				156	126
133	CdI_2	hP15	P3m1	4.240		34.170				156	126
134	CdI_2	hP33	P3m1	4.240		75.170				156	126
135	CdI_2	hP36	P3m1	4.240		82.020				156	126
136	CdI_2	hR6	R-3m	4.240		41.010				166	126
137	CdI_2	hR9	R-3m	4.240		61.510				166	126
138	CdI_2	hR12	R-3m	4.240		82.020				166	126
139	CdI_2	hR15	R-3m	4.240		102.510				166	126
140	CdI_2	hR30	R-3m	4.240		205.020				166	126
141	CdI_2	hR36	R-3m	4.240		246.020				166	126
142	CdI_2	hR42	R-3m	4.240		287.030				166	126
143	CdI_2	hP57	P3m1	4.240		129.850				156	127
144	CdI_2	hR24	R-3m	4.240		164.020				166	127
145	CdI_2	hR27	R-3m	4.240		184.520				166	127
146	CdI_2	hP42	P3m1	4.240		95.690				156	128
147	CdI_2	hP54	P3m1	4.240		123.000				156	128
148	FeS_2	oP6	Pnnm	4.441	5.425	3.387				58	129
149	Al_2Cu	tI12	I4/mcm	6.063		4.872				140	130
150	STl_2	hR27	R3	12.200		18.170				146	131
151	La_2Sb	tI12	I4/mmm	4.626		18.060				139	132
152	O_8P_4	mS48	C2/c	9.660	10.100	6.930		96.8		15	133
153	Sb_2Sm	oS24	Cmca	6.171	6.051	17.890				64	134
154	Co_2Sb	mP12	$P2_1/c$	6.520	6.380	6.505		118.2		14	135
155	Ag_2S	mP12	$P2_1/c$	4.230	6.910	8.291		110.6		14	136
156	PRe_2	oP12	Pnma	5.540	2.900	10.039				62	137
157	O_2Si	hP102	P6/mmm	13.783		11.190				191	138
158	HgO_2	mS6	C2/m	4.470	5.459	3.519		108.4		12	139

159	$Br_{10}Si_5$	mP60	$P2_1/c$	10.279	14.699	14.797		119.7		14	140
160	D_2O	tI24	$I4_1/amd$	4.669		6.810				141	141
161	NbS_2	oS6	Amm2	14.081	3.327	5.795				38	142
162	Dy_2Te	oP36	Pnma	21.860	4.060	11.420				62	143
163	$InMg_2$	hP9	P-62m	8.270		3.420				189	144
164	Cu_2O	cP6	Pn-3m	4.268						224	145
165	S_2Ta	hR6	R3m	3.315		36.200				160	146
166	Se_2Ta	aP39	P-1	12.523	12.523	9.358	101.9	43.9	120.0	2	147
167	$CaSi_2$	hR6	R-3m	3.887		30.526				166	148
168	CdI_2	hP3	P-3m1	4.250		6.850				164	149
169	C_2Ca	tI6	I4/mmm	3.890		6.380				139	150
170	O_2Te	tP6	$P4_2/mnm$	4.799		3.778				136	151
171	Ge_2Tb	oS24	Cmmm	4.096	29.834	3.987				65	152
172	O_2Ti	oP24	Pbca	5.135	9.166	5.436				61	153
173	O_2Si	mP12	$P2_1$	4.708	5.528	5.006		107.8		4	154
174	Ag_2Nd	hP3	P6/mmm	4.789		7.060				191	155
175	Au_2Ti	tI6	I4/mmm	3.430		8.538				139	156, 157
176	$CaIn_2$	hP6	$P6_3/mmc$	4.891		7.736				194	158
177	$CaHg_2$	hP3	P6/mmm	4.887		3.573				191	159
178	Cd_2Ce	hP3	P-3m1	5.073		3.450				164	160-162
179	$InNi_2$	hP6	$P6_3/mmc$	4.171		5.121				194	163
180	O_2Se	oP24	Pbam	8.134	8.146	4.928				55	164
181	P_2Zn	mP24	$P2_1/c$	8.866	7.291	7.561		102.3		14	43, 165
182	CaF_2	cF12	Fm-3m	5.462						225	166
183	I_2Pt	mP12	$P2_1/c$	6.587	8.715	6.889				14	167
184	O_2Si	oS72	$Cmc2_1$	13.836	17.415	5.042				36	168
185	I_2O_4	mP24	$P2_1/c$	7.807	6.699	8.341		116.6		14	169
186	$AuTe_2$	mS6	C2/m	7.194	4.414	5.070		90.0		12	170
187	O_2Si	oS336	Cmma	13.695	22.326	20.178				67	171
188	$SeTa_2$	tP6	P4/nmm	3.375		9.832				129	172
189	Nb_2P	oP54	Pmma	18.079	3.425	13.858				51	173
190	$ReSe_2$	aP12	P-1	6.716	6.602	6.728	104.9	91.8	118.9	2	174
191	O_2Zr	tP6	$P4_2/nmc$	3.592		5.179				137	175
192	S_2Ta	oF12	Fmm2	3.301	23.119	5.724				42	176
193	ClO_2	oP24	Pbca	5.538	10.783	6.674				61	177
194	O_2Si	mS36	I2/a	8.758	4.876	10.715		90.1		15	178
195	S_2Ta	hP6	$P6_3/mmc$	3.314		12.097				194	179
196	NSr_2	hR3	R-3m	3.856		20.695				166	180
197	Fe_2P	hP9	P-62m	5.868		3.456				189	181
198	NbS_2	oF12	Fmm2	3.314	5.714	22.511				42	182
199	O_2Si	oP108	Pnnm	18.575	13.995	7.391				58	183

200	O_2Si	tI12	I-42d	4.7481		7.488				122	184
201	O_2Si	aP12	P1	5.098	5.295	6.959	110.9	107.5	83.9	1	184
202	CFe_2	oP6	Pnnm	4.704	4.318	2.830				58	185
203	Cu_2Te	hP6	P6/mmm	4.237		7.274				191	186
204	Si_2Th	tI12	$I4_1$/amd	4.134		14.375				141	187
205	O_2Si	cF24	Fd-3m	7.131						227	188
206	CTi_2	cF48	Fd-3m	8.600						227	189
207	$NbSb_2$	mS12	C2/m	10.218	3.630	8.315		120.0		12	190
208	Pt_2Si	tI6	I4/mmm	3.933		5.910				139	191
209	$BaCl_2$	mP24	$P2_1$/c	8.613	4.604	11.901		92.5		14	192
210	IrS_2	oP24	Pnma	19.791	5.624	3.567				62	193
211	KSb_2	mS12	C2/m	14.055	4.233	7.053		95.0		12	194
212	O_2Si	mS24	Cc	5.007	5.007	8.217		91.5		9	195
213	Cr_2P	oI36	Imm2	91.512	10.402	6.337				44	196
214	Ge_2U	oS12	Cmmm	4.008	15.088	4.095				65	197
215	$O_{144}Si_{72}$	hP216	P6/mmm	14.208		24.945				191	198
216	$CdCl_2$	hR3	R-3m	3.845		17.493				166	199
217	KO_2	mS12	C2/c	7.880	4.036	7.968		122.8		15	200
218	HfO_2	oP12	Pmnb	3.302	5.569	6.453				62	201
219	$O_{48}Si_{24}$	mS72	C2/m	14.018	13.612	7.418		102.1		12	202
220	O_2Si	hP9	$P6_222$	4.996		5.457				180	203
221	O_2V	mP6	P2/m	4.506	2.899	4.617		91.8		10	204
222	$IrTe_2$	mS18	C2/m	19.975	4.001	5.312		90.8		12	205
223	D_2Zr	tI6	I4/mmm	3.506		4.455				139	206
224	Ge_2Ni	oS24	Cmca	10.830	5.763	5.762				64	207
225	O_2Si	mP24	$P2_1$/c	8.377	4.602	9.058		124.9		14	208
226	C_2Ca	mS12	C2/m	7.207	3.828	7.367		107.2		12	209
227	Si_2Zr	oS12	Cmcm	3.706	14.735	3.672				63	210
228	$GaLi_2$	oS12	Cmcm	4.562	9.542	4.364				63	211
229	O_2Si	mS48	C2/c	7.135	12.372	7.173		120.4		15	212
230	Fe_2Si	hP6	P-3m1	4.052		5.086				164	213
231	O_2Si	oP72	$P2_12_12_1$	26.163	4.987	8.199				19	214
232	F_2Pd	cP12	Pa-3	5.329						205	215
233	$CeCu_2$	oI12	Imma	4.430	7.050	7.540				74	216
234	$CuMg_2$	oF48	Fddd	9.070	5.284	18.250				70	217
235	Cu_2Mg	cF24	Fd-3m	7.021						227	218
236	$CuZr_2$	tI6	I4/mmm	3.220		11.183				139	219
237	Ga_2Hf	tI24	$I4_1$/amd	4.046		25.446				141	220
238	$GaMg_2$	hP18	P-62c	7.794		6.893				190	221
239	Ga_2Zr	oS12	Cmmm	12.894	3.994	4.123				65	220
240	Hg_2Pt	tP3	P4/mmm	4.687		2.913				123	222

241	$MgNi_2$	hP24	$P6_3/mmc$	4.824		15.826				194	223
242	$MgZn_2$	hP12	$P6_3/mmc$	5.221		8.567				194	223
243	$MoPt_2$	oI6	Immm	2.765	8.296	3.938				71	224
244	Na_2Tl	oS48	$C222_1$	13.935	8.87	11.693				20	225
245	$NiTi_2$	cF96	Fd-3m	11.278						227	226
246	Ni_2Tm	cF192	F-43m	14.193						216	227
247	Re_2U	oS24	Cmcm	5.600	9.180	8.460				63	228
248	Br_2Hg	hP9	P3	6.757		5.658				143	229
249	$O_{128}Si_{64}$	mS192	C2/c	5.019	33.743	21.165		90.5		15	230
250	Co_2Nd	tI12	$I4_1/amd$	5.153		7.277				141	231
251	Co_2Nd	oI12	Imma	5.150	5.145	7.296				74	231
252	N_2Rh	mP12	$P2_1/c$	4.772	4.795	4.806		108.5		14	232
253	H_2Be	oI36	Ibam	8.967	4.141	7.643				72	233
254	O_2Si	mP48	$P2_1/c$	7.235	12.485	7.241		120.2		14	234
255	$O_{128}Si_{64}$	tI192	$I4_1/amd$	10.232		34.364				141	235
256	Co_2Si	oP12	Pnma	4.906	3.729	7.090				62	236
257	C_2Os	hP3	P-6m2	2.870		4.020				187	237
258	NRe_2	hP6	$P6_3/mmc$	2.776		9.741				194	238
259	$ScSn_2$	tI24	$I4_1/amd$	4.233		31.039				141	239
260	BeF_2	cP36	P-43n	8.529						218	240
261	$BeCl_2$	cI144	I-43m	19.791						217	240
262	$H_{0.5}Si$	cF12	Fd-3m	5.479						227	241
263	H_2Mg	tP6	$P4_2/mnm$	4.512		3.017				136	242
264	N_2O_4	cI36	Im-3	7.694						204	243
265	O_2Si	cF408	Fd-3m	19.360						227	244
266	I_2Sr	oP12	Pnma	12.328	4.920	8.384				62	245
267	I_4P_2	aP6	P-1	4.461	7.044	7.346	80.7	73.8	81.7	2	246
268	IrN_2	oP6	Pnnm	3.805	4.508	2.434				58	247
269	$CaCl_2$	oP6	Pnnm	6.437	6.287	4.178				58	248
270	H_2O	aP36	P1	8.116	8.318	3.964	90.1	89.9	90.0	1	249
271	$EuGe_2$	hP3	P-3m1	4.235		4.589				164	250
272	Ag_2Se	oP12	$P2_12_12_1$	4.337	7.070	7.773				19	251
273	N_2Os	hP3	P6/mmm	2.829		4.972				191	252
274	N_2Os	tP6	P4/mbm	3.981		2.439				127	252
275	Ag_2S	oP12	$P2_12_12_1$	6.779	4.326	7.115				19	253
276	As_2La	mS48	Cc	12.864	14.422	9.083		134.8		9	254
277	O_2Si	mS96	I2/m	18.628	13.478	7.630		101.9		12	255
278	$O_{72}Si_{36}$	oI108	Immm	7.425	14.056	18.755				71	256
279	Pt_2N_4	hR6	$P6_3/mmc$	3.276		7.596				194	257
280	$Cl_{12}Mo_6$	oS72	Cmca	11.253	11.277	14.068				64	258
281	O_2Si	aP48	P-1	5.023	12.735	14.722	103.4	90.5	100.9	2	259

282	Cu_2Ti	oS12	Amma	4.363	7.977	4.478	63	260
283	LaS_2	tP24	P-4b2	8.185		8.280	117	261
284	Mn_2P	hP9	P321	6.082		3.457	150	262
285	$NbSe_2$	hP12	P-6m2	3.480		25.450	187	263

Table S2. Calculated lattice constants (Å), Pugh ratio G/B, minimum ideal tensile strength σ_{min} (GPa) and ideal shear strength τ_{min} (GPa) and their corresponding paths of 5d TMB_2 (TM=Hf, Ta, W, Re, Os and Ir) in four structures at 0 GPa.

Structure	Compound	Lattice constants			Pugh ratio	Tensile	σ_{min}	Shear	τ_{min}	NOTE
		a	b	c						
hP3[191]	HfB_2	3.142	-	3.489	0.907	[10-10]	35.2	(10-10)[-12-10]	37.3	This work
		3.144	-	3.502	-	-	-	-	-	Ref. 264
		-	-	-	0.869	[10-10]	37.3	(10-10)[-12-10]	33.3	Ref. 265
	TaB_2	3.098	-	3.328	0.641	[10-10]	32.6	(0001)[-12-10]	29.4	This work
		3.096	-	3.346	0.71	-	-	-	-	Ref. 266
	WB_2	3.018	-	3.363	0.500	[-12-10]	20.9	(0001)[10-10]	11.5	This work
		2.998	-	3.334	-	-	-	-	-	Ref. 264
	ReB_2	2.952	-	3.494	0.415	-	-	-	-	This work
	OsB_2	2.988	-	3.439	0.339	-	-	-	-	This work
	IrB_2	3.106	-	3.255	0.472	-	-	-	-	This work
		3.107	-	3.259	-	-	-	-	-	Ref. 266
hP12[194]	HfB_2	3.130	-	15.345	0.809	[10-10]	35.6	(0001)[10-10]	6.0	This work
	TaB_2	3.048	-	14.638	0.809	[10-10]	36.0	(0001)[10-10]	23.4	This work
	WB_2	3.017	-	14.037	0.731	[10-10]	45.2	(0001)[10-10]	25.9	This work
	ReB_2	2.979	-	14.098	0.591	-	-	-	-	This work
	OsB_2	2.927	-	14.908	0.898	-	-	-	-	This work
	IrB_2	2.980	-	15.021	-	-	-	-	-	This work
		2.979	-	15.045	-	-	-	-	-	Ref. 267
hP6[194]	HfB_2	3.064	-	8.456	0.403	-	-	-	-	This work
		3.084	-	8.535	-	-	-	-	-	Ref. 268
	TaB_2	2.993	-	8.080	-	-	-	-	-	This work
		2.993	-	8.081	-	-	-	-	-	Ref. 266
	WB_2	2.926	-	7.750	0.867	[10-10]	54.3	(0001)[10-10]	32.9	This work
		2.929	-	7.757	-	-	-	-	-	Ref. 269
	ReB_2	2.912	-	7.507	0.831	[-12-10]	60.4	(0001)[10-10]	35.3	This work
		2.920	-	7.515	-	[-12-10]	58.5	(0001)[10-10]	34.4	Ref. 270
	OsB_2	2.942	-	7.333	0.629	[-12-10]	32.6	(10-10)[-12-10]	21.8	This work
		2.930	-	7.330	-	-	-	-	-	Ref. 268
	IrB_2	3.069	-	7.067	0.489	[10-10]	29.1	(0001)[10-10]	13.9	This work
		3.072	-	7.074	-	-	-	-	-	Ref. 266
oP6[59]	HfB_2	5.039	3.076	4.532	-	-	-	-	-	This work
	TaB_2	4.821	3.001	4.356	0.635	-	-	-	-	This work

	4.824	3.002	4.355	-	-	-	-	-	Ref. 266
WB_2	4.651	2.920	4.231	0.809	[100]	48.1	(001)[010]	28.6	This work
ReB_2	4.627	2.906	4.130	0.805	[100]	49.2	(001)[010]	28.3	This work
OsB_2	4.702	2.890	4.093	0.667	[010]	23.8	(001)[010]	9.1	This work
	4.71	2.89	4.10	-	-	-	(001)[010]	9.1	Ref. 271
IrB_2	4.547	3.149	4.038	0.448	[100]	11.6	(001)[010]	7.3	This work
	4.55	3.16	4.05	-	-	-	(001)[010]	7.9	Ref. 271

Table S3. Calculated lattice constants (Å), Pugh ratio G/B, minimum ideal tensile strength σ_{min} (GPa) and ideal shear strength τ_{min} (GPa) and their corresponding paths of 5d TMB_2 (TM=Hf, Ta, W, Re, Os and Ir) in four structures at 100 GPa.

Structure	Compound	Lattice constants			Pugh ratio	Tensile	σ_{min}	Shear	τ_{min}	NOTE
		a	b	c						
hP3[191]	HfB_2	2.908	-	3.209	0.701	[10-10]	82.5	(10-10)[-12-10]	91.3	This work
	TaB_2	2.899	-	3.083	0.572	[10-10]	73.1	(0001)[-12-10]	74.2	This work
	WB_2	2.846	-	3.097	0.414	[-12-10]	45.9	(0001)[10-10]	40.2	This work
	ReB_2	2.775	-	3.235	0.393	[-12-10]	44.0	(0001)[10-10]	12.4	This work
	OsB_2	2.799	-	3.185	0.125	-	-	-	-	This work
	IrB_2	2.913	-	2.980	0.167	-	-	-	-	This work
hP12[194]	HfB_2	2.826	-	14.309	0.579	[10-10]	83.7	(0001)[-12-10]	10.0	This work
	TaB_2	2.813	-	13.774	0.632	[10-10]	105.7	(0001)[10-10]	37.9	This work
	WB_2	2.798	-	13.328	0.598	[-12-10]	103.7	(0001)[10-10]	43.5	This work
	ReB_2	2.770	-	13.350	0.517	[-12-10]	60.0	(0001)[10-10]	30.1	This work
	OsB_2	2.730	-	13.726	-	-	-	-	-	This work
	IrB_2	2.743	-	13.841	-	-	-	-	-	This work
hP6[194]	HfB_2	2.717	-	7.846	-	-	-	-	-	This work
	TaB_2	2.719	-	7.590	-	-	-	-	-	This work
	WB_2	2.706	-	7.353	0.661	[-12-10]	89.5	(0001)[10-10]	53.5	This work
	ReB_2	2.702	-	7.163	0.638	[-12-10]	98.8	(0001)[10-10]	59.8	This work
	OsB_2	2.703	-	7.082	0.552	[-12-10]	42.1	(10-10)[-12-10]	33.3	This work
	IrB_2	2.743	-	6.988	0.398	[-12-10]	42.9	(0001)[10-10]	16.9	This work
oP6[59]	HfB_2	4.945	2.295	4.293	0.584	-	-	-	-	This work
	TaB_2	4.475	2.668	4.107	0.210	-	-	-	-	This work
	WB_2	4.315	2.697	4.006	0.616	[010]	103.5	(001)[010]	32.4	This work
	ReB_2	4.306	2.686	3.925	0.623	[010]	83.0	(001)[010]	42.2	This work
	OsB_2	4.373	2.662	3.884	0.540	[010]	44.5	(001)[010]	9.8	This work
	IrB_2	4.490	2.639	3.852	0.365	[010]	9.3	(001)[010]	9.6	This work

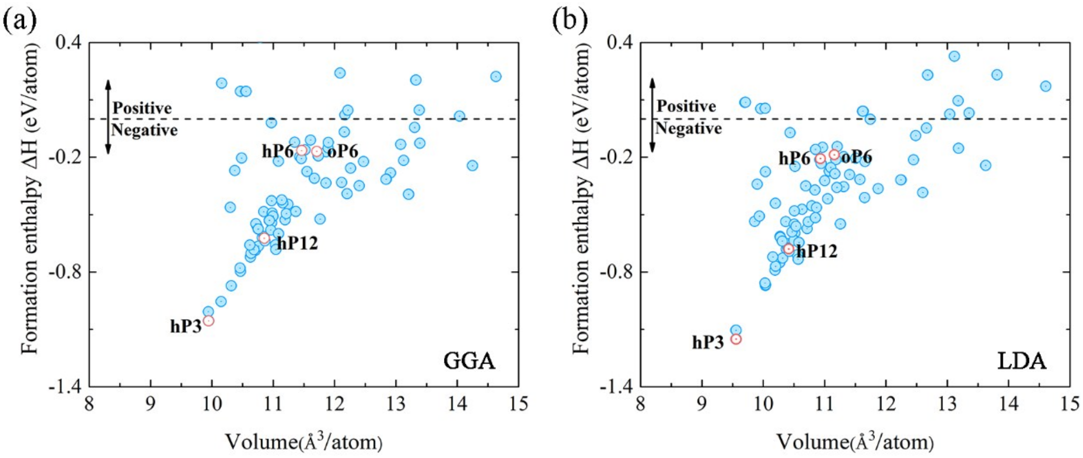

Figure S1. Formation enthalpies of HfB_2 at 0 GPa calculated by means of the projector augmented wave (PAW) method with (a) generalized gradient approximation (GGA) and (b) local density approximation (LDA) as the exchange-correlation functional to determine the possible ground-state phases based on the ICSD structure prototypes and the newly reported diborides.

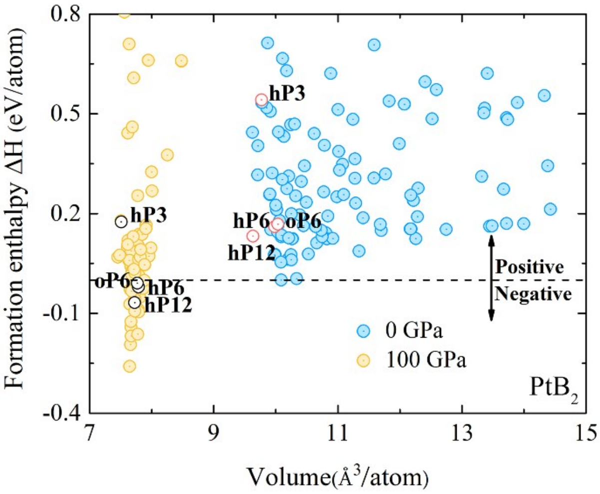

Figure S2. Formation enthalpies of PtB_2 at 0 and 100 GPa calculated by DFT to determine the possible ground-state phases based on the ICSD structure prototypes and the newly reported diborides.

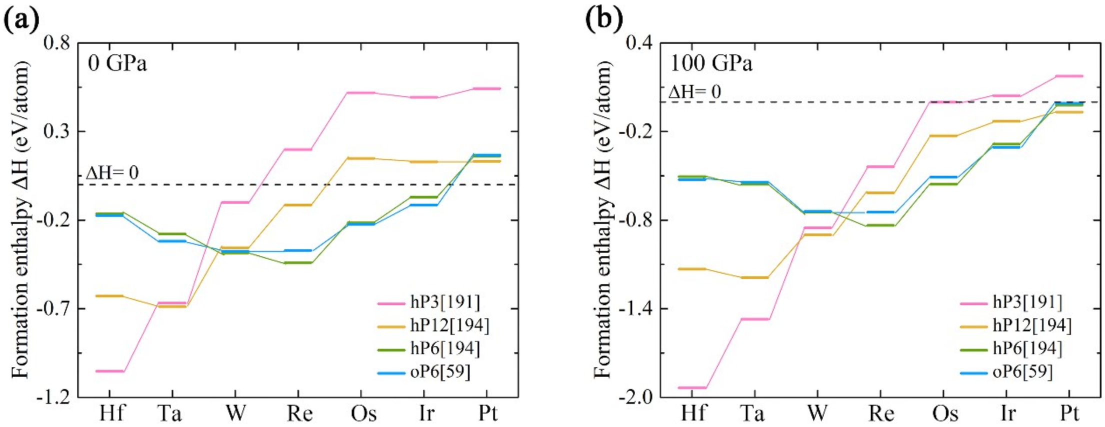

Figure S3. Calculated formation enthalpies of 5d TMB_2 (TM=Hf, Ta, W, Re, Os, Ir and Pt) in four observed structures at (a) 0 GPa and (b) 100 GPa, and the corresponding 5d TMB_2 are represented by the transition metal elements.

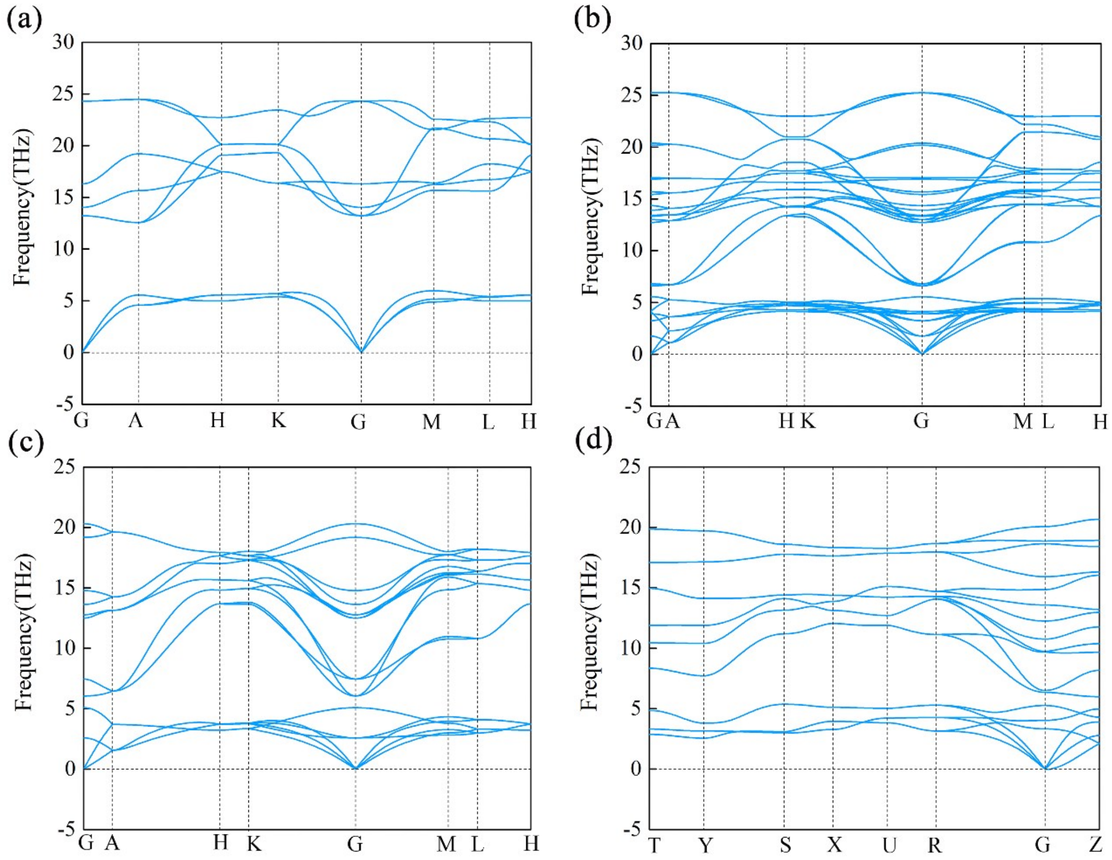

Figure S4. Calculated phonon dispersion curves of HfB_2 at 0 GPa in four structures: (a) hP3[191], (b) hP12[194], (c) hP6[194], and (d) oP6[59].

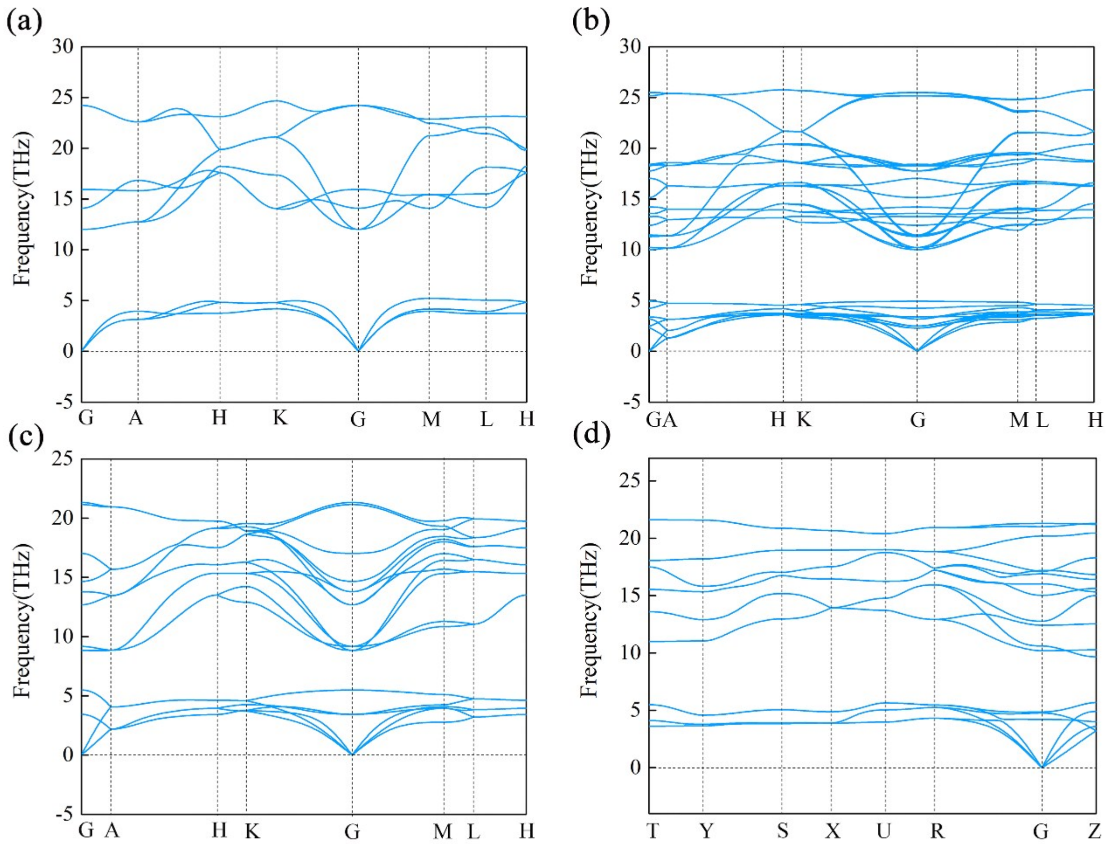

Figure S5. Calculated phonon dispersion curves of TaB_2 at 0 GPa in four structures: (a) hP3[191], (b) hP12[194], (c) hP6[194] and (d) oP6[59].

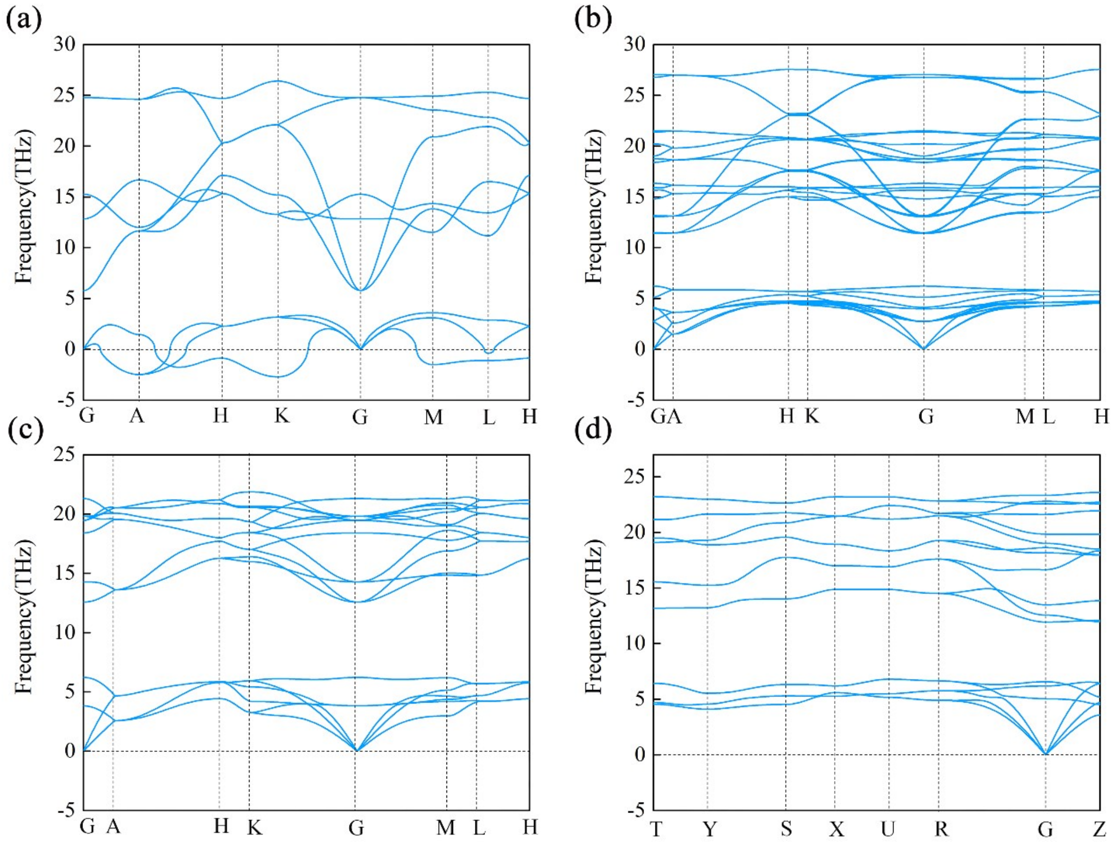

Figure S6. Calculated phonon dispersion curves of WB_2 at 0 GPa in four structures: (a) hP3[191], (b) hP12[194], (c) hP6[194] and (d) oP6[59].

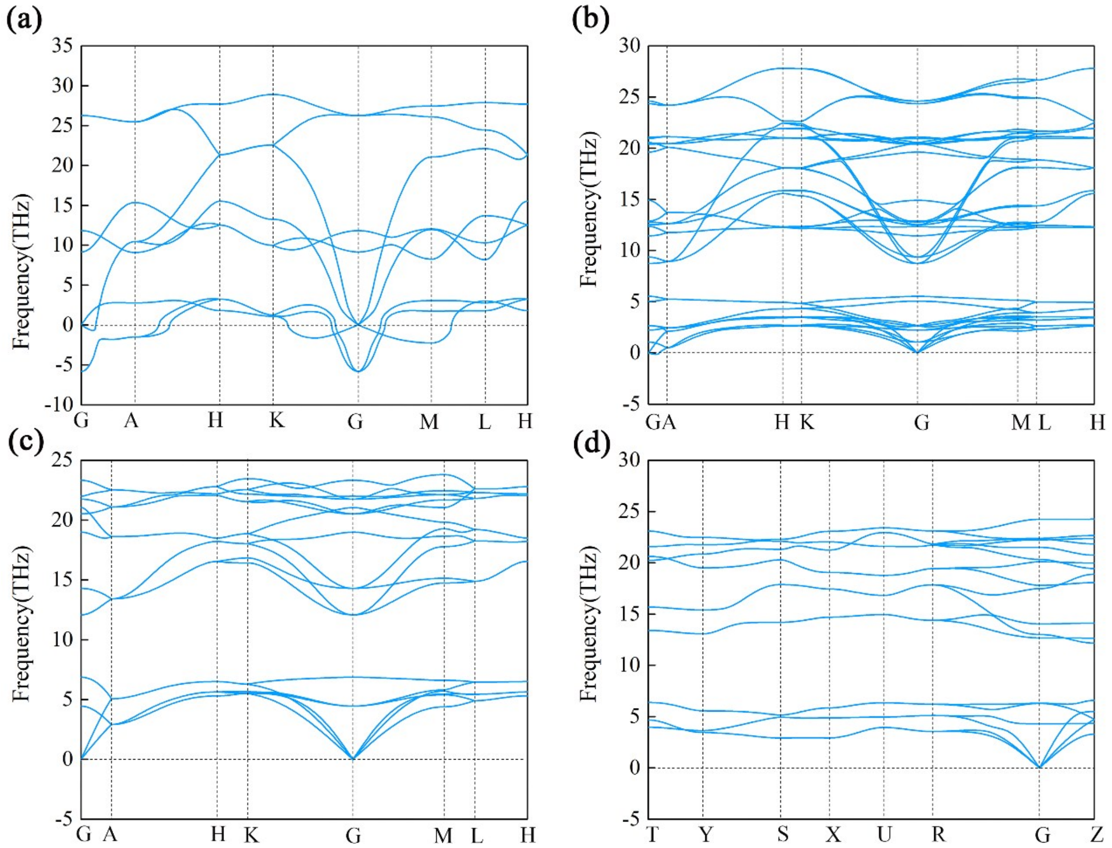

Figure S7. Calculated phonon dispersion curves of ReB_2 at 0 GPa in four structures: (a) hP3[191], (b) hP12[194], (c) hP6[194], and (d) oP6[59].

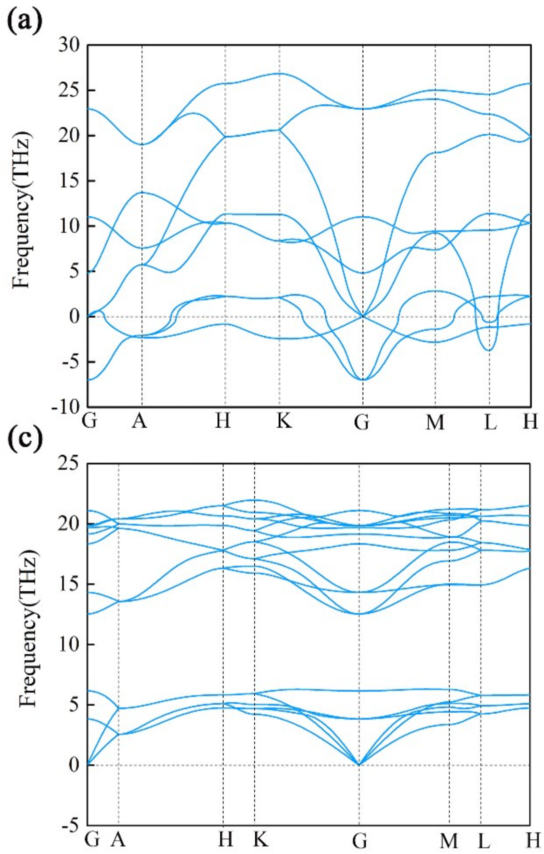

Figure S8. Calculated phonon dispersion curves of OsB_2 at 0 GPa in four structures: (a) hP3[191], (b) hP12[194], (c) hP6[194], and (d) oP6[59].

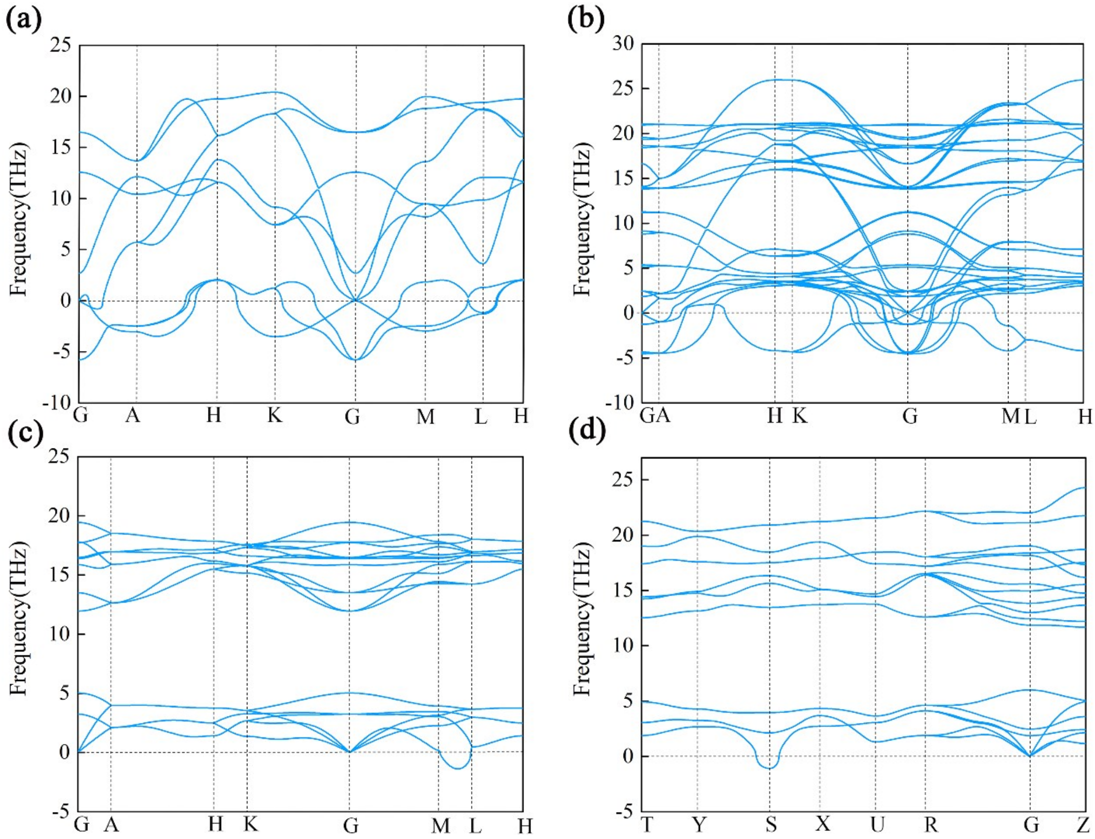

Figure S9. Calculated phonon dispersion curves of IrB_2 at 0 GPa in four structures: (a) hP3[191], (b) hP12[194], (c) hP6[194], and (d) oP6[59].

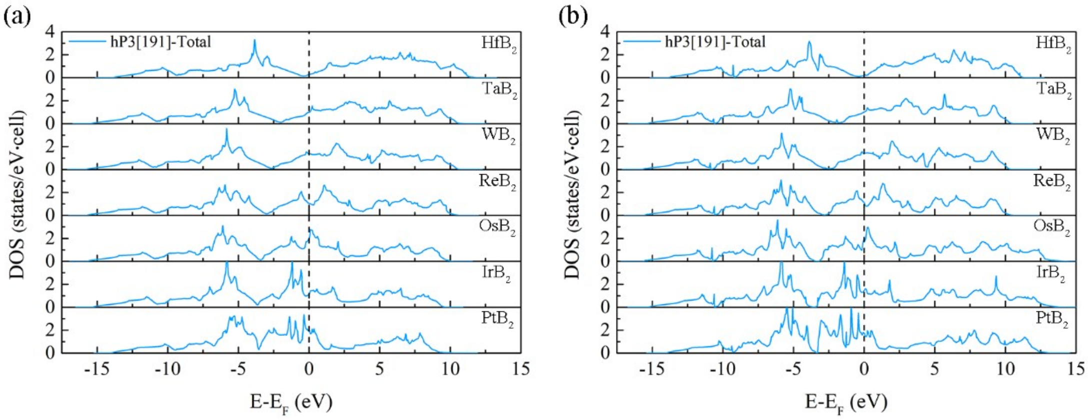

Figure S10. Calculated density of states (DOS) (a) without and (b) within the spin orbit coupling (SOC) interaction effect for 5d TMB_2 (TM = Hf, Ta, W, Re, Os, Ir and Pt) in hP3[191] structure at 0 GPa.

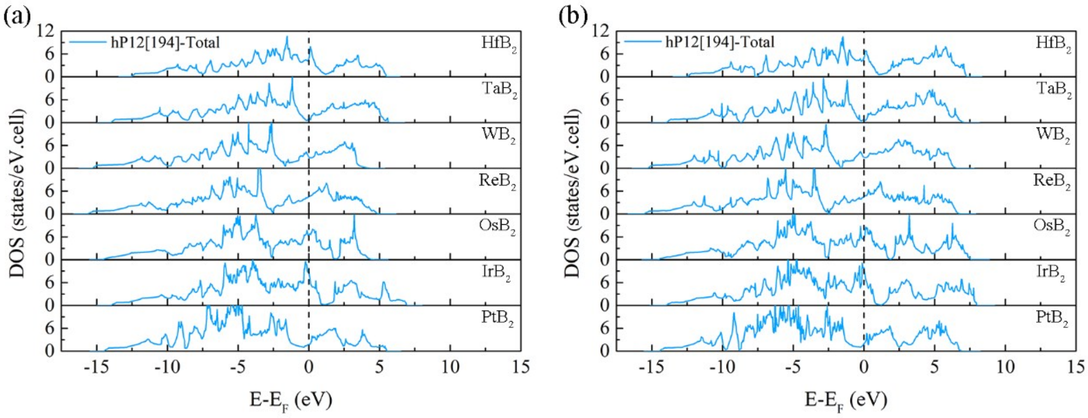

Figure S11. Calculated density of states (DOS) (a) without and (b) within the spin orbit coupling (SOC) interaction effect for 5d TMB_2 (TM = Hf, Ta, W, Re, Os, Ir and Pt) in hP12[194] structure at 0 GPa.

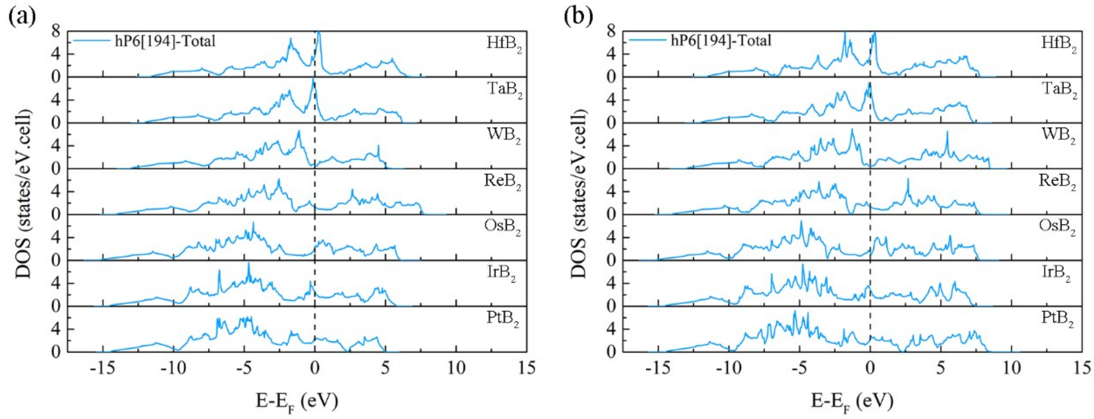

Figure S12. Calculated density of states (DOS) (a) without and (b) within the spin orbit coupling (SOC) interaction effect for 5d TMB_2 (TM = Hf, Ta, W, Re, Os, Ir and Pt) in hP6[194] structure at 0 GPa.

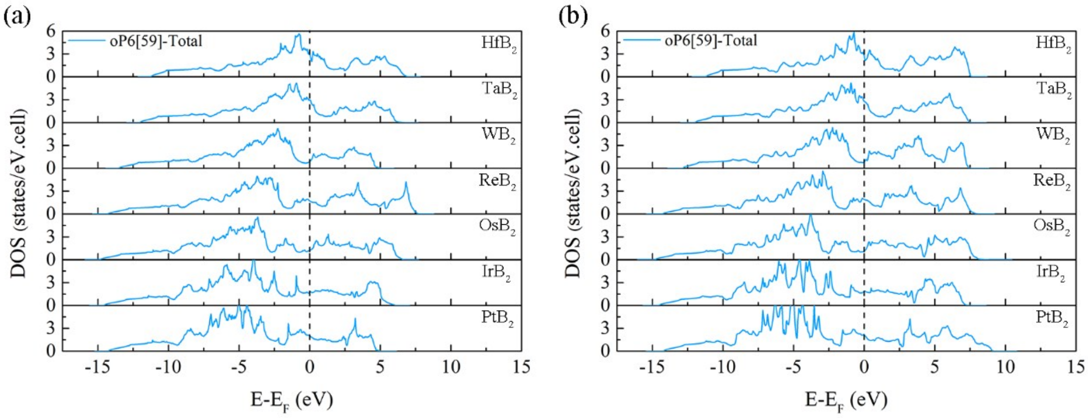

Figure S13. Calculated density of states (DOS) (a) without and (b) within the spin orbit coupling (SOC) interaction effect for 5d TMB_2 (TM = Hf, Ta, W, Re, Os, Ir and Pt) in oP6[59] structure at 0 GPa.

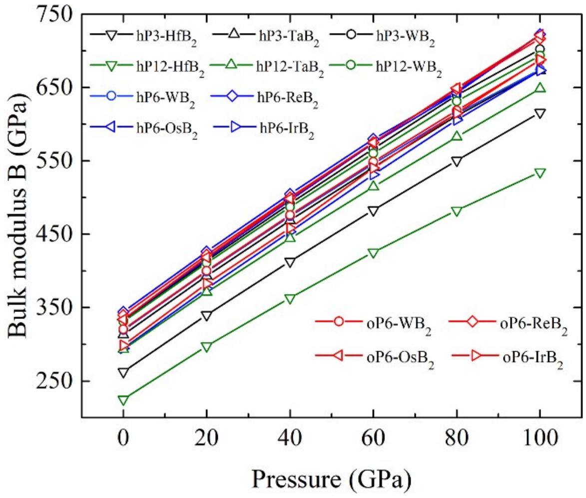

Figure S14. Calculated bulk modulus vs. pressure curves of 5d TMB_2 in four observed structures: hP3[191], hP12[194], hP6[194] and oP6[59].

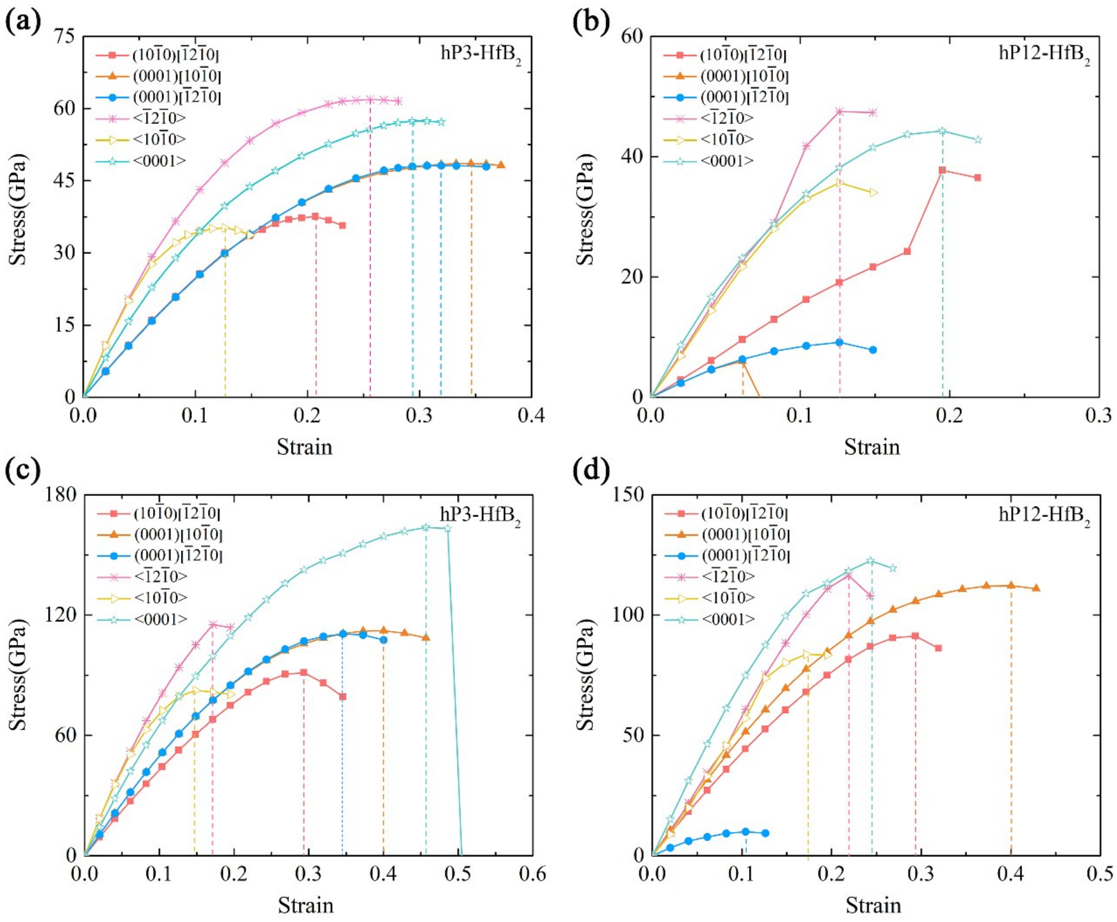

Figure S15. The stress-strain curves of HfB_2 in different structures: (a) hP3[191] and (b) hP12[194] at 0 GPa, and (c) hP3[191] and (d) hP12[194] at 100 GPa.

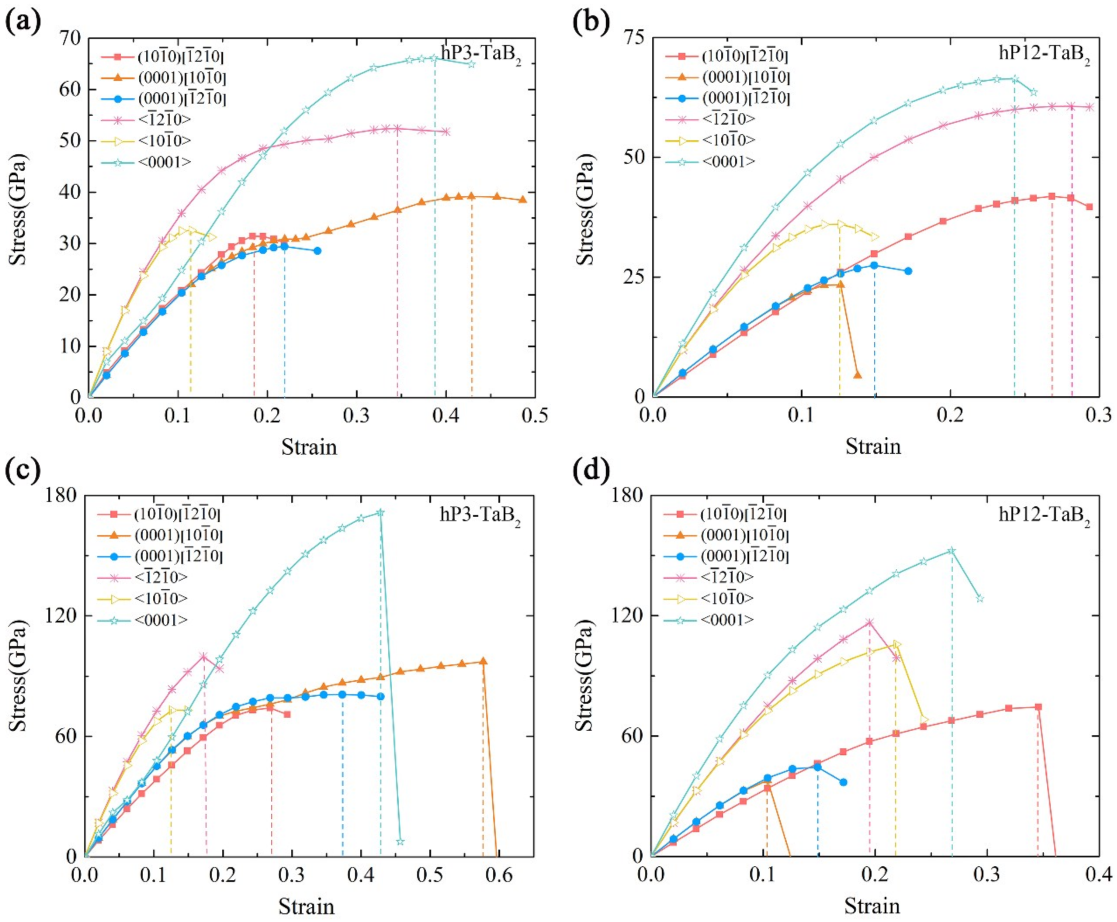

Figure S16. The stress-strain curves of TaB_2 in different structures: (a) hP3[191] and (b) hP12[194] at 0 GPa, and (c) hP3[191] and (d) hP12[194] at 100 GPa.

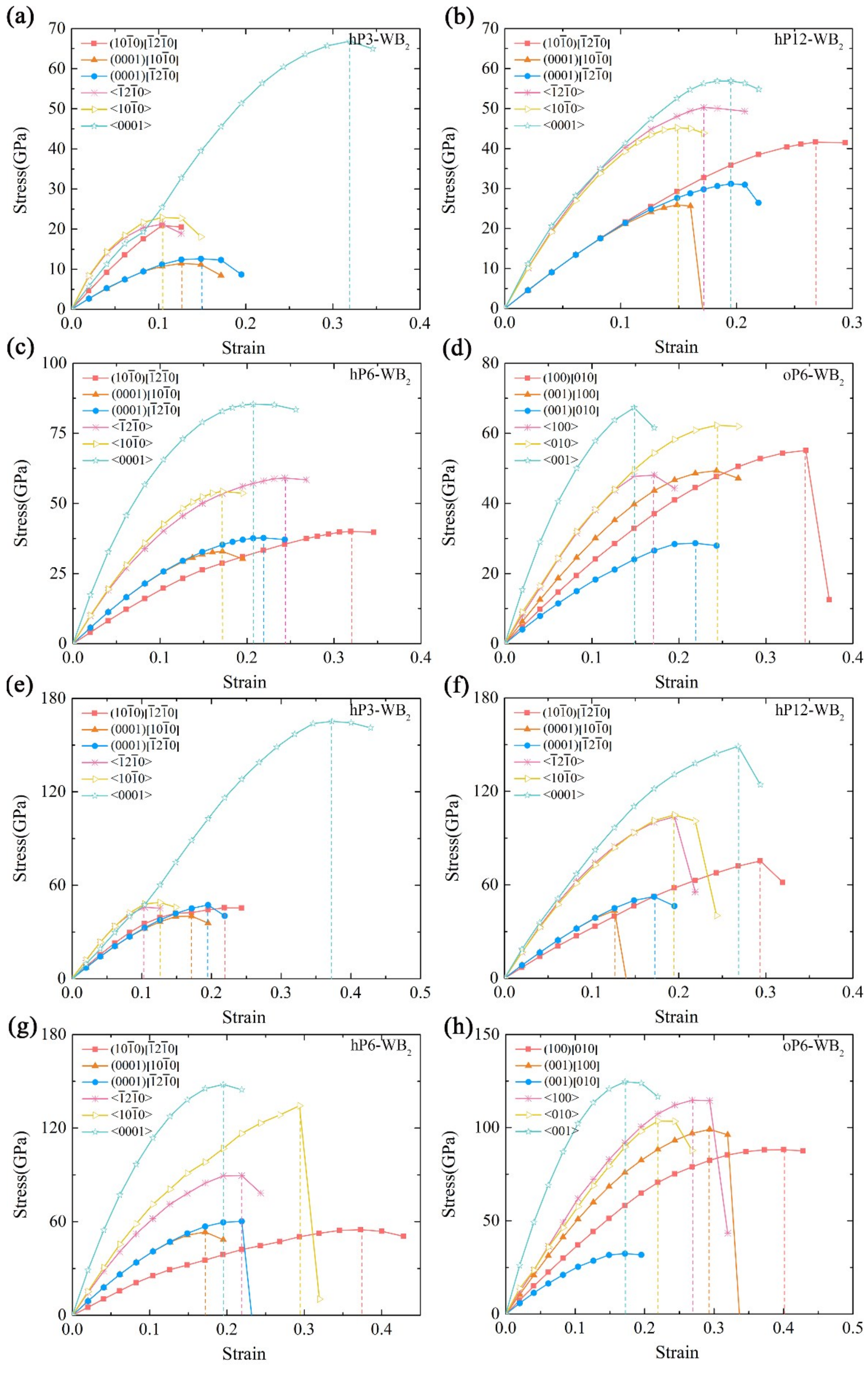

Figure S17. The stress-strain curves of WB_2 in different structures: (a) hP3[191], (b) hP12[194], (c) hP6[194] and (d) oP6[59] at 0 GPa, and (e) hP3[191], (f) hP12[194], (g) hP6[194] and (h) oP6[59] at 100 GPa.

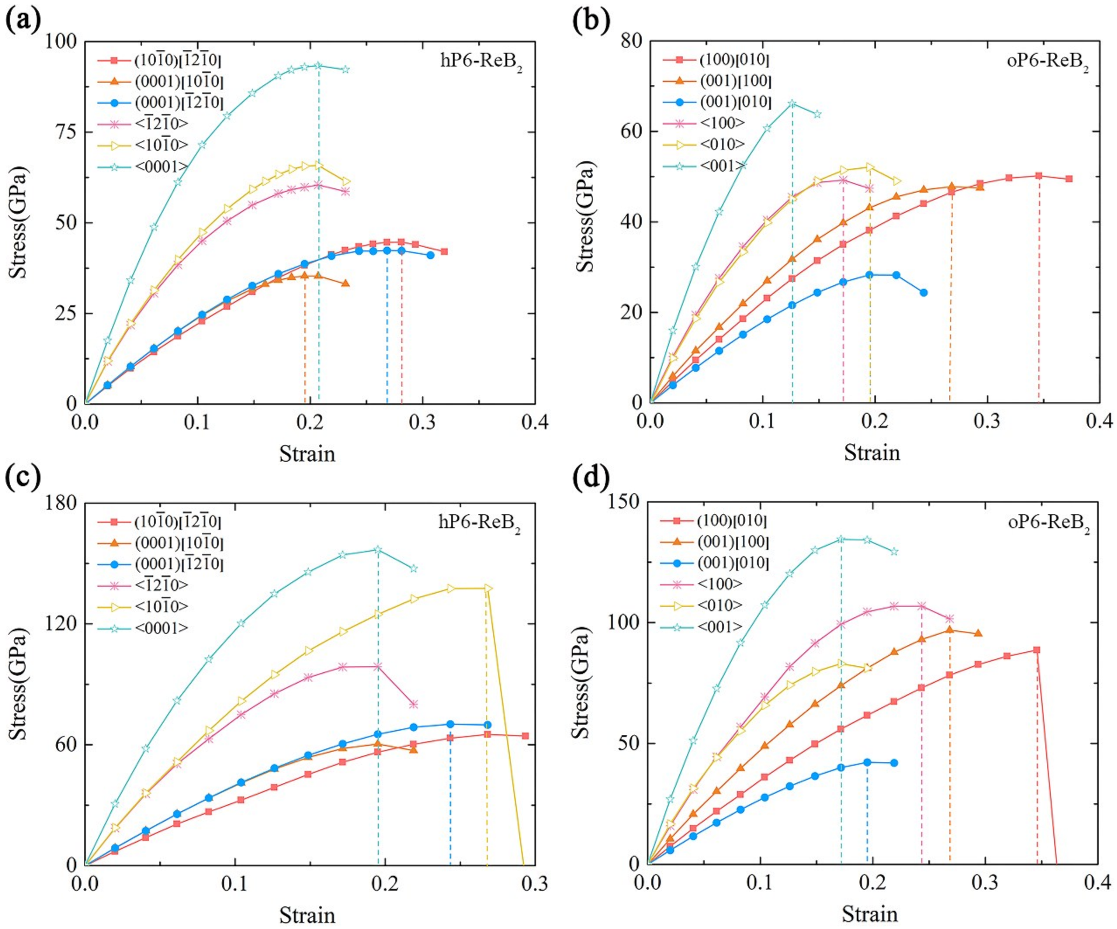

Figure S18. The stress-strain curves of ReB_2 in different structures: (a) hP6[194] and (b) oP6[59] at 0 GPa, and (c) hP6[194] and (d) oP6[59] at 100 GPa.

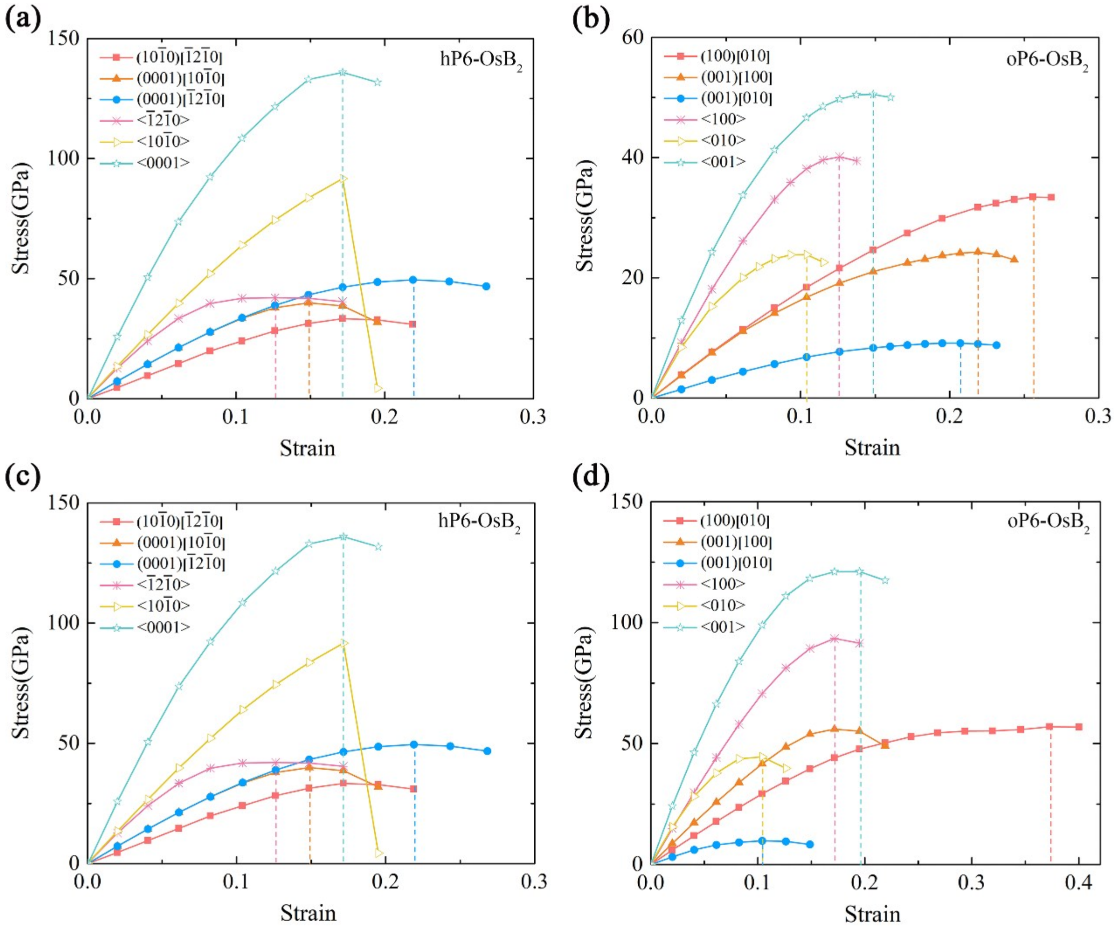

Figure S19. The stress-strain curves of OsB_2 in different structures: (a) hP6[194] and (b) oP6[59] at 0 GPa, and (c) hP6[194] and (d) oP6[59] at 100 GPa.

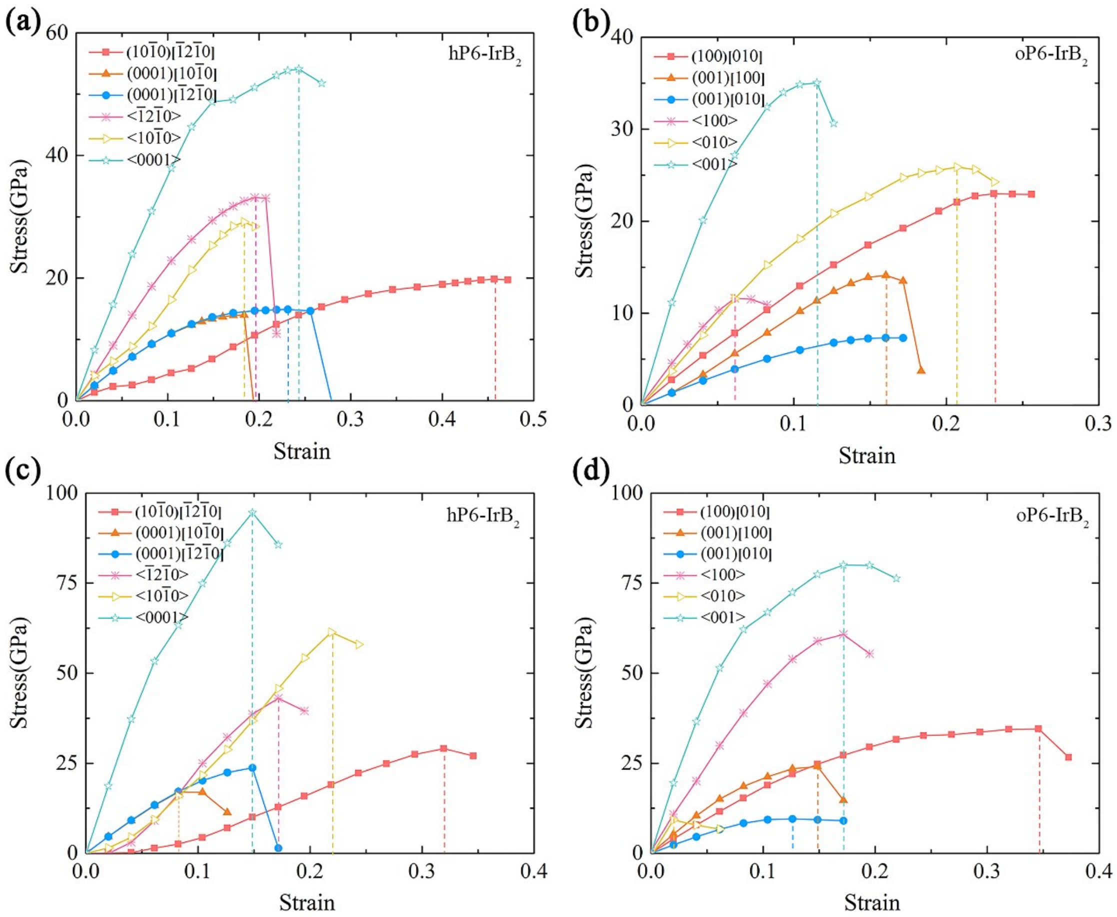

Figure S20. The stress-strain curves of IrB_2 in different structures: (a) hP6[194] and (b) oP6[59] at 0 GPa, and (c) hP6[194] and (d) oP6[59] at 100 GPa.

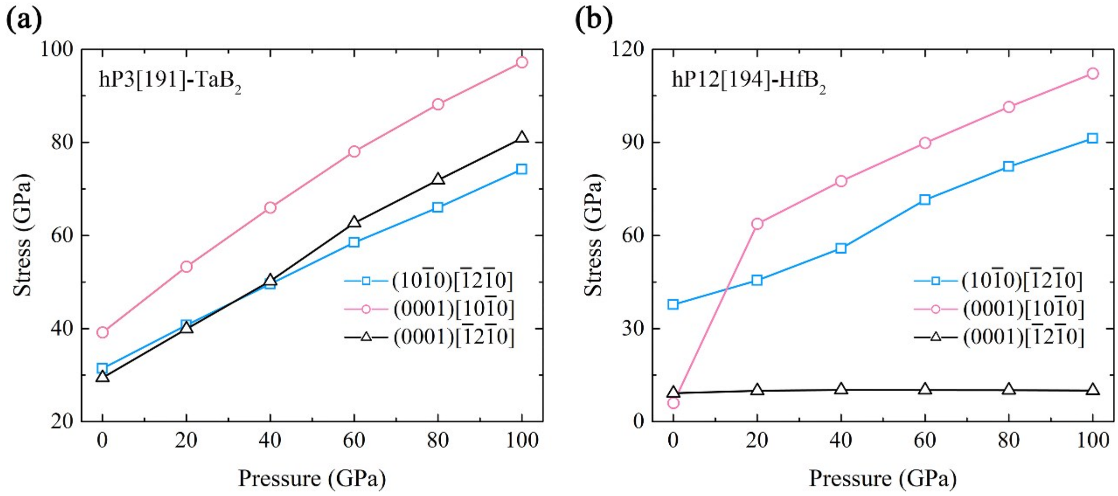

Figure S21. Calculated stress vs. pressure curves of (a) TaB_2 in hP3[191] structure and (b) HfB_2 in hP12[194] structure along the (10-10)[-12-10], (0001)[10-10] and (0001)[-12-10] shearing paths under different pressure ranging from 0 to 100 GPa.

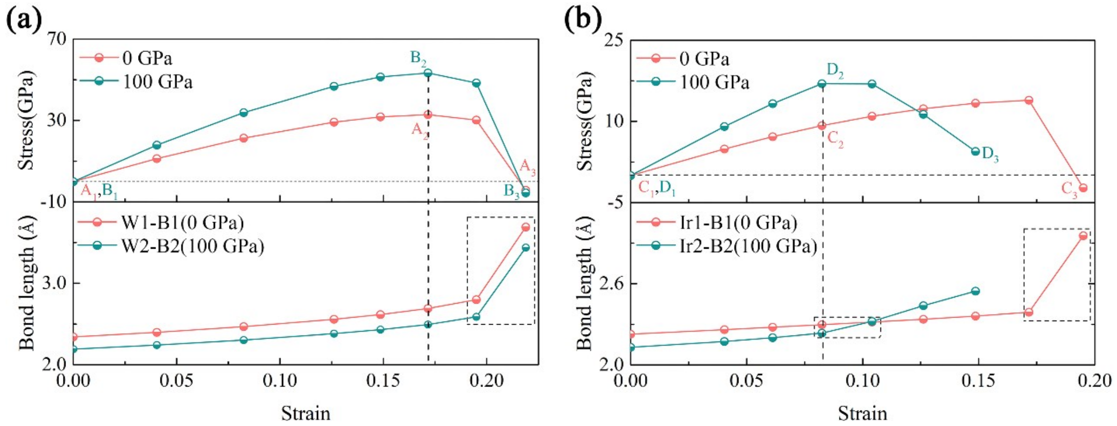

Figure S22. Calculated stress/bond length vs. strain curves of (a) WB_2 and (b) IrB_2 in hP6[194] structure at 0 and 100 GPa.

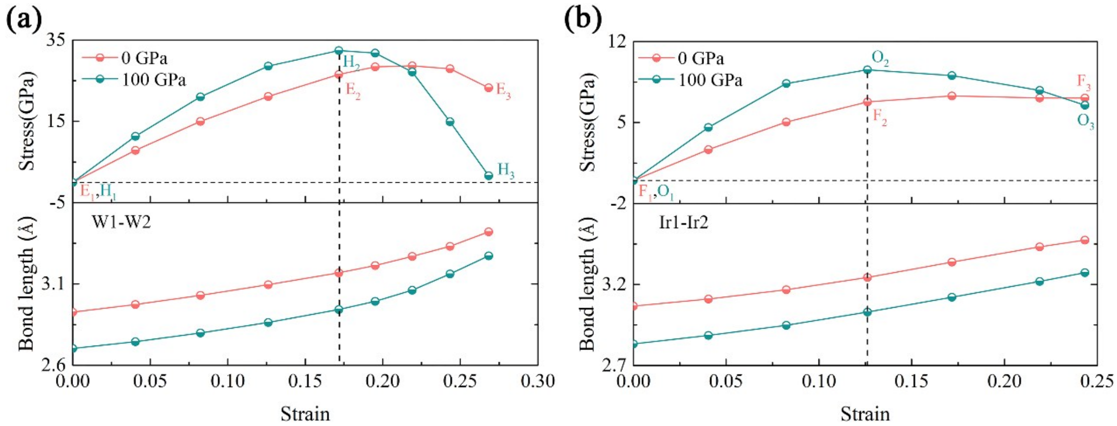

Figure S23. Calculated stress/bond length vs. strain curves of (a) WB_2 and (b) IrB_2 in oP6[59] structure at 0 and 100 GPa.

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