

Supplementary Information: Machine Learning guided high-throughput search of non-oxide garnets

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I. CUTOFF FOR THE MACHINE-LEARNING PREDICTIONS

We would like to discuss further our choice of the cutoff for the machine learning predictions. For that purpose, we depict in the figures the distribution of distances to the convex hull or all compounds predicted to be below or above 100 meV/atom. It is clear from the figures that using the lowest cutoff increases the efficiency of the method, especially in rounds 2 and 3 where the machine exhibited much lower errors. However, lowering the cutoff also increases considerably the amount of false negatives, which can be confirmed from the numerical information in Supplementary Table I.

There is another aspect that we have to take into consideration. The lower cutoff leads to a smaller number of systems validated with DFT. As these calculations are used, within a transfer learning methodology, as a training set for subsequent rounds, less data will inevitably lead to larger errors and worse predictions.

We can therefore conclude that the relatively high cutoff of 200 meV/atom is required for a fully comprehensive search despite the high cost of the extra DFT calculations.

Supplementary Table I. For each round of transfer learning the table shows the total number of systems selected for validation, the number of systems for which DFT validated E_{Hull} is less than 50 ($N_{<50}$), less than 100 ($N_{<100}$), and less than 200 meV/atom ($N_{<200}$). For each round, the first line is for compounds with ML predicted E_{Hull} less than 100 meV/atom, and the second line is for compounds with ML predicted E_{Hull} between 100 and 200 meV/atom. Note for each round the numbers only include compounds not calculated during the previous rounds. We also list the mean value of ML predicted E_{Hull} ($\bar{E}_{\text{Hull}}^{\text{ML}}$), and the mean absolute error of the prediction (MAE) for these systems, both in the unit of meV/atom.

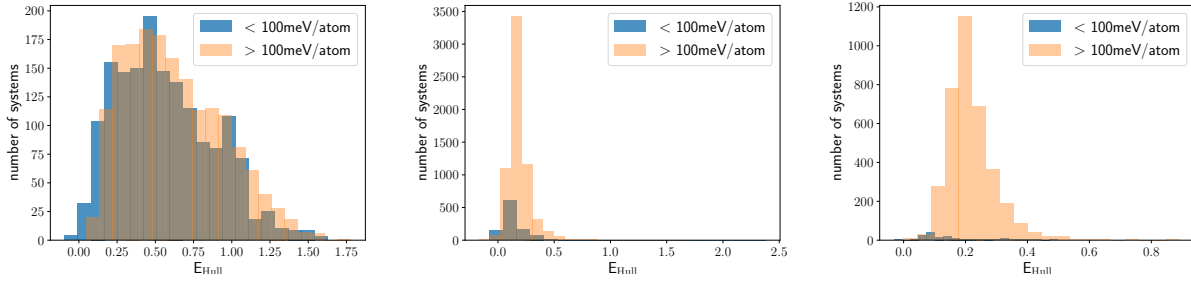
Round	N_{total}	$N_{<50}$	$N_{<100}$	$N_{<200}$	$\bar{E}_{\text{Hull}}^{\text{ML}}$	MAE
1	1604	14	60	209	565	520
	1716	1	9	101	626	475
2	1025	194	488	832	134	85
	6311	159	764	4223	186	61
3	167	10	71	123	158	86
	3677	13	82	1720	218	57

II. SUPPLEMENTARY TABLES

Supplementary Table 2. The full list of (meta-)stable non-oxide garnets with a distance to the convex hull of stability (E_{hull} (in meV/Atom) below 100 meV/atom, and their calculated lattice constant (a , in Å), band gap with the PBE approximation (Gap^{PBE} , in eV), and the decomposition channel (Channel). Note for systems on the hull ($E_{\text{hull}}=0$) the channels represent the second most stable composition(s).

Formula	a	Gap^{PBE}	E_{hull}	Channel
$\text{Bi}_3\text{Al}_5\text{S}_{12}$	15.121	2.11	24	$\text{Bi}_2\text{S}_3, \text{Al}_2\text{S}_3$
$\text{Sb}_3\text{Al}_5\text{S}_{12}$	14.987	1.76	76	$\text{Sb}_2\text{S}_3, \text{Al}_2\text{S}_3$
$\text{Ba}_3\text{Sb}_5\text{S}_{12}$	16.850	0.00	98	$\text{SbS}_2, \text{Ba}(\text{SbS}_2)_2, \text{BaS}_3$
$\text{Ba}_3\text{Sn}_5\text{S}_{12}$	16.602	0.00	39	$\text{Ba}_6\text{Sn}_7\text{S}_{20}, \text{SnS}_2, \text{SnS}$
$\text{Ca}_3\text{Sn}_5\text{S}_{12}$	15.971	0.00	72	$\text{Ca}_2\text{SnS}_4, \text{SnS}, \text{SnS}_2$
$\text{Ce}_3\text{Al}_5\text{S}_{12}$	15.117	0.00	0	$\text{Ce}_2\text{S}_3, \text{Al}_2\text{S}_3$
$\text{Ce}_3\text{Ga}_5\text{S}_{12}$	15.239	0.00	33	$\text{Ga}_2\text{S}_3, \text{Ce}_2\text{S}_3$
$\text{Ce}_3\text{Ge}_5\text{S}_{12}$	15.508	0.00	52	$\text{GeS}, \text{Ce}_3\text{GeS}_6, \text{GeS}_2$
$\text{Ce}_3\text{In}_5\text{S}_{12}$	15.905	0.00	24	$\text{In}_2\text{S}_3, \text{Ce}_2\text{S}_3$
$\text{Dy}_3\text{Al}_5\text{S}_{12}$	14.916	2.07	0	$\text{Dy}_9\text{Al}_5\text{S}_{21}, \text{Al}_2\text{S}_3$
$\text{Dy}_3\text{Ga}_5\text{S}_{12}$	15.057	1.32	48	$\text{Dy}_3\text{GaS}_6, \text{Ga}_2\text{S}_3$
$\text{Dy}_3\text{Ge}_5\text{S}_{12}$	15.305	0.00	82	$\text{GeS}_2, \text{Dy}_2\text{S}_3, \text{GeS}$
$\text{Dy}_3\text{In}_5\text{S}_{12}$	15.692	1.35	48	$\text{Dy}_2\text{S}_3, \text{In}_2\text{S}_3$
$\text{Er}_3\text{Al}_5\text{S}_{12}$	14.868	2.12	8	$\text{Er}_3\text{AlS}_6, \text{Al}_2\text{S}_3$
$\text{Er}_3\text{Ga}_5\text{S}_{12}$	15.006	1.34	54	$\text{Er}_3\text{GaS}_6, \text{Ga}_2\text{S}_3$
$\text{Er}_3\text{Ge}_5\text{S}_{12}$	15.254	0.00	98	$\text{GeS}_2, \text{Er}_2\text{S}_3, \text{GeS}$
$\text{Er}_3\text{In}_5\text{S}_{12}$	15.643	1.70	65	$\text{In}_2\text{S}_3, \text{Er}_2\text{S}_3$
$\text{Eu}_3\text{Al}_5\text{S}_{12}$	15.107	0.06	58	$\text{EuS}_3, \text{Eu}(\text{AlS}_2)_2, \text{Al}_2\text{S}_3$
$\text{Eu}_3\text{As}_5\text{S}_{12}$	15.688	0.00	96	$\text{As}_2\text{S}_3, \text{Eu}_3\text{S}_4, \text{AsS}_2$
$\text{Eu}_3\text{Ge}_5\text{S}_{12}$	15.494	0.00	33	$\text{EuGeS}_3, \text{GeS}_2, \text{GeS}$
$\text{Eu}_3\text{In}_5\text{S}_{12}$	15.919	0.00	50	$\text{Eu}_3\text{S}_4, \text{EuS}_3, \text{In}_2\text{S}_3$
$\text{Eu}_3\text{Sn}_5\text{S}_{12}$	16.145	0.04	31	$\text{Eu}_2\text{SnS}_4, \text{SnS}_2, \text{SnS}$
$\text{Eu}_3\text{Ti}_5\text{S}_{12}$	15.408	0.00	91	$\text{Ti}_7\text{S}_{12}, \text{TiS}_2, \text{EuS}$
$\text{Bi}_3\text{Ga}_5\text{S}_{12}$	15.262	1.94	66	$\text{Ga}_2\text{S}_3, \text{Bi}_2\text{S}_3$
$\text{Gd}_3\text{Al}_5\text{S}_{12}$	14.983	1.57	0	$\text{Gd}_2\text{S}_3, \text{Al}_2\text{S}_3$
$\text{Gd}_3\text{Ga}_5\text{S}_{12}$	15.124	1.24	32	$\text{Ga}_2\text{S}_3, \text{Gd}_2\text{S}_3$
$\text{Gd}_3\text{Ge}_5\text{S}_{12}$	15.376	0.00	64	$\text{GeS}_2, \text{Gd}_2\text{S}_3, \text{GeS}$
$\text{Gd}_3\text{In}_5\text{S}_{12}$	15.762	1.21	32	$\text{Gd}_3\text{InS}_6, \text{In}_2\text{S}_3$
$\text{Ho}_3\text{Al}_5\text{S}_{12}$	14.891	2.09	5	$\text{Ho}_3\text{AlS}_6, \text{Al}_2\text{S}_3$
$\text{Ho}_3\text{Ga}_5\text{S}_{12}$	15.033	1.33	51	$\text{Ho}_3\text{GaS}_6, \text{Ga}_2\text{S}_3$
$\text{Ho}_3\text{In}_5\text{S}_{12}$	15.667	1.36	56	$\text{In}_2\text{S}_3, \text{Ho}_2\text{S}_3$
$\text{Bi}_3\text{In}_5\text{S}_{12}$	15.904	1.90	55	$\text{InBiS}_3, \text{In}_2\text{S}_3$
$\text{La}_3\text{Al}_5\text{S}_{12}$	15.223	2.05	0	$\text{La}_9\text{Al}_5\text{S}_{21}, \text{Al}_2\text{S}_3$
$\text{La}_3\text{Ga}_5\text{S}_{12}$	15.371	1.24	36	$\text{LaGaS}_3, \text{Ga}_2\text{S}_3$
$\text{La}_3\text{Ge}_5\text{S}_{12}$	15.639	0.00	49	$\text{GeS}, \text{La}_2\text{GeS}_5, \text{GeS}_2$
$\text{La}_3\text{In}_5\text{S}_{12}$	16.002	1.49	2	$\text{La}_3\text{InS}_6, \text{In}_2\text{S}_3$
$\text{La}_3\text{Sc}_5\text{S}_{12}$	15.828	2.20	97	$\text{LaScS}_3, \text{Sc}_2\text{S}_3$
$\text{La}_3\text{Sn}_5\text{S}_{12}$	16.282	0.00	79	$\text{La}_2\text{SnS}_5, \text{SnS}_2, \text{SnS}$
$\text{Lu}_3\text{Al}_5\text{S}_{12}$	14.804	2.15	27	$\text{Lu}_2\text{S}_3, \text{Al}_2\text{S}_3$
$\text{Lu}_3\text{Ga}_5\text{S}_{12}$	14.941	1.36	73	$\text{Lu}_2\text{S}_3, \text{Ga}_2\text{S}_3$
$\text{Lu}_3\text{In}_5\text{S}_{12}$	15.578	1.37	93	$\text{Lu}_2\text{S}_3, \text{In}_2\text{S}_3$
$\text{Nd}_3\text{Al}_5\text{S}_{12}$	15.120	1.91	0	$\text{Nd}_9\text{Al}_5\text{S}_{21}, \text{Al}_2\text{S}_3$
$\text{Nd}_3\text{Ga}_5\text{S}_{12}$	15.266	1.21	33	$\text{Nd}_3\text{GaS}_6, \text{Ga}_2\text{S}_3$

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Supplementary Figure 1. The distribution of the distances to the convex hull for all compounds predicted to be below 100 meV/atom in blue and above 100 meV/atom in orange for the first, second, and third rounds of calculations. This evaluation uses the hull used during the training data creation of the models.

Nd ₃ Ge ₅ S ₁₂	15.524	0.00	57	GeS ₂ ,Nd ₆ Ge ₃ S ₁₄ ,GeS	Eu ₃ Ge ₅ Se ₁₂	16.308	0.00	38	GeSe,GeSe ₂ ,EuSe
Nd ₃ In ₅ S ₁₂	15.900	1.36	14	Nd ₃ InS ₆ ,In ₂ S ₃	Eu ₃ In ₅ Se ₁₂	16.714	0.00	65	Eu(InSe ₂) ₂ ,EuSe,Se
Nd ₃ Sn ₅ S ₁₂	16.156	0.00	95	Nd ₂ SnS ₅ ,SnS ₂ ,SnS	Eu ₃ Sb ₅ Se ₁₂	17.112	0.00	88	Eu ₃ Sb ₄ Se ₉ ,Sb ₂ Se ₃ ,Se
Pr ₃ Al ₅ S ₁₂	15.167	1.89	0	Pr ₉ Al ₅ S ₂₁ ,Al ₂ S ₃	Eu ₃ Sn ₅ Se ₁₂	16.923	0.00	23	SnSe ₂ ,SnSe,EuSe
Pr ₃ Ga ₅ S ₁₂	15.314	1.18	31	Pr ₃ GaS ₆ ,Ga ₂ S ₃	Gd ₃ Al ₅ Se ₁₂	15.812	1.15	21	Gd ₂ Se ₃ ,Al ₂ Se ₃
Pr ₃ Ge ₅ S ₁₂	15.575	0.00	55	GeS ₂ ,Pr ₆ Ge ₃ S ₁₄ ,GeS	Gd ₃ Ga ₅ Se ₁₂	15.949	0.45	66	Ga ₂ Se ₃ ,Gd ₂ Se ₃
Pr ₃ In ₅ S ₁₂	15.947	1.36	8	Pr ₃ InS ₆ ,In ₂ S ₃	Gd ₃ Ge ₅ Se ₁₂	16.167	0.00	67	GeSe ₂ ,Gd ₂ Se ₃ ,GeSe
Pr ₃ Sn ₅ S ₁₂	16.209	0.00	89	Pr ₂ SnS ₅ ,SnS ₂ ,SnS	Gd ₃ In ₅ Se ₁₂	16.546	0.56	57	Gd ₂ Se ₃ ,In ₂ Se ₃
Sc ₃ Al ₅ S ₁₂	14.631	1.55	86	Sc ₂ S ₃ ,Al ₂ S ₃	Gd ₃ Sn ₅ Se ₁₂	16.771	0.00	97	GdSe ₂ ,SnSe ₂ ,SnSe
Sm ₃ Al ₅ S ₁₂	15.043	1.96	0	Sm ₃ AlS ₆ ,Al ₂ S ₃	Ho ₃ Al ₅ Se ₁₂	15.730	1.47	44	Ho ₂ Se ₃ ,Al ₂ Se ₃
Sm ₃ Ga ₅ S ₁₂	15.187	1.27	37	Sm ₃ GaS ₆ ,Ga ₂ S ₃	Ho ₃ Ga ₅ Se ₁₂	15.860	0.51	88	Ga ₂ Se ₃ ,Ho ₂ Se ₃
Sm ₃ Ge ₅ S ₁₂	15.442	0.00	61	Sm ₆ Ge ₃ S ₁₄ ,GeS ₂ ,GeS	Ho ₃ Ge ₅ Se ₁₂	16.077	0.00	97	GeSe ₂ ,Ho ₂ Se ₃ ,GeSe
Sm ₃ In ₅ S ₁₂	15.821	1.35	25	Sm ₃ InS ₆ ,In ₂ S ₃	Ho ₃ In ₅ Se ₁₂	16.462	0.58	88	Ho ₂ Se ₃ ,In ₂ Se ₃
Sr ₃ Ge ₅ S ₁₂	15.600	0.00	80	Sr ₂ GeS ₄ ,GeS,GeS ₂	Bi ₃ In ₅ Se ₁₂	16.697	1.23	93	Bi ₂ Se ₃ ,In ₂ Se ₃
Sr ₃ Sn ₅ S ₁₂	16.259	0.00	26	Sr ₂ SnS ₄ ,SnS ₂ ,SnS	La ₃ Al ₅ Se ₁₂	16.039	1.38	18	La ₉ Al ₅ Se ₂₁ ,Al ₂ Se ₃
Sr ₃ Ti ₅ S ₁₂	15.577	0.00	95	Sr ₈ (TiS ₃) ₇ ,Ti ₇ S ₁₂ ,TiS ₂	La ₃ Ga ₅ Se ₁₂	16.182	0.49	54	La ₃ GaSe ₆ ,Ga ₂ Se ₃
Tb ₃ Al ₅ S ₁₂	14.942	2.04	0	Tb ₃ AlS ₆ ,Al ₂ S ₃	La ₃ Ge ₅ Se ₁₂	16.414	0.00	54	La ₁₀ Se ₁₉ ,GeSe ₂ ,GeSe ₂
Tb ₃ Ga ₅ S ₁₂	15.084	1.31	45	Tb ₃ GaS ₆ ,Ga ₂ S ₃	La ₃ In ₅ Se ₁₂	16.778	0.73	24	La ₃ InSe ₆ ,In ₂ Se ₃
Tb ₃ Ge ₅ S ₁₂	15.333	0.00	76	GeS ₂ ,Tb ₂ S ₃ ,GeS	La ₃ Sc ₅ Se ₁₂	16.568	1.87	100	La ₂ Se ₃ ,Sc ₂ Se ₃
Tb ₃ In ₅ S ₁₂	15.718	1.35	42	Tb ₂ S ₃ ,In ₂ S ₃	La ₃ Sn ₅ Se ₁₂	17.015	0.00	76	SnSe ₂ ,LaSe ₂ ,SnSe
Tm ₃ Al ₅ S ₁₂	14.842	2.13	15	Tm ₂ S ₃ ,Al ₂ S ₃	Lu ₃ Al ₅ Se ₁₂	15.652	1.51	70	Lu ₂ Se ₃ ,Al ₂ Se ₃
Tm ₃ Ga ₅ S ₁₂	14.980	1.35	62	Tm ₂ S ₃ ,Ga ₂ S ₃	Nd ₃ Al ₅ Se ₁₂	15.942	1.29	16	Nd ₉ Al ₅ Se ₂₁ ,Al ₂ Se ₃
Tm ₃ In ₅ S ₁₂	15.617	1.36	78	In ₂ S ₃ ,Tm ₂ S ₃	Nd ₃ Ga ₅ Se ₁₂	16.084	0.46	56	Nd ₃ GaSe ₆ ,Ga ₂ Se ₃
Y ₃ Al ₅ S ₁₂	14.932	2.08	1	Y ₃ AlS ₆ ,Al ₂ S ₃	Nd ₃ Ge ₅ Se ₁₂	16.301	0.00	62	Nd ₁₀ Se ₁₉ ,GeSe ₂ ,GeSe
Y ₃ Ga ₅ S ₁₂	15.073	1.32	46	Y ₃ GaS ₆ ,Ga ₂ S ₃	Nd ₃ In ₅ Se ₁₂	16.681	0.60	36	Nd ₃ InSe ₆ ,In ₂ Se ₃
Y ₃ Ge ₅ S ₁₂	15.324	0.00	81	GeS ₂ ,Y ₂ S ₃ ,GeS	Nd ₃ Sn ₅ Se ₁₂	16.907	0.00	91	Nd ₁₀ Se ₁₉ ,SnSe ₂ ,SnSe
Y ₃ In ₅ S ₁₂	15.709	1.35	46	Y ₂ S ₃ ,In ₂ S ₃	Pr ₃ Al ₅ Se ₁₂	15.987	1.27	15	Pr ₉ Al ₅ Se ₂₁ ,Al ₂ Se ₃
Bi ₃ Al ₅ Se ₁₂	15.958	1.61	71	Bi ₂ Se ₃ ,Al ₂ Se ₃	Pr ₃ Ga ₅ Se ₁₂	16.126	0.44	56	Ga ₂ Se ₃ ,Pr ₂ Se ₃
Ba ₃ Sb ₅ Se ₁₂	17.596	0.00	86	Ba ₃ Sb ₂ Se ₇ ,Ba(SbSe ₂) ₂ ,Se	Pr ₃ Ge ₅ Se ₁₂	16.352	0.00	60	GeSe ₂ ,Pr ₆ Ge ₃ Se ₁₄ ,GeSe
Ba ₃ Sn ₅ Se ₁₂	17.383	0.00	38	SnSe ₂ ,Ba ₂ SnSe ₅ ,SnSe	Pr ₃ In ₅ Se ₁₂	16.726	0.61	34	Pr ₃ InSe ₆ ,In ₂ Se ₃
Ca ₃ Ge ₅ Se ₁₂	16.148	0.00	90	GeSe,GeSe ₂ ,CaSe	Pr ₃ Sn ₅ Se ₁₂	16.954	0.00	85	Pr ₁₀ Se ₁₉ ,SnSe ₂ ,SnSe
Ca ₃ Sn ₅ Se ₁₂	16.777	0.00	69	SnSe ₂ ,CaSe,SnSe	Sm ₃ Al ₅ Se ₁₂	15.870	1.34	18	Sm ₃ AlSe ₆ ,Al ₂ Se ₃
Ce ₃ Al ₅ Se ₁₂	15.944	0.00	19	Ce ₂ Se ₃ ,Al ₂ Se ₃	Sm ₃ Ga ₅ Se ₁₂	16.008	0.49	63	Ga ₂ Se ₃ ,Sm ₂ Se ₃
Ce ₃ Cu ₅ Se ₁₂	15.530	0.00	97	CeSe ₃ ,CeSe ₂ ,CuSe	Sm ₃ Ge ₅ Se ₁₂	16.225	0.00	65	Sm ₂ Se ₃ ,GeSe ₂ ,GeSe
Ce ₃ Ga ₅ Se ₁₂	16.055	0.00	63	Ga ₂ Se ₃ ,CeSe ₂ ,GaSe	Sm ₃ In ₅ Se ₁₂	16.607	0.59	50	Sm ₂ Se ₃ ,In ₂ Se ₃
Ce ₃ Ge ₅ Se ₁₂	16.283	0.00	73	GeSe ₂ ,CeSe ₂ ,GeSe	Sm ₃ Sn ₅ Se ₁₂	16.831	0.00	97	SmSe ₂ ,SnSe ₂ ,SnSe
Ce ₃ In ₅ Se ₁₂	16.682	0.00	52	In ₂ Se ₃ ,CeSe ₂ ,InSe	Pb ₃ Sn ₅ Se ₁₂	16.997	0.00	67	SnSe ₂ ,SnSe,PbSe
Dy ₃ Al ₅ Se ₁₂	15.752	1.46	35	Dy ₂ Se ₃ ,Al ₂ Se ₃	Sr ₃ Ge ₅ Se ₁₂	16.433	0.00	79	Sr ₂ GeS ₄ ,GeSe ₂ ,GeSe
Dy ₃ Ga ₅ Se ₁₂	15.883	0.51	80	Ga ₂ Se ₃ ,Dy ₂ Se ₃	Sr ₃ Sb ₅ Se ₁₂	17.271	0.00	99	SrSbSe ₃ ,Sb ₂ Se ₃
Dy ₃ Ge ₅ Se ₁₂	16.101	0.00	88	GeSe ₂ ,Dy ₂ Se ₃ ,GeSe	Sr ₃ Sn ₅ Se ₁₂	17.053	0.00	32	SnSe ₂ ,SnSe,SrSe
Dy ₃ In ₅ Se ₁₂	16.485	0.58	78	Dy ₂ Se ₃ ,In ₂ Se ₃	Tb ₃ Al ₅ Se ₁₂	15.776	1.43	29	Tb ₂ Se ₃ ,Al ₂ Se ₃
Er ₃ Al ₅ Se ₁₂	15.708	1.49	50	Er ₂ Se ₃ ,Al ₂ Se ₃	Tb ₃ Ga ₅ Se ₁₂	15.907	0.50	74	Ga ₂ Se ₃ ,Tb ₂ Se ₃
Er ₃ Ga ₅ Se ₁₂	15.837	0.52	94	Ga ₂ Se ₃ ,Er ₂ Se ₃	Tb ₃ Ge ₅ Se ₁₂	16.123	0.00	80	GeSe ₂ ,Tb ₂ Se ₃ ,GeSe
Er ₃ In ₅ Se ₁₂	16.439	0.57	96	In ₂ Se ₃ ,Er ₂ Se ₃	Tb ₃ In ₅ Se ₁₂	16.509	0.58	70	Tb ₂ Se ₃ ,In ₂ Se ₃
Eu ₃ Al ₅ Se ₁₂	15.957	0.04	88	Eu(AlSe ₂) ₂ ,Se,EuSe	Tm ₃ Al ₅ Se ₁₂	15.685	1.50	57	Al ₂ Se ₃ ,Tm ₂ Se ₃
Eu ₃ As ₅ Se ₁₂	16.472	0.00	81	Se,EuSe,As ₂ Se ₃	Y ₃ Al ₅ Se ₁₂	15.766	1.45	36	Y ₂ Se ₃ ,Al ₂ Se ₃

Y ₃ Ga ₅ Se ₁₂	15.898	0.51	81	Y ₂ Se ₃ ,Ga ₂ Se ₃	La ₃ Ta ₅ N ₁₂	13.276	0.00	85	Ta ₃ N ₅ ,La ₃ (Ta ₃ N ₃) ₂ ,N ₂
Y ₃ Ge ₅ Se ₁₂	16.116	0.00	88	GeSe ₂ ,Y ₂ Se ₃ ,GeSe	La ₃ W ₅ N ₁₂	13.141	0.00	50	W ₂ N ₃ ,LaWN ₃
Y ₃ In ₅ Se ₁₂	16.499	0.59	78	Y ₂ Se ₃ ,In ₂ Se ₃	Lu ₃ Re ₅ N ₁₂	12.618	0.00	0	ReN,N ₂ ,LuN
Ba ₃ Sn ₅ Te ₁₂	18.652	0.00	83	Ba ₂ SnTe ₅ ,SnTe,Te	Nd ₃ Mo ₅ N ₁₂	12.990	0.00	24	MoN ₂ ,NdMoN ₃ ,MoN
Dy ₃ Al ₅ Te ₁₂	17.120	0.58	86	Dy ₂ Te ₃ ,Al ₂ Te ₃	Nd ₃ Os ₅ N ₁₂	12.902	0.00	48	N ₂ ,Os,NdN
Er ₃ Al ₅ Te ₁₂	17.080	0.59	98	Er ₂ Te ₃ ,Al ₂ Te ₃	Nd ₃ Re ₅ N ₁₂	12.956	0.00	0	ReN,NdReN ₃ ,N ₂
Eu ₃ Al ₅ Te ₁₂	17.336	0.00	100	Al ₂ Te ₅ ,EuTe,Eu(AlTe ₂) ₂	Nd ₃ Ta ₅ N ₁₂	13.169	0.00	80	Nd(Ta ₂ N ₂) ₂ ,Nd ₃ (Ta ₃ N ₃) ₂ ,N ₂
Eu ₃ Ge ₅ Te ₁₂	17.575	0.00	79	Te,EuTe,GeTe	Nd ₃ W ₅ N ₁₂	13.020	0.00	40	NdWN ₃ ,W ₂ N ₃
Eu ₃ In ₅ Te ₁₂	18.019	0.00	99	In ₂ Te ₅ ,In ₇ Te ₁₀ ,EuTe	Pr ₃ Mo ₅ N ₁₂	13.040	0.00	21	PrMoN ₃ ,MoN ₂ ,MoN
Eu ₃ Si ₅ Te ₁₂	17.267	0.00	97	EuTe,Si ₂ SiTe ₂	Pr ₃ Os ₅ N ₁₂	12.947	0.00	36	PrN ₂ ,N ₂ ,Os
Eu ₃ Sn ₅ Te ₁₂	18.186	0.00	83	SnTe,EuTe,Te	Pr ₃ Re ₅ N ₁₂	13.002	0.00	0	ReN,PrReN ₃ ,N ₂
Gd ₃ Al ₅ Te ₁₂	17.176	0.55	63	Gd ₂ Te ₃ ,Al ₂ Te ₃	Pr ₃ Ta ₅ N ₁₂	13.218	0.00	81	Pr ₃ (Ta ₃ N ₃) ₂ ,Ta ₃ N ₅ ,N ₂
Gd ₃ Ga ₅ Te ₁₂	17.262	0.00	93	GdTe ₂ ,GdTe ₃ ,GaTe	Pr ₃ W ₅ N ₁₂	13.068	0.00	41	PrWN ₃ ,W ₂ N ₃
Gd ₃ Ge ₅ Te ₁₂	17.403	0.00	93	GdTe ₂ ,GdTe ₃ ,GeTe	Pb ₃ Re ₅ N ₁₂	13.202	0.00	75	ReN,N ₂ ,Pb
Gd ₃ In ₅ Te ₁₂	17.823	0.00	86	GdTe ₂ ,In ₇ Te ₁₀ ,Gd ₂ Te ₃	Sm ₃ Mo ₅ N ₁₂	12.908	0.00	32	MoN ₂ ,SmMoN ₃ ,MoN
Ho ₃ Al ₅ Te ₁₂	17.098	0.59	92	Ho ₂ Te ₃ ,Al ₂ Te ₃	Sm ₃ Os ₅ N ₁₂	12.826	0.00	76	N ₂ ,Os,SmN
La ₃ Al ₅ Te ₁₂	17.385	0.58	49	La ₂ Te ₃ ,Al ₂ Te ₃	Sm ₃ Re ₅ N ₁₂	12.880	0.00	0	ReN,SmReN ₃ ,N ₂
La ₃ Ge ₅ Te ₁₂	17.634	0.00	99	La ₂ Te ₅ ,LaTe ₂ ,GeTe	Sm ₃ Ta ₅ N ₁₂	13.087	0.00	96	Sm ₃ (Ta ₃ N ₃) ₂ ,Sm(Ta ₂ N ₂) ₂ ,N ₂
La ₃ In ₅ Te ₁₂	18.052	0.11	74	In ₇ Te ₁₀ ,InTe,LaTe ₂	Sm ₃ W ₅ N ₁₂	12.939	0.00	45	SmWN ₃ ,W ₂ N ₃
Nd ₃ Al ₅ Te ₁₂	17.292	0.50	58	Nd ₂ Te ₃ ,Al ₂ Te ₃	Sr ₃ Mo ₅ N ₁₂	13.158	0.32	97	Sr ₅ Mo ₂ N ₇ ,SrN ₆ ,MoN ₂
Nd ₃ Ga ₅ Te ₁₂	17.384	0.00	98	NdTe ₂ ,Nd ₂ Te ₅ ,GaTe	Sr ₃ Re ₅ N ₁₂	13.126	0.00	8	ReN,SrN ₆ ,SrReN ₃
Nd ₃ In ₅ Te ₁₂	17.955	0.00	78	NdTe ₂ ,In ₇ Te ₁₀ ,InTe	Sr ₃ W ₅ N ₁₂	13.174	0.89	0	Sr ₂ W ₂ N ₅ ,SrN ₆ ,W ₂ N ₃
Pr ₃ Al ₅ Te ₁₂	17.334	0.49	50	Pr ₂ Te ₃ ,Al ₂ Te ₃	Tb ₃ Mo ₅ N ₁₂	12.795	0.00	50	TbMoN ₃ ,MoN ₂ ,MoN
Pr ₃ Ga ₅ Te ₁₂	17.430	0.00	98	Pr ₂ Te ₅ ,PrTe ₂ ,GaTe	Tb ₃ Re ₅ N ₁₂	12.773	0.00	0	ReN,TbReN ₃ ,N ₂
Pr ₃ In ₅ Te ₁₂	17.999	0.00	76	PrTe ₂ ,In ₇ Te ₁₀ ,InTe	Tb ₃ W ₅ N ₁₂	12.828	0.00	65	TbWN ₃ ,W ₂ N ₃
Sm ₃ Al ₅ Te ₁₂	17.226	0.54	63	Sm ₂ Te ₃ ,Al ₂ Te ₃	Tm ₃ Mo ₅ N ₁₂	12.678	0.00	76	TmMoN ₃ ,MoN ₂ ,MoN
Sm ₃ Ga ₅ Te ₁₂	17.313	0.00	98	Sm ₂ Te ₃ ,Sm ₂ Te ₅ ,GaTe	Tm ₃ Re ₅ N ₁₂	12.661	0.00	0	ReN,N ₂ ,TmN
Sm ₃ In ₅ Te ₁₂	17.886	0.00	85	Sm ₂ Te ₅ ,In ₇ Te ₁₀ ,Sm ₂ Te ₃	Tm ₃ W ₅ N ₁₂	12.713	0.00	93	TmWN ₃ ,W ₂ N ₃
Sr ₃ Sn ₅ Te ₁₂	18.345	0.00	97	SnTe,SrTe,Te	Y ₃ Mo ₅ N ₁₂	12.787	0.00	68	YMoN ₃ ,MoN ₂ ,MoN
Tb ₃ Al ₅ Te ₁₂	17.141	0.58	80	Tb ₂ Te ₃ ,Al ₂ Te ₃	Y ₃ Re ₅ N ₁₂	12.767	0.00	0	ReN,YReN ₃ ,N ₂
Y ₃ Al ₅ Te ₁₂	17.131	0.60	84	Y ₂ Te ₃ ,Al ₂ Te ₃	Y ₃ W ₅ N ₁₂	12.820	0.00	72	YWN ₃ ,W ₂ N ₃
Ba ₃ Re ₅ N ₁₂	13.414	0.00	58	ReN,BaN ₆ ,BaReN ₃	Ag ₃ Hg ₅ F ₁₂	14.122	0.00	75	Ag ₂ F,HgF ₂ ,AgF
Ba ₃ W ₅ N ₁₂	13.485	0.56	45	BaN ₆ ,W ₂ N ₃ ,Ba ₃ WN ₄	Hg ₃ Ag ₅ F ₁₂	13.814	0.04	70	Ag ₅ F ₆ ,HgF ₂
Ca ₃ Re ₅ N ₁₂	12.896	0.00	9	ReN,CaReN ₃ ,N ₂	Pb ₃ Ag ₅ F ₁₂	14.198	0.00	44	Ag ₃ PbF ₆ ,AgF,PbF ₂
Ca ₃ W ₅ N ₁₂	12.928	0.93	0	Ca ₃ WN ₄ ,CaN ₆ ,W ₂ N ₃	Ba ₃ Ag ₅ F ₁₂	14.580	0.00	40	BaAg ₇ F ₁₂ ,AgF,BaF ₂
Ce ₃ Mo ₅ N ₁₂	12.882	0.03	16	CeMoN ₃ ,MoN ₂ ,MoN	Ba ₃ Li ₅ F ₁₂	13.385	0.00	79	LiF,LiF ₃ ,BaF ₂
Ce ₃ Nb ₅ N ₁₂	13.063	0.00	14	Ce(NbN ₂) ₂ ,CeN ₂ ,N ₂	Ba ₃ Na ₅ F ₁₂	14.281	0.00	63	NaF ₃ ,NaF,BaF ₂
Ce ₃ Os ₅ N ₁₂	12.800	0.00	92	CeN ₂ ,N ₂ ,Os	Cs ₃ Ag ₅ F ₁₂	14.924	0.00	91	CsAg ₇ F ₁₂ ,CsAgF ₃
Ce ₃ Re ₅ N ₁₂	12.878	0.00	0	ReN,Ce ₃ ReN ₆ ,N ₂	Cs ₃ Cd ₅ F ₁₂	15.055	0.00	98	CsCdF ₃ ,CdF ₂ ,Cd
Ce ₃ Ta ₅ N ₁₂	13.051	0.00	0	Ce ₃ (Ta ₃ N ₃) ₂ ,Ce ₃ N ₄ ,Ta ₃ N ₅	Cs ₃ Cu ₅ F ₁₂	13.942	0.00	92	CsCu ₂ F ₅ ,CsCuF ₃ ,Cu
Ce ₃ W ₅ N ₁₂	12.943	0.00	48	CeWN ₃ ,W ₂ N ₃	Cs ₃ Hg ₅ F ₁₂	15.331	0.00	70	CsHgF ₃ ,HgF,HgF ₂
Dy ₃ Mo ₅ N ₁₂	12.766	0.00	56	DyMoN ₃ ,MoN ₂ ,MoN	Cs ₃ In ₅ F ₁₂	15.557	2.82	27	Cs ₂ InF ₅ ,InF,InF ₂
Dy ₃ Re ₅ N ₁₂	12.746	0.00	0	ReN,N ₂ ,DyN	Cs ₃ Tl ₅ F ₁₂	15.831	2.51	14	TlF ₂ ,CsTlF ₃ ,TlF
Dy ₃ W ₅ N ₁₂	12.799	0.00	71	DyWN ₃ ,W ₂ N ₃	Hg ₃ Cs ₅ F ₁₂	16.374	0.00	45	Cs ₃ HgF ₆ ,CsHgF ₃
Er ₃ Mo ₅ N ₁₂	12.710	0.00	69	ErMoN ₃ ,MoN ₂ ,MoN	Ag ₃ Cu ₅ F ₁₂	13.133	0.00	53	CuAgF ₃ ,Ag ₂ F,CuF ₂
Er ₃ Re ₅ N ₁₂	12.693	0.00	0	ErReN ₃ ,ReN,N ₂	Eu ₃ Ag ₅ F ₁₂	14.052	0.00	63	AgF,Ag ₂ F,EuF ₃
Er ₃ W ₅ N ₁₂	12.745	0.00	85	ErWN ₃ ,W ₂ N ₃	Eu ₃ Tl ₅ F ₁₂	14.945	0.00	84	TlF,EuF ₃ ,EuF ₂
Eu ₃ Mo ₅ N ₁₂	12.990	0.00	0	EuMoN ₃ ,MoN ₂ ,MoN	K ₃ Ag ₅ F ₁₂	14.354	0.03	71	KAgF ₃ ,KAg ₇ F ₁₂
Eu ₃ Os ₅ N ₁₂	12.910	0.00	74	EuN ₂ ,N ₂ ,Os	K ₃ Cd ₅ F ₁₂	14.437	0.00	75	KCdF ₃ ,CdF ₂ ,Cd
Eu ₃ Re ₅ N ₁₂	12.985	0.00	0	ReN,EuReN ₃ ,N ₂	K ₃ Cu ₅ F ₁₂	13.389	0.00	51	KCuF ₃ ,CuF ₂ ,Cu
Eu ₃ W ₅ N ₁₂	13.038	0.00	0	EuN ₂ ,W ₂ N ₃ ,EuN	K ₃ Hg ₅ F ₁₂	14.694	0.00	64	KHgF ₃ ,HgF ₂ ,HgF
Gd ₃ Mo ₅ N ₁₂	12.851	0.00	43	GdMoN ₃ ,MoN ₂ ,MoN	K ₃ In ₅ F ₁₂	14.898	2.41	59	InF,K ₅ In ₃ F ₁₄ ,InF ₂
Gd ₃ Nb ₅ N ₁₂	13.037	0.00	69	Nb ₅ N ₆ ,GdN,N ₂	K ₃ Tl ₅ F ₁₂	15.157	2.28	29	K ₃ TlF ₆ ,TlF ₂ ,TlF
Gd ₃ Os ₅ N ₁₂	12.776	0.00	99	N ₂ ,Os,GdN	K ₃ Zn ₅ F ₁₂	13.592	0.00	84	KZnF ₃ ,ZnF ₂ ,Zn
Gd ₃ Re ₅ N ₁₂	12.829	0.00	0	ReN,GdReN ₃ ,N ₂	Ba ₃ K ₅ F ₁₂	15.276	0.00	92	KF ₂ ,KF,BaF ₂
Gd ₃ Ta ₅ N ₁₂	13.015	0.00	69	Ta ₃ N ₅ ,GdN,N ₂	Eu ₃ K ₅ F ₁₂	14.547	0.00	68	K ₃ EuF ₆ ,KF,EuF ₂
Gd ₃ W ₅ N ₁₂	12.888	0.00	56	GdWN ₃ ,W ₂ N ₃	Hg ₃ K ₅ F ₁₂	15.221	0.00	54	K ₃ HgF ₆ ,KHgF ₃
Ho ₃ Mo ₅ N ₁₂	12.739	0.00	63	HoMoN ₃ ,MoN ₂ ,MoN	Li ₃ Cu ₅ F ₁₂	12.795	0.00	88	CuF ₂ ,LiF,Cu
Ho ₃ Re ₅ N ₁₂	12.720	0.00	0	HoReN ₃ ,ReN,N ₂	Ca ₃ Li ₅ F ₁₂	12.444	0.00	47	LiF ₃ ,LiF,CaF ₂
Ho ₃ W ₅ N ₁₂	12.772	0.00	79	HoWN ₃ ,W ₂ N ₃	Cd ₃ Li ₅ F ₁₂	12.362	0.00	33	LiF ₃ ,CdF ₂ ,LiF
La ₃ Mo ₅ N ₁₂	13.108	0.00	43	MoN ₂ ,LaMoN ₃ ,MoN	Ce ₃ Li ₅ F ₁₂	12.794	0.00	75	LiCeF ₄ ,LiF,Ce
La ₃ Nb ₅ N ₁₂	13.297	0.00	99	La(NbN ₂) ₂ ,La ₃ (NbN ₃) ₂ ,N ₂	Eu ₃ Li ₅ F ₁₂	12.742	0.00	0	LiEuF ₄ ,EuF ₂ ,LiF
La ₃ Os ₅ N ₁₂	13.008	0.00	42	LaN ₂ ,N ₂ ,Os	Gd ₃ Li ₅ F ₁₂	12.565	0.00	85	LiGdF ₄ ,LiF,Gd
La ₃ Re ₅ N ₁₂	13.069	0.00	0	ReN,LaReN ₃ ,N ₂	Hg ₃ Li ₅ F ₁₂	12.583	0.00	19	LiHgF ₄ ,HgF ₂ ,LiF

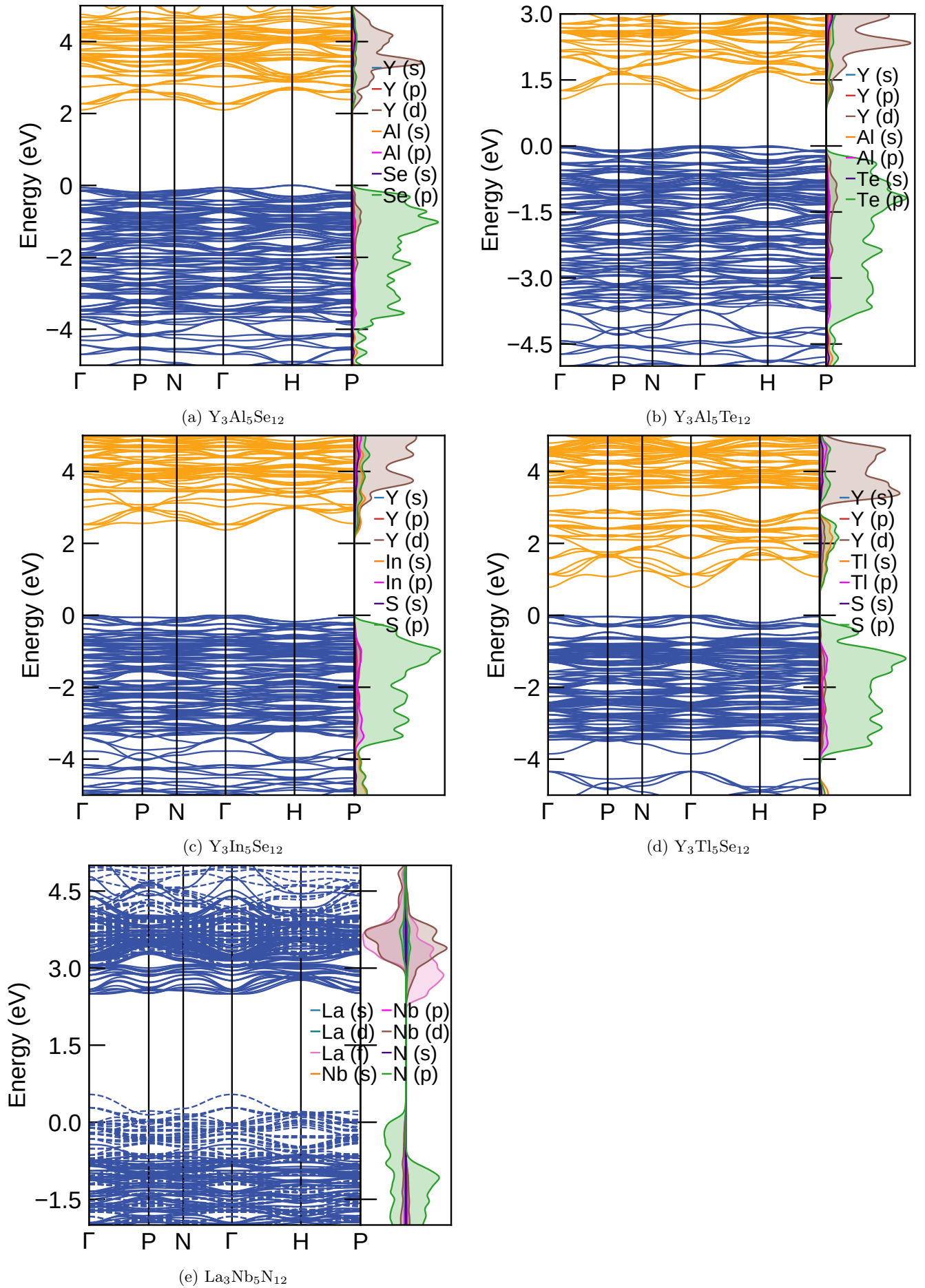
In ₃ Li ₅ F ₁₂	12.434	0.00	100	LiInF ₄ ,InF ₂ ,LiF	Ce ₃ Li ₅ Cl ₁₂	15.549	0.00	25	Ce ₂ Cl ₅ ,LiCl,Ce
La ₃ Li ₅ F ₁₂	12.793	0.00	87	LiLaF ₄ ,LiF,La	Eu ₃ Li ₅ Cl ₁₂	15.530	0.00	0	EuCl ₃ ,EuCl ₂ ,LiCl
Pb ₃ Li ₅ F ₁₂	12.883	0.00	52	PbF ₃ ,LiF,PbF ₂	Gd ₃ Li ₅ Cl ₁₂	15.343	0.00	44	Gd ₂ Cl ₃ ,GdCl ₃ ,LiCl
Tl ₃ Li ₅ F ₁₂	12.662	0.00	61	LiTiF ₄ ,TiF ₂ ,LiF	La ₃ Li ₅ Cl ₁₂	15.546	0.00	46	LaCl ₃ ,La,LiCl
Na ₃ Ag ₅ F ₁₂	14.202	0.00	77	NaAgF ₂ ,Na ₂ AgF ₄ ,AgF ₂	Nd ₃ Li ₅ Cl ₁₂	15.357	0.00	68	Nd ₂ Cl ₃ ,NdCl ₃ ,LiCl
Na ₃ Cu ₅ F ₁₂	12.879	0.00	33	NaCuF ₃ ,Cu,CuF ₂	Pb ₃ Li ₅ Cl ₁₂	15.651	0.00	52	LiCl ₂ ,PbCl ₂ ,LiCl
Na ₃ Hg ₅ F ₁₂	14.074	0.00	98	NaHgF ₃ ,HgF ₂ ,HgF	Pr ₃ Li ₅ Cl ₁₂	15.414	0.00	62	Pr ₂ Cl ₃ ,PrCl ₃ ,LiCl
Na ₃ Zn ₅ F ₁₂	13.040	0.00	75	NaZnF ₃ ,ZnF ₂ ,Zn	Sm ₃ Li ₅ Cl ₁₂	15.262	0.00	83	Sm ₂ Cl ₃ ,LiCl,SmCl ₃
Eu ₃ Na ₅ F ₁₂	13.575	0.00	0	NaEuF ₄ ,EuF ₂ ,NaF	Sn ₃ Li ₅ Cl ₁₂	15.507	0.00	90	SnCl ₄ ,LiCl,SnCl ₂
Hg ₃ Na ₅ F ₁₂	13.375	0.00	86	Na ₂ HgF ₅ ,NaHgF ₃ ,NaF	Na ₃ Ag ₅ Cl ₁₂	16.278	0.00	41	Na(AgCl ₂) ₃ ,AgCl ₂ ,NaCl
Pb ₃ Na ₅ F ₁₂	13.723	0.00	74	Na ₂ PbF ₆ ,NaF,PbF ₂	Na ₃ Cd ₅ Cl ₁₂	16.520	0.00	85	Na ₆ CdCl ₈ ,CdCl ₂ ,Cd
Sr ₃ Na ₅ F ₁₂	13.788	0.00	76	NaF ₃ ,NaF,SrF ₂	Na ₃ Cu ₅ Cl ₁₂	15.343	0.00	26	CuCl ₂ ,Cu ₃ Cl ₄ ,NaCl
Rb ₃ Ag ₅ F ₁₂	14.617	0.01	83	RbAg ₇ F ₁₂ ,RbAgF ₃	Na ₃ Hg ₅ Cl ₁₂	16.702	0.00	89	HgCl,HgCl ₂ ,NaCl
Rb ₃ Cd ₅ F ₁₂	14.716	0.00	81	RbCdF ₃ ,CdF ₂ ,Cd	Ce ₃ Na ₅ Cl ₁₂	16.438	0.00	92	Na ₃ Ce ₅ Cl ₁₈ ,NaCl,Ce
Rb ₃ Cu ₅ F ₁₂	13.644	0.00	62	RbCuF ₃ ,CuF ₂ ,Cu	Eu ₃ Na ₅ Cl ₁₂	16.373	0.00	42	NaEu ₂ Cl ₆ ,NaCl,EuCl ₂
Rb ₃ Hg ₅ F ₁₂	14.977	0.00	58	RbHgF ₃ ,HgF ₂ ,HgF	Hg ₃ Na ₅ Cl ₁₂	16.891	0.00	96	NaCl ₃ ,HgCl ₂ ,NaCl
Rb ₃ In ₅ F ₁₂	15.204	2.56	35	RbInF ₃ ,InF ₂	Rb ₃ Ag ₅ Cl ₁₂	16.899	0.00	58	RbAgCl ₃ ,Ag ₂ Cl ₃
Rb ₃ Tl ₅ F ₁₂	15.466	2.34	6	Rb ₃ TlF ₆ ,TlF ₂ ,TlF ₂	Rb ₃ Ca ₅ Cl ₁₂	17.797	0.00	98	CaCl ₂ ,RbCaCl ₃ ,Ca
Rb ₃ Zn ₅ F ₁₂	13.862	0.00	97	RbZnF ₃ ,ZnF ₂ ,Zn	Rb ₃ Cd ₅ Cl ₁₂	17.229	0.00	46	Rb ₂ Cd ₃ Cl ₈ ,Cd
Hg ₃ Rb ₅ F ₁₂	15.714	0.00	46	Rb ₃ HgF ₆ ,RbHgF ₃	Rb ₃ Cu ₅ Cl ₁₂	16.027	0.00	51	RbCuCl ₃ ,Cu ₃ Cl ₄ ,CuCl ₂
Sr ₃ Ag ₅ F ₁₂	14.113	0.00	65	Ag ₅ F ₆ ,SrF ₂	Rb ₃ Eu ₅ Cl ₁₂	18.271	0.00	93	RbEuCl ₃ ,RbEu ₂ Cl ₅ ,Eu
Sr ₃ Li ₅ F ₁₂	12.879	0.00	57	LiF ₃ ,LiF,SrF ₂	Rb ₃ Hg ₅ Cl ₁₂	17.400	0.00	41	Rb ₂ Hg ₃ Cl ₈ ,Rb ₂ HgCl ₄ ,HgCl
Tl ₃ Ag ₅ F ₁₂	13.940	0.00	90	TlAgF ₄ ,AgF,TlF ₂	Rb ₃ Sr ₅ Cl ₁₂	18.390	0.00	96	RbSr ₂ Cl ₅ ,RbCl,Sr
Tl ₃ Cd ₅ F ₁₂	14.674	0.00	92	TlCdF ₃ ,Cd,CdF ₂	Rb ₃ Tl ₅ Cl ₁₂	18.260	0.00	72	Tl ₂ Cl ₃ ,Rb ₃ TlCl ₆
Tl ₃ Cu ₅ F ₁₂	13.647	0.00	58	TlCuF ₃ ,CuF ₂ ,Cu	Eu ₃ Rb ₅ Cl ₁₂	19.508	0.00	75	RbEuCl ₃ ,RbEu ₂ Cl ₇ ,RbCl
Tl ₃ Hg ₅ F ₁₂	14.916	0.00	84	HgF ₂ ,TlF ₂ ,HgF	Hg ₃ Rb ₅ Cl ₁₂	18.448	0.00	60	Rb ₂ Hg ₃ Cl ₈ ,Rb ₂ HgCl ₄ ,RbCl ₃
Tl ₃ In ₅ F ₁₂	15.071	2.38	42	TlInF ₄ ,In	Sr ₃ Ag ₅ Cl ₁₂	16.384	0.00	25	Ag ₅ Cl ₆ ,SrCl ₂
Tl ₃ Zn ₅ F ₁₂	13.852	0.00	95	TlZnF ₃ ,ZnF ₂ ,Zn	Sr ₃ Cu ₅ Cl ₁₂	15.585	0.00	41	Cu ₃ Cl ₄ ,Cu,SrCl ₂
Ag ₃ Tl ₅ F ₁₂	14.576	1.70	72	AgF,Ag ₂ F,TlF ₂	Sr ₃ Li ₅ Cl ₁₂	15.757	0.00	66	LiCl ₂ ,LiCl,SrCl ₂
Hg ₃ Ag ₅ Cl ₁₂	16.772	0.00	83	Ag ₅ Cl ₆ ,HgCl ₂	Tl ₃ Ag ₅ Cl ₁₂	16.722	0.00	63	TlCl ₃ ,TlCl ₂ ,AgCl
Pb ₃ Ag ₅ Cl ₁₂	16.364	0.00	22	Ag ₅ Cl ₆ ,PbCl ₂	Tl ₃ Cd ₅ Cl ₁₂	17.098	0.00	58	TlCdCl ₃ ,CdCl ₂ ,Cd
Sn ₃ Ag ₅ Cl ₁₂	16.252	0.00	75	Ag ₂ SnCl ₆ ,AgSnCl ₃ ,AgCl	Tl ₃ Cu ₅ Cl ₁₂	15.905	0.00	34	TlCuCl ₃ ,Cu ₃ Cl ₄ ,CuCl ₂
Ba ₃ Ag ₅ Cl ₁₂	16.772	0.00	15	Ag ₅ Cl ₆ ,BaCl ₂	Tl ₃ Hg ₅ Cl ₁₂	17.262	0.00	54	TlHgCl ₃ ,HgCl ₂ ,HgCl
Ba ₃ Cu ₅ Cl ₁₂	15.976	0.00	50	Cu ₃ Cl ₄ ,BaCl ₂ ,Cu	Au ₃ Ag ₅ Br ₁₂	17.007	0.00	86	AgAuBr ₄ ,AuBr,AgBr
Ba ₃ Li ₅ Cl ₁₂	16.193	0.00	74	LiCl ₂ ,LiCl,BaCl ₂	Hg ₃ Ag ₅ Br ₁₂	17.623	0.00	92	HgBr ₂ ,Br,AgBr
Ba ₃ Na ₅ Cl ₁₂	17.112	0.00	91	NaCl ₃ ,NaCl,BaCl ₂	Pb ₃ Ag ₅ Br ₁₂	17.162	0.00	39	PbBr ₂ ,Br,AgBr
Ca ₃ Ag ₅ Cl ₁₂	16.060	0.00	68	Ag ₅ Cl ₆ ,CaCl ₂	Sn ₃ Ag ₅ Br ₁₂	17.060	0.00	80	SnBr ₄ ,SnBr ₂ ,AgBr
Ca ₃ Cu ₅ Cl ₁₂	15.271	0.00	65	Cu ₃ Cl ₄ ,CaCl ₂ ,Cu	Ba ₃ Ag ₅ Br ₁₂	17.602	0.00	18	AgBr,BaBr ₂ ,Br
In ₃ Cd ₅ Cl ₁₂	17.067	0.00	65	CdInCl ₃ ,Cd,CdCl ₂	Ba ₃ Cu ₅ Br ₁₂	16.847	0.00	53	Cu ₃ Br ₄ ,BaBr ₂ ,Cu
Cs ₃ Ag ₅ Cl ₁₂	17.198	0.00	79	Ag ₂ Cl ₃ ,CsAgCl ₃	Ba ₃ Li ₅ Br ₁₂	17.125	0.00	65	LiBr,Br,BaBr ₂
Cs ₃ Cd ₅ Cl ₁₂	17.549	0.00	58	CsCdCl ₃ ,CdCl ₂ ,Cd	Ba ₃ Na ₅ Br ₁₂	18.053	0.00	87	BaBr ₂ ,NaBr,Br
Cs ₃ Cu ₅ Cl ₁₂	16.344	0.00	89	CsCuCl ₃ ,Cu ₃ Cl ₄ ,CuCl ₂	Ba ₃ Tl ₅ Br ₁₂	18.995	0.00	97	TlBr ₂ ,TlBr,BaBr ₂
Cs ₃ Hg ₅ Cl ₁₂	17.724	0.00	54	CsHg ₅ Cl ₁₁ ,CsHgCl ₃ ,HgCl	Ca ₃ Ag ₅ Br ₁₂	16.923	0.00	82	AgBr,Br,CaBr ₂
Cs ₃ Sr ₅ Cl ₁₂	18.711	0.00	99	CsSrCl ₃ ,SrCl ₂ ,Sr	Ca ₃ Cu ₅ Br ₁₂	16.186	0.00	86	Cu ₃ Br ₄ ,Cu,CaBr ₂
Cs ₃ Tl ₅ Cl ₁₂	18.609	0.00	72	Tl ₂ Cl ₃ ,CsTlCl ₃	Ga ₃ Cd ₅ Br ₁₂	17.556	0.00	93	CdBr ₂ ,Ga,GaBr
Eu ₃ Cs ₅ Cl ₁₂	20.205	0.00	62	CsEuCl ₃ ,CsCl ₂ ,CsCl	In ₃ Cd ₅ Br ₁₂	17.868	0.00	58	InBr,Cd,CdBr ₂
Cu ₃ Ag ₅ Cl ₁₂	15.819	0.00	41	Ag ₅ Cl ₆ ,CuCl ₂	Cs ₃ Ag ₅ Br ₁₂	18.073	0.00	73	CsAgBr ₃ ,AgBr,Br
Ag ₃ Cu ₅ Cl ₁₂	15.337	0.00	49	AgCl,Cu ₃ Cl ₄ ,CuCl ₂	Cs ₃ Ca ₅ Br ₁₂	18.984	0.00	99	CsCaBr ₃ ,CaBr ₂ ,Ca
Hg ₃ Cu ₅ Cl ₁₂	15.452	0.03	98	HgCl ₂ ,Cu ₃ Cl ₄ ,HgCl	Cs ₃ Cd ₅ Br ₁₂	18.416	0.00	48	CsCdBr ₃ ,CdBr ₂ ,Cd
Pb ₃ Cu ₅ Cl ₁₂	15.598	0.00	34	Cu ₃ Cl ₄ ,PbCl ₂ ,Cu	Cs ₃ Cu ₅ Br ₁₂	17.262	0.00	85	Cu ₃ Br ₄ ,CsCuBr ₃ ,CuBr ₂
Sn ₃ Cu ₅ Cl ₁₂	15.484	0.00	47	Cu ₃ Cl ₄ ,SnCl ₂ ,Cu	Cs ₃ Hg ₅ Br ₁₂	18.583	0.00	43	CsHg ₂ Br ₅ ,Cs ₂ HgBr ₄ ,HgBr
Eu ₃ Ag ₅ Cl ₁₂	16.255	0.00	0	Eu(AgCl ₂) ₃ ,AgCl,EuCl ₂	Cs ₃ In ₅ Br ₁₂	19.273	0.00	75	In ₂ Br ₃ ,CsInBr ₃
Eu ₃ Cu ₅ Cl ₁₂	15.457	0.00	16	Cu ₃ Cl ₄ ,EuCl ₂ ,Cu	Cs ₃ Pb ₅ Br ₁₂	19.488	0.00	99	CsPbBr ₃ ,PbBr ₂ ,Pb
Hg ₃ Ga ₅ Cl ₁₂	17.510	0.00	96	Ga ₂ Hg ₃ Cl ₈ ,GaCl ₂ ,Hg	Cs ₃ Sr ₅ Br ₁₂	19.585	0.00	88	CsSrBr ₃ ,SrBr ₂ ,Sr
K ₃ Ag ₅ Cl ₁₂	16.656	0.00	43	KAgCl ₃ ,Ag ₂ Cl ₃	Cs ₃ Tl ₅ Br ₁₂	19.458	0.00	49	CsTlBr ₃ ,CsTlBr ₄ ,TlBr
K ₃ Cd ₅ Cl ₁₂	16.983	0.00	51	K ₂ Cd ₃ Cl ₈ ,Cd	Ag ₃ Cu ₅ Br ₁₂	16.313	0.00	67	Cu ₃ Br ₄ ,AgBr,CuBr ₂
K ₃ Cu ₅ Cl ₁₂	15.783	0.00	24	KCuCl ₃ ,Cu ₃ Cl ₄ ,CuCl ₂	Pb ₃ Cu ₅ Br ₁₂	16.444	0.00	52	Cu ₃ Br ₄ ,PbBr ₂ ,Cu
K ₃ Hg ₅ Cl ₁₂	17.145	0.00	39	K ₂ HgCl ₄ ,HgCl,HgCl ₂	Sn ₃ Cu ₅ Br ₁₂	16.340	0.00	62	Cu ₃ Br ₄ ,SnBr ₂ ,Cu
K ₃ Mg ₅ Cl ₁₂	16.485	0.00	92	K ₂ Mg ₃ Cl ₈ ,Mg ₁₄₉ Cl,KMgCl ₃	Eu ₃ Ag ₅ Br ₁₂	17.100	0.00	1	EuBr ₃ ,AgBr,EuBr ₂
K ₃ Tl ₅ Cl ₁₂	17.993	0.00	80	Tl ₂ Cl ₃ ,K ₃ TlCl ₆	Eu ₃ Cu ₅ Br ₁₂	16.356	0.00	36	Cu ₃ Br ₄ ,EuBr ₂ ,Cu
K ₃ Zn ₅ Cl ₁₂	16.224	0.00	92	K ₂ ZnCl ₄ ,ZnCl ₂ ,Zn	Hg ₃ Ga ₅ Br ₁₂	18.161	0.00	95	GaBr ₃ ,GaBr ₂ ,Hg
Li ₃ Ag ₅ Cl ₁₂	16.198	0.00	72	AgCl ₂ ,Ag ₂ Cl ₃ ,LiCl	Hg ₃ In ₅ Br ₁₂	18.832	0.00	93	InBr ₂ ,InBr ₃ ,Hg
Li ₃ Cu ₅ Cl ₁₂	15.192	0.00	82	Cu ₃ Cl ₄ ,CuCl ₂ ,LiCl	K ₃ Ag ₅ Br ₁₂	17.508	0.00	44	KAgBr ₃ ,AgBr,Br
Ca ₃ Li ₅ Cl ₁₂	15.390	0.00	90	LiCl ₂ ,CaCl ₂ ,LiCl	K ₃ Cd ₅ Br ₁₂	17.880	0.00	34	CdBr ₂ ,Cd,KBr

K ₃ Cu ₅ Br ₁₂	16.714	0.00	29	CuBr ₂ ,Cu ₃ Br ₄ ,KBr	Hg ₃ Ga ₅ I ₁₂	19.164	0.00	87	GaI ₂ ,GaI ₃ ,Hg
K ₃ Eu ₅ Br ₁₂	18.907	0.00	97	KEuBr ₃ ,Eu,EuBr ₂	In ₃ Hg ₅ I ₁₂	19.096	0.00	88	InI ₃ ,HgI,InI ₂
K ₃ Hg ₅ Br ₁₂	18.012	0.00	28	K ₂ Hg ₃ Br ₈ ,HgBr,KBr	Hg ₃ In ₅ I ₁₂	19.857	0.00	75	HgI,InI ₂ ,Hg
K ₃ In ₅ Br ₁₂	18.685	0.00	86	In ₂ Br ₃ ,KInBr ₃	K ₃ Ag ₅ I ₁₂	18.703	0.00	82	AgI,I,KI
K ₃ Mg ₅ Br ₁₂	17.489	0.00	84	Mg ₁₄₉ Br,MgBr ₂ ,KBr	K ₃ Au ₅ I ₁₂	18.647	0.00	88	KAuI ₃ ,AuI ₃ ,AuI
K ₃ Sr ₅ Br ₁₂	19.066	0.00	95	KSr ₂ Br ₅ ,Sr,KBr	K ₃ Cd ₅ I ₁₂	19.204	0.00	48	CdI ₂ ,KI,Cd
K ₃ Tl ₅ Br ₁₂	18.849	0.00	65	KTlBr ₄ ,KTlBr ₂ ,TlBr	K ₃ Cu ₅ I ₁₂	17.963	0.00	46	KI,I,CuI
K ₃ Zn ₅ Br ₁₂	17.154	0.00	95	K ₂ ZnBr ₄ ,ZnBr ₂ ,Zn	K ₃ Ga ₅ I ₁₂	19.305	0.00	98	KGaI ₃ ,Ga ₂ I ₃
Li ₃ Ag ₅ Br ₁₂	17.136	0.00	80	AgBr,Br,LiBr	K ₃ Hg ₅ I ₁₂	19.285	0.00	44	HgI ₂ ,KI,HgI
Li ₃ Cu ₅ Br ₁₂	16.204	0.00	86	CuBr ₂ ,Cu ₃ Br ₄ ,LiBr	K ₃ In ₅ I ₁₂	19.977	0.00	61	InI ₂ ,KInI ₂ ,KI
Ce ₃ Li ₅ Br ₁₂	16.505	0.00	56	LiBr,Ce ₂ Br ₅ ,Ce	K ₃ Mg ₅ I ₁₂	18.946	0.00	86	Mg ₁₄₉ I,MgI ₂ ,KI
Eu ₃ Li ₅ Br ₁₂	16.495	0.00	0	EuBr ₃ ,EuBr ₂ ,LiBr	K ₃ Tl ₅ I ₁₂	20.120	0.00	77	I,KI,TlI
Gd ₃ Li ₅ Br ₁₂	16.314	0.00	76	GdBr ₃ ,LiBr,GdBr ₂	Hg ₃ K ₅ I ₁₂	20.209	0.00	94	HgI ₂ ,KI,I
La ₃ Li ₅ Br ₁₂	16.495	0.00	68	La ₂ Br ₅ ,La,LiBr	Ce ₃ Li ₅ I ₁₂	17.882	0.00	74	CeI ₂ ,CeI ₃ ,LiI
Nd ₃ Li ₅ Br ₁₂	16.328	0.00	92	NdBr ₃ ,LiBr,NdBr ₂	Eu ₃ Li ₅ I ₁₂	17.909	0.00	34	EuI ₂ ,I,LiI
Pb ₃ Li ₅ Br ₁₂	16.620	0.00	76	PbBr ₂ ,Br,LiBr	La ₃ Li ₅ I ₁₂	17.857	0.00	98	La ₂ I ₅ ,LaI ₂ ,LiI
Pr ₃ Li ₅ Br ₁₂	16.377	0.00	86	Pr ₂ Br ₅ ,PrBr ₂ ,LiBr	Na ₃ Ag ₅ I ₁₂	18.672	0.00	98	NaI,AgI,I
Na ₃ Ag ₅ Br ₁₂	17.233	0.00	58	AgBr,NaBr,Br	Na ₃ Au ₅ I ₁₂	18.456	0.00	91	NaAuI ₄ ,NaI,AuI
Na ₃ Cd ₅ Br ₁₂	17.455	0.00	81	Na ₆ CdBr ₈ ,CdBr ₂ ,Cd	Na ₃ Cd ₅ I ₁₂	18.788	0.00	90	NaI,CdI ₂ ,Cd
Na ₃ Cu ₅ Br ₁₂	16.293	0.00	40	NaBr,Cu ₃ Br ₄ ,CuBr ₂	Na ₃ Cu ₅ I ₁₂	17.579	0.00	53	CuI,NaI,I
Na ₃ Hg ₅ Br ₁₂	17.581	0.00	75	HgBr ₂ ,NaBr,HgBr	Na ₃ Hg ₅ I ₁₂	18.872	0.00	85	HgI,HgI ₂ ,NaI
Cu ₃ Na ₅ Br ₁₂	17.052	0.00	64	NaBr,Br,CuBr ₂	Eu ₃ Na ₅ I ₁₂	18.783	0.00	84	EuI ₂ ,I,NaI
Eu ₃ Na ₅ Br ₁₂	17.343	0.00	32	EuBr ₃ ,NaBr,EuBr ₂	Rb ₃ Ag ₅ I ₁₂	18.945	0.00	90	RbI ₃ ,Rb ₂ AgI ₃ ,AgI
Rb ₃ Ag ₅ Br ₁₂	17.774	0.00	51	RbAgBr ₃ ,AgBr,Br	Rb ₃ Au ₅ I ₁₂	18.873	0.00	100	AuI ₃ ,AuI,RbAuI ₃
Rb ₃ Ca ₅ Br ₁₂	18.702	0.00	94	Rb ₂ Ca ₃ Br ₈ ,Ca	Rb ₃ Cd ₅ I ₁₂	19.427	0.00	47	Rb ₂ CdI ₄ ,CdI ₂ ,Cd
Rb ₃ Cd ₅ Br ₁₂	18.116	0.00	36	Rb ₂ CdBr ₄ ,CdBr ₂ ,Cd	Rb ₃ Cu ₅ I ₁₂	18.192	0.00	63	RbI ₃ ,RbCu ₂ I ₃ ,CuI
Rb ₃ Cu ₅ Br ₁₂	16.951	0.00	50	RbCuBr ₃ ,Cu ₃ Br ₄ ,CuBr ₂	Rb ₃ Ga ₅ I ₁₂	19.504	0.00	69	RbGaI ₄ ,Ga
Rb ₃ Hg ₅ Br ₁₂	18.278	0.00	30	Rb ₂ Hg ₃ Br ₈ ,Rb ₂ HgBr ₄ ,HgBr	Rb ₃ Hg ₅ I ₁₂	19.524	0.00	41	Rb ₂ HgI ₄ ,HgI ₂ ,HgI
Rb ₃ In ₅ Br ₁₂	18.957	0.00	79	In ₂ Br ₃ ,RbInBr ₃	Rb ₃ In ₅ I ₁₂	20.218	0.00	63	RbInI ₄ ,InI,RbI
Rb ₃ Mg ₅ Br ₁₂	17.723	0.00	89	RbMgBr ₃ ,Mg ₁₄₉ Br,MgBr ₂	Rb ₃ Mg ₅ I ₁₂	19.179	0.00	82	Mg ₁₄₉ I,Rb ₂ MgI ₄ ,MgI ₂
Rb ₃ Sr ₅ Br ₁₂	19.271	0.00	87	RbSr ₂ Br ₅ ,RbSrBr ₃ ,Sr	Rb ₃ Sr ₅ I ₁₂	20.716	0.00	100	RbSrI ₃ ,SrI ₂ ,Sr
Rb ₃ Tl ₅ Br ₁₂	19.141	0.00	48	RbTlBr ₄ ,Rb ₄ TlBr ₅ ,TlBr	Rb ₃ Tl ₅ I ₁₂	20.389	0.00	69	RbI ₃ ,TlI,RbI
Eu ₃ Rb ₅ Br ₁₂	20.331	0.00	78	RbBr ₃ ,RbBr,EuBr ₂	Hg ₃ Rb ₅ I ₁₂	20.730	0.00	98	Rb ₂ HgI ₄ ,RbI ₃ ,HgI ₂
Sr ₃ Ag ₅ Br ₁₂	17.238	0.00	30	AgBr,Br,SrBr ₂	Sr ₃ Ag ₅ I ₁₂	18.405	0.00	62	AgI,SrI ₂ ,I
Sr ₃ Cu ₅ Br ₁₂	16.486	0.00	50	Cu ₃ Br ₄ ,Cu,SrBr ₂	Sr ₃ Cu ₅ I ₁₂	17.701	0.00	59	CuI,SrI ₂ ,I
Sr ₃ Li ₅ Br ₁₂	16.721	0.00	66	LiBr,Br,SrBr ₂	Sr ₃ Li ₅ I ₁₂	18.132	0.00	78	SrI ₂ ,I,LiI
Tl ₃ Ag ₅ Br ₁₂	17.530	0.00	62	TlBr ₂ ,AgBr,Br	Tl ₃ Ag ₅ I ₁₂	18.613	0.00	89	AgI,I,TlI
Tl ₃ Cd ₅ Br ₁₂	17.907	0.00	48	TlCdBr ₃ ,CdBr ₂ ,Cd	Tl ₃ Au ₅ I ₁₂	18.550	0.00	77	AuI ₃ ,TlI,AuI
Tl ₃ Cu ₅ Br ₁₂	16.764	0.00	43	TlBr ₂ ,Cu ₃ Br ₄ ,TlBr	Tl ₃ Cd ₅ I ₁₂	19.089	0.00	59	TlI,CdI ₂ ,Cd
Tl ₃ Hg ₅ Br ₁₂	18.058	0.00	40	HgBr,HgBr ₂ ,TlBr	Tl ₃ Cu ₅ I ₁₂	17.916	0.00	49	CuI,TlI,I
Tl ₃ In ₅ Br ₁₂	18.639	0.00	77	In ₂ Br ₃ ,InBr ₂ ,TlBr	Tl ₃ Ga ₅ I ₁₂	19.117	0.00	81	TlGaI ₄ ,Ga
Pb ₃ Ag ₅ I ₁₂	18.251	0.00	88	PbI ₂ ,I,AgI	Tl ₃ Hg ₅ I ₁₂	19.173	0.00	55	HgI ₂ ,TlI,HgI
Ba ₃ Ag ₅ I ₁₂	18.731	0.00	35	AgI,I,BaI ₂	Tl ₃ In ₅ I ₁₂	19.793	0.00	72	InI,InI ₂ ,TlI
Ba ₃ Au ₅ I ₁₂	18.638	0.00	98	AuI ₃ ,BaI ₂ ,AuI	Ag ₃ Tl ₅ I ₁₂	19.569	0.00	82	AgI,I,TlI
Ba ₃ Cu ₅ I ₁₂	18.028	0.00	44	CuI,BaI ₂ ,I	Au ₃ Tl ₅ I ₁₂	19.583	0.00	48	AuI ₃ ,TlI,AuI
Ba ₃ Ga ₅ I ₁₂	19.525	0.00	93	Ba(GaI ₃) ₂ ,BaI ₂ ,Ga	Ag ₃ Pt ₅ H ₁₂	11.540	0.00	90	AgHPt,AgPt ₄ ,H ₂
Ba ₃ In ₅ I ₁₂	20.102	0.00	97	InI ₂ ,BaI ₂ ,InI	Ca ₃ Cu ₅ H ₁₂	11.635	0.00	86	CaH ₂ ,H ₂ ,Cu
Ba ₃ Li ₅ I ₁₂	18.492	0.00	54	BaI ₂ ,I,LiI	Cu ₃ Rh ₅ H ₁₂	10.686	0.00	95	CuH ₄ Rh,Cu,H ₂ Rh
Ba ₃ Na ₅ I ₁₂	19.424	0.00	79	BaI ₂ ,I,NaI	Dy ₃ Rh ₅ H ₁₂	11.560	0.26	94	H ₂ Rh,DyH ₃ Rh,Rh
Ba ₃ Tl ₅ I ₁₂	20.247	0.00	90	TlI,BaI ₂ ,I	Er ₃ Rh ₅ H ₁₂	11.490	0.25	94	H ₂ Rh,ErH ₃ Rh,Rh
In ₃ Cd ₅ I ₁₂	19.029	0.00	66	CdI ₂ ,Cd,InI	Gd ₃ Pd ₅ H ₁₂	11.937	0.00	98	GdH ₃ Pd,HPd,GdH ₃
Cs ₃ Cd ₅ I ₁₂	19.701	0.00	54	Cs ₂ CdI ₄ ,CdI ₂ ,Cd	Gd ₃ Rh ₅ H ₁₂	11.645	0.06	89	H ₂ Rh,GdH ₃ Rh,Rh
Cs ₃ Cu ₅ I ₁₂	18.488	0.00	97	Cs(CuI ₂) ₂ ,CsI ₄	Pd ₃ Pt ₅ H ₁₂	11.154	0.00	71	HPd,H ₂ ,Pt
Cs ₃ Ga ₅ I ₁₂	19.797	0.00	72	CsGaI ₄ ,Ga	Pt ₃ Pd ₅ H ₁₂	11.091	0.00	100	HPd,H ₂ ,Pt
Cs ₃ Hg ₅ I ₁₂	19.803	0.00	54	HgI,Cs ₂ Hg ₃ I ₈ ,Cs ₂ HgI ₄	Rh ₃ Pd ₅ H ₁₂	10.879	0.00	79	H ₂ Rh,H ₂ ,HPd
Cs ₃ In ₅ I ₁₂	20.504	0.00	52	CsInI ₄ ,InI,CsI	Pb ₃ Rh ₅ H ₁₂	11.850	0.15	95	H ₂ Pb,RhPb ₂ ,H ₂ Rh
Cs ₃ Mg ₅ I ₁₂	19.470	0.00	89	CsMgI ₃ ,Mg ₁₄₉ I,MgI ₂	Hf ₃ Mo ₅ H ₁₂	11.195	0.00	85	HfMoH ₄ ,Mo
Cs ₃ Pb ₅ I ₁₂	20.741	0.00	100	CsPbI ₃ ,PbI ₂ ,Pb	Hf ₃ Nb ₅ H ₁₂	11.455	0.00	38	HfNbH ₄ ,HfH ₂ ,NbH
Cs ₃ Sr ₅ I ₁₂	20.999	0.00	97	CsSrI ₃ ,SrI ₂ ,Sr	Hf ₃ Ta ₅ H ₁₂	11.394	0.00	32	Ta ₅ H ₄ ,HfH ₂ ,TaH ₂
Cs ₃ Tl ₅ I ₁₂	20.690	0.00	65	CsI ₃ ,TlI,CsI	Hf ₃ Ti ₅ H ₁₂	11.277	0.00	42	Hf ₂ TiH ₆ ,Hf(TiH ₂) ₂ ,TiH ₂
Pb ₃ Cu ₅ I ₁₂	17.581	0.00	74	CuI,PbI ₂ ,I	Hf ₃ Zr ₅ H ₁₂	11.884	0.00	61	HfH,ZrH ₂ ,Hf
Sn ₃ Cu ₅ I ₁₂	17.465	0.00	90	SnI ₄ ,SnI ₂ ,CuI	Ti ₃ Hf ₅ H ₁₂	11.480	0.00	80	Hf ₂ TiH ₆ ,HfH,Hf(TiH ₂) ₂
Eu ₃ Ag ₅ I ₁₂	18.253	0.00	52	AgI,I,EuI ₂	Zr ₃ Hf ₅ H ₁₂	11.844	0.00	57	HfZrH ₄ ,HfH,ZrH ₂
Eu ₃ Cu ₅ I ₁₂	17.552	0.00	53	EuI ₂ ,CuI,I	Ho ₃ Rh ₅ H ₁₂	11.525	0.26	94	H ₂ Rh,HoH ₃ Rh,Rh

K ₃ Cd ₅ H ₁₂	13.468	0.00	81	K ₃ CdH ₅ ,H ₂ ,Cd	Eu ₃ Na ₅ H ₁₂	13.335	0.00	84	NaH,EuH ₂ ,H ₂
K ₃ Mg ₅ H ₁₂	13.152	0.00	91	KMgH ₃ ,KMg ₁₄₉ ,MgH ₂	Rb ₃ Cd ₅ H ₁₂	13.772	0.00	94	Rb ₃ CdH ₅ ,H ₂ ,Cd
Li ₃ Ca ₅ H ₁₂	12.766	0.00	97	CaH ₂ ,LiH,Li	Sc ₃ Cu ₅ H ₁₂	11.068	0.00	83	ScH ₂ ,H ₂ ,Cu
Li ₃ Pd ₅ H ₁₂	10.986	0.00	72	LiH ₃ Pd,HPd,H ₂	Sc ₃ Pd ₅ H ₁₂	11.356	0.00	73	ScH ₃ Pd,ScHPd ₃ ,H ₂
Li ₃ Pt ₅ H ₁₂	11.102	0.00	89	LiH ₃ Pt,Pt,H ₂	Sc ₃ Rh ₅ H ₁₂	11.138	0.15	72	ScH ₄ Rh ₃ ,H ₂ Rh,ScH ₃ Rh
Li ₃ Ta ₅ H ₁₂	11.055	0.00	93	Ta ₅ H ₄ ,TaH ₂ ,LiH	Sc ₃ Ru ₅ H ₁₂	11.010	0.00	70	ScH ₃ Ru,Ru,H ₂
Li ₃ Zn ₅ H ₁₂	11.432	0.00	94	LiH,H ₂ ,Zn	Sc ₃ Nb ₅ H ₁₂	11.458	0.00	94	NbH ₂ ,ScH ₂ ,NbH
Dy ₃ Li ₅ H ₁₂	11.841	0.00	96	DyH ₃ ,LiH,DyH ₂	Sc ₃ Ta ₅ H ₁₂	11.380	0.00	83	ScTaH ₄ ,Ta ₃ H ₂ ,ScH ₂
Er ₃ Li ₅ H ₁₂	11.734	0.00	99	LiH,ErH ₃ ,ErH ₂	Sc ₃ Ti ₅ H ₁₂	11.321	0.00	95	ScH ₂ ,Ti,TiH ₂
Eu ₃ Li ₅ H ₁₂	12.370	0.00	82	LiH,LiEuH ₃ ,H ₂	Ta ₃ Mo ₅ H ₁₂	11.027	0.10	98	Ta ₂ MoH ₆ ,TaMo ₇ ,MoH
Gd ₃ Li ₅ H ₁₂	11.970	0.00	91	GdH ₃ ,LiH,GdH ₂	Ta ₃ Nb ₅ H ₁₂	11.274	0.00	98	Ta ₃ H ₂ ,NbH ₂
Hf ₃ Li ₅ H ₁₂	11.085	0.00	92	LiHfH ₄ ,LiH,HfH ₂	Nb ₃ Ta ₅ H ₁₂	11.256	0.00	79	Ta(NbH ₃) ₂ ,Ta ₂ NbH ₆ ,Ta ₅ H ₄
Ho ₃ Li ₅ H ₁₂	11.786	0.00	98	HoH ₃ ,LiH,HoH ₂	Ti ₃ Ta ₅ H ₁₂	11.089	0.00	43	Ta(TiH ₃) ₂ ,Ta ₂ TiH ₆ ,Ta ₃ H ₂
Nd ₃ Li ₅ H ₁₂	12.276	0.00	91	LiH,NdH ₃ ,NdH ₂	Tb ₃ Rh ₅ H ₁₂	11.597	0.23	98	TbH ₄ Rh,Rh
Pr ₃ Li ₅ H ₁₂	12.355	0.00	84	PrH ₃ ,LiH,PrH ₂	Ti ₃ Mo ₅ H ₁₂	10.867	0.00	97	TiMoH ₄ ,Mo
Sc ₃ Li ₅ H ₁₂	11.218	0.00	92	ScH ₂ ,LiH,H ₂	Ti ₃ Nb ₅ H ₁₂	11.148	0.00	59	Ti(NbH ₃) ₂ ,NbH,TiH ₂
Sm ₃ Li ₅ H ₁₂	12.113	0.00	92	SmH ₃ ,LiH,SmH ₂	Nb ₃ Ti ₅ H ₁₂	11.085	0.00	96	Nb ₃ H ₂ ,TiH ₂
Tb ₃ Li ₅ H ₁₂	11.900	0.00	95	TbH ₃ ,TbH ₂ ,LiH	Tm ₃ Rh ₅ H ₁₂	11.453	0.24	94	H ₂ Rh,TmH ₃ Rh,Rh
Y ₃ Li ₅ H ₁₂	11.859	0.00	93	YH ₃ ,YH ₂ ,LiH	Y ₃ Pd ₅ H ₁₂	11.824	0.00	99	YHPd ₃ ,YH ₄ Pd,HPd
Zr ₃ Li ₅ H ₁₂	11.237	0.00	95	LiH,ZrH ₂ ,H ₂	Y ₃ Rh ₅ H ₁₂	11.581	0.27	93	H ₂ Rh,YH ₃ Rh,Rh
Lu ₃ Rh ₅ H ₁₂	11.393	0.23	94	H ₂ Rh,LuH ₃ Rh,Rh	Zr ₃ Pd ₅ H ₁₂	11.434	0.05	87	ZrH ₃ Pd,ZrPd ₃ ,H ₂
Lu ₃ Zr ₅ H ₁₂	12.204	0.00	97	ZrH ₂ ,Zr,LuH ₂	Zr ₃ Nb ₅ H ₁₂	11.543	0.00	63	ZrH ₂ ,NbH ₂ ,NbH
Mg ₃ Pd ₅ H ₁₂	11.305	0.00	90	MgHPd,MgHPd ₃ ,H ₂	Zr ₃ Ta ₅ H ₁₂	11.480	0.00	56	Ta ₅ H ₄ ,TaH ₂ ,ZrH ₂
Mg ₃ Rh ₅ H ₁₂	11.008	0.00	51	MgH ₃ Rh,H ₂ Rh,MgH ₂ Rh	Zr ₃ Ti ₅ H ₁₂	11.378	0.00	63	Zr(TiH ₂) ₂ ,TiH ₂ ,ZrH ₂
Na ₃ Mg ₅ H ₁₂	12.421	0.00	82	NaMg ₁₄₉ ,MgH ₂ ,NaMgH ₃					
Na ₃ Zn ₅ H ₁₂	11.955	0.00	64	Na ₂ ZnH ₄ ,H ₂ ,Zn					

Supplementary Table III. The VASP 5.2 version pseudopotentials chosen for calculation. Note the W_pv should be replaced by the more accurate W_sv (VASP 5.4 or later version) in future calculations.

Elements	Choice	Elements	Choice	Elements	Choice		
Ac	Ac	Eu	Eu	Na	Na_pv	Sc	Sc_sv
Ag	Ag	F	F	Nb	Nb_pv	Se	Se
Al	Al	Fe	Fe_pv	Nd	Nd_3	Si	Si
As	As	Ga	Ga_d	Ni	Ni_pv	Sm	Sm_3
Au	Au	Gd	Gd	Np	Np	Sn	Sn_d
B	B	Ge	Ge_d	O	O	Sr	Sr_sv
Ba	Ba_sv	H	H	Os	Os_pv	Ta	Ta_pv
Be	Be_sv	Hf	Hf_pv	P	P	Tb	Tb_3
Bi	Bi	Hg	Hg	Pa	Pa	Tc	Tc_pv
Br	Br	Ho	Ho_3	Pb	Pb_d	Te	Te
C	C	I	I	Pd	Pd	Th	Th
Ca	Ca_sv	In	In_d	Pm	Pm_3	Ti	Ti_pv
Cd	Cd	Ir	Ir	Pr	Pr_3	Tl	Tl_d
Ce	Ce	K	K_sv	Pt	Pt	Tm	Tm_3
Cl	Cl	La	La	Pu	Pu	U	U
Co	Co	Li	Li_sv	Rb	Rb_sv	V	V_sv
Cr	Cr_pv	Lu	Lu_3	Re	Re_pv	W	W_pv
Cs	Cs_sv	Mg	Mg_pv	Rh	Rh_pv	Y	Y_sv
Cu	Cu_pv	Mn	Mn_pv	Ru	Ru_pv	Zr	Zr_sv
Dy	Dy_3	Mo	Mo_pv	S	S	Zn	Zn
Er	Er_3	N	N	Sb	Sb		



Supplementary Figure 2. The calculated mBJ electronic band structures of (a) $\text{Y}_3\text{Al}_5\text{Se}_{12}$, (b) $\text{Y}_3\text{Al}_5\text{Te}_{12}$, (c) $\text{Y}_3\text{In}_5\text{Se}_{12}$, (d) $\text{Y}_3\text{Tl}_5\text{Se}_{12}$, and (e) $\text{La}_3\text{Nb}_5\text{N}_{12}$.