Supplementary Information

1. Overview of paper

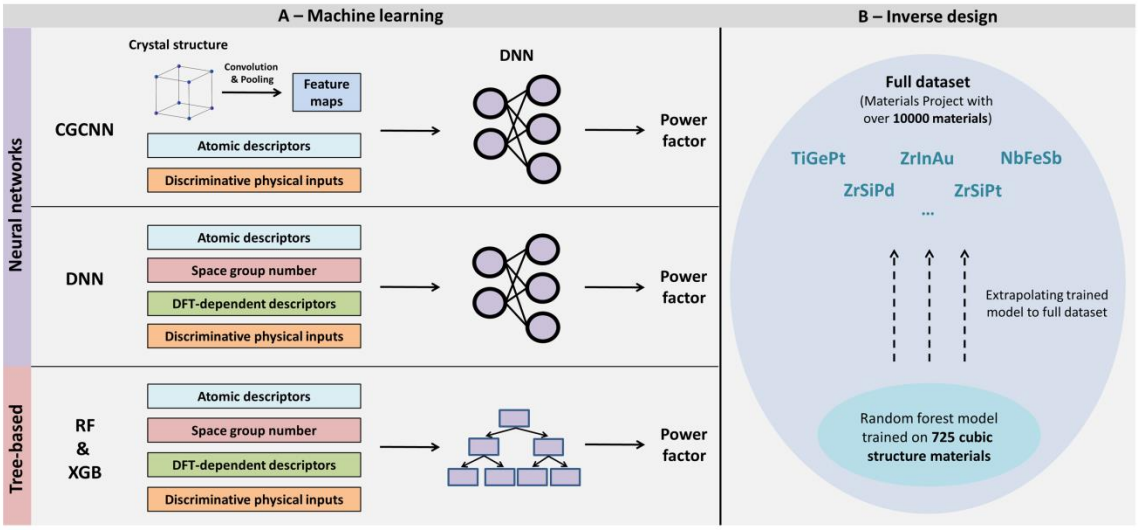

Figure S1. **(A)** 4 machine learning models: Crystal Graph Convolutional Neural Network (CGCNN), Deep Neural Network (DNN), Random Forest (RF) and XG Boost (XGB) were trained independently for predicting power factor of thermoelectric materials. These models differ in terms of their architecture and inputs as shown. **(B)** Random forest model, being the most accurate among the 4, was used to discover numerous new materials with good thermoelectric property (e.g. TiGePt, ZrInAu, NbFeSb, ZrSiPd and ZrSiPt) outside the training set.

2. Methodology

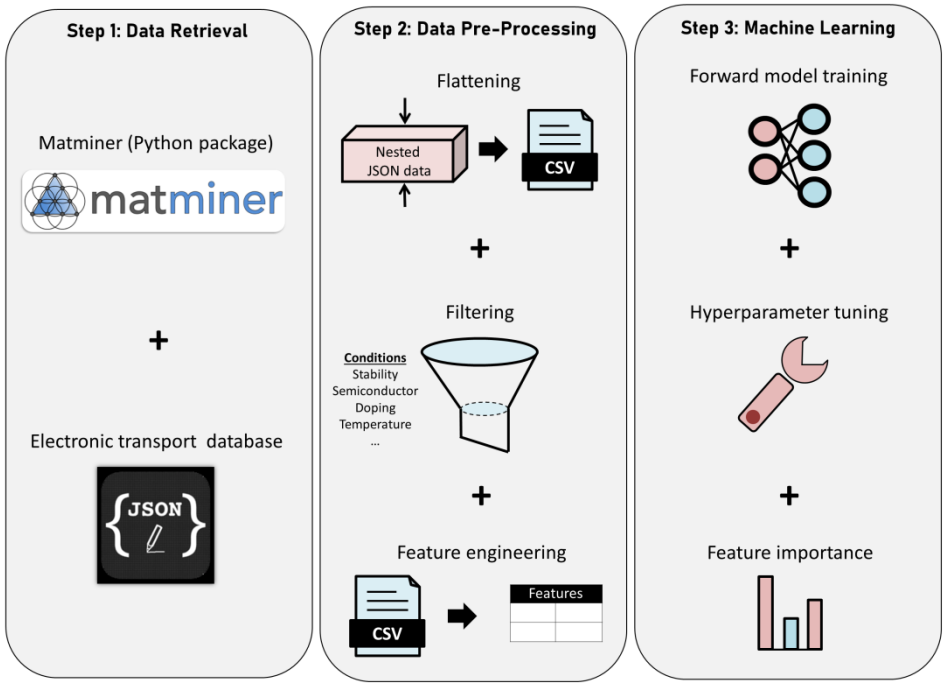

Figure S2: The 3 phases involved in the forward model training are retrieving data from open-source material databases, processing the retrieved data to obtain the necessary features and developing optimized forward machine learning models based on these features

3. Box cox transformation

The following diagram illustrates the impact of box-cox transformation on the prediction accuracy of a machine learning model.

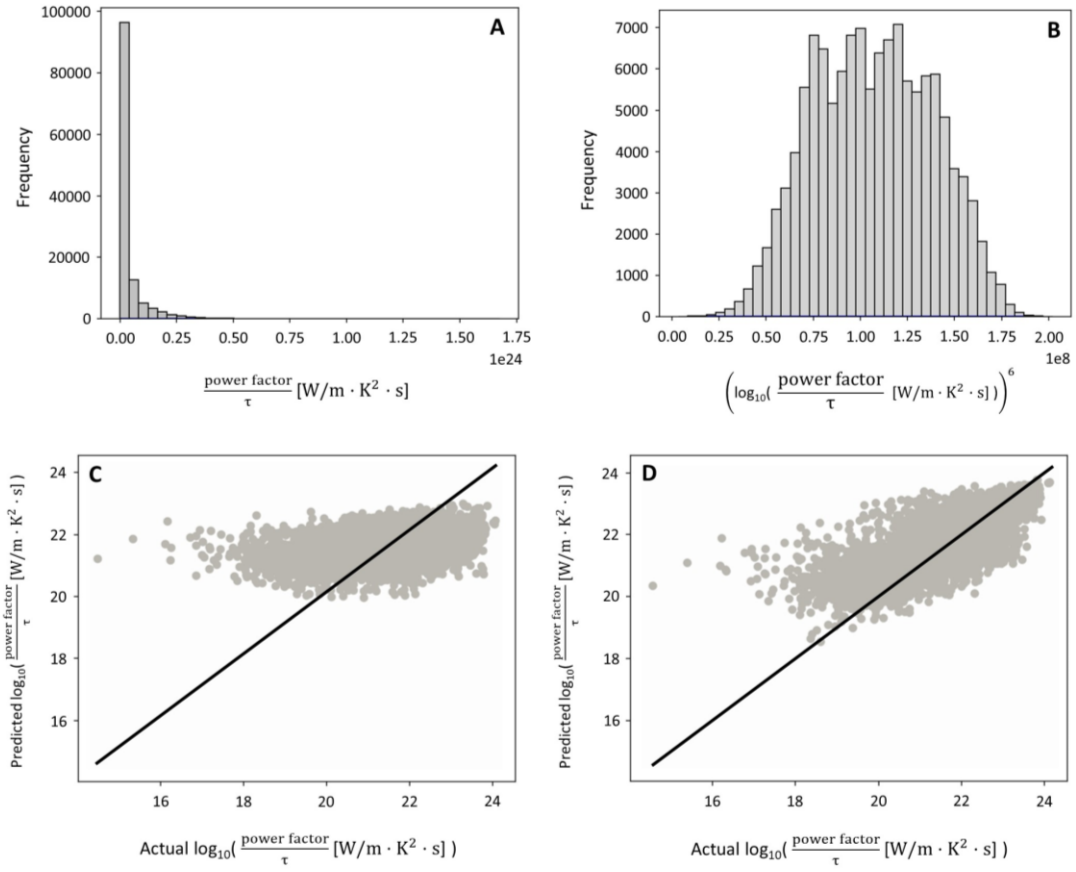

Figure S3: Box-cox transformation. (**A)** Distribution of power factor (before transformation). (**B)** Distribution of power factor (after transformation). (**C)** Plot of prediction against actual $\log_{10}(\frac{\text{power factor}}{\tau}\ [\mathrm{W/m \cdot K^2 \cdot s}])$ values (before transformation). (**D)** Plot of prediction against actual $\log_{10}(\frac{\text{power factor}}{\tau}\ [\mathrm{W/m \cdot K^2}]\ ) \cdot \mathrm{s}])$ values (after transformation)

As seen in Figure S3, the variance of the data is increased when box-cox transformation is applied. This is essential for the neural networks to learn the intricacies of the data; otherwise, the predictions by the neural networks will also have high bias and low variance.

4. Statistics of the reduced training set

Supplementary Table 1: Statistics of reduced training set

Parameter	Value
Number of unique materials	8059
Range of Atomic Weight	0 to 207.97
Mean Atomic Weight	1.01 to 176.24
Standard deviation of Atomic Weight	0 to 95.6
Range of Covalent Radius	0 to 213
Mean Covalent Radius	31.0 to 217.75
Standard deviation of Covalent Radius	0 to 94.5
Range of Electronegativity	0 to 3.19
Mean Electronegativity	1.11 to 3.82
Standard deviation of Electronegativity	0 to 1.60
Number of elements	1 to 7
Molecular weight	2.02 to 7253.08
n/p type (One-hot encoded)	1 or 0
Temperature	100 to 1300
Doping	1e18 to 1e20
Crystal structure	Cubic, Hexagonal, Monoclinic, Orthorhombic, Tetragonal, Triclinic, Trigonal
Number of sites in the unit cell (n_{sites})	2 to 192
s fraction	0.0164 to 0.927
d fraction	0.068 to 0.940
p fraction	0 to 0.868
Formation energy per atom	-4.49 to 0.0448
Energy above hull	0 to 0.0498
Final energy per atom	-10.70 to -1.12
Volume	13.98 to 5047.21
Density	0.0400 to 13.16
Band gap	0.161 to 9.06
Fermi energy	-8.37 to 10.93
Direct/indirect (One-hot encoded)	1 or 0

5. Machine Learning models

5.1 Crystal graph convolutional neural network (CGCNN)

The CGCNN model was developed in PyTorch. The following custom loss function was used to compute the loss.

$$\text{Loss} = 10^{\frac{1}{n}\sum(\text{prediction}-\text{actual})^2} = 10^{\text{mean squared error}} \quad \text{(S1)}$$

This loss function was used in place of standard mean squared error as this amplifies the error value which was back-propagated during training. In this way, the CGCNN model was better able to learn from the data.

Since the training of CGCNN model involves assembling atomic features from the crystal structure of a material using Pymatgen package for each training datapoint, the time needed for training the forward model significantly increased. Hence, randomized search of hyper parameters was used for finding the best hyper parameters of CGCNN model.

Feature importance was employed in a similar fashion like hyperparameter tuning such that random combinations of atomic descriptors were experimented. Finally, the smallest combination of atomic descriptors which gives the highest accuracy on test set was determined to be most important features.

5.2 Deep neural network (DNN)

Deep neural network (DNN) was implemented in Python using a deep learning library called Keras was used which is a high level neural networks API capable of running on top of Tensorflow and Theano. The loss function used for DNN was standard mean squared error. This standard loss function was sufficient for DNN to be trained effectively. Hyperparameter tuning of DNN was done by an optimizer called GridSearchCV. Since the training of DNN was significantly faster than CGCNN, grid search was implemented in place of random search. An open-source Python-based library called eli5 was used to perform permutation feature importance on DNN model. eli5 permutation importance does not require training the model again for every new combination of features. Instead, it makes use of the trained model to predict the output value using only a subset of features from the test set. In this way, it quantifies the importance of that subset of features.

5.3 XG Boost (XGB)

A Python library called ‘xgboost’ was used to train the XG boost (XGB) model. The procedure for hyperparameter tuning is same as that for DNN. There is no additional package needed for computing the feature importance of XGB model as feature importance will automatically be computed during model training based on the information of the splits in the decision trees. Total gain was used as the metric for quantifying the importance of the features. There are other metrics such as average gain, cover and total cover available for quantifying the importance of features in a XGB model. However, total gain being the most useful metric was used in this project.

5.4 Random Forest (RF)

Training of random forest (RF) model was done by a class called ‘RandomForestRegressor’ available in Scikit-learn machine learning library. Apart from that, forward model training, hyperparameter tuning as well as feature importance was carried out in a similar fashion as XGB.

6. Hyperparameters

Supplementary Table 2: Hyperparameters for CGCNN

Hyperparameter	**Range**	**Best**
No. of conv layers	1-5	3
No. of neurons (conv layer)	{50,100,150}	50
No. of fully connected (FC) layers	1-5	2
No. of neurons (FC layer)	{50,100,150}	100
Learning rate	{0.1,0.001, 0.0001}	0.0001
Batch size	{128, 256}	128
Optimizer	Adam, SGD	Adam

Supplementary Table 3: Hyperparameters for DNN

Hyperparameter	**Range**	**Best**
Number of hidden layers	1-5	3
Number of neurons	20-100	100
Activation function	Relu, sigmoid, tanh	Relu
Drop out rate	0-0.8	0
Batch size	{16, 32, 64, 128, 256}	16
Optimizer	SGD, RMSprop, Adam	Adam

Supplementary Table 4: Hyperparameters for XG Boost

Hyper parameter	**Range**	**Best**
n_estimators	1 - 500	319
max_depth	1 - 10	10
min_child_weight	1 - 10	10
Learning rate	0.01 - 0.2	0.2
gamma	0 - 1	1
alpha	1e-10 - 1	0.75
lambda	0.1 - 10	10
scale_pos_weight	0.1 - 10	3.4
subsample	0 - 1	1

Supplementary Table 5: Hyperparameters for random forest

Hyperparameter	**Range**	**Best**
n_estimators	1-500	391
max_features	auto or sqrt	sqrt
max_depth	10-110	100
min_samples_split	{2,5,10}	2
min_samples_leaf	{1,2,4}	1
bootstrap	True or False	False

7. Variation of error

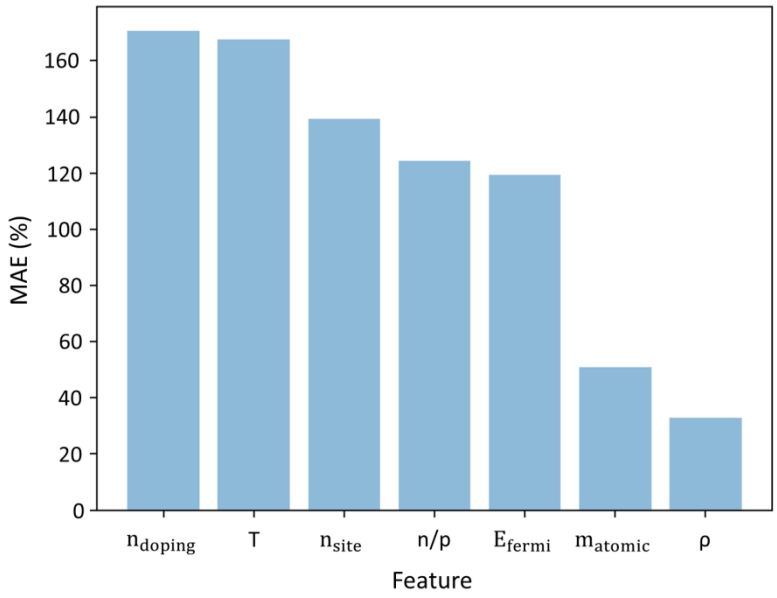

Figure S4. Variation of error for random forest model trained with only 7 features (all crystal structures)

8. Random Forest model (no filters on power factor)

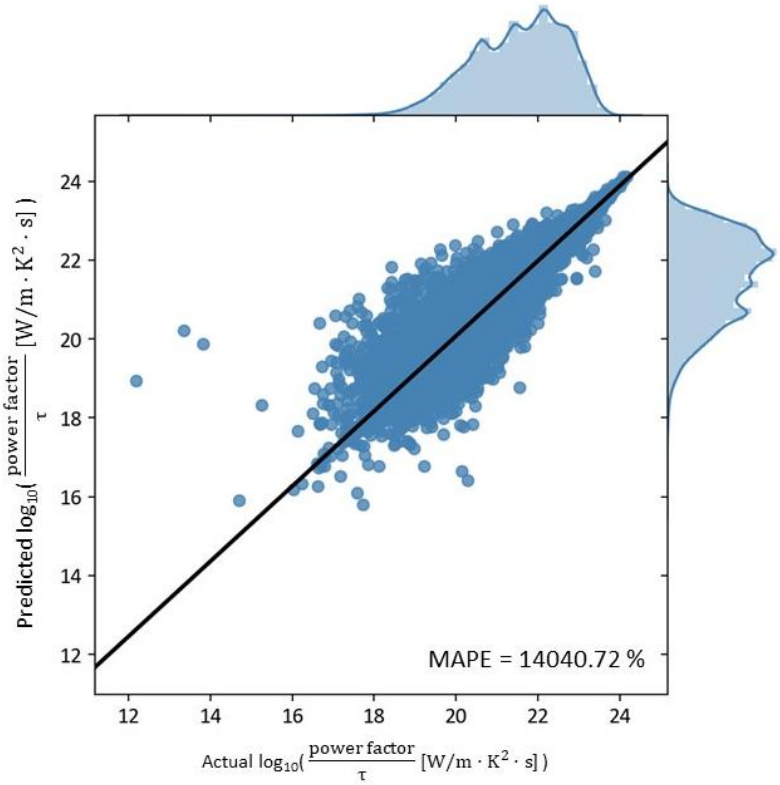

Figure S5. Test results of random forest model trained on all crystal structures (no filters on power factor)

9. Prediction of fermi energy

The following diagram shows the performance of the pre-trained CGCNN model in predicting fermi energy.

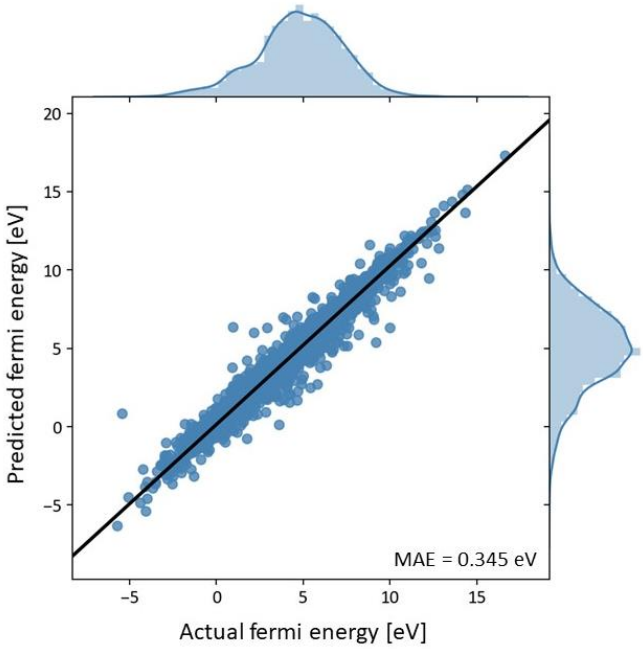

Figure S6. Plot of prediction against actual fermi energy (eV).

As shown in Figure S6, the MAE of the Fermi energy prediction model is 0.345 eV, which is consistent with the performance of the original CGCNN model [Phys. Rev. Lett. 120, 145301, MAE (E_fermi) = 0.363 eV]. This value informs our choice of E_fermi, as displayed in Figure 4 of the main manuscript.

10. Random Forest model (cubic structure with all features)

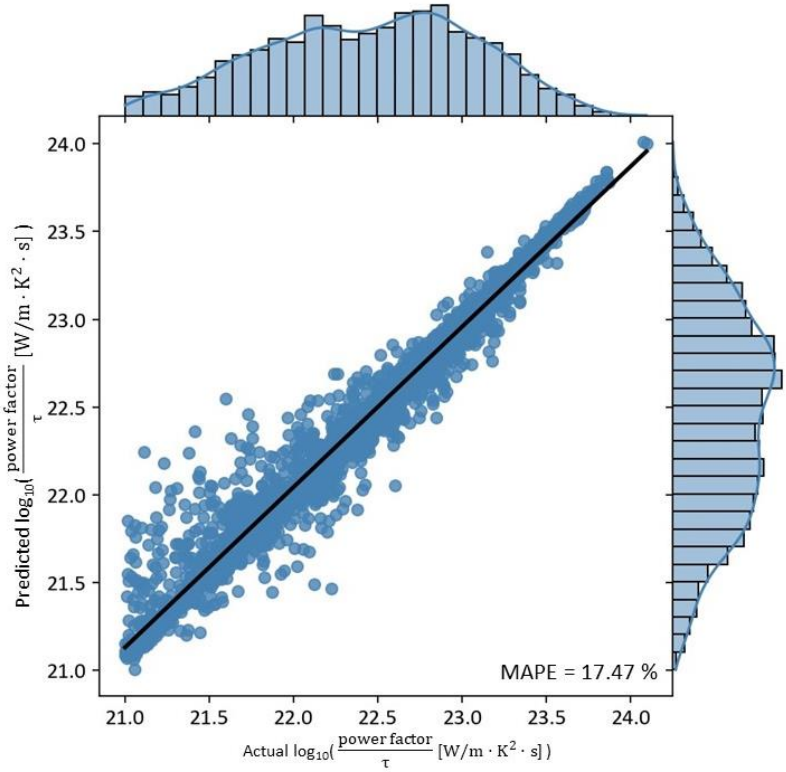

Figure S7. Test results of random forest model trained on cubic structure materials (all features).

11. Random Forest model (different Seebeck coefficient values)

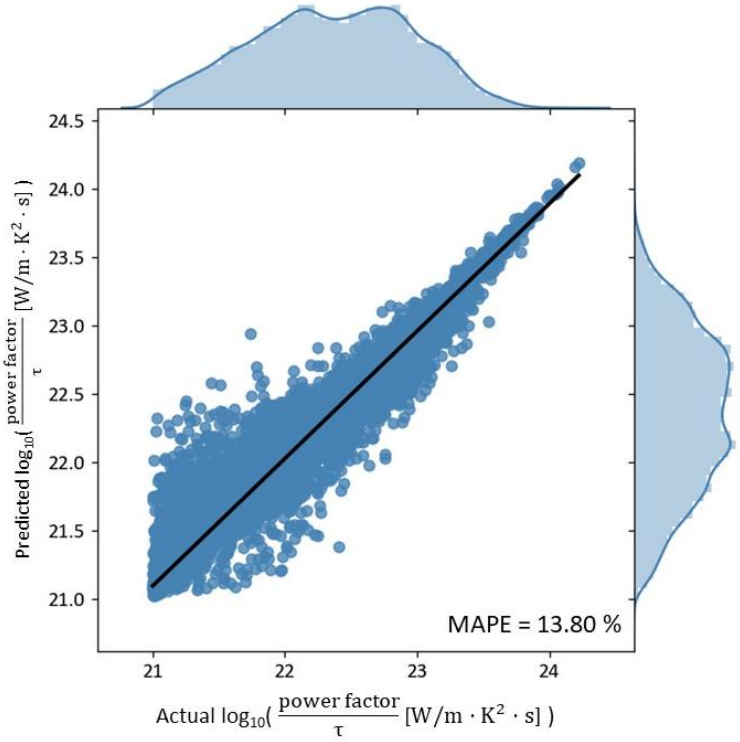

Figure S8. Test results of random forest model trained on all structure materials (different Seebeck coefficient values)

12. Inverse design predictions

The target power factor values were benchmarked using the theoretical power factor values of NbFeSb computed using BoltzTrap BTE package at different physical conditions. The predictions for the different crystal structures can be found in the excel file attached.

Supplementary Table 6: Nomenclature of the letters representing physical conditions

Category	Temperature (K)	Doping concentration (cm^{-3})	n/p type	Target power factor ($mW/m \cdot K^2$)
A	300	1e20	n-type	0.714
B	300	1e19	n-type	0.543
C	300	1e18	n-type	0.17
D	500	1e20	n-type	1.57
E	500	1e19	n-type	0.809
F	500	1e18	n-type	0.197
G	300	1e20	p-type	2.24
H	300	1e19	p-type	0.64
I	300	1e18	p-type	0.128
J	500	1e20	p-type	3.29
K	500	1e19	p-type	0.789
L	500	1e18	p-type	0.084

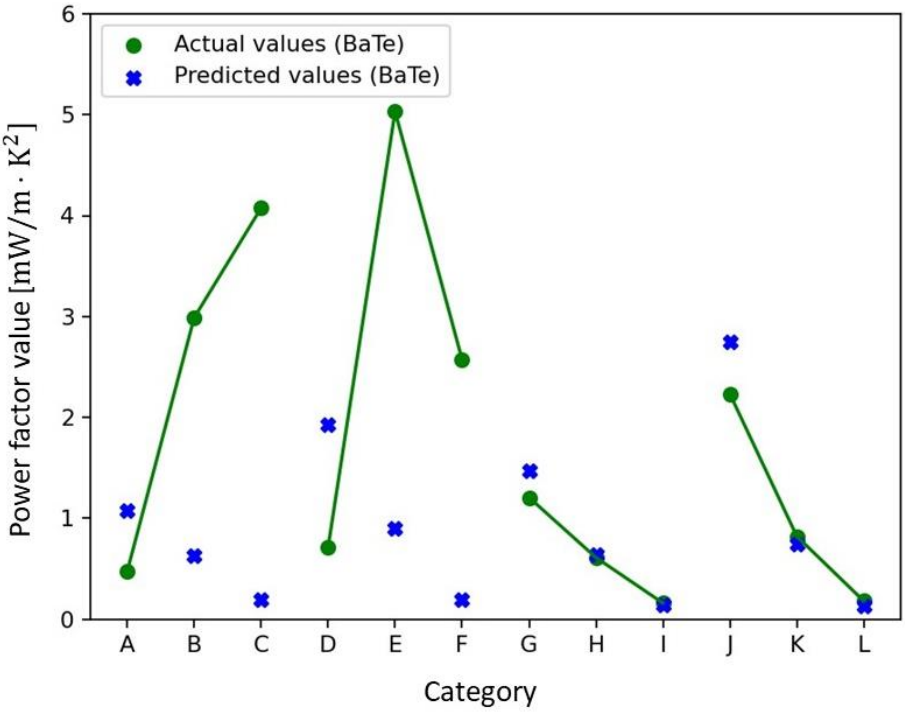

Figure S9: Plot of actual & predicted power factor values (BaTe)

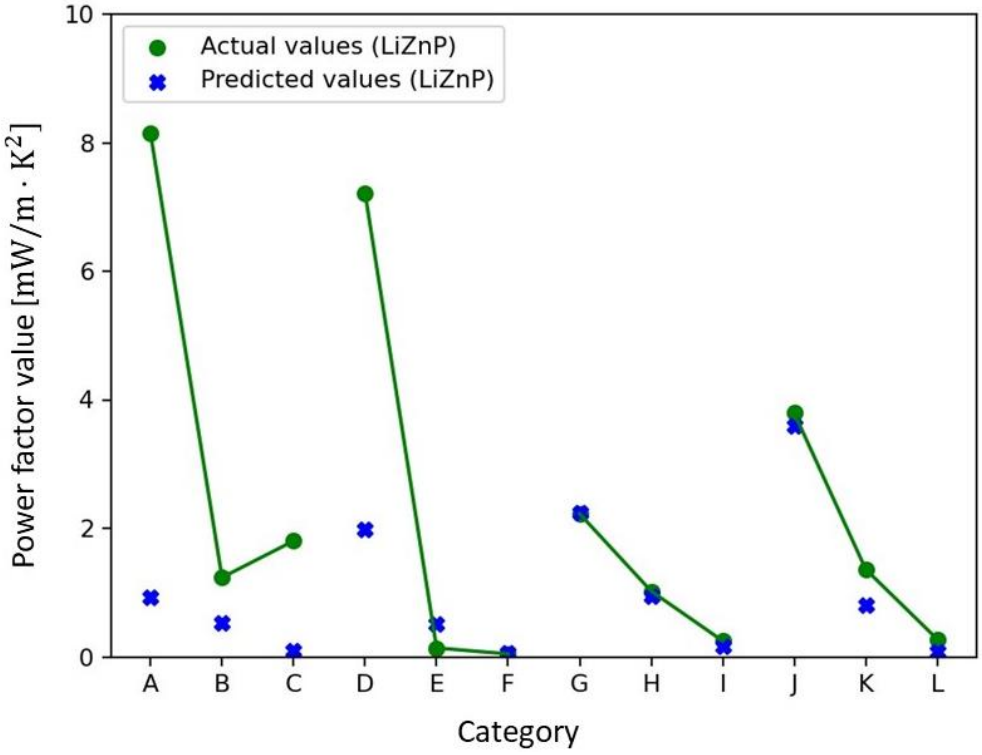

Figure S10: Plot of actual & predicted power factor values (LiZnP)

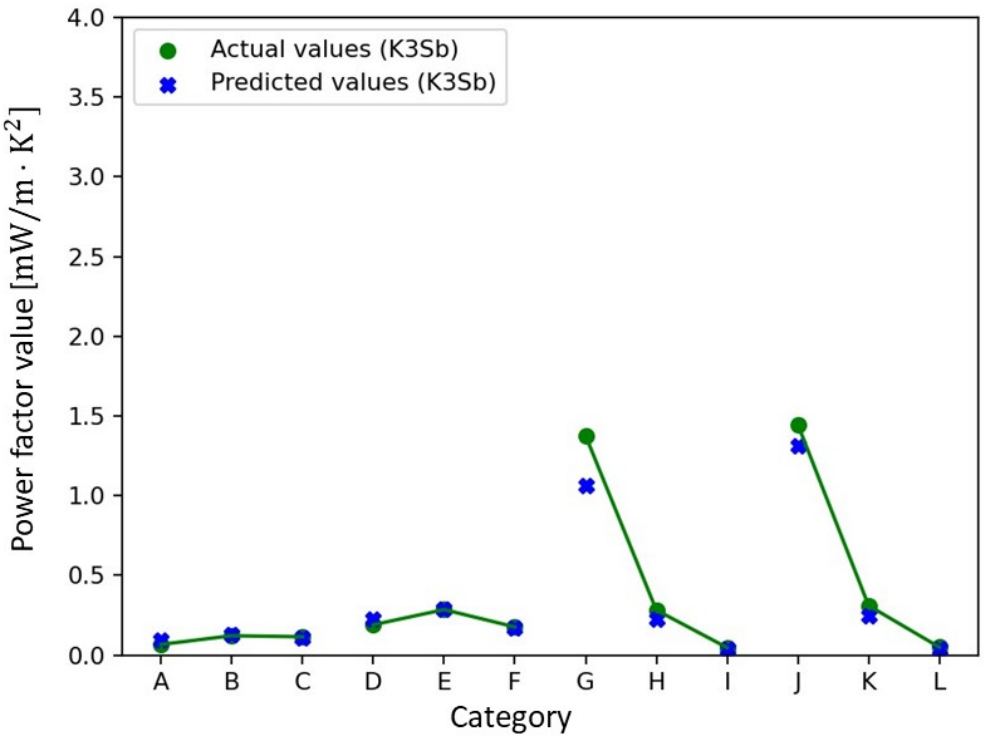

Figure S11: Plot of actual & predicted power factor values (K_3Sb)

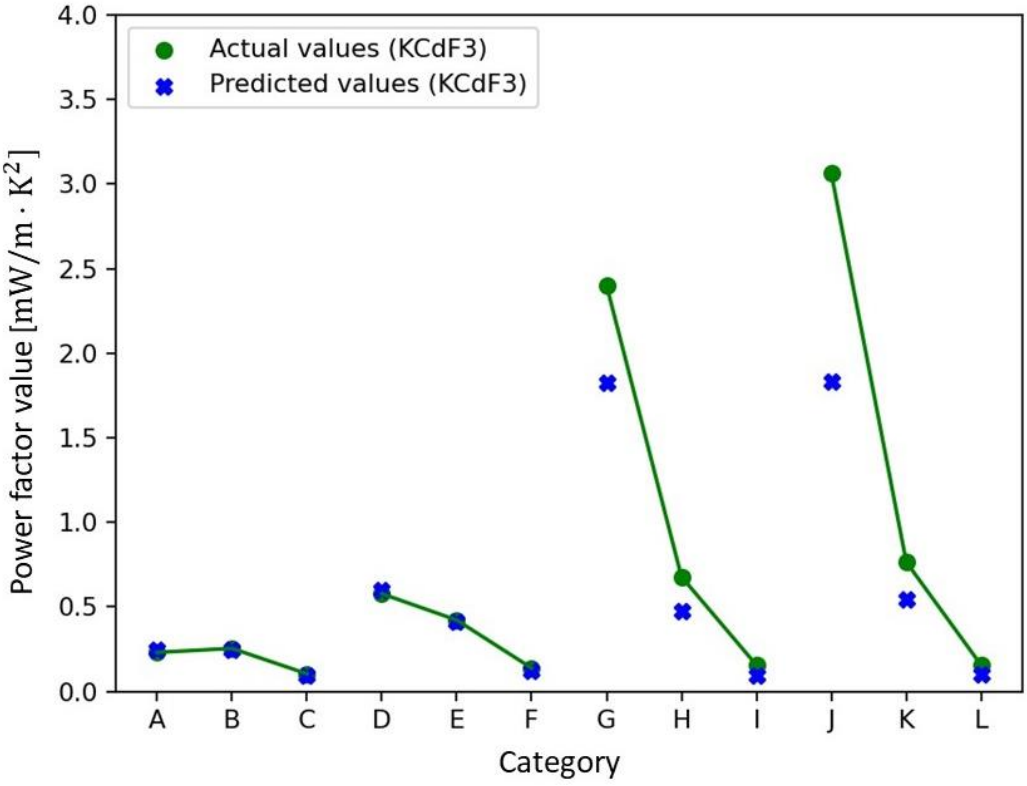

Figure S12: Plot of actual & predicted power factor values ($KCdF_3$)

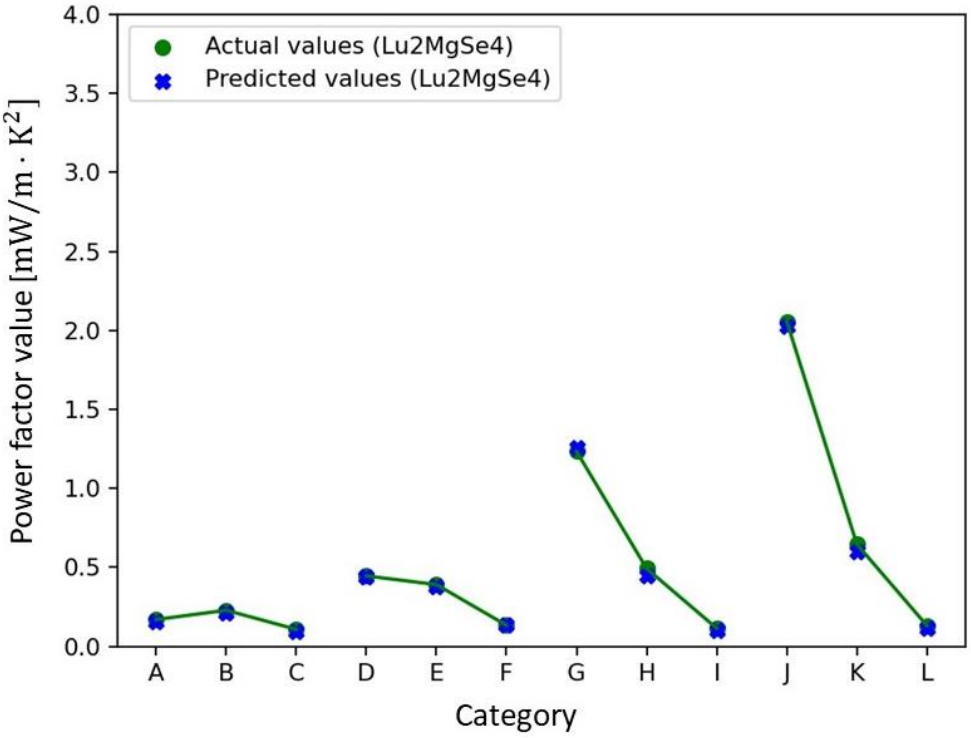

Figure S13: Plot of actual & predicted power factor values (Lu_2MgSe_4)

There is a relatively large mismatch between the predicted vs. actual values for two sets of points (conditions A, B and C) for two materials, BaTe and LiZnP at 300K for n-doping. This indicates that the ML has lower accuracy in this region, since it misses the optimally doped point but Boltztrap captures.

Supplementary Table 7. Candidate list predicted by the algorithm.

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
1	mp-648	Na2S	1	1	1	1	1	1	1	1	1	1	1	1	12	2.4399
2	mp-252	BeTe	1	1	1	1	1	1	1	1	1	1	1	1	12	2.0173
3	mp-961683	LiMgP	1	1	1	1	1	1	1	1	1	1	1	1	12	1.8107
4	mp-971	K2O	1	1	1	1	1	1	1	1	1	1	1	1	12	1.7072
5	mp-1002164	GeC	1	1	1	1	1	1	1	1	1	1	1	1	12	1.6502
6	mp-961685	NaCaAs	1	1	1	1	1	1	1	1	1	1	1	1	12	1.5819
7	mp-961698	LiZnP	1	1	1	1	1	1	1	1	1	1	1	1	12	1.2971
8	mp-961660	TiFeSe	1	1	1	1	1	1	1	1	1	1	1	1	12	0.987
9	mp-961661	ZrSiPd	1	1	1	1	1	1	1	1	1	1	1	1	12	0.7448
10	mp-10623	ThSbRh	1	1	1	1	1	1	1	1	1	1	1	1	12	0.7444
11	mp-1009730	Ca2Sn	1	1	1	1	1	1	1	1	1	1	1	1	12	0.664
12	mp-962057	SrCaSi	1	1	1	1	1	1	1	1	1	1	1	1	12	0.5002
13	mp-1008786	MgTe	1	1	1	1	1	1	1	1	1	1	1	1	12	0.4343
14	mp-2612	GeTe	1	1	1	1	1	1	1	1	1	1	1	1	12	0.3631
15	mp-1018118	TmSbPd	1	1	1	1	1	1	1	1	1	1	1	1	12	0.3569

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
16	mp-865101	NaLi2Bi	1	1	1	1	1	1	1	1	1	1	1	1	12	0.3251
17	mp-1002124	HfC	1	1	1	1	1	1	1	1	1	1	1	1	12	0.2957
18	mp-11390	LiGaSi	1	1	1	1	1	1	1	1	1	1	1	1	12	0.1909
19	mp-962065	SrCaSn	1	1	1	1	1	1	1	1	1	1	1	1	12	0.1582
20	mp-3161	LiAlSi	1	1	1	1	1	1	1	1	1	1	1	1	12	0.1121
21	mp-962064	NaYSn	1	1	1	1	1	1	1	1	1	1	1	1	12	0.1018
22	mp-1000	BaTe	1	1	1	1	1	1	1	1	1	1	1	1	12	1.593
23	mp-1779	YbTe	1	1	1	1	1	1	1	1	1	1	1	1	12	1.4688
24	mp-10182	LiZnP	1	1	1	1	1	1	1	1	1	1	1	1	12	1.3386
25	mp-1394	Rb2O	1	1	1	1	1	1	1	1	1	1	1	1	12	1.3192
26	mp-19717	TePb	1	1	1	1	1	1	1	1	1	1	1	1	12	0.8072
27	mp-2074	Li3Sb	1	1	1	1	1	1	1	1	1	1	1	1	12	0.6961
28	mp-5077	NaLi2Sb	1	1	1	1	1	1	1	1	1	1	1	1	12	0.68
29	mp-149	Si	1	1	1	1	1	1	1	1	1	1	1	1	12	0.6119
30	mp-20351	InP	1	1	1	1	1	1	1	1	1	1	1	1	12	0.4679
31	mp-505297	NbSbRu	1	1	1	1	1	1	1	1	1	1	1	1	12	0.3749
32	mp-30373	RbAu	1	1	1	1	1	1	1	1	1	1	1	1	12	0.3714
33	mp-23222	Li3Bi	1	1	1	1	1	1	1	1	1	1	1	1	12	0.3429
34	mp-1367	Mg2Si	1	1	1	1	1	1	1	1	1	1	1	1	12	0.2169
35	mp-408	Mg2Ge	1	1	1	1	1	1	1	1	1	1	1	1	12	0.1689
36	mp-1876	SnS	1	1	1	1	1	1	1	1	1	1	1	1	12	0.0894
37	mp-631505	BeCuBr	1	1	1	1	1	1	1	1	1	1	1	1	12	0.077
38	mp-5920	LiAlGe	1	1	1	1	1	1	1	1	1	1	1	1	12	0.0564
39	mp-961665	MgScGa	1	1	1	1	1	1	1	1	1	1	1	1	12	0.0554
40	mp-867912	Ba2SnHg	1	1	1	1	1	1	1	1	1	1	1	1	12	0.0498
41	mp-962062	BaSrSn	1	1	1	1	1	1	1	1	1	1	1	1	12	0.0028
42	mp-12719	LiNdSn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
43	mp-961676	HfGePt	1	1	1	1	1	1	1	1	1	1	1	1	12	0
44	mp-865142	DyMgZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
45	mp-631387	SnRuW	1	1	1	1	1	1	1	1	1	1	1	1	12	0
46	mp-1766	TmS	1	1	1	1	1	1	1	1	1	1	1	1	12	0
47	mp-862755	PrCd3	1	1	1	1	1	1	1	1	1	1	1	1	12	0
48	mp-974253	HoErZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
49	mp-712	YCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0
50	mp-631570	BaTaB	1	1	1	1	1	1	1	1	1	1	1	1	12	0
51	mp-631429	ZrCrFe	1	1	1	1	1	1	1	1	1	1	1	1	12	0
52	mp-972	MnSe	1	1	1	1	1	1	1	1	1	1	1	1	12	0
53	mp-1352	ZrN	1	1	1	1	1	1	1	1	1	1	1	1	12	0
54	mp-213	CaPd	1	1	1	1	1	1	1	1	1	1	1	1	12	0
55	mp-972630	SmErZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
56	mp-961725	CrGeRh	1	1	1	1	1	1	1	1	1	1	1	1	12	0
57	mp-631568	AlAgB	1	1	1	1	1	1	1	1	1	1	1	1	12	0
58	mp-2861	CaTl	1	1	1	1	1	1	1	1	1	1	1	1	12	0
59	mp-12718	LiPrSn	1	1	1	1	1	1	1	1	1	1	1	1	12	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
60	mp-1018106	YbBiPt	1	1	1	1	1	1	1	1	1	1	1	1	12	0
61	mp-2459	YbIn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
62	mp-962068	CaMgSn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
63	mp-11566	ScZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
64	mp-2054	TbHg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
65	mp-962078	CaCdSi	1	1	1	1	1	1	1	1	1	1	1	1	12	0
66	mp-861948	LiPm2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0
67	mp-973841	LiHo2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0
68	mp-1008727	Ti2Ge	1	1	1	1	1	1	1	1	1	1	1	1	12	0
69	mp-10902	PrAl	1	1	1	1	1	1	1	1	1	1	1	1	12	0
70	mp-2434	SrTl	1	1	1	1	1	1	1	1	1	1	1	1	12	0
71	mp-983425	Li2PmGe	1	1	1	1	1	1	1	1	1	1	1	1	12	0
72	mp-866017	LiNd2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0
73	mp-631562	SiBAu	1	1	1	1	1	1	1	1	1	1	1	1	12	0
74	mp-975789	PrTmMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
75	mp-11475	TmHg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
76	mp-1014230	TiZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
77	mp-295	HoAs	1	1	1	1	1	1	1	1	1	1	1	1	12	0
78	mp-861955	LiPm2Ge	1	1	1	1	1	1	1	1	1	1	1	1	12	0
79	mp-631521	BaHfMo	1	1	1	1	1	1	1	1	1	1	1	1	12	0
80	mp-12753	GdAl	1	1	1	1	1	1	1	1	1	1	1	1	12	0
81	mp-631471	YScBe	1	1	1	1	1	1	1	1	1	1	1	1	12	0
82	mp-460	PrZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
83	mp-2823	NdP	1	1	1	1	1	1	1	1	1	1	1	1	12	0
84	mp-975822	PrNdZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
85	mp-978512	SmTmMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
86	mp-972456	Sm3V	1	1	1	1	1	1	1	1	1	1	1	1	12	0
87	mp-977551	ErLuMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
88	mp-631544	BaSiB	1	1	1	1	1	1	1	1	1	1	1	1	12	0
89	mp-1156	GaSb	1	1	1	1	1	1	1	1	1	1	1	1	12	0
90	mp-20389	Na2CdPb	1	1	1	1	1	1	1	1	1	1	1	1	12	0
91	mp-2597	InTe	1	1	1	1	1	1	1	1	1	1	1	1	12	0
92	mp-754545	NdO	1	1	1	1	1	1	1	1	1	1	1	1	12	0
93	mp-2796	TmAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
94	mp-865426	YbNdAg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
95	mp-631554	Na2TiAu	1	1	1	1	1	1	1	1	1	1	1	1	12	0
96	mp-631422	CuSiBr	1	1	1	1	1	1	1	1	1	1	1	1	12	0
97	mp-864799	HoLuMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
98	mp-12793	NdAl	1	1	1	1	1	1	1	1	1	1	1	1	12	0
99	mp-976151	PrErMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
100	mp-11469	PrHg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
101	mp-2988	Li2GaRh	1	1	1	1	1	1	1	1	1	1	1	1	12	0
102	mp-2696	MgAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
103	mp-631531	NbBW	1	1	1	1	1	1	1	1	1	1	1	1	12	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
104	mp-24650	YH2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
105	mp-981311	SrTlHg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
106	mp-2857	ScN	1	1	1	1	1	1	1	1	1	1	1	1	12	0
107	mp-862902	PmDyMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
108	mp-2167	DyAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
109	mp-1955	ErCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0
110	mp-23171	PrBi	1	1	1	1	1	1	1	1	1	1	1	1	12	0
111	mp-2249	HoZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
112	mp-972522	SmTmZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
113	mp-976008	NdTmMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
114	mp-1586	NdSb	1	1	1	1	1	1	1	1	1	1	1	1	12	0
115	mp-866015	CaPrZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
116	mp-656	LuS	1	1	1	1	1	1	1	1	1	1	1	1	12	0
117	mp-2302	AsRh2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
118	mp-11313	ZrCd3	1	1	1	1	1	1	1	1	1	1	1	1	12	0
119	mp-30648	LiMg2Ga	1	1	1	1	1	1	1	1	1	1	1	1	12	0
120	mp-972156	TbY3	1	1	1	1	1	1	1	1	1	1	1	1	12	0
121	mp-961645	LiAlGe	1	1	1	1	1	1	1	1	1	1	1	1	12	0
122	mp-983126	HoTmZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
123	mp-2525	PrAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
124	mp-11503	MnZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
125	mp-631317	NaIrPb	1	1	1	1	1	1	1	1	1	1	1	1	12	0
126	mp-862740	Sr2TlCd	1	1	1	1	1	1	1	1	1	1	1	1	12	0
127	mp-979937	Yb3Ru	1	1	1	1	1	1	1	1	1	1	1	1	12	0
128	mp-862964	PmSmMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
129	mp-631314	KTaPt	1	1	1	1	1	1	1	1	1	1	1	1	12	0
130	mp-979417	DyYCd2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
131	mp-999484	YTi	1	1	1	1	1	1	1	1	1	1	1	1	12	0
132	mp-24287	CrH	1	1	1	1	1	1	1	1	1	1	1	1	12	0
133	mp-1837	TbCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0
134	mp-1008753	Ti2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0
135	mp-1009538	PdC	1	1	1	1	1	1	1	1	1	1	1	1	12	0
136	mp-614455	GdCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0
137	mp-978513	SmErMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
138	mp-972640	SmDyZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
139	mp-2343	Mg2Sn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
140	mp-631311	IrOsW	1	1	1	1	1	1	1	1	1	1	1	1	12	0
141	mp-631542	BaZrNi	1	1	1	1	1	1	1	1	1	1	1	1	12	0
142	mp-862937	PmMgZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
143	mp-1009458	NbC	1	1	1	1	1	1	1	1	1	1	1	1	12	0
144	mp-2532	PrTe	1	1	1	1	1	1	1	1	1	1	1	1	12	0
145	mp-1236	NdAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
146	mp-631492	BaScIr	1	1	1	1	1	1	1	1	1	1	1	1	12	0
147	mp-962069	LiAgTe	1	1	1	1	1	1	1	1	1	1	1	1	12	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
148	mp-2470	DyS	1	1	1	1	1	1	1	1	1	1	1	1	12	0
149	mp-2334	DyCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0
150	mp-1008876	MnCoS	1	1	1	1	1	1	1	1	1	1	1	1	12	0
151	mp-2497	GdZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
152	mp-11274	BePd	1	1	1	1	1	1	1	1	1	1	1	1	12	0
153	mp-11563	TiRh	1	1	1	1	1	1	1	1	1	1	1	1	12	0
154	mp-631534	NaSrRe2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
155	mp-631383	MnCrRe	1	1	1	1	1	1	1	1	1	1	1	1	12	0
156	mp-972601	SmLuMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
157	mp-1971	HoCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0
158	mp-631541	BeGeB	1	1	1	1	1	1	1	1	1	1	1	1	12	0
159	mp-861886	LiDyHg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
160	mp-11344	PrO	1	1	1	1	1	1	1	1	1	1	1	1	12	0
161	mp-1008901	MgH2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
162	mp-631337	NaTaNi	1	1	1	1	1	1	1	1	1	1	1	1	12	0
163	mp-836	TbZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
164	mp-865911	YbPmHg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
165	mp-865896	YbPmAg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
166	mp-978823	SmY3	1	1	1	1	1	1	1	1	1	1	1	1	12	0
167	mp-24724	TbH2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
168	mp-1008920	Mn2Ge	1	1	1	1	1	1	1	1	1	1	1	1	12	0
169	mp-2195	LuMg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
170	mp-2268	TbAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
171	mp-631394	CaZrPd	1	1	1	1	1	1	1	1	1	1	1	1	12	0
172	mp-631349	ZnTcMo	1	1	1	1	1	1	1	1	1	1	1	1	12	0
173	mp-631319	LiTiRe	1	1	1	1	1	1	1	1	1	1	1	1	12	0
174	mp-962071	MgScTl	1	1	1	1	1	1	1	1	1	1	1	1	12	0
175	mp-982388	HoTmMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
176	mp-973276	HoLuCd2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
177	mp-34611	ZnAgAs	1	1	1	1	1	1	1	1	1	1	1	1	12	0
178	mp-867222	LiCa2Ir	1	1	1	1	1	1	1	1	1	1	1	1	12	0
179	mp-1001844	HoN	1	1	1	1	1	1	1	1	1	1	1	1	12	0
180	mp-1014219	HfZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
181	mp-22873	SmBi	1	1	1	1	1	1	1	1	1	1	1	1	12	0
182	mp-631440	BiTeIr	1	1	1	1	1	1	1	1	1	1	1	1	12	0
183	mp-542779	GdAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
184	mp-980198	TmLuZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
185	mp-978094	NdHo3	1	1	1	1	1	1	1	1	1	1	1	1	12	0
186	mp-980055	YErMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
187	mp-1240	HoS	1	1	1	1	1	1	1	1	1	1	1	1	12	0
188	mp-961688	VGaPt	1	1	1	1	1	1	1	1	1	1	1	1	12	0
189	mp-861913	LiDy2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0
190	mp-975997	NaLi2Pb	1	1	1	1	1	1	1	1	1	1	1	1	12	0
191	mp-961671	TiGePt	1	1	1	1	1	1	1	1	1	1	1	1	12	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
192	mp-23300	NdBi	1	1	1	1	1	1	1	1	1	1	1	1	12	0
193	mp-979419	Dy3Y	1	1	1	1	1	1	1	1	1	1	1	1	12	0
194	mp-571059	YCd3	1	1	1	1	1	1	1	1	1	1	1	1	12	0
195	mp-866063	NdDyMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
196	mp-2165	SmZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
197	mp-2516	YZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
198	mp-976030	PrHoMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
199	mp-1008911	LiMnAs	1	1	1	1	1	1	1	1	1	1	1	1	12	0
200	mp-862918	PmHoMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
201	mp-31453	NbSbRh	1	1	1	1	1	1	1	1	1	1	1	1	12	0
202	mp-1008	NiHg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
203	mp-570276	ZrZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
204	mp-24289	HPd	1	1	1	1	1	1	1	1	1	1	1	1	12	0
205	mp-20300	EuP	1	1	1	1	1	1	1	1	1	1	1	1	12	0
206	mp-1007776	TlP	1	1	1	1	1	1	1	1	1	1	1	1	12	0
207	mp-866220	CaNdZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
208	mp-2502	TmCd	1	1	1	1	1	1	1	1	1	1	1	1	12	0
209	mp-11467	NdHg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
210	mp-631322	KSnOs	1	1	1	1	1	1	1	1	1	1	1	1	12	0
211	mp-11478	GaAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
212	mp-962061	YMgTl	1	1	1	1	1	1	1	1	1	1	1	1	12	0
213	mp-631382	YMgCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0
214	mp-972997	HoErCd2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
215	mp-2636	GdMg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
216	mp-864598	LiMg2Ag	1	1	1	1	1	1	1	1	1	1	1	1	12	0
217	mp-11240	DyAu	1	1	1	1	1	1	1	1	1	1	1	1	12	0
218	mp-615	YMg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
219	mp-1001837	MoP	1	1	1	1	1	1	1	1	1	1	1	1	12	0
220	mp-972062	YbTmHg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
221	mp-2732	PRh2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
222	mp-126	Pt	1	1	1	1	1	1	1	1	1	1	1	1	12	0
223	mp-631324	HfMnTl	1	1	1	1	1	1	1	1	1	1	1	1	12	0
224	mp-861479	PrYMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
225	mp-760381	CuS	1	1	1	1	1	1	1	1	1	1	1	1	12	0
226	mp-437	MgAu	1	1	1	1	1	1	1	1	1	1	1	1	12	0
227	mp-1009663	ReC	1	1	1	1	1	1	1	1	1	1	1	1	12	0
228	mp-631482	BiMoRh	1	1	1	1	1	1	1	1	1	1	1	1	12	0
229	mp-11279	TiBe	1	1	1	1	1	1	1	1	1	1	1	1	12	0
230	mp-2474	YAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
231	mp-976426	LiLuHg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
232	mp-961680	NbAlPt	1	1	1	1	1	1	1	1	1	1	1	1	12	0
233	mp-867873	LiTm2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0
234	mp-631395	CaTaTc	1	1	1	1	1	1	1	1	1	1	1	1	12	0
235	mp-980942	YTmMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
236	mp-11576	YbTl	1	1	1	1	1	1	1	1	1	1	1	1	12	0
237	mp-631484	TaTiAl	1	1	1	1	1	1	1	1	1	1	1	1	12	0
238	mp-961669	NbGaPt	1	1	1	1	1	1	1	1	1	1	1	1	12	0
239	mp-1013549	Ba3BiN	1	1	1	1	1	1	1	1	1	1	1	1	12	0
240	mp-973232	NdTm3	1	1	1	1	1	1	1	1	1	1	1	1	12	0
241	mp-1660	ErZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
242	mp-2778	HoAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
243	mp-976143	PrDyZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
244	mp-980082	YHo3	1	1	1	1	1	1	1	1	1	1	1	1	12	0
245	mp-975886	PrSmZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
246	mp-975972	PrLuMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
247	mp-24152	HoH2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
248	mp-631546	TlCoBi	1	1	1	1	1	1	1	1	1	1	1	1	12	0
249	mp-2475	SmAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
250	mp-1211	ScCd	1	1	1	1	1	1	1	1	1	1	1	1	12	0
251	mp-1174	MgSc	1	1	1	1	1	1	1	1	1	1	1	1	12	0
252	mp-30779	SmMg3	1	1	1	1	1	1	1	1	1	1	1	1	12	0
253	mp-2283	ZrCo	1	1	1	1	1	1	1	1	1	1	1	1	12	0
254	mp-978514	SmTm3	1	1	1	1	1	1	1	1	1	1	1	1	12	0
255	mp-631381	TeRuSe	1	1	1	1	1	1	1	1	1	1	1	1	12	0
256	mp-867149	Sr2CdSn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
257	mp-1008726	Ti2Ga	1	1	1	1	1	1	1	1	1	1	1	1	12	0
258	mp-12586	SmCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0
259	mp-20724	Mg2Pb	1	1	1	1	1	1	1	1	1	1	1	1	12	0
260	mp-865210	TmLuMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
261	mp-631373	TiVW	1	1	1	1	1	1	1	1	1	1	1	1	12	0
262	mp-862555	LiY2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0
263	mp-639675	EuCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0
264	mp-866158	YLuMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
265	mp-631479	CaHfBe	1	1	1	1	1	1	1	1	1	1	1	1	12	0
266	mp-1785	PrSb	1	1	1	1	1	1	1	1	1	1	1	1	12	0
267	mp-976032	PrHoZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
268	mp-867159	SmDyMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
269	mp-2640	TbAs	1	1	1	1	1	1	1	1	1	1	1	1	12	0
270	mp-973058	LiLu2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0
271	mp-974517	NdErMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
272	mp-631365	TeRuPb	1	1	1	1	1	1	1	1	1	1	1	1	12	0
273	mp-1432	Be2B	1	1	1	1	1	1	1	1	1	1	1	1	12	0
274	mp-973333	HoLuZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
275	mp-862493	LiEr2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0
276	mp-631552	SrBiB	1	1	1	1	1	1	1	1	1	1	1	1	12	0
277	mp-11237	ScAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
278	mp-7381	TbMg3	1	1	1	1	1	1	1	1	1	1	1	1	12	0
279	mp-864630	LiMg2Hg	1	1	1	1	1	1	1	1	1	1	1	1	12	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
280	mp-976147	PrEr3	1	1	1	1	1	1	1	1	1	1	1	1	12	0
281	mp-866191	Li2YbSi	1	1	1	1	1	1	1	1	1	1	1	1	12	0
282	mp-985	TmCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0
283	mp-974527	NdSmZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
284	mp-973759	Lu2MgCd	1	1	1	1	1	1	1	1	1	1	1	1	12	0
285	mp-975848	PrNdMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
286	mp-11221	SmAl	1	1	1	1	1	1	1	1	1	1	1	1	12	0
287	mp-976129	PrErZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
288	mp-2303	DyZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
289	mp-961726	NbGeRh	1	1	1	1	1	1	1	1	1	1	1	1	12	0
290	mp-754940	Ba3SiO	1	1	1	1	1	1	1	1	1	1	1	1	12	0
291	mp-31168	Li2AlAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
292	mp-867163	Sr2AgPt	1	1	1	1	1	1	1	1	1	1	1	1	12	0
293	mp-1053	NdZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
294	mp-631335	MgTaZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0
295	mp-961699	NaMgP	1	1	1	1	1	1	1	1	1	1	1	1	12	0
296	mp-12087	Cu2S	1	1	1	1	1	1	1	1	1	1	1	1	12	0
297	mp-631506	SrZrCo	1	1	1	1	1	1	1	1	1	1	1	1	12	0
298	mp-867158	SmCd3	1	1	1	1	1	1	1	1	1	1	1	1	12	0
299	mp-1007819	CoW	1	1	1	1	1	1	1	1	1	1	1	1	12	0
300	mp-1009135	MnP	1	1	1	1	1	1	1	1	1	1	1	1	12	0
301	mp-867130	SmHoMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
302	mp-24192	ErH2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
303	mp-934	LiTl	1	1	1	1	1	1	1	1	1	1	1	1	12	0
304	mp-710	SmP	1	1	1	1	1	1	1	1	1	1	1	1	12	0
305	mp-975880	PrSmMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
306	mp-2621	ErAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0
307	mp-2724	TbSb	1	1	1	1	1	1	1	1	1	1	1	1	12	0
308	mp-631410	CdNiP	1	1	1	1	1	1	1	1	1	1	1	1	12	0
309	mp-24237	ScH2	1	1	1	1	1	1	1	1	1	1	1	1	12	0
310	mp-631269	LiIrRh	1	1	1	1	1	1	1	1	1	1	1	1	12	0
311	mp-973060	MgCr	1	1	1	1	1	1	1	1	1	1	1	1	12	0
312	mp-8062	SiC	1	1	1	1	1	1	0	1	1	1	1	1	11	1.3704
313	mp-961711	ZrSiPt	1	1	1	1	1	1	0	1	1	1	1	1	11	1.3298
314	mp-1569	Be2C	1	1	1	1	1	1	0	1	1	1	1	1	11	1.1637
315	mp-961649	ZrFeTe	1	1	1	1	1	1	0	1	1	1	1	1	11	1.1558
316	mp-961706	TiSiPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0.993
317	mp-1008680	TiGePt	1	1	1	1	1	1	0	1	1	1	1	1	11	0.8819
318	mp-997618	BSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0.7513
319	mp-961774	BaNaSb	1	1	0	1	1	1	1	1	1	1	1	1	11	0.7372
320	mp-961657	YNiP	1	1	1	1	1	1	0	1	1	1	1	1	11	0.7214
321	mp-19886	ThSnPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0.6738
322	mp-7173	ScSbPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0.6441
323	mp-1009820	SnC	1	1	1	1	1	1	0	1	1	1	1	1	11	0.6257

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
324	mp-961675	ScNiP	1	1	1	1	1	1	0	1	1	1	1	1	11	0.5921
325	mp-9437	NbFeSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0.5138
326	mp-961693	ZrInAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0.4532
327	mp-1009813	SiSn	1	1	1	1	1	1	1	1	1	0	1	1	11	0.4113
328	mp-866132	Na2TlSb	1	1	0	1	1	1	1	1	1	1	1	1	11	0.3844
329	mp-961663	SrTePd	1	1	1	1	1	1	0	1	1	1	1	1	11	0.3215
330	mp-961697	ScGeAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0.2804
331	mp-1315	MgS	1	1	1	1	1	1	0	1	1	1	1	1	11	2.7628
332	mp-1550	AlP	1	1	1	1	1	1	1	1	1	0	1	1	11	1.6302
333	mp-2490	GaP	1	1	1	1	1	1	0	1	1	1	1	1	11	1.5928
334	mp-36111	LiMgP	1	1	0	1	1	1	1	1	1	1	1	1	11	1.5391
335	mp-1479	BP	1	1	1	1	1	0	1	1	1	1	1	1	11	1.2435
336	mp-2624	AlSb	1	1	1	1	1	1	1	1	1	0	1	1	11	1.2273
337	mp-30847	TiSnPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0.7908
338	mp-31454	TaSbRu	1	1	1	1	1	1	0	1	1	1	1	1	11	0.6669
339	mp-11836	ErSbPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0.2096
340	mp-2114	YN	1	1	1	1	1	1	0	1	1	1	1	1	11	0.151
341	mp-1008858	NdBiPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0.1051
342	mp-13305	SmSnAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0.097
343	mp-631550	CaBiB	1	1	1	1	1	1	0	1	1	1	1	1	11	0.0821
344	mp-961653	FeSiW	1	1	1	1	1	1	0	1	1	1	1	1	11	0.065
345	mp-1883	SnTe	1	1	1	1	1	1	0	1	1	1	1	1	11	0.0428
346	mp-30390	HoSnAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0.0235
347	mp-5640	ErSnAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0.0072
348	mp-631466	KSc2Co	1	1	0	1	1	1	1	1	1	1	1	1	11	0
349	mp-1009459	NbC	1	1	1	1	1	1	0	1	1	1	1	1	11	0
350	mp-971702	YbNdCd2	1	1	0	1	1	1	1	1	1	1	1	1	11	0
351	mp-124	Ag	1	1	1	1	1	1	0	1	1	1	1	1	11	0
352	mp-1546	DyMg3	1	1	0	1	1	1	1	1	1	1	1	1	11	0
353	mp-10624	USbRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0
354	mp-12599	PrTl	1	1	1	1	1	1	0	1	1	1	1	1	11	0
355	mp-1502	Al2Pt	1	1	1	1	1	1	0	1	1	1	1	1	11	0
356	mp-1006884	CoMo	1	1	1	1	1	1	0	1	1	1	1	1	11	0
357	mp-75	Nb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
358	mp-961721	HfBiRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0
359	mp-961696	MnCoSi	1	1	1	1	1	1	0	1	1	1	1	1	11	0
360	mp-428	PrMg3	1	1	0	1	1	1	1	1	1	1	1	1	11	0
361	mp-1009878	ZrC	1	1	1	1	1	1	0	1	1	1	1	1	11	0
362	mp-961694	TiNiGe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
363	mp-22682	In2Pt	1	1	1	1	1	1	0	1	1	1	1	1	11	0
364	mp-4846	MnSbRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0
365	mp-863705	Pm2MgGa	1	1	0	1	1	1	1	1	1	1	1	1	11	0
366	mp-961690	VGaNi	1	1	1	1	1	1	0	1	1	1	1	1	11	0
367	mp-631353	MnRePt	1	1	1	1	1	1	0	1	1	1	1	1	11	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
368	mp-770	DyCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
369	mp-5549	MgSnAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
370	mp-30479	Ca3Pb	1	1	0	1	1	1	1	1	1	1	1	1	11	0
371	mp-961720	ZrAsRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0
372	mp-1009494	NpN	1	1	1	1	1	0	1	1	1	1	1	1	11	0
373	mp-1453	NdSe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
374	mp-11843	DyAl	1	1	1	1	1	1	0	1	1	1	1	1	11	0
375	mp-1018132	AlBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0
376	mp-2050	HoSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
377	mp-23245	ErBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0
378	mp-1406	MnTe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
379	mp-961681	ZrGePt	1	1	1	1	1	1	0	1	1	1	1	1	11	0
380	mp-1008689	Ti2Si	1	1	1	1	1	1	0	1	1	1	1	1	11	0
381	mp-1001785	MoP	1	1	1	1	1	1	0	1	1	1	1	1	11	0
382	mp-631379	ZnCuMo	1	1	1	1	1	1	0	1	1	1	1	1	11	0
383	mp-31456	HfSbRu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
384	mp-2316	TmZn	1	1	1	1	1	1	0	1	1	1	1	1	11	0
385	mp-961709	ZrPtPb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
386	mp-867145	LiHo2Ga	1	1	0	1	1	1	1	1	1	1	1	1	11	0
387	mp-961702	LaSbPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0
388	mp-436	SmRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0
389	mp-30377	ErPbAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
390	mp-11516	NbRu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
391	mp-1408	MgHg	1	1	1	1	1	1	0	1	1	1	1	1	11	0
392	mp-1013545	Ca3BiAs	1	1	1	1	1	0	1	1	1	1	1	1	11	0
393	mp-2563	CeSe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
394	mp-1001834	HfN	1	1	1	1	1	1	0	1	1	1	1	1	11	0
395	mp-866180	Li2YbPb	1	1	0	1	1	1	1	1	1	1	1	1	11	0
396	mp-2210	ZrCu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
397	mp-776	LaCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
398	mp-2163	HoRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0
399	mp-1006883	CoNi	1	1	1	1	1	1	0	1	1	1	1	1	11	0
400	mp-979989	Yb2AgPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
401	mp-1009132	HoBiPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
402	mp-1002165	GeC	1	1	1	1	1	1	0	1	1	1	1	1	11	0
403	mp-631555	MnVNi	1	1	1	1	1	1	0	1	1	1	1	1	11	0
404	mp-170	HoCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
405	mp-1009731	ReC	1	1	1	1	1	1	0	1	1	1	1	1	11	0
406	mp-621592	YPbAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
407	mp-24096	NdH2	1	1	1	1	1	1	0	1	1	1	1	1	11	0
408	mp-12564	LiSbAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
409	mp-1925	ZrS	1	1	1	1	1	1	0	1	1	1	1	1	11	0
410	mp-865579	Li2ErIn	1	1	0	1	1	1	1	1	1	1	1	1	11	0
411	mp-29242	Ba3PbO	1	1	1	1	1	1	0	1	1	1	1	1	11	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
412	mp-510403	GdSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
413	mp-542065	CdAgSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
414	mp-1738	SmAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0
415	mp-11471	ScHg	1	1	1	1	1	1	0	1	1	1	1	1	11	0
416	mp-834	ThN	1	1	1	1	1	1	0	1	1	1	1	1	11	0
417	mp-961679	TaAlPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0
418	mp-721	TbCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
419	mp-1176	TbTe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
420	mp-1018029	CuPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
421	mp-232	DyRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0
422	mp-13308	HoGeAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
423	mp-631371	TlCuIr	1	1	1	1	1	1	0	1	1	1	1	1	11	0
424	mp-1164	ThC	1	1	1	1	1	1	0	1	1	1	1	1	11	0
425	mp-961710	VSiPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0
426	mp-1059	NdCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
427	mp-22907	DyBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0
428	mp-2052	ScAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0
429	mp-568398	CaBiAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
430	mp-865882	Li2SmIn	1	1	0	1	1	1	1	1	1	1	1	1	11	0
431	mp-631405	ZrTcCl	1	1	1	1	1	1	0	1	1	1	1	1	11	0
432	mp-20952	TiNiSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
433	mp-631754	ReSnGe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
434	mp-1031	GdCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
435	mp-2014	DyP	1	1	1	1	1	1	0	1	1	1	1	1	11	0
436	mp-631294	HfMoSe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
437	mp-30413	TbPbAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
438	mp-30466	YbBiPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
439	mp-568931	YbNiSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
440	mp-1009822	SnC	1	1	1	1	1	1	0	1	1	1	1	1	11	0
441	mp-2444	GaRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0
442	mp-1008702	Ti2In	1	1	1	1	1	1	0	1	1	1	1	1	11	0
443	mp-979073	TmMg2Sc	1	1	0	1	1	1	1	1	1	1	1	1	11	0
444	mp-978528	SmMg2Sc	1	1	0	1	1	1	1	1	1	1	1	1	11	0
445	mp-998890	Cu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
446	mp-22866	HoBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0
447	mp-915	YCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
448	mp-2443	DyHg	1	1	1	1	1	1	0	1	1	1	1	1	11	0
449	mp-13	Fe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
450	mp-631320	TcIrOs	1	1	1	1	1	1	0	1	1	1	1	1	11	0
451	mp-24092	GdH2	1	1	1	1	1	1	0	1	1	1	1	1	11	0
452	mp-933	YAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0
453	mp-574283	GdTe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
454	mp-2082	PIr2	1	1	1	1	1	1	0	1	1	1	1	1	11	0
455	mp-1013733	Ca3BiSb	1	1	1	1	1	0	1	1	1	1	1	1	11	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
456	mp-11242	DyPbAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
457	mp-10755	TiFeSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
458	mp-24727	TmH2	1	1	1	1	1	1	0	1	1	1	1	1	11	0
459	mp-961716	VSnPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0
460	mp-510374	GdAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0
461	mp-11286	CaHg	1	1	1	1	1	1	0	1	1	1	1	1	11	0
462	mp-1018162	CeBiPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0
463	mp-631366	TcSnSe	1	1	1	1	1	0	1	1	1	1	1	1	11	0
464	mp-910	NbC	1	1	1	1	1	1	0	1	1	1	1	1	11	0
465	mp-865661	YbMgCd2	1	1	0	1	1	1	1	1	1	1	1	1	11	0
466	mp-961666	MnNbAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0
467	mp-5318	MnCoSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
468	mp-568466	LiInSn	1	1	1	1	1	1	0	1	1	1	1	1	11	0
469	mp-20263	CaIn	1	1	1	1	1	1	0	1	1	1	1	1	11	0
470	mp-1092	HoHg	1	1	1	1	1	1	0	1	1	1	1	1	11	0
471	mp-862681	ErMg3	1	1	0	1	1	1	1	1	1	1	1	1	11	0
472	mp-1008631	VCoTe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
473	mp-961658	VFeSe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
474	mp-978273	Mg3Cd	1	1	0	1	1	1	1	1	1	1	1	1	11	0
475	mp-631497	BeInBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0
476	mp-11256	ScAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
477	mp-631288	LaGeOs	1	1	1	1	1	1	0	1	1	1	1	1	11	0
478	mp-572	SmCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
479	mp-20415	GdPbAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
480	mp-2795	ZrC	1	1	1	1	1	1	0	1	1	1	1	1	11	0
481	mp-2637	YSe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
482	mp-1007	DySb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
483	mp-102	Co	1	1	1	1	1	1	0	1	1	1	1	1	11	0
484	mp-11255	PrAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
485	mp-22921	TbBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0
486	mp-2781	ScPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
487	mp-961719	HfAsRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0
488	mp-631526	SiBPb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
489	mp-1006150	Eu3Re	1	1	0	1	1	1	1	1	1	1	1	1	11	0
490	mp-129	Mo	1	1	1	1	1	1	0	1	1	1	1	1	11	0
491	mp-2602	NdAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0
492	mp-23241	YBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0
493	mp-24147	AcH2	1	1	1	1	1	1	0	1	1	1	1	1	11	0
494	mp-2281	SmSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
495	mp-2642	CdAg	1	1	1	1	1	1	0	1	1	1	1	1	11	0
496	mp-1008928	EuSe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
497	mp-1902	MnPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
498	mp-571405	NdTl	1	1	1	1	1	1	0	1	1	1	1	1	11	0
499	mp-191	YRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
500	mp-21005	GdIn	1	1	1	1	1	1	0	1	1	1	1	1	11	0
501	mp-510401	GdP	1	1	1	1	1	1	0	1	1	1	1	1	11	0
502	mp-133	Sb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
503	mp-1008734	ThH2	1	1	1	1	1	1	0	1	1	1	1	1	11	0
504	mp-1623	ErS	1	1	1	1	1	1	0	1	1	1	1	1	11	0
505	mp-30	Cu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
506	mp-2399	YHg	1	1	1	1	1	1	0	1	1	1	1	1	11	0
507	mp-12594	TiIr	1	1	1	1	1	1	0	1	1	1	1	1	11	0
508	mp-377	LuRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0
509	mp-1009582	NiC	1	1	1	1	1	1	0	1	1	1	1	1	11	0
510	mp-1009222	MnTe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
511	mp-865580	Li2DyIn	1	1	0	1	1	1	1	1	1	1	1	1	11	0
512	mp-24151	DyH2	1	1	1	1	1	1	0	1	1	1	1	1	11	0
513	mp-24288	LuH2	1	1	1	1	1	1	0	1	1	1	1	1	11	0
514	mp-1008650	CeSe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
515	mp-961677	TaGaPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0
516	mp-20298	SmIn	1	1	1	1	1	1	0	1	1	1	1	1	11	0
517	mp-631464	KBePt	1	0	1	1	1	1	1	1	1	1	1	1	11	0
518	mp-867	ErCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
519	mp-20012	InSb	1	1	1	1	1	1	1	1	1	0	1	1	11	0
520	mp-542583	EuTe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
521	mp-1009543	DyBiPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
522	mp-1787	NdMg3	1	1	0	1	1	1	1	1	1	1	1	1	11	0
523	mp-11561	TbRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0
524	mp-1008624	YBiPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
525	mp-15694	PaAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0
526	mp-506	MgPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
527	mp-11495	LuRu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
528	mp-631538	NiBiB	1	1	1	1	1	1	0	1	1	1	1	1	11	0
529	mp-601	PrP	1	1	1	1	1	1	0	1	1	1	1	1	11	0
530	mp-1018119	VCoSn	1	1	1	1	1	1	0	1	1	1	1	1	11	0
531	mp-12674	MnAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
532	mp-981545	Ho3Zr	1	1	0	1	1	1	1	1	1	1	1	1	11	0
533	mp-631254	KMnRu	1	0	1	1	1	1	1	1	1	1	1	1	11	0
534	mp-984713	Dy3Ga	1	1	0	1	1	1	1	1	1	1	1	1	11	0
535	mp-2090	FeCo	1	1	1	1	1	1	0	1	1	1	1	1	11	0
536	mp-866196	Li2PrIn	1	1	0	1	1	1	1	1	1	1	1	1	11	0
537	mp-866199	AcAg	1	1	1	1	1	1	0	1	1	1	1	1	11	0
538	mp-961718	TiAsRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0
539	mp-2520	TmSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
540	mp-631421	CrGaTe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
541	mp-11374	DyTl	1	1	1	1	1	1	0	1	1	1	1	1	11	0
542	mp-631561	ZrAgMo	1	1	1	1	1	1	0	1	1	1	1	1	11	0
543	mp-2350	LaS	1	1	1	1	1	1	0	1	1	1	1	1	11	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
544	mp-862930	Li2PmIn	1	1	0	1	1	1	1	1	1	1	1	1	11	0
545	mp-331	ScAl	1	1	1	1	1	1	0	1	1	1	1	1	11	0
546	mp-8640	Hf	1	1	1	1	1	1	0	1	1	1	1	1	11	0
547	mp-2191	ErSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
548	mp-1093	ThGe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
549	mp-2627	DyAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0
550	mp-24658	SmH2	1	1	1	1	1	1	0	1	1	1	1	1	11	0
551	mp-117	Sn	1	1	1	1	1	1	1	1	1	0	1	1	11	0
552	mp-646	PrCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
553	mp-2381	ErRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0
554	mp-10622	PrAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0
555	mp-492	TiN	1	1	1	1	1	1	0	1	1	1	1	1	11	0
556	mp-20997	InNi	1	1	1	1	1	1	0	1	1	1	1	1	11	0
557	mp-2065	MnS	1	1	1	1	1	1	0	1	1	1	1	1	11	0
558	mp-979950	AcYbMg2	1	1	0	1	1	1	1	1	1	1	1	1	11	0
559	mp-542569	AlRu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
560	mp-1008642	UC2	1	1	1	1	1	1	0	1	1	1	1	1	11	0
561	mp-30389	HoPbAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
562	mp-875	AlOs	1	1	1	1	1	1	0	1	1	1	1	1	11	0
563	mp-1534	YS	1	1	1	1	1	1	0	1	1	1	1	1	11	0
564	mp-6933	MnN	1	1	1	1	1	1	0	1	1	1	1	1	11	0
565	mp-1002206	SiC	1	1	1	1	1	1	0	1	1	1	1	1	11	0
566	mp-631302	ScVFe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
567	mp-2212	ScCo	1	1	1	1	1	1	0	1	1	1	1	1	11	0
568	mp-24154	NbH2	1	1	1	1	1	1	0	1	1	1	1	1	11	0
569	mp-866181	Li2NdIn	1	1	0	1	1	1	1	1	1	1	1	1	11	0
570	mp-23234	TmBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0
571	mp-1009128	MnN	1	1	1	1	1	1	0	1	1	1	1	1	11	0
572	mp-11621	ZnNiSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
573	mp-364	AlRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0
574	mp-13496	ZrPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
575	mp-570632	ScBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0
576	mp-1169	ScCu	1	1	1	1	1	1	0	1	1	1	1	1	11	0
577	mp-645	TbP	1	1	1	1	1	1	0	1	1	1	1	1	11	0
578	mp-570	NdTe	1	1	1	1	1	1	0	1	1	1	1	1	11	0
579	mp-631364	TaOsPb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
580	mp-5676	MnSbPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0
581	mp-1941	GaNi	1	1	1	1	1	1	0	1	1	1	1	1	11	0
582	mp-215	YSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
583	mp-631572	GaReAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0
584	mp-11564	TmRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0
585	mp-977386	LiLu2Tc	1	1	0	1	1	1	1	1	1	1	1	1	11	0
586	mp-1008903	MgAgSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0
587	mp-2379	CoSi2	1	1	1	1	1	1	0	1	1	1	1	1	11	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
588	mp-631342	MnTcPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0
589	mp-30848	USnPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0
590	mp-515	TmTl	1	1	1	1	1	1	0	1	1	1	1	1	11	0
591	mp-2828	HfN	1	1	1	1	1	1	0	1	1	1	1	1	11	0
592	mp-994	YP	1	1	1	1	1	1	0	1	1	1	1	1	11	0
593	mp-961684	LiCaAs	1	1	1	1	1	1	0	1	1	0	1	1	10	1.8116
594	mp-961648	KBaP	1	1	1	1	1	1	0	1	1	0	1	1	10	1.1622
595	mp-5967	TiCoSb	1	1	1	1	1	1	0	1	1	0	1	1	10	1.052
596	mp-961713	ZrSnPt	1	1	1	1	1	1	0	1	1	0	1	1	10	0.9628
597	mp-961678	ScCoTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0.8678
598	mp-962072	KYSn	1	0	0	1	1	1	1	1	1	1	1	1	10	0.7193
599	mp-1009733	Ca2Si	1	0	0	1	1	1	1	1	1	1	1	1	10	0.5549
600	mp-961703	NaLiPt	1	1	1	1	1	1	0	1	1	0	1	1	10	0.5526
601	mp-9124	LiZnAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0.5475
602	mp-924129	ZrNiSn	1	1	1	1	1	1	0	1	1	0	1	1	10	0.4954
603	mp-1009894	ZrC	1	1	1	1	1	1	0	1	1	0	1	1	10	0.484
604	mp-961682	TiSnPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0.4691
605	mp-961646	TiTeOs	1	1	1	1	1	1	0	1	1	0	1	1	10	0.4298
606	mp-924128	HfNiSn	1	1	1	1	1	1	0	1	1	0	1	1	10	0.3854
607	mp-570213	LiMgBi	1	0	0	1	1	1	1	1	1	1	1	1	10	0.3619
608	mp-567636	VFeSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0.3487
609	mp-22786	ThNiSn	1	1	1	1	1	1	0	1	1	0	1	1	10	0.2714
610	mp-23703	LiH	1	1	0	1	1	1	1	1	0	1	1	1	10	2.9737
611	mp-1266	Na2Se	1	1	0	1	1	1	1	1	1	0	1	1	10	2.0162
612	mp-1958	SrTe	1	0	1	1	1	1	0	1	1	1	1	1	10	1.7623
613	mp-2172	AlAs	1	1	1	1	1	1	0	1	1	0	1	1	10	1.5037
614	mp-22895	CuI	1	1	1	1	0	1	0	1	1	1	1	1	10	1.1363
615	mp-4510	DyNiSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0.3133
616	mp-3432	ScNiSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0.268
617	mp-4025	TmNiSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0.2527
618	mp-31455	VSbRu	1	1	1	1	1	1	0	1	1	0	1	1	10	0.2161
619	mp-20185	LuNiSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0.2159
620	mp-30459	ScNiBi	1	1	1	1	1	1	0	1	1	0	1	1	10	0.1844
621	mp-19962	Sn2Pt	1	1	1	1	1	1	0	1	1	0	1	1	10	0
622	mp-20305	InAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0
623	mp-10183	MgSbPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0
624	mp-979963	Yb3Ti	1	0	0	1	1	1	1	1	1	1	1	1	10	0
625	mp-867811	TaMnRu2	1	1	0	1	0	1	1	1	1	1	1	1	10	0
626	mp-20340	EuN	1	1	1	1	1	1	0	1	1	0	1	1	10	0
627	mp-1002114	VH	1	1	1	1	1	1	0	1	1	0	1	1	10	0
628	mp-11488	LaTl	1	1	1	1	1	1	0	1	1	0	1	1	10	0
629	mp-11573	TiTc	1	1	1	1	1	1	0	1	1	0	1	1	10	0
630	mp-1086	TaC	1	1	1	1	1	1	0	1	1	0	1	1	10	0
631	mp-11258	TbAu	1	1	1	1	1	1	0	1	1	0	1	1	10	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
632	mp-1335	VFe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
633	mp-510404	GdSe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
634	mp-30455	HoBiPt	1	1	1	1	1	1	0	1	1	0	1	1	10	0
635	mp-974310	In3Ge	1	1	0	1	0	1	1	1	1	1	1	1	10	0
636	mp-1018136	LaBiPt	1	1	1	1	1	1	0	1	1	0	1	1	10	0
637	mp-865843	YbNdZn2	1	0	0	1	1	1	1	1	1	1	1	1	10	0
638	mp-8638	Tc	1	1	1	1	1	1	0	1	1	0	1	1	10	0
639	mp-631463	CuTcBi	1	1	1	1	1	1	0	1	1	0	1	1	10	0
640	mp-592	TiRu	1	1	1	1	1	1	0	1	1	0	1	1	10	0
641	mp-1101	TmAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0
642	mp-1144	ErP	1	1	1	1	1	1	0	1	1	0	1	1	10	0
643	mp-39	Tl	1	1	1	1	1	1	0	1	1	0	1	1	10	0
644	mp-24153	LaH2	1	1	1	1	1	1	0	1	1	0	1	1	10	0
645	mp-631301	HgPRh	1	1	1	1	1	1	0	1	1	0	1	1	10	0
646	mp-2186	NpAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0
647	mp-972352	YbMg	1	1	1	1	1	1	0	1	1	0	1	1	10	0
648	mp-867224	CaNdCd2	1	0	0	1	1	1	1	1	1	1	1	1	10	0
649	mp-861892	DyInRh2	1	1	0	1	0	1	1	1	1	1	1	1	10	0
650	mp-41	Zr	1	1	1	1	1	1	0	1	1	0	1	1	10	0
651	mp-865471	VGaTc2	1	1	0	1	0	1	1	1	1	1	1	1	10	0
652	mp-2197	BaHg	1	1	1	1	1	1	0	1	1	0	1	1	10	0
653	mp-962073	KBaSn	1	1	1	1	1	1	0	1	1	0	1	1	10	0
654	mp-631	TiC	1	1	1	1	1	1	0	1	1	0	1	1	10	0
655	mp-1009217	MnSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0
656	mp-980006	Yb3Os	1	1	0	1	0	1	1	1	1	1	1	1	10	0
657	mp-1009131	MnAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0
658	mp-977409	NbTc2Ge	1	1	0	1	0	1	1	1	1	1	1	1	10	0
659	mp-631338	LiZrSc	1	1	1	1	1	1	0	1	1	0	1	1	10	0
660	mp-1073	CaCd	1	1	1	1	1	1	0	1	1	0	1	1	10	0
661	mp-519	USb	1	1	1	1	1	1	0	1	1	0	1	1	10	0
662	mp-1172	MgRh	1	1	1	1	1	1	0	1	1	0	1	1	10	0
663	mp-571	TiNi	1	1	1	1	1	1	0	1	1	0	1	1	10	0
664	mp-4076	VCoSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0
665	mp-1009079	CrTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
666	mp-2442	ErAu	1	1	1	1	1	1	0	1	1	0	1	1	10	0
667	mp-1008728	Ni	1	1	1	1	1	1	0	1	1	0	1	1	10	0
668	mp-976793	LiEr2Ga	1	0	0	1	1	1	1	1	1	1	1	1	10	0
669	mp-866157	TiGaRh2	1	1	0	1	0	1	1	1	1	1	1	1	10	0
670	mp-20582	LaIn	1	1	1	1	1	1	0	1	1	0	1	1	10	0
671	mp-631503	ZrAlW	1	1	1	0	1	1	0	1	1	1	1	1	10	0
672	mp-2012	LiHg	1	1	1	1	1	1	0	1	1	0	1	1	10	0
673	mp-85	In	1	1	1	1	1	1	0	1	1	0	1	1	10	0
674	mp-985806	Al2Cu	1	1	1	1	1	1	0	1	1	0	1	1	10	0
675	mp-631468	SrScBe	1	1	1	1	1	1	0	1	1	0	1	1	10	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
676	mp-979259	V2ReMo	1	1	0	1	0	1	1	1	1	1	1	1	10	0
677	mp-984791	CaTmCd2	1	0	0	1	1	1	1	1	1	1	1	1	10	0
678	mp-1009206	MnSn	1	1	1	1	1	1	0	1	1	0	1	1	10	0
679	mp-2	Pd	1	1	1	1	1	1	0	1	1	0	1	1	10	0
680	mp-2743	LiPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0
681	mp-1009207	MnSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0
682	mp-981384	ScOs3	1	1	0	1	0	1	1	1	1	1	1	1	10	0
683	mp-1688	ErAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0
684	mp-284	AlCo	1	1	1	1	1	1	0	1	1	0	1	1	10	0
685	mp-980052	Yb3In	1	0	0	1	1	1	1	1	1	1	1	1	10	0
686	mp-980062	YbErZn2	1	0	0	1	1	1	1	1	1	1	1	1	10	0
687	mp-961722	TiBiRh	1	1	1	1	1	1	0	1	1	0	1	1	10	0
688	mp-604453	CeBiPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0
689	mp-31459	TaCoSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0
690	mp-22320	GaRu	1	1	1	1	1	1	0	1	1	0	1	1	10	0
691	mp-631515	CaHfZn	1	1	1	1	1	1	0	1	1	0	1	1	10	0
692	mp-1009264	NbCo	1	1	1	1	1	1	0	1	1	0	1	1	10	0
693	mp-21215	InPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0
694	mp-24719	NiH	1	1	1	1	1	1	0	1	1	0	1	1	10	0
695	mp-631299	NbCrCo	1	1	1	0	1	1	0	1	1	1	1	1	10	0
696	mp-865992	YbSnRh2	1	1	0	1	0	1	1	1	1	1	1	1	10	0
697	mp-291	TiOs	1	1	1	1	1	1	0	1	1	0	1	1	10	0
698	mp-1018155	MnSn	1	1	1	1	1	1	0	1	1	0	1	1	10	0
699	mp-979939	Yb3W	1	1	0	1	0	1	1	1	1	1	1	1	10	0
700	mp-10054	ZrAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0
701	mp-1610	TbS	1	1	1	1	1	1	0	1	1	0	1	1	10	0
702	mp-567389	Li2ZnGe	1	0	0	1	1	1	1	1	1	1	1	1	10	0
703	mp-862713	BeGeRu2	1	1	0	1	0	1	1	1	1	1	1	1	10	0
704	mp-864620	CaSmCd2	1	0	0	1	1	1	1	1	1	1	1	1	10	0
705	mp-11375	EuHg	1	0	1	1	1	1	0	1	1	1	1	1	10	0
706	mp-862774	LiInPt2	1	1	0	1	0	1	1	1	1	1	1	1	10	0
707	mp-926	PuP	1	1	1	1	1	1	0	1	1	0	1	1	10	0
708	mp-829	AlPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0
709	mp-635426	GdAu	1	1	1	1	1	1	0	1	1	0	1	1	10	0
710	mp-8642	Re	1	1	1	1	1	1	0	1	1	0	1	1	10	0
711	mp-1009885	ZrN	1	1	1	1	1	1	0	1	1	0	1	1	10	0
712	mp-1008926	CrTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
713	mp-1912	ZnAg	1	1	1	1	1	1	0	1	1	0	1	1	10	0
714	mp-7163	Tb	1	1	1	1	1	1	0	1	1	0	1	1	10	0
715	mp-1018074	GaFeNi2	1	1	0	1	0	1	1	1	1	1	1	1	10	0
716	mp-980905	ZnSn3	1	1	0	1	0	1	1	1	1	1	1	1	10	0
717	mp-980947	SrCaHg2	1	0	0	1	1	1	1	1	1	1	1	1	10	0
718	mp-1002122	HfIr	1	1	1	1	1	1	0	1	1	0	1	1	10	0
719	mp-2545	YbHg	1	1	1	1	1	1	0	1	1	0	1	1	10	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
720	mp-7171	TmP	1	1	1	1	1	1	0	1	1	0	1	1	10	0
721	mp-2493	CeN	1	1	1	1	1	1	0	1	1	0	1	1	10	0
722	mp-864883	MgSnPd2	1	1	0	1	0	1	1	1	1	1	1	1	10	0
723	mp-832	HoPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0
724	mp-31458	TiSbRu	1	1	1	1	1	1	0	1	1	0	1	1	10	0
725	mp-631452	NbCrW	1	1	1	0	1	1	0	1	1	1	1	1	10	0
726	mp-864734	HfInPd2	1	1	0	1	0	1	1	1	1	1	1	1	10	0
727	mp-980049	Yb3Re	1	0	0	1	1	1	1	1	1	1	1	1	10	0
728	mp-571363	YbSbPd	1	1	1	0	1	1	0	1	1	1	1	1	10	0
729	mp-11261	YAu	1	1	1	1	1	1	0	1	1	0	1	1	10	0
730	mp-2226	DyPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0
731	mp-867902	LiSiRh2	1	1	0	1	0	1	1	1	1	1	1	1	10	0
732	mp-868003	LaInAu2	1	1	0	1	0	1	1	1	1	1	1	1	10	0
733	mp-12086	Cu3Pt	1	1	0	1	0	1	1	1	1	1	1	1	10	0
734	mp-1009592	CrFeTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
735	mp-631543	AlInB	1	1	1	1	1	1	0	1	1	0	1	1	10	0
736	mp-31460	NbCoSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0
737	mp-1395	VRu	1	1	1	1	1	1	0	1	1	0	1	1	10	0
738	mp-962067	BaNaSn	1	1	1	1	1	1	0	1	1	0	1	1	10	0
739	mp-10154	MnSbIr	1	1	1	1	1	1	0	1	1	0	1	1	10	0
740	mp-631462	BeTcSe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
741	mp-2548	PuAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0
742	mp-8635	Zr	1	1	1	1	1	1	0	1	1	0	1	1	10	0
743	mp-15778	MgNiSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0
744	mp-1008874	MnCoTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
745	mp-30658	VGaNi2	1	1	0	1	0	1	1	1	1	1	1	1	10	0
746	mp-1007657	HfRu3	1	1	0	1	0	1	1	1	1	1	1	1	10	0
747	mp-12558	LiMgAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0
748	mp-631255	InSiIr	1	1	1	1	1	1	0	1	1	0	1	1	10	0
749	mp-31457	ZrSbRu	1	1	1	1	1	1	0	1	1	0	1	1	10	0
750	mp-475	SnP	1	1	1	1	1	1	0	1	1	0	1	1	10	0
751	mp-2323	BeCu	1	1	1	1	1	1	0	1	1	0	1	1	10	0
752	mp-631384	Sr2VW	1	0	0	1	1	1	1	1	1	1	1	1	10	0
753	mp-1008872	MnFeTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
754	mp-2104	UAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0
755	mp-744	HoP	1	1	1	1	1	1	0	1	1	0	1	1	10	0
756	mp-600124	MnNiSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0
757	mp-11388	GaIr	1	1	1	1	1	1	0	1	1	0	1	1	10	0
758	mp-865920	YbPmZn2	1	0	0	1	1	1	1	1	1	1	1	1	10	0
759	mp-567089	YbRh	1	1	1	1	1	1	0	1	1	0	1	1	10	0
760	mp-2547	YbPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0
761	mp-12778	VOs	1	1	1	1	1	1	0	1	1	0	1	1	10	0
762	mp-2658	AlFe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
763	mp-11452	HfOs	1	1	1	1	1	1	0	1	1	0	1	1	10	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
764	mp-1018145	MnSn	1	1	1	1	1	1	0	1	1	0	1	1	10	0
765	mp-1703	YbZn	1	1	1	1	1	1	0	1	1	0	1	1	10	0
766	mp-1476	ScS	1	1	1	1	1	1	0	1	1	0	1	1	10	0
767	mp-631540	NiBTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
768	mp-50	Ta	1	1	1	1	1	1	0	1	1	0	1	1	10	0
769	mp-1008875	Mn2Sb	1	1	1	1	1	1	0	1	1	0	1	1	10	0
770	mp-3201	Li2GaPd	1	0	0	1	1	1	1	1	1	1	1	1	10	0
771	mp-2802	HfRu	1	1	1	1	1	1	0	1	1	0	1	1	10	0
772	mp-1486	ZnNi	1	1	1	1	1	1	0	1	1	0	1	1	10	0
773	mp-631430	LaInW	1	1	1	1	1	1	0	1	1	0	1	1	10	0
774	mp-864876	TbInRh2	1	1	0	1	0	1	1	1	1	1	1	1	10	0
775	mp-961656	VFeTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
776	mp-2818	YbAu	1	1	1	1	1	1	0	1	1	0	1	1	10	0
777	mp-1561	TbSe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
778	mp-1009593	CrCoTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
779	mp-1129	ScIr	1	1	1	1	1	1	0	1	1	0	1	1	10	0
780	mp-4262	BeAlB	1	1	1	1	1	1	0	1	1	0	1	1	10	0
781	mp-930	ZrP	1	1	1	1	1	1	0	1	1	0	1	1	10	0
782	mp-865577	Li2CdAu	1	1	0	1	0	1	1	1	1	1	1	1	10	0
783	mp-2288	PuSe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
784	mp-931	ThP	1	1	1	1	1	1	0	1	1	0	1	1	10	0
785	mp-899	InRh	1	1	1	1	1	1	0	1	1	0	1	1	10	0
786	mp-2011	UP	1	1	1	1	1	1	0	1	1	0	1	1	10	0
787	mp-1161	LaSe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
788	mp-10194	LuSbPt	1	1	1	1	1	1	0	1	1	0	1	1	10	0
789	mp-851	ErPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0
790	mp-1282	VC	1	1	1	1	1	1	0	1	1	0	1	1	10	0
791	mp-2083	Sn2Ir	1	1	1	1	1	1	0	1	1	0	1	1	10	0
792	mp-2183	ThSe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
793	mp-976596	LiLu2Ga	1	0	0	1	1	1	1	1	1	1	1	1	10	0
794	mp-1018161	CrNiSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0
795	mp-12110	TaRu	1	1	1	1	1	1	0	1	1	0	1	1	10	0
796	mp-11245	HoAu	1	1	1	1	1	1	0	1	1	0	1	1	10	0
797	mp-10635	SnSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0
798	mp-23	Ni	1	1	1	1	1	1	0	1	1	0	1	1	10	0
799	mp-348	TmPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0
800	mp-21418	MnSnPt	1	1	1	1	1	1	0	1	1	0	1	1	10	0
801	mp-2179	TiRe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
802	mp-1487	AlNi	1	1	1	1	1	1	0	1	1	0	1	1	10	0
803	mp-31452	ZrNiBi	1	1	1	1	1	1	0	1	1	0	1	1	10	0
804	mp-2540	VTc	1	1	1	1	1	1	0	1	1	0	1	1	10	0
805	mp-631274	KFeP	1	1	1	1	1	1	0	1	1	0	1	1	10	0
806	mp-631449	LiTaBe	1	1	1	1	1	1	0	1	1	0	1	1	10	0
807	mp-1008999	LaSe	1	1	1	1	1	1	0	1	1	0	1	1	10	0

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap
808	mp-987	ZnCu	1	1	1	1	1	1	0	1	1	0	1	1	10	0
809	mp-256	LaN	1	1	1	1	1	1	0	1	1	0	1	1	10	0

Supplementary Table 8. True positive candidate list for E_fermi <=0.4eV.

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap	pred_Ef	actual_Ef
1	mp-648	Na2S	1	1	1	1	1	1	1	1	1	1	1	1	12	2.4399	0.2652	0.2843
2	mp-961683	LiMgP	1	1	1	1	1	1	1	1	1	1	1	1	12	1.8107	3.1024	2.7892
3	mp-971	K2O	1	1	1	1	1	1	1	1	1	1	1	1	12	1.7072	0.4962	0.3983
4	mp-961660	TiFeSe	1	1	1	1	1	1	1	1	1	1	1	1	12	0.987	7.245	6.8588
5	mp-961661	ZrSiPd	1	1	1	1	1	1	1	1	1	1	1	1	12	0.7448	5.2604	5.1529
6	mp-10623	ThSbRh	1	1	1	1	1	1	1	1	1	1	1	1	12	0.7444	7.2799	7.0322
7	mp-2612	GeTe	1	1	1	1	1	1	1	1	1	1	1	1	12	0.3631	4.8339	5.1041
8	mp-1018118	TmSbPd	1	1	1	1	1	1	1	1	1	1	1	1	12	0.3569	5.0512	5.0181
9	mp-865101	NaLi2Bi	1	1	1	1	1	1	1	1	1	1	1	1	12	0.3251	3.1734	2.9574
10	mp-11390	LiGaSi	1	1	1	1	1	1	1	1	1	1	1	1	12	0.1909	4.3002	4.3938
11	mp-3161	LiAlSi	1	1	1	1	1	1	1	1	1	1	1	1	12	0.1121	4.8157	4.9571
12	mp-962064	NaYSn	1	1	1	1	1	1	1	1	1	1	1	1	12	0.1018	2.9243	2.6526
13	mp-1779	YbTe	1	1	1	1	1	1	1	1	1	1	1	1	12	1.4688	3.2703	3.1704
14	mp-10182	LiZnP	1	1	1	1	1	1	1	1	1	1	1	1	12	1.3386	3.3371	3.2728
15	mp-19717	TePb	1	1	1	1	1	1	1	1	1	1	1	1	12	0.8072	4.8376	5.0414
16	mp-2074	Li3Sb	1	1	1	1	1	1	1	1	1	1	1	1	12	0.6961	3.5173	3.3089
17	mp-5077	NaLi2Sb	1	1	1	1	1	1	1	1	1	1	1	1	12	0.68	3.51	3.2153
18	mp-20351	InP	1	1	1	1	1	1	1	1	1	1	1	1	12	0.4679	4.8848	4.6896
19	mp-505297	NbSbRu	1	1	1	1	1	1	1	1	1	1	1	1	12	0.3749	7.3196	6.9668
20	mp-30373	RbAu	1	1	1	1	1	1	1	1	1	1	1	1	12	0.3714	0.4183	0.6106
21	mp-23222	Li3Bi	1	1	1	1	1	1	1	1	1	1	1	1	12	0.3429	3.2173	2.9226
22	mp-1367	Mg2Si	1	1	1	1	1	1	1	1	1	1	1	1	12	0.2169	4.2855	4.2152
23	mp-408	Mg2Ge	1	1	1	1	1	1	1	1	1	1	1	1	12	0.1689	3.3123	3.2815
24	mp-1876	SnS	1	1	1	1	1	1	1	1	1	1	1	1	12	0.0894	6.5547	6.5138
25	mp-5920	LiAlGe	1	1	1	1	1	1	1	1	1	1	1	1	12	0.0564	3.9252	3.8344
26	mp-867912	Ba2SnHg	1	1	1	1	1	1	1	1	1	1	1	1	12	0.0498	3.1841	3.1876
27	mp-961676	HfGePt	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.165	4.2578
28	mp-865142	DyMgZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3187	3.3628
29	mp-862755	PrCd3	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.1755	3.2451
30	mp-974253	HoErZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2725	3.0863
31	mp-712	YCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.6197	4.5059
32	mp-631570	BaTaB	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.7945	3.7217
33	mp-631429	ZrCrFe	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.7023	4.3951
34	mp-1352	ZrN	1	1	1	1	1	1	1	1	1	1	1	1	12	0	7.3777	7.3603
35	mp-213	CaPd	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.6951	3.5913
36	mp-972630	SmErZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2708	3.0957
37	mp-631568	AlAgB	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.0033	4.6668
38	mp-2861	CaTl	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.8534	4.8663
39	mp-12718	LiPrSn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.2832	4.0986

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap	pred_Ef	actual_Ef
40	mp-962068	CaMgSn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.4581	4.3148
41	mp-11566	ScZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.9805	3.6343
42	mp-2054	TbHg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.7396	3.8293
43	mp-962078	CaCdSi	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.5702	3.6518
44	mp-861948	LiPm2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3899	3.1732
45	mp-973841	LiHo2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4061	3.0956
46	mp-1008727	Ti2Ge	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.6178	4.3671
47	mp-2434	SrTl	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.1963	4.0709
48	mp-983425	Li2PmGe	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.368	3.4629
49	mp-866017	LiNd2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.171	3.2315
50	mp-631562	SiBAu	1	1	1	1	1	1	1	1	1	1	1	1	12	0	6.6072	6.4142
51	mp-975789	PrTmMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4184	3.203
52	mp-11475	TmHg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.715	3.7645
53	mp-1014230	TiZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.8677	4.65
54	mp-295	HoAs	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.1586	3.8571
55	mp-861955	LiPm2Ge	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3307	3.417
56	mp-631521	BaHfMo	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.9175	3.8222
57	mp-631471	YScBe	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2016	3.133
58	mp-460	PrZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3627	3.2964
59	mp-2823	NdP	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.24	4.0306
60	mp-975822	PrNdZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4053	3.2342
61	mp-978512	SmTmMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2869	3.1013
62	mp-972456	Sm3V	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4497	3.4442
63	mp-977551	ErLuMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3049	3.0245
64	mp-631544	BaSiB	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2496	3.1485
65	mp-1156	GaSb	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.6943	3.7747
66	mp-20389	Na2CdPb	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2668	3.4387
67	mp-2796	TmAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4281	3.5227
68	mp-865426	YbNdAg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2532	3.0912
69	mp-631554	Na2TiAu	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.218	3.1713
70	mp-631422	CuSiBr	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.6023	5.3149
71	mp-864799	HoLuMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2999	3.0318
72	mp-12793	NdAl	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.0322	4.7465
73	mp-976151	PrErMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4319	3.2164
74	mp-11469	PrHg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.7211	3.6894
75	mp-2988	Li2GaRh	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.1671	3.139
76	mp-2696	MgAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.0674	3.9911
77	mp-24650	YH2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4711	3.378
78	mp-981311	SrTlHg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2824	3.6621
79	mp-2857	ScN	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.7665	5.516
80	mp-862902	PmDyMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3366	3.1782
81	mp-2167	DyAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.7544	3.5891
82	mp-1955	ErCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.5955	4.4461
83	mp-23171	PrBi	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.1732	4.37

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap	pred_Ef	actual_Ef
84	mp-2249	HoZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2665	3.0679
85	mp-972522	SmTmZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2843	3.0675
86	mp-976008	NdTmMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3412	3.1592
87	mp-1586	NdSb	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.8819	4.7092
88	mp-866015	CaPrZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.1382	2.915
89	mp-656	LuS	1	1	1	1	1	1	1	1	1	1	1	1	12	0	7.1375	6.896
90	mp-11313	ZrCd3	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2682	2.9675
91	mp-30648	LiMg2Ga	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4309	3.5287
92	mp-972156	TbY3	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3557	3.2027
93	mp-983126	HoTmZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2364	3.0329
94	mp-2525	PrAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.8799	3.5918
95	mp-11503	MnZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.3216	4.292
96	mp-631317	NaIrPb	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.9502	4.705
97	mp-862740	Sr2TlCd	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.0467	3.0867
98	mp-979937	Yb3Ru	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.1789	3.1569
99	mp-862964	PmSmMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2862	3.1832
100	mp-631314	KTaPt	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.8022	3.5448
101	mp-979417	DyYCd2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.131	3.1235
102	mp-999484	YTi	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.2916	4.0322
103	mp-24287	CrH	1	1	1	1	1	1	1	1	1	1	1	1	12	0	7.2458	7.0124
104	mp-1837	TbCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.8254	4.5458
105	mp-1008753	Ti2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.739	4.4213
106	mp-1009538	PdC	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.1523	4.7999
107	mp-978513	SmErMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2767	3.1299
108	mp-972640	SmDyZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2577	3.1205
109	mp-631311	IrOsW	1	1	1	1	1	1	1	1	1	1	1	1	12	0	6.7325	6.4455
110	mp-631542	BaZrNi	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2369	3.4405
111	mp-862937	PmMgZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3116	3.3279
112	mp-1009458	NbC	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.0072	4.7239
113	mp-1236	NdAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.583	3.514
114	mp-631492	BaScIr	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.1979	3.8697
115	mp-2334	DyCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.7132	4.5112
116	mp-1008876	MnCoS	1	1	1	1	1	1	1	1	1	1	1	1	12	0	7.2915	6.9389
117	mp-2497	GdZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2807	2.9191
118	mp-11563	TiRh	1	1	1	1	1	1	1	1	1	1	1	1	12	0	7.1493	7.2107
119	mp-631534	NaSrRe2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2494	3.2633
120	mp-631383	MnCrRe	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.0061	4.7507
121	mp-972601	SmLuMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2927	3.0997
122	mp-1971	HoCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.5822	4.4552
123	mp-631541	BeGeB	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.275	5.1763
124	mp-861886	LiDyHg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.1945	2.8112
125	mp-11344	PrO	1	1	1	1	1	1	1	1	1	1	1	1	12	0	6.7417	6.5295
126	mp-631337	NaTaNi	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.6374	3.4858
127	mp-836	TbZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3642	3.2052

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap	pred_Ef	actual_Ef
128	mp-865911	YbPmHg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2071	3.2187
129	mp-865896	YbPmAg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.1242	3.0786
130	mp-978823	SmY3	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.276	3.1308
131	mp-24724	TbH2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4564	3.2313
132	mp-2195	LuMg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2922	3.0198
133	mp-2268	TbAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.5333	3.638
134	mp-631394	CaZrPd	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4108	3.3652
135	mp-631349	ZnTcMo	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.0035	4.6481
136	mp-962071	MgScTl	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.7623	3.7303
137	mp-982388	HoTmMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2857	3.0487
138	mp-973276	HoLuCd2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.1205	3.0768
139	mp-34611	ZnAgAs	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.5985	3.3492
140	mp-867222	LiCa2Ir	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.5017	3.3786
141	mp-1014219	HfZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.3148	4.2543
142	mp-22873	SmBi	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.5447	4.4017
143	mp-542779	GdAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.697	3.2987
144	mp-980198	TmLuZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2979	3.0928
145	mp-978094	NdHo3	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2739	3.1524
146	mp-980055	YErMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2697	3.0946
147	mp-861913	LiDy2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.466	3.1446
148	mp-961671	TiGePt	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.3129	5.0225
149	mp-23300	NdBi	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.5109	4.3712
150	mp-979419	Dy3Y	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2658	3.1677
151	mp-571059	YCd3	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2976	3.3042
152	mp-866063	NdDyMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3749	3.2117
153	mp-2165	SmZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2728	3.1214
154	mp-2516	YZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4325	3.1441
155	mp-976030	PrHoMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4227	3.2137
156	mp-1008911	LiMnAs	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.064	3.2213
157	mp-862918	PmHoMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2883	3.1521
158	mp-1008	NiHg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.0576	5.3042
159	mp-570276	ZrZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.783	3.8634
160	mp-866220	CaNdZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.1507	2.8702
161	mp-2502	TmCd	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2527	3.0585
162	mp-11467	NdHg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.7703	3.6354
163	mp-631322	KSnOs	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.4045	4.1273
164	mp-962061	YMgTl	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.0899	3.3273
165	mp-972997	HoErCd2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.1334	3.0894
166	mp-2636	GdMg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2689	2.9839
167	mp-864598	LiMg2Ag	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.1055	3.0678
168	mp-11240	DyAu	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.8839	4.6045
169	mp-615	YMg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2792	3.1415
170	mp-1001837	MoP	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.7182	5.4497
171	mp-972062	YbTmHg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2454	3.2159

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap	pred_Ef	actual_Ef
172	mp-2732	PRh2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	7.2678	7.6429
173	mp-631324	HfMnTl	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.8896	5.1903
174	mp-861479	PrYMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3661	3.2544
175	mp-437	MgAu	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.0401	5.1908
176	mp-631482	BiMoRh	1	1	1	1	1	1	1	1	1	1	1	1	12	0	6.7508	6.491
177	mp-2474	YAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.703	3.5978
178	mp-976426	LiLuHg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2134	2.8329
179	mp-961680	NbAlPt	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.1711	5.2047
180	mp-867873	LiTm2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2999	3.1115
181	mp-631395	CaTaTc	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.8622	4.0717
182	mp-980942	YTmMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2068	3.0714
183	mp-11576	YbTl	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.6774	4.5373
184	mp-631484	TaTiAl	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.5154	4.302
185	mp-961669	NbGaPt	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.3151	4.151
186	mp-1013549	Ba3BiN	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3785	3.2323
187	mp-973232	NdTm3	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.1749	3.1189
188	mp-1660	ErZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2735	3.0789
189	mp-2778	HoAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.5796	3.5528
190	mp-976143	PrDyZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2502	3.2428
191	mp-980082	YHo3	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.258	3.0769
192	mp-975886	PrSmZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3153	3.1795
193	mp-975972	PrLuMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4678	3.1954
194	mp-24152	HoH2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4619	3.1836
195	mp-631546	TlCoBi	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.8257	4.9163
196	mp-2475	SmAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.612	3.4686
197	mp-1211	ScCd	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.539	3.5494
198	mp-1174	MgSc	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.7673	3.5238
199	mp-30779	SmMg3	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.5021	3.3912
200	mp-2283	ZrCo	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.218	5.1044
201	mp-978514	SmTm3	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.1595	3.0505
202	mp-631381	TeRuSe	1	1	1	1	1	1	1	1	1	1	1	1	12	0	7.3803	7.1396
203	mp-867149	Sr2CdSn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4995	3.5142
204	mp-1008726	Ti2Ga	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.7951	3.7464
205	mp-12586	SmCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.6212	4.3522
206	mp-865210	TmLuMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2313	2.9988
207	mp-631373	TiVW	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.9418	4.7089
208	mp-862555	LiY2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3264	3.2089
209	mp-866158	YLuMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2975	3.0593
210	mp-631479	CaHfBe	1	1	1	1	1	1	1	1	1	1	1	1	12	0	2.949	2.7717
211	mp-1785	PrSb	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.772	4.6852
212	mp-976032	PrHoZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2704	3.2329
213	mp-867159	SmDyMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2991	3.1691
214	mp-2640	TbAs	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.2123	3.8887
215	mp-973058	LiLu2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3562	3.1363

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap	pred_Ef	actual_Ef
216	mp-974517	NdErMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3252	3.1752
217	mp-973333	HoLuZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2616	3.0648
218	mp-862493	LiEr2Al	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4429	3.1262
219	mp-11237	ScAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.1438	4.0697
220	mp-7381	TbMg3	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.5108	3.42
221	mp-864630	LiMg2Hg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3338	3.359
222	mp-976147	PrEr3	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3207	3.2068
223	mp-866191	Li2YbSi	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.0808	3.4012
224	mp-985	TmCu	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.6247	4.4514
225	mp-974527	NdSmZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3456	3.1397
226	mp-973759	Lu2MgCd	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.1936	3.1219
227	mp-975848	PrNdMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4282	3.2511
228	mp-11221	SmAl	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.095	4.7243
229	mp-976129	PrErZn2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2699	3.2209
230	mp-2303	DyZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2617	3.1439
231	mp-961726	NbGeRh	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.3969	4.1615
232	mp-754940	Ba3SiO	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.1826	3.2181
233	mp-31168	Li2AlAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2704	3.0633
234	mp-867163	Sr2AgPt	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2977	3.3584
235	mp-1053	NdZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.432	3.2121
236	mp-631335	MgTaZn	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2711	3.548
237	mp-961699	NaMgP	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.0592	2.8238
238	mp-12087	Cu2S	1	1	1	1	1	1	1	1	1	1	1	1	12	0	7.3435	6.9671
239	mp-631506	SrZrCo	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.23	3.1425
240	mp-867158	SmCd3	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.1514	3.2057
241	mp-1007819	CoW	1	1	1	1	1	1	1	1	1	1	1	1	12	0	6.9553	6.5964
242	mp-867130	SmHoMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.2666	3.1265
243	mp-24192	ErH2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.4558	3.2383
244	mp-934	LiTl	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.5238	4.8548
245	mp-710	SmP	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.2294	4.0539
246	mp-975880	PrSmMg2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.3943	3.2134
247	mp-2621	ErAg	1	1	1	1	1	1	1	1	1	1	1	1	12	0	3.6062	3.5529
248	mp-2724	TbSb	1	1	1	1	1	1	1	1	1	1	1	1	12	0	5.0229	5.0018
249	mp-24237	ScH2	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.3563	4.0224
250	mp-631269	LiIrRh	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.9948	4.7661
251	mp-973060	MgCr	1	1	1	1	1	1	1	1	1	1	1	1	12	0	4.2194	3.9464
252	mp-961711	ZrSiPt	1	1	1	1	1	1	0	1	1	1	1	1	11	1.3298	5.5778	5.5489
253	mp-961649	ZrFeTe	1	1	1	1	1	1	0	1	1	1	1	1	11	1.1558	7.194	7.3318
254	mp-961706	TiSiPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0.993	6.8589	6.47
255	mp-1008680	TiGePt	1	1	1	1	1	1	0	1	1	1	1	1	11	0.8819	5.5039	5.2294
256	mp-997618	BSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0.7513	7.4827	7.402
257	mp-961774	BaNaSb	1	1	0	1	1	1	1	1	1	1	1	1	11	0.7372	2.641	2.6824
258	mp-961657	YNiP	1	1	1	1	1	1	0	1	1	1	1	1	11	0.7214	5.7735	5.8012
259	mp-19886	ThSnPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0.6738	7.0743	6.8919

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap	pred_Ef	actual_Ef
260	mp-7173	ScSbPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0.6441	6.8712	6.9454
261	mp-961675	ScNiP	1	1	1	1	1	1	0	1	1	1	1	1	11	0.5921	7.0468	7.1642
262	mp-9437	NbFeSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0.5138	7.4875	7.1629
263	mp-961693	ZrInAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0.4532	5.8168	5.4322
264	mp-866132	Na2TlSb	1	1	0	1	1	1	1	1	1	1	1	1	11	0.3844	3.7245	3.5985
265	mp-961663	SrTePd	1	1	1	1	1	1	0	1	1	1	1	1	11	0.3215	4.8325	4.6799
266	mp-961697	ScGeAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0.2804	4.4951	4.5931
267	mp-1550	AlP	1	1	1	1	1	1	1	1	1	0	1	1	11	1.6302	4.1081	4.3526
268	mp-2490	GaP	1	1	1	1	1	1	0	1	1	1	1	1	11	1.5928	3.3661	3.4498
269	mp-36111	LiMgP	1	1	0	1	1	1	1	1	1	1	1	1	11	1.5391	2.6744	2.7368
270	mp-2624	AlSb	1	1	1	1	1	1	1	1	1	0	1	1	11	1.2273	4.0331	4.4141
271	mp-31454	TaSbRu	1	1	1	1	1	1	0	1	1	1	1	1	11	0.6669	7.4924	7.2965
272	mp-11836	ErSbPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0.2096	5.8143	5.9523
273	mp-2114	YN	1	1	1	1	1	1	0	1	1	1	1	1	11	0.151	4.4608	4.1988
274	mp-1008858	NdBiPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0.1051	5.2871	5.0598
275	mp-13305	SmSnAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0.097	5.6064	5.2119
276	mp-631550	CaBiB	1	1	1	1	1	1	0	1	1	1	1	1	11	0.0821	3.1419	3.0328
277	mp-961653	FeSiW	1	1	1	1	1	1	0	1	1	1	1	1	11	0.065	6.9207	6.7925
278	mp-1883	SnTe	1	1	1	1	1	1	0	1	1	1	1	1	11	0.0428	6.6076	6.3219
279	mp-30390	HoSnAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0.0235	5.7215	5.5328
280	mp-5640	ErSnAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0.0072	5.7315	5.5847
281	mp-1009459	NbC	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.0352	6.7194
282	mp-971702	YbNdCd2	1	1	0	1	1	1	1	1	1	1	1	1	11	0	2.6218	2.6114
283	mp-124	Ag	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.2334	3.0638
284	mp-1546	DyMg3	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.5441	3.4075
285	mp-12599	PrTl	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.561	5.3363
286	mp-1502	Al2Pt	1	1	1	1	1	1	0	1	1	1	1	1	11	0	6.8257	6.7538
287	mp-1006884	CoMo	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.596	7.2444
288	mp-75	Nb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.9676	4.8562
289	mp-428	PrMg3	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.5991	3.4756
290	mp-22682	In2Pt	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.3414	7.1868
291	mp-863705	Pm2MgGa	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.6977	3.5164
292	mp-770	DyCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.083	3.1041
293	mp-5549	MgSnAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.766	5.4858
294	mp-30479	Ca3Pb	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.7504	3.5001
295	mp-961720	ZrAsRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.4448	4.4423
296	mp-11843	DyAl	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.2906	4.9916
297	mp-1018132	AlBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.33	3.7003
298	mp-2050	HoSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.172	5.0264
299	mp-23245	ErBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.5628	4.6886
300	mp-961681	ZrGePt	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.9917	3.9417
301	mp-1008689	Ti2Si	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.4382	5.3887
302	mp-631379	ZnCuMo	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.5584	4.171
303	mp-31456	HfSbRu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	6.9886	6.6448

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap	pred_Ef	actual_Ef
304	mp-2316	TmZn	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.146	3.0531
305	mp-961709	ZrPtPb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.4618	5.2237
306	mp-867145	LiHo2Ga	1	1	0	1	1	1	1	1	1	1	1	1	11	0	2.7124	2.7381
307	mp-961702	LaSbPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.407	7.1184
308	mp-436	SmRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.0014	4.681
309	mp-30377	ErPbAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.6985	5.4104
310	mp-1408	MgHg	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.9916	3.9863
311	mp-1013545	Ca3BiAs	1	1	1	1	1	0	1	1	1	1	1	1	11	0	3.2567	3.0414
312	mp-866180	Li2YbPb	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.7041	3.9326
313	mp-2210	ZrCu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.4706	5.2258
314	mp-776	LaCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.6972	5.6551
315	mp-2163	HoRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.0509	4.8763
316	mp-1006883	CoNi	1	1	1	1	1	1	0	1	1	1	1	1	11	0	6.8227	6.6365
317	mp-979989	Yb2AgPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.1238	2.9114
318	mp-1009132	HoBiPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.5263	5.3856
319	mp-631555	MnVNi	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.4372	5.3176
320	mp-170	HoCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.1112	3.0452
321	mp-1009731	ReC	1	1	1	1	1	1	0	1	1	1	1	1	11	0	9.3175	9.3828
322	mp-621592	YPbAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.6869	5.3626
323	mp-24096	NdH2	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.0415	3.0047
324	mp-12564	LiSbAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.8734	4.055
325	mp-1925	ZrS	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.487	7.7692
326	mp-865579	Li2ErIn	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.7769	3.8581
327	mp-510403	GdSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.8937	4.5984
328	mp-542065	CdAgSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.4733	4.1606
329	mp-1738	SmAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.7812	3.663
330	mp-11471	ScHg	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.469	4.2923
331	mp-834	ThN	1	1	1	1	1	1	0	1	1	1	1	1	11	0	8.4741	8.6131
332	mp-961679	TaAlPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.5232	5.4099
333	mp-721	TbCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.1198	3.1047
334	mp-232	DyRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.1733	4.9481
335	mp-13308	HoGeAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.9911	3.9146
336	mp-1164	ThC	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.3285	6.9516
337	mp-961710	VSiPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.082	7.2823
338	mp-1059	NdCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.1678	3.0984
339	mp-22907	DyBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.671	4.6575
340	mp-2052	ScAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.0754	4.8075
341	mp-568398	CaBiAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.5718	4.6605
342	mp-865882	Li2SmIn	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.6063	3.6066
343	mp-20952	TiNiSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	9.0042	8.844
344	mp-631754	ReSnGe	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.3889	7.1367
345	mp-1031	GdCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.1114	2.8861
346	mp-30413	TbPbAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.6988	5.3247
347	mp-568931	YbNiSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.134	5.0064

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap	pred_Ef	actual_Ef
348	mp-2444	GaRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0	6.5857	6.6048
349	mp-1008702	Ti2In	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.4227	5.1408
350	mp-979073	TmMg2Sc	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.5826	3.2528
351	mp-978528	SmMg2Sc	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.5345	3.2945
352	mp-22866	HoBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.5016	4.6453
353	mp-915	YCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.1963	3.1393
354	mp-2443	DyHg	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.8865	3.8038
355	mp-13	Fe	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.3824	5.2186
356	mp-631320	TcIrOs	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.3597	7.0927
357	mp-24092	GdH2	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.1051	2.8994
358	mp-933	YAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.9698	3.998
359	mp-574283	GdTe	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.7469	6.0798
360	mp-2082	PIr2	1	1	1	1	1	1	0	1	1	1	1	1	11	0	9.7965	9.5109
361	mp-1013733	Ca3BiSb	1	1	1	1	1	0	1	1	1	1	1	1	11	0	3.1498	2.9838
362	mp-11242	DyPbAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.6293	5.339
363	mp-10755	TiFeSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.4379	7.0863
364	mp-961716	VSnPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0	6.955	7.2512
365	mp-510374	GdAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.8974	3.6276
366	mp-11286	CaHg	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.1554	3.0196
367	mp-631366	TcSnSe	1	1	1	1	1	0	1	1	1	1	1	1	11	0	6.2673	6.1283
368	mp-865661	YbMgCd2	1	1	0	1	1	1	1	1	1	1	1	1	11	0	2.7025	2.5413
369	mp-961666	MnNbAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.0412	4.9135
370	mp-568466	LiInSn	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.4723	5.499
371	mp-20263	CaIn	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.2229	4.9765
372	mp-1092	HoHg	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.7961	3.7531
373	mp-862681	ErMg3	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.5619	3.3711
374	mp-961658	VFeSe	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.6305	7.4476
375	mp-978273	Mg3Cd	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.6829	3.4504
376	mp-11256	ScAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.4615	5.258
377	mp-572	SmCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.0368	2.9943
378	mp-2795	ZrC	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.5106	5.4347
379	mp-2637	YSe	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.6675	5.882
380	mp-1007	DySb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.1465	5.0263
381	mp-102	Co	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.7004	5.4433
382	mp-11255	PrAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.5464	4.4923
383	mp-22921	TbBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.6999	4.6467
384	mp-2781	ScPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.2341	5.1743
385	mp-961719	HfAsRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.6094	4.7655
386	mp-631526	SiBPb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.5908	5.9829
387	mp-1006150	Eu3Re	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.6723	3.6964
388	mp-129	Mo	1	1	1	1	1	1	0	1	1	1	1	1	11	0	8.7109	8.4313
389	mp-2602	NdAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.9536	3.6034
390	mp-23241	YBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.507	4.7053
391	mp-24147	AcH2	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.3823	5.4202

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap	pred_Ef	actual_Ef
392	mp-2281	SmSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.8393	4.763
393	mp-2642	CdAg	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.3321	3.1453
394	mp-1902	MnPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.3416	5.001
395	mp-571405	NdTl	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.6838	5.3499
396	mp-191	YRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.0619	4.934
397	mp-21005	GdIn	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.7897	5.4105
398	mp-510401	GdP	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.3296	4.1296
399	mp-133	Sb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.4967	7.1582
400	mp-1008734	ThH2	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.0958	6.7238
401	mp-1623	ErS	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.0763	6.7264
402	mp-30	Cu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.2356	6.8571
403	mp-2399	YHg	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.853	3.8157
404	mp-377	LuRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.9902	4.9321
405	mp-1009222	MnTe	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.2806	3.5504
406	mp-865580	Li2DyIn	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.788	3.7969
407	mp-961677	TaGaPt	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.6004	4.4598
408	mp-20298	SmIn	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.7512	5.5601
409	mp-867	ErCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.1465	3.0782
410	mp-20012	InSb	1	1	1	1	1	1	1	1	1	0	1	1	11	0	4.0818	4.3194
411	mp-542583	EuTe	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.4228	4.5791
412	mp-1009543	DyBiPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.6198	5.376
413	mp-1787	NdMg3	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.5359	3.4389
414	mp-11561	TbRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.0358	4.9615
415	mp-1008624	YBiPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.425	5.3985
416	mp-15694	PaAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0	9.1347	9.0277
417	mp-506	MgPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.0661	4.9127
418	mp-11495	LuRu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.0151	4.6559
419	mp-631538	NiBiB	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.3628	7.0516
420	mp-981545	Ho3Zr	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.5218	3.3714
421	mp-984713	Dy3Ga	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.7467	3.4778
422	mp-2090	FeCo	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.815	5.6096
423	mp-866196	Li2PrIn	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.7108	3.6045
424	mp-866199	AcAg	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.3626	5.4226
425	mp-961718	TiAsRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.5651	5.6778
426	mp-2520	TmSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.9082	5.1036
427	mp-11374	DyTl	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.7799	5.6909
428	mp-2350	LaS	1	1	1	1	1	1	0	1	1	1	1	1	11	0	9.0285	8.8139
429	mp-862930	Li2PmIn	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.7667	3.5909
430	mp-2191	ErSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.2548	5.0951
431	mp-1093	ThGe	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.918	5.0499
432	mp-2627	DyAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.7993	3.8924
433	mp-24658	SmH2	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.059	2.9611
434	mp-646	PrCd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.051	3.1736
435	mp-2381	ErRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.0866	4.923

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap	pred_Ef	actual_Ef
436	mp-10622	PrAs	1	1	1	1	1	1	0	1	1	1	1	1	11	0	3.9728	3.6191
437	mp-20997	InNi	1	1	1	1	1	1	0	1	1	1	1	1	11	0	9.7164	9.6157
438	mp-2065	MnS	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.7697	6.0307
439	mp-979950	AcYbMg2	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.5568	3.4829
440	mp-30389	HoPbAu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.6858	5.3528
441	mp-1534	YS	1	1	1	1	1	1	0	1	1	1	1	1	11	0	6.8449	6.6989
442	mp-631302	ScVFe	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.8414	4.5206
443	mp-2212	ScCo	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.401	5.0701
444	mp-24154	NbH2	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.5119	5.1812
445	mp-866181	Li2NdIn	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.7302	3.596
446	mp-23234	TmBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.6163	4.6993
447	mp-11621	ZnNiSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	6.9728	6.6777
448	mp-364	AlRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0	9.3289	8.9573
449	mp-13496	ZrPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.2784	5.1342
450	mp-570632	ScBi	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.458	5.359
451	mp-1169	ScCu	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.6319	5.2973
452	mp-645	TbP	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.4616	4.3457
453	mp-631364	TaOsPb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	6.5984	6.3135
454	mp-1941	GaNi	1	1	1	1	1	1	0	1	1	1	1	1	11	0	6.9143	6.9123
455	mp-215	YSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.2865	5.0871
456	mp-11564	TmRh	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.9327	4.8988
457	mp-977386	LiLu2Tc	1	1	0	1	1	1	1	1	1	1	1	1	11	0	3.5411	3.2563
458	mp-1008903	MgAgSb	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.1877	5.2523
459	mp-2379	CoSi2	1	1	1	1	1	1	0	1	1	1	1	1	11	0	8.9969	8.6951
460	mp-631342	MnTcPd	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.3682	4.9947
461	mp-515	TmTl	1	1	1	1	1	1	0	1	1	1	1	1	11	0	5.8179	5.7586
462	mp-2828	HfN	1	1	1	1	1	1	0	1	1	1	1	1	11	0	7.9435	8.2721
463	mp-994	YP	1	1	1	1	1	1	0	1	1	1	1	1	11	0	4.5482	4.4436
464	mp-961648	KBaP	1	1	1	1	1	1	0	1	1	0	1	1	10	1.1622	2.0358	1.9643
465	mp-961713	ZrSnPt	1	1	1	1	1	1	0	1	1	0	1	1	10	0.9628	6.6782	6.2904
466	mp-961678	ScCoTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0.8678	7.5606	7.3586
467	mp-962072	KYSn	1	0	0	1	1	1	1	1	1	1	1	1	10	0.7193	2.7879	2.5032
468	mp-9124	LiZnAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0.5475	2.5804	2.6476
469	mp-961682	TiSnPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0.4691	6.8067	6.4978
470	mp-961646	TiTeOs	1	1	1	1	1	1	0	1	1	0	1	1	10	0.4298	7.7281	7.6784
471	mp-570213	LiMgBi	1	0	0	1	1	1	1	1	1	1	1	1	10	0.3619	2.8396	2.8871
472	mp-22786	ThNiSn	1	1	1	1	1	1	0	1	1	0	1	1	10	0.2714	7.5183	7.2697
473	mp-1266	Na2Se	1	1	0	1	1	1	1	1	1	0	1	1	10	2.0162	-0.0105	-0.0028
474	mp-1958	SrTe	1	0	1	1	1	1	0	1	1	1	1	1	10	1.7623	2.8976	2.6887
475	mp-2172	AlAs	1	1	1	1	1	1	0	1	1	0	1	1	10	1.5037	3.7511	3.5939
476	mp-22895	CuI	1	1	1	1	0	1	0	1	1	1	1	1	10	1.1363	4.476	4.2801
477	mp-4025	TmNiSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0.2527	6.8923	6.6101
478	mp-20185	LuNiSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0.2159	6.9857	6.7164
479	mp-30459	ScNiBi	1	1	1	1	1	1	0	1	1	0	1	1	10	0.1844	6.9345	6.7971

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap	pred_Ef	actual_Ef
480	mp-19962	Sn2Pt	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.3125	8.0068
481	mp-20305	InAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0	3.8811	3.7986
482	mp-10183	MgSbPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0	5.9122	5.6783
483	mp-867811	TaMnRu2	1	1	0	1	0	1	1	1	1	1	1	1	10	0	7.1489	6.7668
484	mp-20340	EuN	1	1	1	1	1	1	0	1	1	0	1	1	10	0	3.2865	3.0567
485	mp-1002114	VH	1	1	1	1	1	1	0	1	1	0	1	1	10	0	6.6927	6.3637
486	mp-11488	LaTl	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.8989	7.6632
487	mp-11573	TiTc	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.3182	7.1488
488	mp-1086	TaC	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.569	8.2251
489	mp-11258	TbAu	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.8195	4.6289
490	mp-30455	HoBiPt	1	1	1	1	1	1	0	1	1	0	1	1	10	0	5.9127	5.6678
491	mp-865843	YbNdZn2	1	0	0	1	1	1	1	1	1	1	1	1	10	0	2.867	2.6528
492	mp-8638	Tc	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.6361	8.4034
493	mp-592	TiRu	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.8551	7.6303
494	mp-1101	TmAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.2202	3.9088
495	mp-1144	ErP	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.4922	4.3845
496	mp-39	Tl	1	1	1	1	1	1	0	1	1	0	1	1	10	0	5.7307	5.7592
497	mp-24153	LaH2	1	1	1	1	1	1	0	1	1	0	1	1	10	0	6.6201	6.4422
498	mp-631301	HgPRh	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.372	4.1854
499	mp-2186	NpAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.8758	8.6164
500	mp-972352	YbMg	1	1	1	1	1	1	0	1	1	0	1	1	10	0	2.1738	1.973
501	mp-867224	CaNdCd2	1	0	0	1	1	1	1	1	1	1	1	1	10	0	2.8818	2.7974
502	mp-861892	DyInRh2	1	1	0	1	0	1	1	1	1	1	1	1	10	0	7.1763	6.8642
503	mp-41	Zr	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.2678	4.1525
504	mp-865471	VGaTc2	1	1	0	1	0	1	1	1	1	1	1	1	10	0	7.2677	6.9201
505	mp-2197	BaHg	1	1	1	1	1	1	0	1	1	0	1	1	10	0	2.1413	2.4789
506	mp-962073	KBaSn	1	1	1	1	1	1	0	1	1	0	1	1	10	0	2.2929	2.0259
507	mp-1009217	MnSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0	6.8763	6.654
508	mp-980006	Yb3Os	1	1	0	1	0	1	1	1	1	1	1	1	10	0	3.1191	3.3668
509	mp-1009131	MnAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0	3.1289	2.862
510	mp-977409	NbTc2Ge	1	1	0	1	0	1	1	1	1	1	1	1	10	0	7.3043	7.0512
511	mp-1073	CaCd	1	1	1	1	1	1	0	1	1	0	1	1	10	0	2.4777	2.4264
512	mp-519	USb	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.8383	8.5018
513	mp-1172	MgRh	1	1	1	1	1	1	0	1	1	0	1	1	10	0	5.3385	5.0274
514	mp-571	TiNi	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.6396	7.2451
515	mp-4076	VCoSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.3316	7.9606
516	mp-1009079	CrTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0	6.7209	6.4731
517	mp-2442	ErAu	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.7633	4.5573
518	mp-976793	LiEr2Ga	1	0	0	1	1	1	1	1	1	1	1	1	10	0	2.7248	2.7743
519	mp-866157	TiGaRh2	1	1	0	1	0	1	1	1	1	1	1	1	10	0	7.2172	7.0602
520	mp-2012	LiHg	1	1	1	1	1	1	0	1	1	0	1	1	10	0	2.273	2.1955
521	mp-85	In	1	1	1	1	1	1	0	1	1	0	1	1	10	0	6.919	6.8952
522	mp-985806	Al2Cu	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.0513	6.7848
523	mp-631468	SrScBe	1	1	1	1	1	1	0	1	1	0	1	1	10	0	2.1018	1.9807

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap	pred_Ef	actual_Ef
524	mp-979259	V2ReMo	1	1	0	1	0	1	1	1	1	1	1	1	10	0	7.2644	7.0814
525	mp-984791	CaTmCd2	1	0	0	1	1	1	1	1	1	1	1	1	10	0	2.9163	2.7805
526	mp-1009206	MnSn	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.8128	8.4866
527	mp-2	Pd	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.3412	4.4097
528	mp-2743	LiPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0	2.5516	2.4585
529	mp-1009207	MnSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.472	8.2256
530	mp-981384	ScOs3	1	1	0	1	0	1	1	1	1	1	1	1	10	0	7.2469	7.0026
531	mp-1688	ErAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.1383	3.9159
532	mp-284	AlCo	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.5392	8.3049
533	mp-980052	Yb3In	1	0	0	1	1	1	1	1	1	1	1	1	10	0	2.726	2.9783
534	mp-980062	YbErZn2	1	0	0	1	1	1	1	1	1	1	1	1	10	0	2.7611	2.5707
535	mp-604453	CeBiPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0	6.9418	6.5488
536	mp-31459	TaCoSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.2165	8.5572
537	mp-22320	GaRu	1	1	1	1	1	1	0	1	1	0	1	1	10	0	6.6381	6.4373
538	mp-631515	CaHfZn	1	1	1	1	1	1	0	1	1	0	1	1	10	0	2.5109	2.5015
539	mp-1009264	NbCo	1	1	1	1	1	1	0	1	1	0	1	1	10	0	5.7025	5.5509
540	mp-21215	InPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.2624	8.0576
541	mp-865992	YbSnRh2	1	1	0	1	0	1	1	1	1	1	1	1	10	0	7.1259	7.0727
542	mp-979939	Yb3W	1	1	0	1	0	1	1	1	1	1	1	1	10	0	2.6725	2.6853
543	mp-1610	TbS	1	1	1	1	1	1	0	1	1	0	1	1	10	0	6.7187	6.6019
544	mp-864620	CaSmCd2	1	0	0	1	1	1	1	1	1	1	1	1	10	0	2.8426	2.7516
545	mp-11375	EuHg	1	0	1	1	1	1	0	1	1	1	1	1	10	0	2.8454	2.9072
546	mp-926	PuP	1	1	1	1	1	1	0	1	1	0	1	1	10	0	9.3065	8.9739
547	mp-829	AlPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.9077	7.7534
548	mp-8642	Re	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.7739	7.4711
549	mp-1008926	CrTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0	3.9949	3.8599
550	mp-1912	ZnAg	1	1	1	1	1	1	0	1	1	0	1	1	10	0	3.3466	3.4195
551	mp-1018074	GaFeNi2	1	1	0	1	0	1	1	1	1	1	1	1	10	0	7.158	6.7585
552	mp-980947	SrCaHg2	1	0	0	1	1	1	1	1	1	1	1	1	10	0	2.8683	2.7672
553	mp-1002122	HfIr	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.8337	7.4415
554	mp-2545	YbHg	1	1	1	1	1	1	0	1	1	0	1	1	10	0	2.5723	2.6373
555	mp-7171	TmP	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.5311	4.3817
556	mp-2493	CeN	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.7606	8.6302
557	mp-864883	MgSnPd2	1	1	0	1	0	1	1	1	1	1	1	1	10	0	7.2126	7.0531
558	mp-832	HoPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.6041	4.4118
559	mp-631452	NbCrW	1	1	1	0	1	1	0	1	1	1	1	1	10	0	4.6635	4.3453
560	mp-864734	HfInPd2	1	1	0	1	0	1	1	1	1	1	1	1	10	0	7.3103	6.9487
561	mp-980049	Yb3Re	1	0	0	1	1	1	1	1	1	1	1	1	10	0	2.8847	2.7422
562	mp-11261	YAu	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.7553	4.6004
563	mp-2226	DyPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.7989	4.4696
564	mp-867902	LiSiRh2	1	1	0	1	0	1	1	1	1	1	1	1	10	0	7.3013	6.9246
565	mp-868003	LaInAu2	1	1	0	1	0	1	1	1	1	1	1	1	10	0	7.2556	7.0483
566	mp-1009592	CrFeTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.1392	7.9973
567	mp-631543	AlInB	1	1	1	1	1	1	0	1	1	0	1	1	10	0	6.7032	6.5333

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap	pred_Ef	actual_Ef
568	mp-31460	NbCoSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.1085	8.0841
569	mp-962067	BaNaSn	1	1	1	1	1	1	0	1	1	0	1	1	10	0	2.4429	2.3264
570	mp-8635	Zr	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.2994	4.2222
571	mp-15778	MgNiSb	1	1	1	1	1	1	0	1	1	0	1	1	10	0	6.971	6.7454
572	mp-30658	VGaNi2	1	1	0	1	0	1	1	1	1	1	1	1	10	0	7.257	7.1086
573	mp-12558	LiMgAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0	2.4763	2.1775
574	mp-31457	ZrSbRu	1	1	1	1	1	1	0	1	1	0	1	1	10	0	6.6699	6.2987
575	mp-475	SnP	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.9427	7.8952
576	mp-631384	Sr2VW	1	0	0	1	1	1	1	1	1	1	1	1	10	0	2.8655	2.8984
577	mp-1008872	MnFeTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.1279	7.902
578	mp-2104	UAs	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.7429	8.4021
579	mp-744	HoP	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.4401	4.2894
580	mp-11388	GaIr	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.878	8.0867
581	mp-865920	YbPmZn2	1	0	0	1	1	1	1	1	1	1	1	1	10	0	2.7911	2.6584
582	mp-567089	YbRh	1	1	1	1	1	1	0	1	1	0	1	1	10	0	3.815	3.594
583	mp-2547	YbPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0	3.3731	3.1314
584	mp-11452	HfOs	1	1	1	1	1	1	0	1	1	0	1	1	10	0	6.8325	6.7506
585	mp-1703	YbZn	1	1	1	1	1	1	0	1	1	0	1	1	10	0	2.1778	1.9687
586	mp-1476	ScS	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.8998	7.5207
587	mp-631540	NiBTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.6992	8.3288
588	mp-50	Ta	1	1	1	1	1	1	0	1	1	0	1	1	10	0	5.3655	5.3872
589	mp-1008875	Mn2Sb	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.0646	6.8742
590	mp-3201	Li2GaPd	1	0	0	1	1	1	1	1	1	1	1	1	10	0	2.8899	2.7852
591	mp-2802	HfRu	1	1	1	1	1	1	0	1	1	0	1	1	10	0	6.8574	6.7614
592	mp-1486	ZnNi	1	1	1	1	1	1	0	1	1	0	1	1	10	0	5.6586	5.4528
593	mp-864876	TbInRh2	1	1	0	1	0	1	1	1	1	1	1	1	10	0	7.1306	6.8478
594	mp-961656	VFeTe	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.763	8.7414
595	mp-2818	YbAu	1	1	1	1	1	1	0	1	1	0	1	1	10	0	3.7608	3.5674
596	mp-1561	TbSe	1	1	1	1	1	1	0	1	1	0	1	1	10	0	5.9	5.8059
597	mp-1129	ScIr	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.1759	7.0315
598	mp-930	ZrP	1	1	1	1	1	1	0	1	1	0	1	1	10	0	6.9408	6.8636
599	mp-865577	Li2CdAu	1	1	0	1	0	1	1	1	1	1	1	1	10	0	2.6311	2.4973
600	mp-2288	PuSe	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.4715	8.7459
601	mp-931	ThP	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.5187	7.4805
602	mp-899	InRh	1	1	1	1	1	1	0	1	1	0	1	1	10	0	9.1282	9.1032
603	mp-2011	UP	1	1	1	1	1	1	0	1	1	0	1	1	10	0	9.6012	9.6418
604	mp-1161	LaSe	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.7598	7.8543
605	mp-10194	LuSbPt	1	1	1	1	1	1	0	1	1	0	1	1	10	0	6.727	6.4308
606	mp-851	ErPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.5888	4.4274
607	mp-1282	VC	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.474	8.2028
608	mp-2083	Sn2Ir	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.6395	8.3859
609	mp-976596	LiLu2Ga	1	0	0	1	1	1	1	1	1	1	1	1	10	0	2.8158	2.7942
610	mp-11245	HoAu	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.7261	4.5265
611	mp-348	TmPd	1	1	1	1	1	1	0	1	1	0	1	1	10	0	4.5763	4.3862

No.	cif_id	Crystal strcture	A	B	C	D	E	F	G	H	I	J	K	L	Total match	Bandgap	pred_Ef	actual_Ef
612	mp-1487	AlNi	1	1	1	1	1	1	0	1	1	0	1	1	10	0	9.3342	9.259
613	mp-31452	ZrNiBi	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.0645	7.3037
614	mp-2540	VTc	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.0455	7.6507
615	mp-631274	KFeP	1	1	1	1	1	1	0	1	1	0	1	1	10	0	2.5679	2.6245
616	mp-631449	LiTaBe	1	1	1	1	1	1	0	1	1	0	1	1	10	0	2.3897	2.2106
617	mp-1008999	LaSe	1	1	1	1	1	1	0	1	1	0	1	1	10	0	8.5973	8.7064
618	mp-987	ZnCu	1	1	1	1	1	1	0	1	1	0	1	1	10	0	5.3672	5.1028
619	mp-256	LaN	1	1	1	1	1	1	0	1	1	0	1	1	10	0	7.8657	7.8908

Supplementary Table 9. Calculations of Mean Absolute Error (MAE) of the power factor for the 5 predicted compounds.

Material	Category	Predicted	Actual	Absolute Error
TiGePt	A	0.895459233	1.0737	0.178240767
	B	0.560856437	0.52287	0.037986437
	C	0.103746524	0.13224	0.028493476
	D	2.00411877	1.9385	0.06561877
	E	0.550344551	0.69027	0.139925449
	F	0.114029471	0.15126	0.037230529
	G	2.125983024	1.7971	0.328883024
	H	0.679412173	0.53511	0.144302173
	I	0.153885805	0.10908	0.044805805
	J	3.132287016	2.6343	0.497987016
	K	0.744137635	0.66957	0.074567635
	L	0.13898344	0.1267	0.01228344
NbFeSb	A	1.710981449	0.714	0.996981449
	B	0.626356905	0.543	0.083356905
	C	0.089616253	0.17	0.080383747
	D	2.754388229	1.57	1.184388229
	E	0.281267197	0.809	0.527732803
	F	0.044741974	0.197	0.152258026
	G	1.861662244	2.24	0.378337756
	H	0.734183821	0.64	0.094183821
	I	0.163543476	0.128	0.035543476
	J	2.715426725	3.29	0.574573275
	K	0.669671469	0.789	0.119328531
	L	0.110717267	0.084	0.026717267
ZrSiPd	A	1.328269412	1.3917	0.063430588
	B	0.638400031	0.56833	0.070070031
	C	0.100808597	0.13109	0.030281403
	D	2.448769615	2.3769	0.071869615

Material	Category	Predicted	Actual	Absolute Error
	E	0.562896882	0.75633	0.193433118
	F	0.105464752	0.1584	0.052935248
	G	2.035492918	1.8622	0.173292918
	H	0.672417178	0.62626	0.046157178
	I	0.150925354	0.13427	0.016655354
	J	3.121642983	2.7486	0.373042983
	K	0.81331712	0.7676	0.04571712
	L	0.148811714	0.15129	0.002478286
ZrSiPt	A	1.886287107	1.2465	0.639787107
	B	0.692162467	0.4283	0.263862467
	C	0.087377421	0.092634	0.005256579
	D	2.915366657	2.1314	0.783966657
	E	0.517761346	0.59274	0.074978654
	F	0.099179566	0.11682	0.017640434
	G	1.953580915	2.1013	0.147719085
	H	0.674642155	0.68564	0.010997845
	I	0.156199547	0.14185	0.014349547
	J	2.949819079	3.0663	0.116480921
	K	0.816606484	0.82369	0.007083516
	L	0.147863506	0.15812	0.010256494
ZrInAu	A	1.10148154	1.0352	0.06628154
	B	0.596133019	0.67747	0.081336981
	C	0.06732609	0.19442	0.12709391
	D	2.126659604	2.0807	0.045959604
	E	0.344720766	0.92321	0.578489234
	F	0.07400919	0.18476	0.11075081
	G	1.69091934	1.9819	0.29098066
	H	0.640531506	0.56401	0.076521506
	I	0.154860651	0.11173	0.043130651
	J	2.355808994	3.0522	0.696391006
	K	0.635544655	0.65474	0.019195345
	L	0.123847472	4.7262E-08	0.123847425
MAE				0.189