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Supplementary Information

Enthalpies of Formation of Transition Metal Diborides: A First Principles Study

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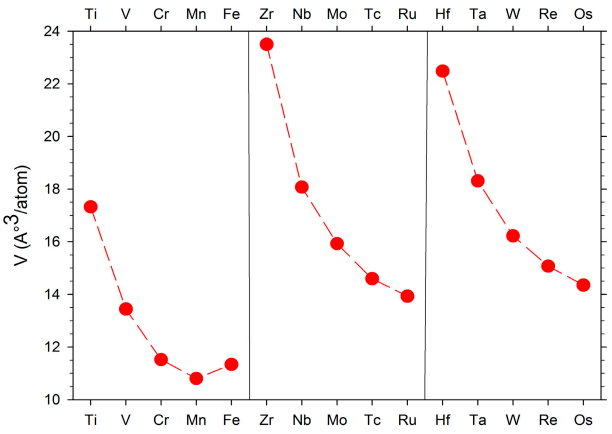

Figure S1. Atomic volumes of the transition metals considered in the present work.

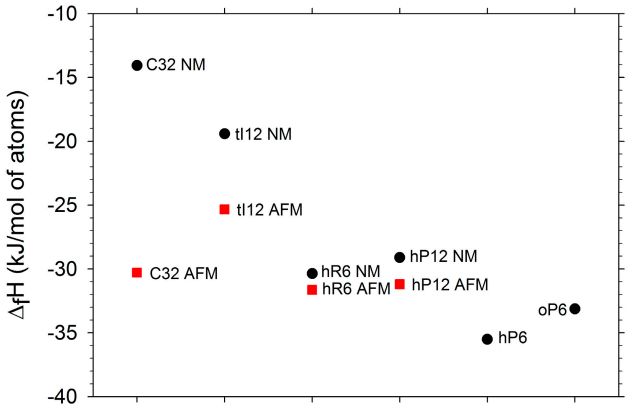

Figure S2. Enthalpies of formation of anti-ferromagnetic and non-magnetic MnB_2 in the hP3, tI12, hP12, hR6, hP6, and oP6 structures.

Table S1. Values of the formation enthalpies and atomic volumes of the early transition metals diborides.

--	TiB_2		VB_2		CrB_2		MnB_2		FeB_2	
	Δ_fH kJ/mol of atoms	V Å³/atom	Δ_fH kJ/mol of atoms	V Å³/atom	Δ_fH kJ/mol of atoms	V Å³/atom	Δ_fH kJ/mol of atoms	V Å³/atom	Δ_fH kJ/mol of atoms	V Å³/atom
hP3-TMB_2	−102.30	8.5705	−71.33	7.8533	−33.64	7.6461	−30.29	7.5443	−4.93	7.2377
tI12-TMB_2	−100.15	8.5139	−70.03	7.8477	−34.29	7.4932	−25.34	7.4908	−7.61	7.3474
hP12-TMB_2	−64.07	9.3724	−61.86	8.3712	−41.13	7.8441	−31.20	7.6839	−15.18	7.5966
hR6-TMB_2	−64.97	9.3703	−61.72	8.3766	−40.99	7.8462	−31.64	7.7146	−16.63	7.7146
hP6-TMB_2	−20.38	10.0008	−23.54	8.9052	−27.07	8.1426	−35.52	7.75	−25.73	7.6304
oP6-TMB_2	−24.01	10.0431	−29.76	8.8623	−29.96	8.0841	−33.13	7.7948	−25.49	7.6745
hR3-TMB_2	−26.48	10.0919	−31.76	8.855	−29.37	8.1236	−33.26	7.7741	−19.68	7.7002
--	ZrB_2		NbB_2		MoB_2		TcB_2		RuB_2	
	Δ_fH kJ/mol of atoms	V Å³/atom	Δ_fH kJ/mol of atoms	V Å³/atom	Δ_fH kJ/mol of atoms	V Å³/atom	Δ_fH kJ/mol of atoms	V Å³/atom	Δ_fH kJ/mol of atoms	V Å³/atom
hP3-TMB_2	−95.87	10.3489	−70.71	9.2755	−26.68	8.8632	−5.40	8.7071	14.27	3.2945
tI12-TMB_2	−90.08	10.351	−68.98	9.2499	−26.69	8.8164	−5.32	8.6273	8.90	10.3578
hP12-TMB_2	−53.37	11.2615	−63.65	9.891	−41.85	9.2396	−24.98	8.9447	−1.96	14.2147
hR6-TMB_2	−54.07	11.247	−62.25	9.8922	−42.19	9.2373	−26.62	8.9317	−3.16	7.1662
hP6-TMB_2	−12.80	11.7646	−23.66	10.4428	−32.80	9.6046	−42.98	9.0923	−26.85	7.2884
oP6-TMB_2	−7.88	12.0197	−24.22	10.5677	−33.62	9.6047	−37.90	9.156	−27.72	4.0582
hR3-TMB_2	−10.20	12.033	−25.58	10.5427	−32.84	9.6315	−37.68	9.1491	−20.10	11.1019
--	HfB_2		TaB_2		WB_2		ReB_2		OsB_2	
	Δ_fH kJ/mol of atoms	V Å³/atom	Δ_fH kJ/mol of atoms	V Å³/atom	Δ_fH kJ/mol of atoms	V Å³/atom	Δ_fH kJ/mol of atoms	V Å³/atom	Δ_fH kJ/mol of atoms	V Å³/atom
hP3-TMB_2	−98.90	9.9623	−62.58	9.2523	−7.45	8.9166	20.18	8.8164	51.14	8.8701
tI12-TMB_2	−94.19	9.949	−61.44	9.2352	−6.31	8.8641	23.23	8.9044	48.07	8.8504
hP12-TMB_2	−58.17	10.8636	−64.32	9.8555	−32.31	9.2741	−9.90	9.0545	14.83	9.2306
hR6-TMB_2	−59.04	10.8743	−63.81	9.8541	−32.93	9.2697	−12.28	9.0443	12.80	9.171
hP6-TMB_2	−14.66	11.4586	−25.95	10.4651	−35.32	9.6528	−41.50	9.2181	−19.93	9.1623
oP6-TMB_2	−14.70	11.7292	−29.58	10.5484	−34.47	9.6476	−34.76	9.276	-20.77	9.2608
hR3-TMB_2	−16.66	11.7519	−31.56	10.5409	−34.02	9.6556	−34.48	9.2708	−12.96	9.1399

Table S2. Comparison of the calculated and experimental values of the lattice parameters and internal parameters of some diborides.The experimental values are the more recent one indicated in the Pearson's Handbook [13]. For the prototypes, the calculated and experimental values are given in Table 1 of the manuscript.

Compound	**Structure**	**--**	**a (Å)**	**b (Å)**	**c (Å)**	**Internal Coordinates**		
ZrB2	hP3, C32	VASP	3.1767	3.1767	3.5525	--	--	--
		exp.	3.1682	3.1682	3.5284	--	--	--
HfB2	hP3, C32	VASP	3.1449	3.1449	3.4892	--	--	--
		exp.	3.1458	3.1458	3.4778	--	--	--
VB2	hP3, C32	VASP	2.9971	2.9971	3.0286	--	--	--
		exp.	2.9980	2.9980	3.0440	--	--	--
NbB2	hP3, C32	VASP	3.1077	3.1077	3.3271	--	--	--
		exp.	3.0890	3.0890	3.3090	--	--	--
TaB2	hP3, C32	VASP	3.1016	3.1016	3.3316	--	--	--
		exp.	3.0728	3.0728	3.2382	--	--	--
CrB2	hP3, C32	VASP	2.9765	2.9765	2.9377	--	--	--
		exp.	2.9680	2.9680	3.0740	--	--	--
MoB2	hP3, C32	VASP	3.0327	3.0327	3.3822	--	--	--
		exp.	3.0430	3.0430	3.0670	--	--	--
WB2	hP3, C32	VASP	3.0233	3.0233	3.3793	--	--	--
		exp.	3.0200	3.0200	3.0500	--	--	--
MnB2	hP3, C32	VASP	2.9764	2.9764	2.8865	--	--	--
		exp.	3.0100	3.0100	3.0380	--	--	--
TcB2	hP6, ReB2-type	VASP	2.9044	2.9044	7.4676	x (B 4f) = 0.54776	--	--
		exp.	2.8920	2.8920	7.4530	x (B 4f) = 0.548	--	--
FeB2	hP3, C32	VASP	3.0433	3.0433	2.6840	--	--	--
		exp.	3.0450	3.0450	3.0350	--	--	--
OsB2	oP6, RuB2-type	VASP	2.8888	4.7023	4.0904	y (B 4e) = 0.05604	z (B 4e) = 0.13813	z (Os 2a) = 0.65502
		exp.	2.8726	4.6841	4.0769	y (B 4e) = 0.0557	z (B 4e) = 0.1325	z (Os 2a) = 0.6545