Supplemental Material for:

Formation criterion for binary metal diboride solid solutions established through combinatorial methods

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Table S1. Calculated lattice parameters (*a* and *c*) and energies (*E*) of $(M_xN_{1-x})B_2$ solid solutions (M, N = Hf, Zr, Ta, Nb, or Ti).

No.	$(M_xN_{1-x})B_2$	*a* (Å)	*c* (Å)	*E* (eV/atom)
1	$(Ta_{0.5}Ti_{0.5})B_2$	3.069	3.273	-8.632
2	$(Nb_{0.5}Ti_{0.5})B_2$	3.073	3.273	-8.391
3	$(Zr_{0.5}Ta_{0.5})B_2$	3.134	3.427	-8.699
4	$(Hf_{0.5}Ta_{0.5})B_2$	3.120	3.401	-8.935
5	$(Ta_{0.5}Nb_{0.5})B_2$	3.106	3.321	-8.835
6	$(Hf_{0.5}Zr_{0.5})B_2$	3.156	3.518	-8.564
7	$(Hf_{0.5}Nb_{0.5})B_2$	3.126	3.402	-8.703
8	$(Zr_{0.5}Nb_{0.5})B_2$	3.140	3.429	-8.465
9	$(Hf_{0.5}Ti_{0.5})B_2$	3.096	3.361	-8.448
10	$(Zr_{0.5}Ti_{0.5})B_2$	3.112	3.390	-8.196
11	$(Hf_{0.9}Ta_{0.1})B_2$	3.138	3.469	-8.830
12	$(Hf_{0.9}Nb_{0.1})B_2$	3.139	3.468	-8.782
13	$(Nb_{0.9}Ti_{0.1})B_2$	3.102	3.311	-8.566
14	$(Nb_{0.8}Ti_{0.2})B_2$	3.096	3.302	-8.524
15	$(Nb_{0.7}Ti_{0.3})B_2$	3.088	3.293	-8.481

16	$(Ta_{0.8}Ti_{0.2})B_2$	3.090	3.304	-8.891
17	$(Ta_{0.6}Ti_{0.4})B_2$	3.076	3.284	-8.720
18	$(Hf_{0.1}Ta_{0.9})B_2$	3.106	3.338	-9.030
19	$(Hf_{0.1}Nb_{0.9})B_2$	3.112	3.337	-8.628
20	$(Nb_{0.1}Ti_{0.9})B_2$	3.042	3.232	-8.197
21	$(Ta_{0.2}Ti_{0.8})B_2$	3.048	3.243	-8.349
22	$(Ta_{0.4}Ti_{0.6})B_2$	3.062	3.263	-8.540

Table S2. The leave-one-out cross validation accuracy of the model and the value of θ_0 - θ_4 when different training data was used (only 1 validation data was used and the rest was used as training data).

No.	Validation data	θ_0	θ_1	θ_2	θ_3	θ_4	Accuracy
1	$(Ta_{0.5}Ti_{0.5})B_2$	56.053	-81.747	-157.377	9.309	11.206	100%
2	$(Nb_{0.5}Ti_{0.5})B_2$	56.365	-82.185	-156.837	8.729	11.446	100%
3	$(Zr_{0.5}Ta_{0.5})B_2$	56.053	-81.747	-157.377	9.309	11.206	100%
4	$(Hf_{0.5}Ta_{0.5})B_2$	56.053	-81.747	-157.377	9.309	11.206	100%
5	$(Ta_{0.5}Nb_{0.5})B_2$	139.830	-219.434	-443.647	49.402	25.569	100%
6	$(Hf_{0.5}Zr_{0.5})B_2$	55.544	-81.578	-158.255	10.386	10.949	100%

7	$(Hf_{0.5}Nb_{0.5})B_2$	56.053	-81.747	-157.377	9.309	11.206	100%
8	$(Zr_{0.5}Nb_{0.5})B_2$	56.053	-81.747	-157.377	9.309	11.206	100%
9	$(Hf_{0.5}Ti_{0.5})B_2$	56.053	-81.747	-157.377	9.309	11.206	100%
10	$(Zr_{0.5}Ti_{0.5})B_2$	56.053	-81.747	-157.377	9.309	11.206	100%
11	$(Hf_{0.9}Ta_{0.1})B_2$	56.123	-81.766	-157.268	9.168	11.235	100%
12	$(Hf_{0.9}Nb_{0.1})B_2$	56.055	-81.757	-157.373	9.303	11.212	100%
13	$(Nb_{0.9}Ti_{0.1})B_2$	56.053	-81.750	-157.381	9.311	11.207	100%
14	$(Nb_{0.8}Ti_{0.2})B_2$	60.561	-84.631	-152.915	1.498	10.180	**0%**
15	$(Nb_{0.7}Ti_{0.3})B_2$	56.502	-84.096	-152.517	7.374	12.884	100%
16	$(Ta_{0.8}Ti_{0.2})B_2$	56.052	-81.756	-157.378	9.309	11.210	100%
17	$(Ta_{0.6}Ti_{0.4})B_2$	56.053	-81.747	-157.377	9.309	11.206	100%
18	$(Hf_{0.1}Ta_{0.9})B_2$	56.053	-81.747	-157.377	9.309	11.206	100%
19	$(Hf_{0.1}Nb_{0.9})B_2$	56.053	-81.747	-157.377	9.309	11.206	100%
20	$(Nb_{0.1}Ti_{0.9})B_2$	65.640	-77.226	-158.810	12.648	-2.401	**0%**
21	$(Ta_{0.2}Ti_{0.8})B_2$	55.052	-81.344	-156.839	8.964	12.262	100%
22	$(Ta_{0.4}Ti_{0.6})B_2$	55.630	-81.668	-157.024	9.047	11.763	100%