Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Predicting Two-Dimensional Semiconductors Using Conductivity Effective Mass - Supplementary Information

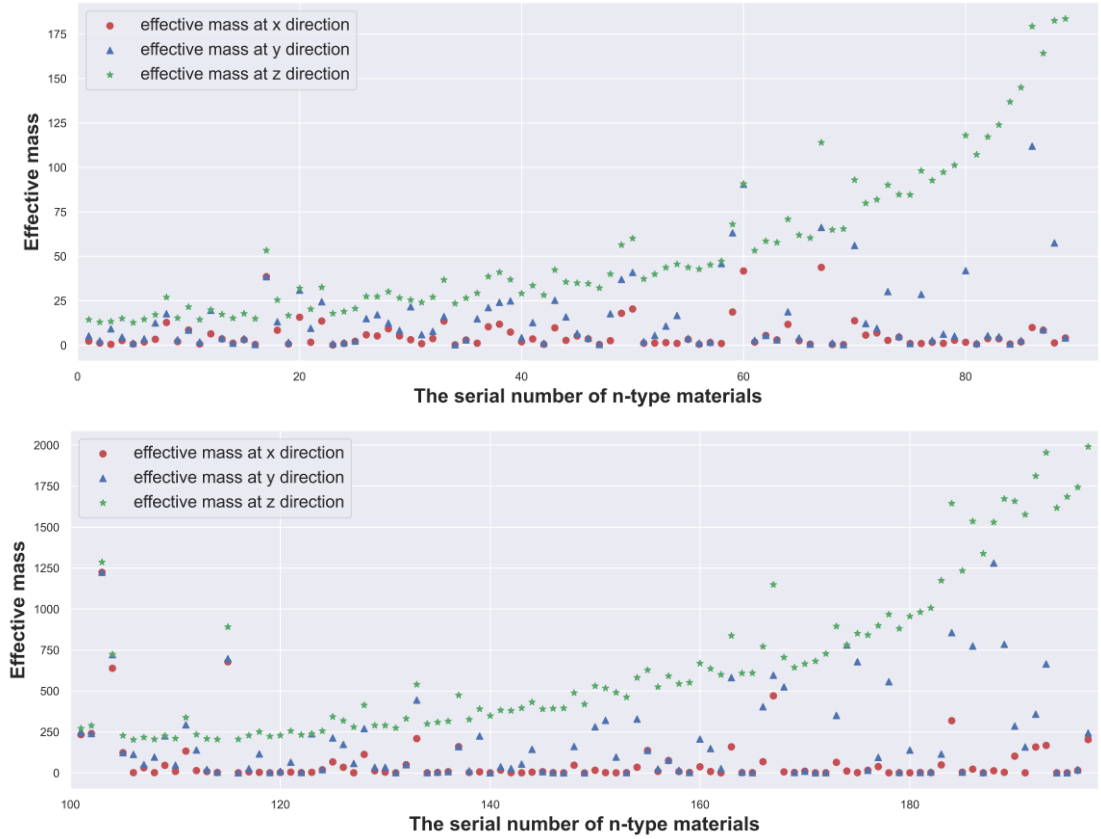


Figure S1 The effective mass distribution in the three crystallographic directions for a sample of materials shown in Figure 5-b of the main text. 186 materials were selected for display using an interval sampling method for the 904 materials with conductivity effective mass less than 2000. 0-100 are displayed in the top panel and 100-186 are displayed in the bottom panel. Please not the large difference in the y axis for the top and bottom plots.

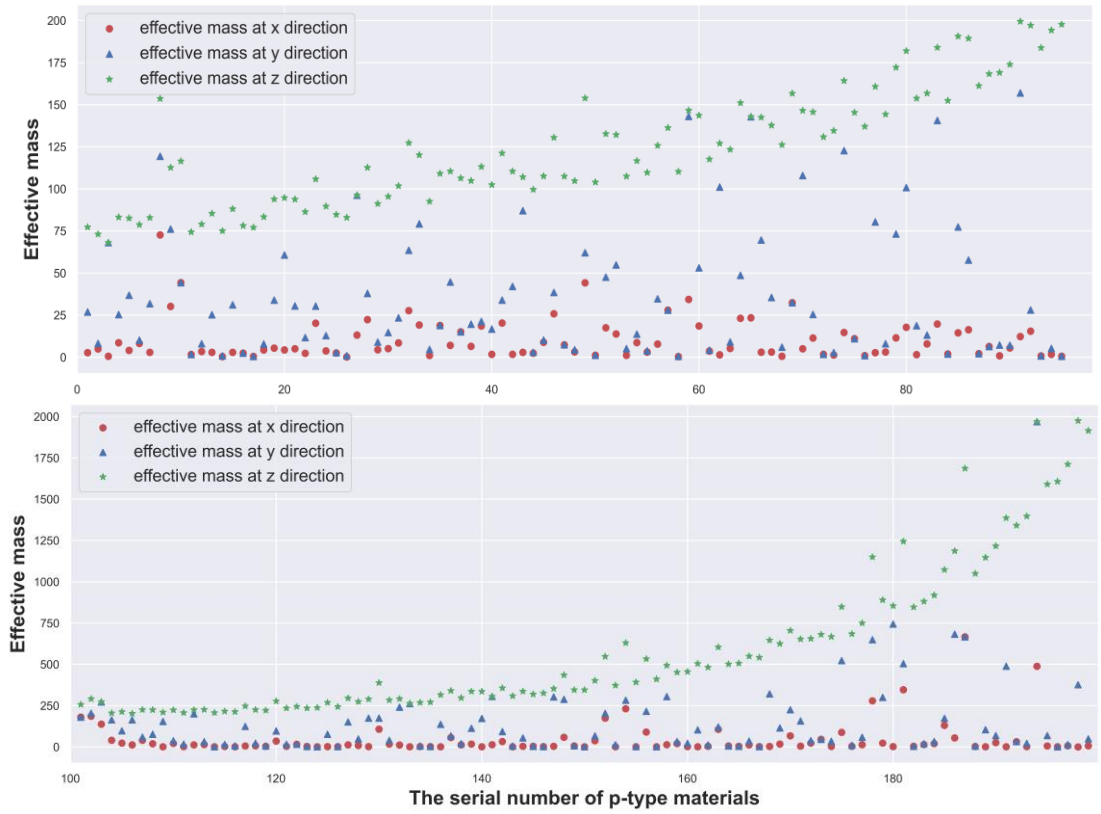
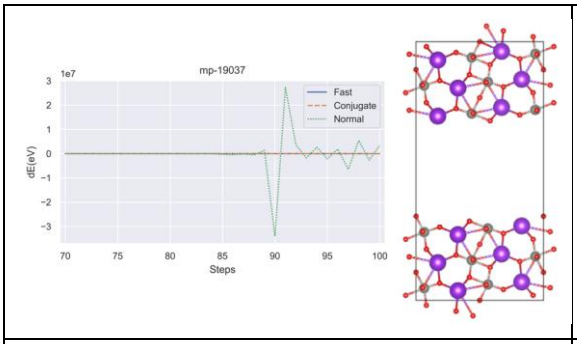
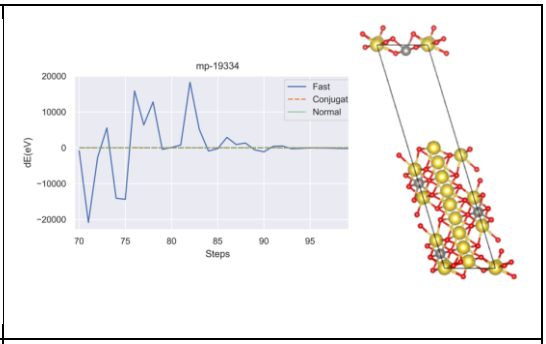


Figure S2 The effective mass distributions in the three crystallographic directions for a sample of materials shown in Figure 5-d of the main text. 194 materials were selected for display using an interval sampling method for the 867 materials with conductivity effective mass less than 2000. 0-100 are displayed in the top panel and 100-194 are displayed in the bottom panel. Please not the large difference in the y axis for the top and bottom plots.

When performing structural optimization and static calculations for a thousand candidate materials of each type p and n, we found that including the spin polarization of electrons made convergence difficult for a significant portion of the materials and so were omitted. For the choice of algorithms, Fast, Conjugate and Normal algorithms were employed sequentially to converge the structure. However, some materials still failed to reach the convergence criteria, and the convergence of the energy of p- and n-type materials at the level of PBE functional as well as the level of PBE-vdW functional calculation, respectively, is shown in the Figures S3 to S6.


mp-19037
1e7
Fast
Conjugate
Normal
dE(eV)
Steps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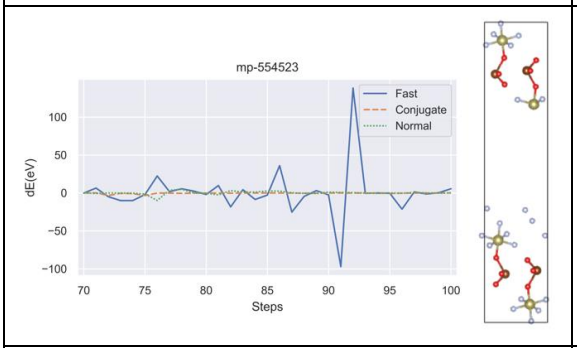
Conjugat
Normal
dE(eV)
Steps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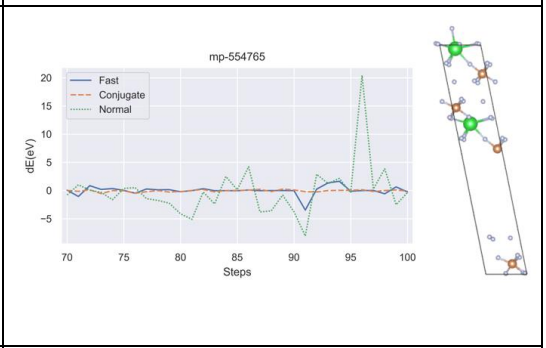
Fast
Conjugate
Normal
dE(eV)
Steps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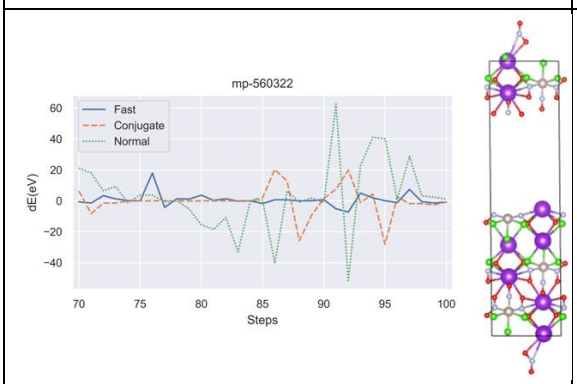
Conjugate
Normal
dE(eV)
Steps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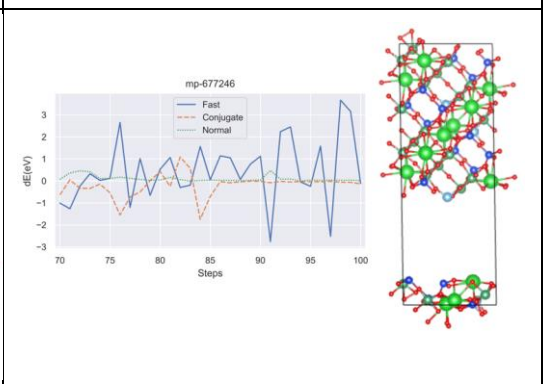
Fast
Conjugate
Normal
dE(eV)
Steps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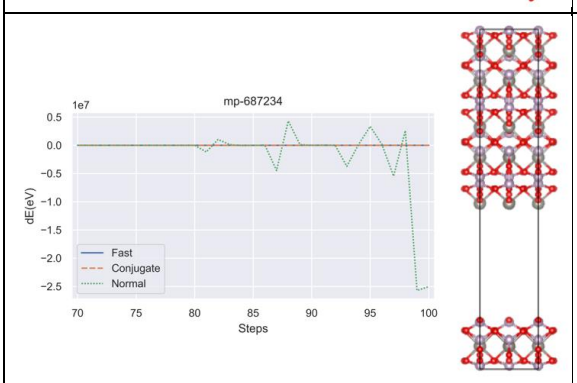
Fast
Conjugate
Normal
dE(eV)
Steps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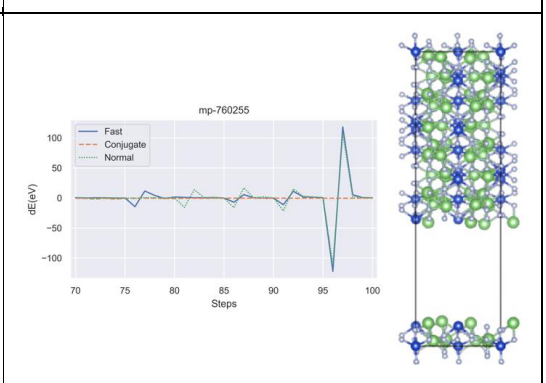
1e7
Fast
Conjugate
Normal
dE(eV)
Steps


mp-760255
Fast
Conjugate
Normal
dE(eV)
Steps

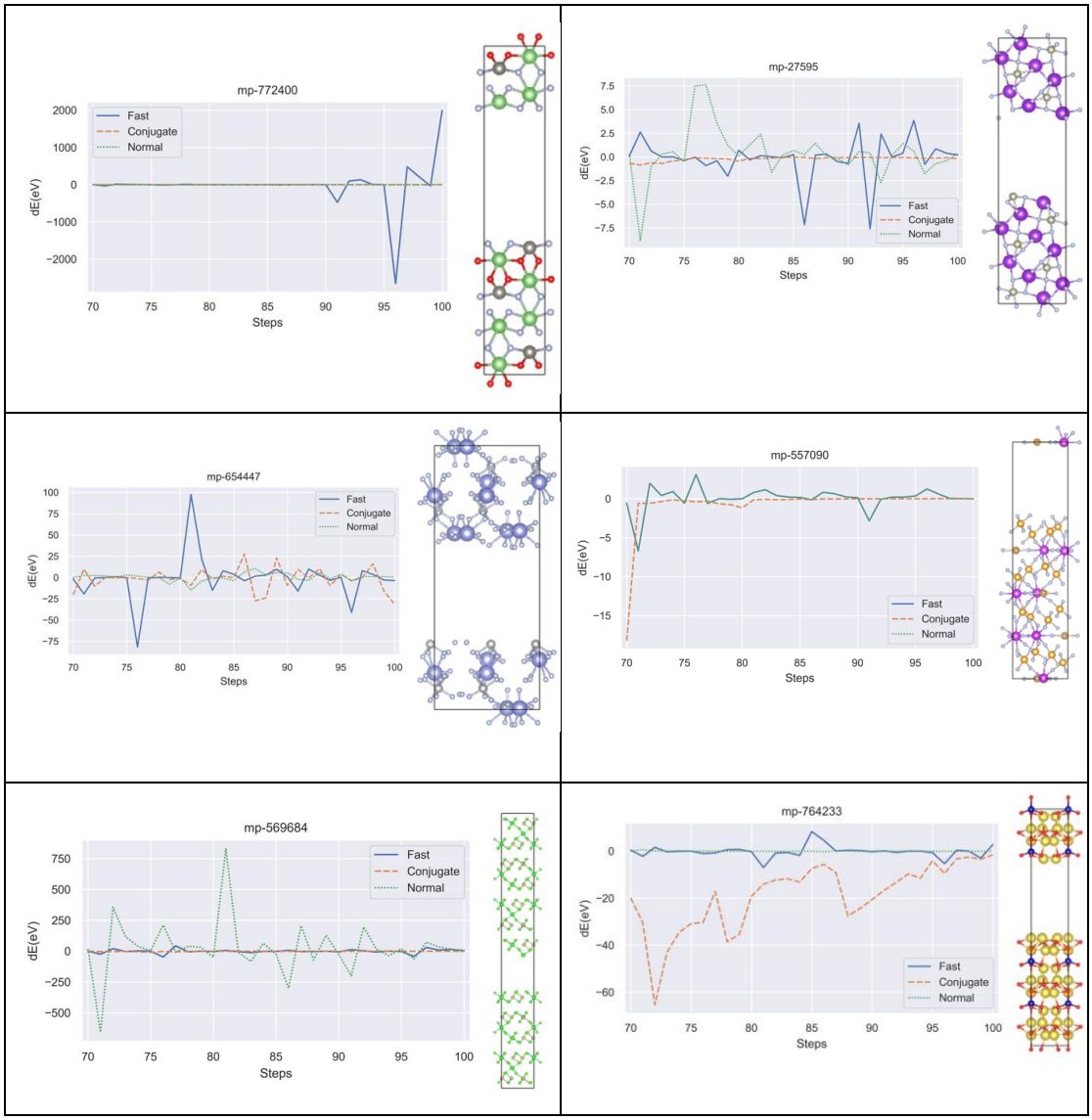
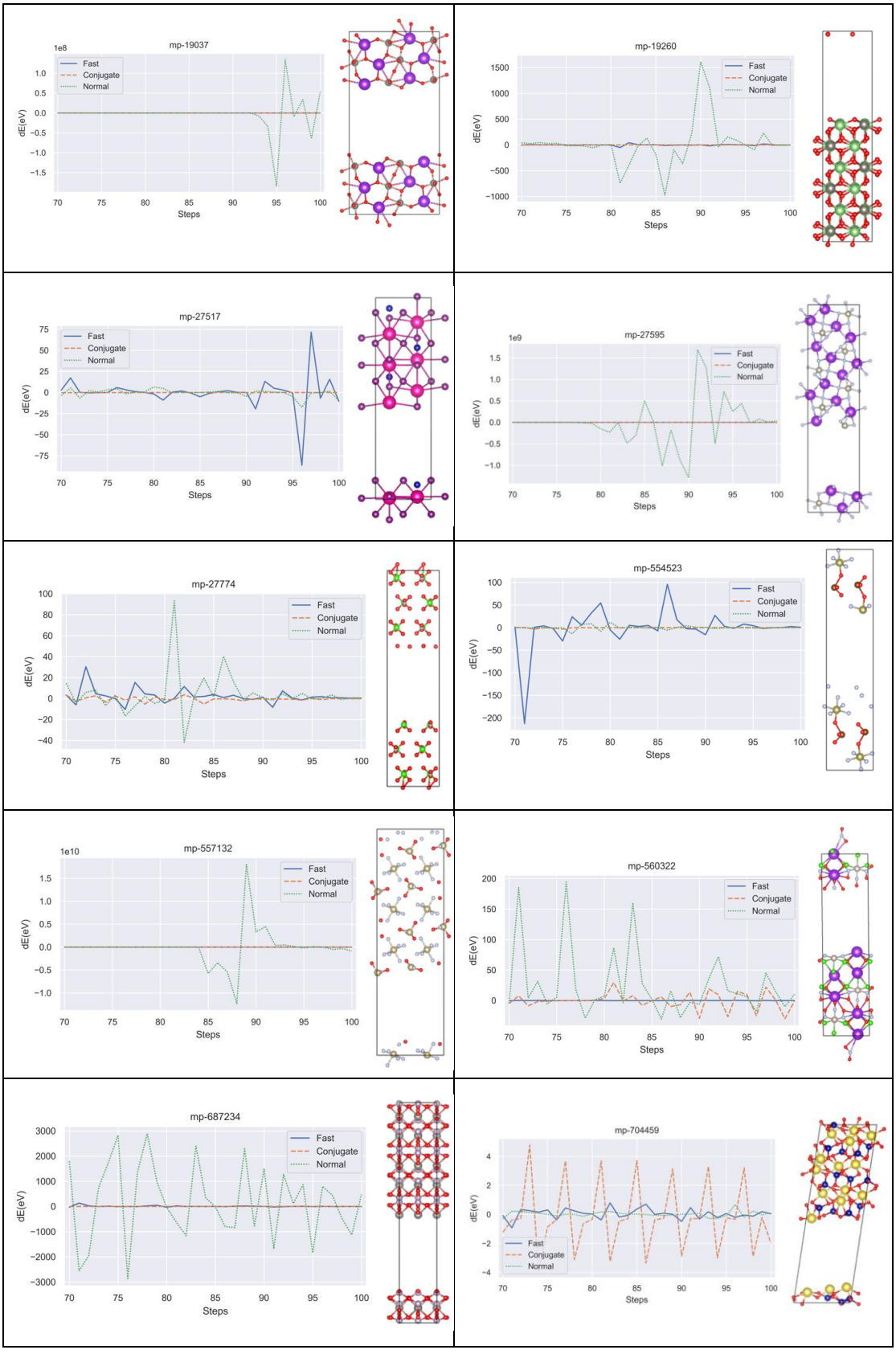


Figure S3 Diagrams depicting the change in energy (dE) during the relaxation of the p-type materials that failed to converge at the PBE level. The horizontal axis of the graph depicts the number of calculation steps and the colours represent the algorithms used during the calculation. The title of each graph is the Materials Project ID number. On the right side, the structure of the slab configuration is shown.


mp-19037
1e8
Fast
Conjugate
Normal
dE(eV)
Steps
mp-19260
mp-27517
mp-27595
1e9
mp-27774
mp-554523
mp-557132
1e10
mp-560322
mp-687234
mp-704459

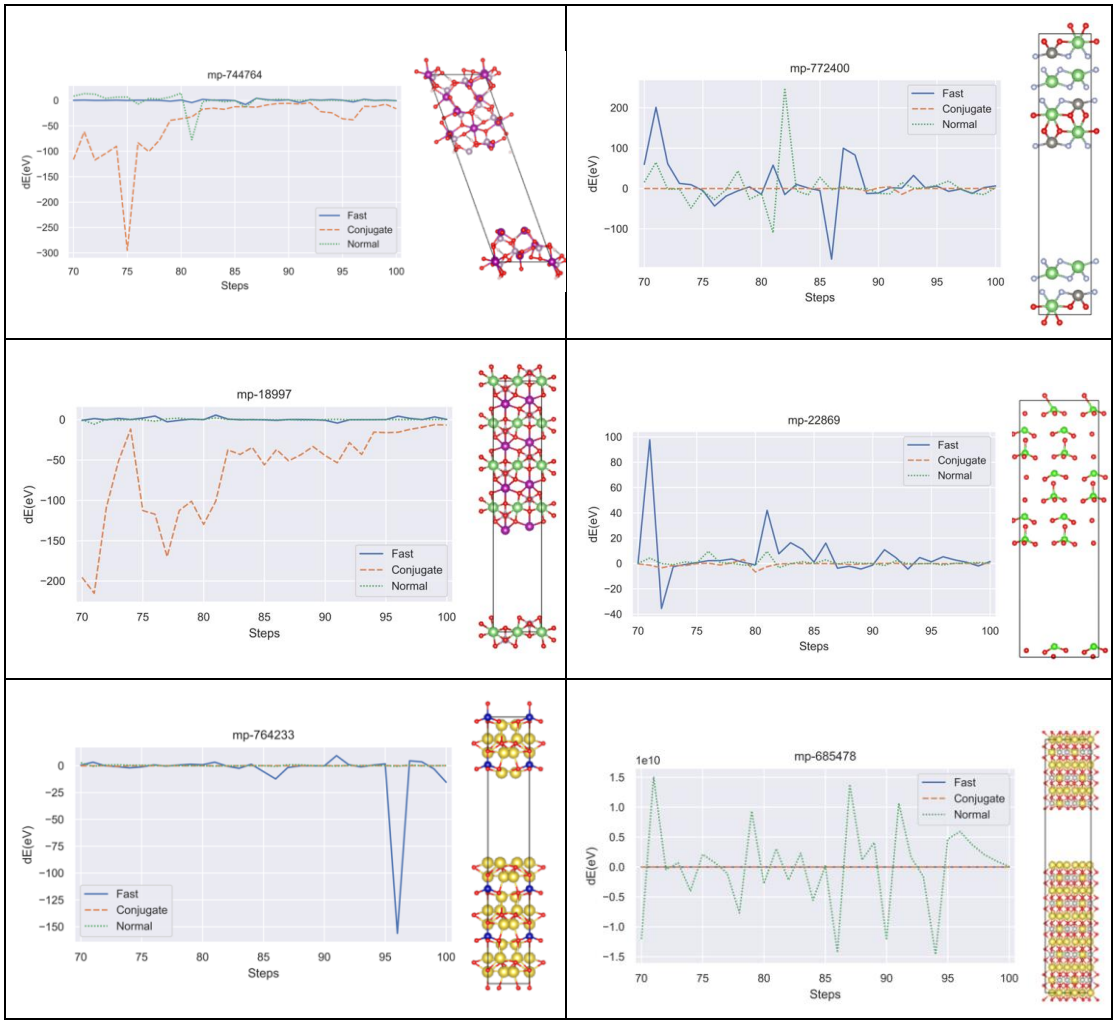


Figure S4 Diagrams depicting the change in energy (dE) during the relaxation of the n-type materials that failed to converge at the PBE level. The horizontal axis of the graph depicts the number of calculation steps and the colours represent the algorithms used during the calculation. The title of each graph is the Materials Project ID number. On the right side, the structure of the slab configuration is shown.

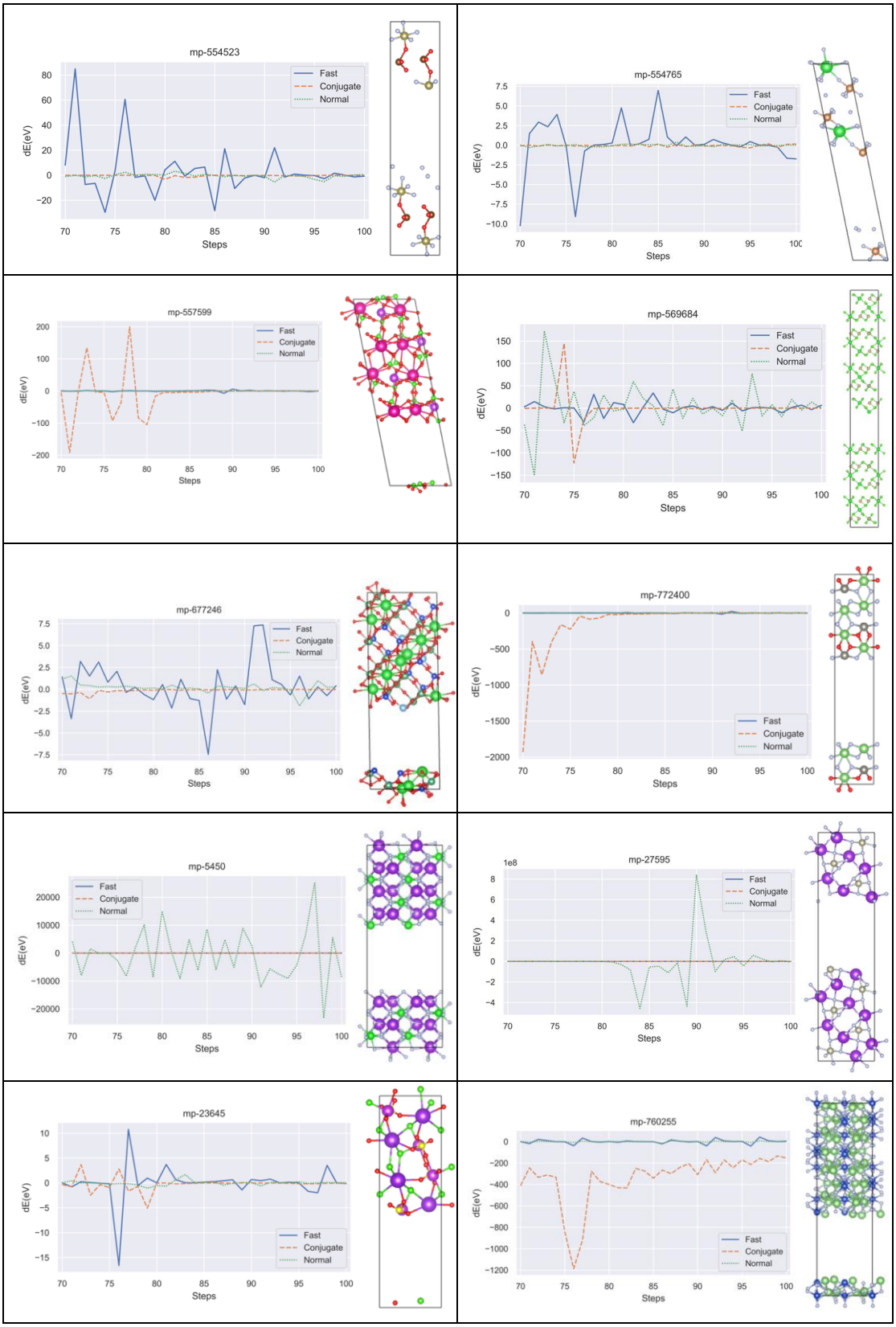
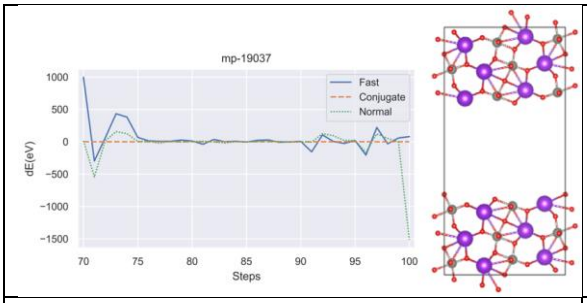
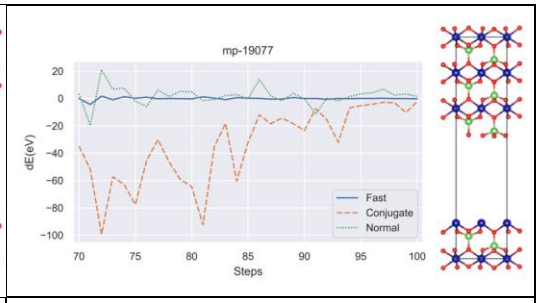
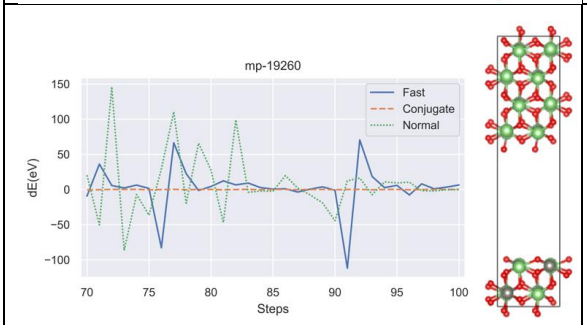


Figure S5 Diagrams depicting the change in energy (dE) during the relaxation of the p-type materials that failed to converge at the PBE+vdW level. The horizontal axis of the graph depicts the number of calculation steps and the colours represent the algorithms used during the calculation. The title of each graph is the Materials Project ID number. On the right side, the structure of the slab configuration is shown.


mp-19037
Fast
Conjugate
Normal
dE(eV)
Steps


mp-19077
Fast
Conjugate
Normal
dE(eV)
Steps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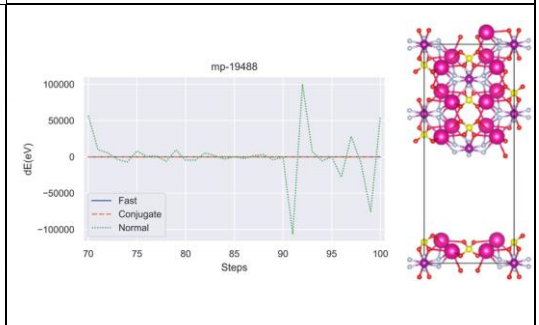
Fast
Conjugate
Normal
dE(eV)
Steps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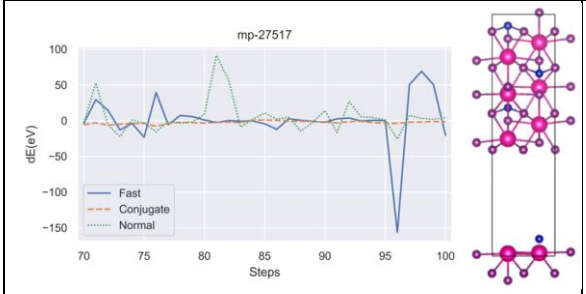
Conjugate
Normal
dE(eV)
Steps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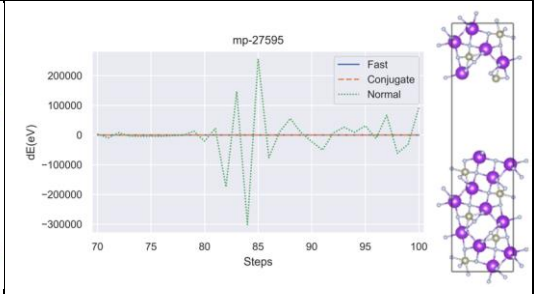
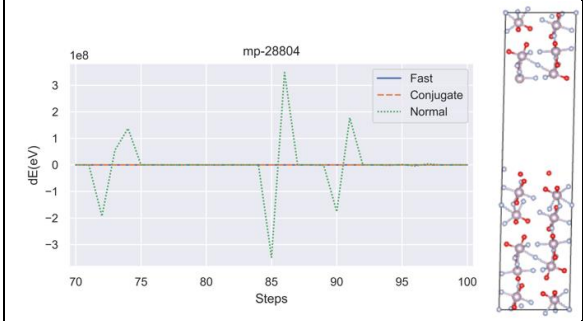
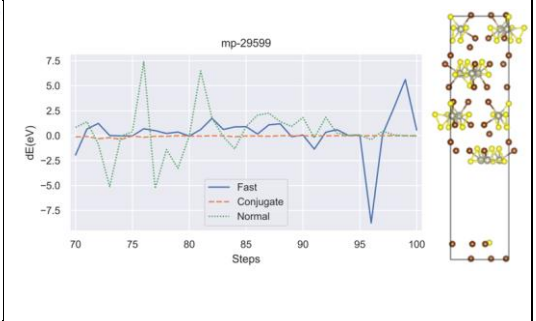
Fast
Conjugate
Normal
dE(eV)
Steps


mp-27595
Fast
Conjugate
Normal
dE(eV)
Steps


mp-28804
1e8
Fast
Conjugate
Normal
dE(eV)
Steps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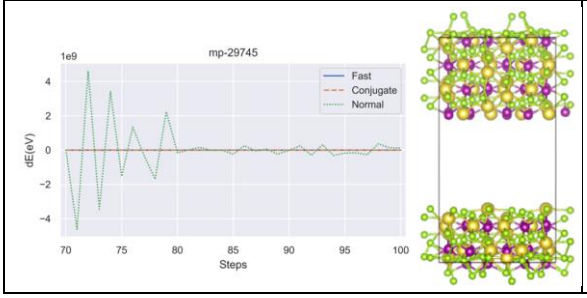
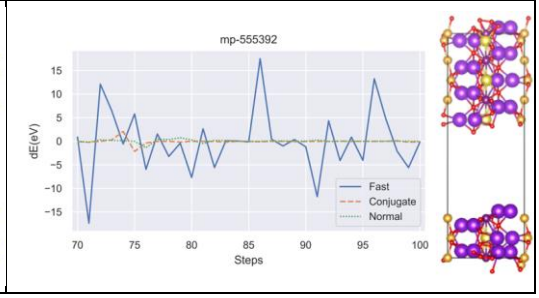
Fast
Conjugate
Normal
dE(eV)
Steps


mp-29745
1e9
Fast
Conjugate
Normal
dE(eV)
Steps


mp-555392
Fast
Conjugate
Normal
dE(eV)
Steps

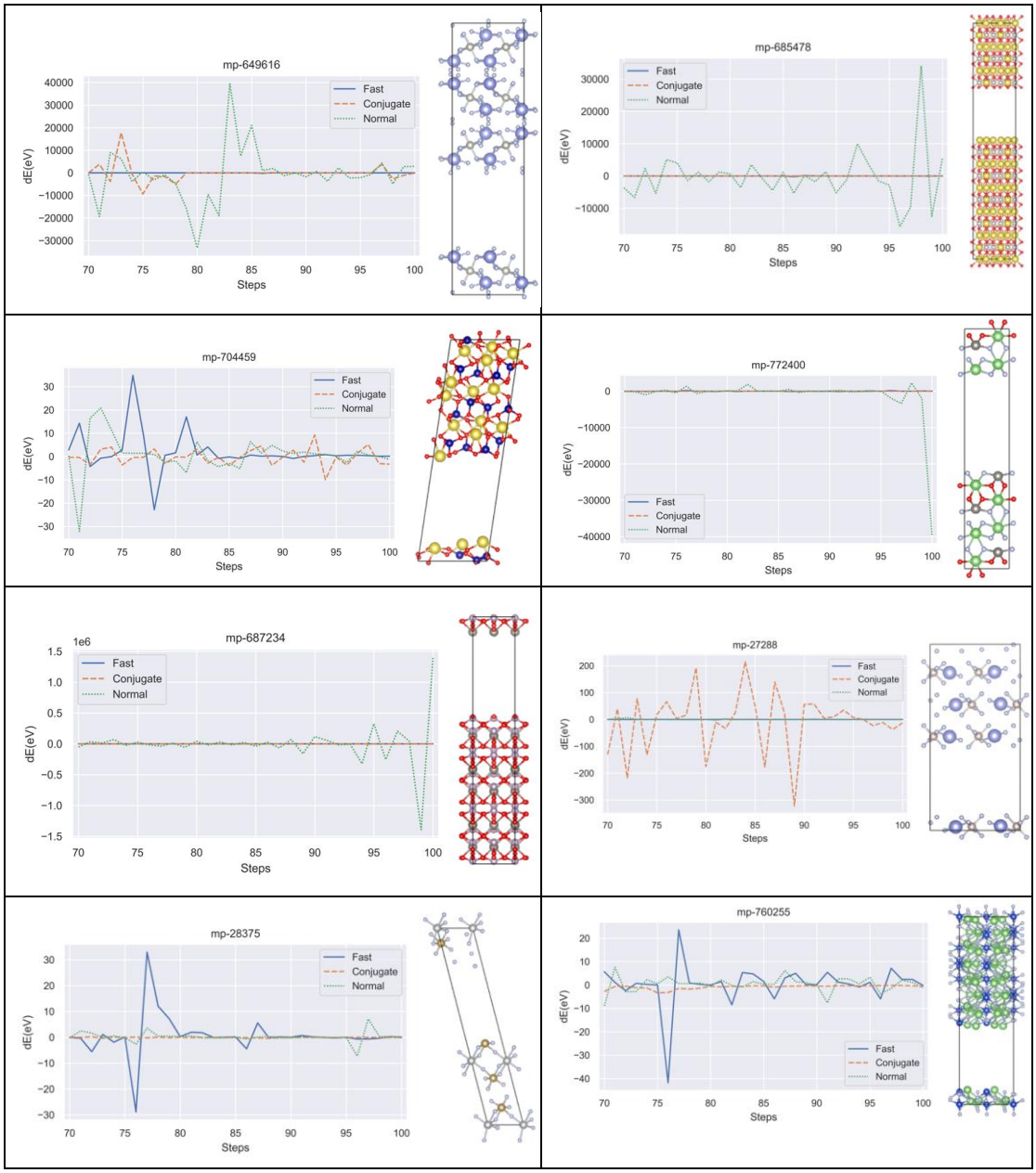


Figure S6 Diagrams depicting the change in energy (dE) during the relaxation of the n-type materials that failed to converge at the PBE+vdW level. The horizontal axis of the graph depicts the number of calculation steps and the colours represent the algorithms used during the calculation. The title of each graph is the Materials Project ID number. On the right side, the structure of the slab configuration is shown.

From the convergence process of the above materials, we can find that the energy change of most of the materials is haphazard, and the difference between the energy obtained from adjacent steps in the convergence process of some structures reaches outlandish extremes such as for mp-28804, mp-29745, mp-27595, mp-685478. There are some materials that have a gradual decrease in energy change during convergence, such as mp-560322, mp-27774, mp-554523, for which it is possible that they may converge eventually given enough calculation steps. However, some materials have been in a state of energy oscillation during the calculation

process and will likely never converge such as: mp-760255, mp-704459, mp-649616, mp-29745, mp-22869, mp-27774. Overall the cases of nonconvergence represent a very small minority of the data represented in this work.

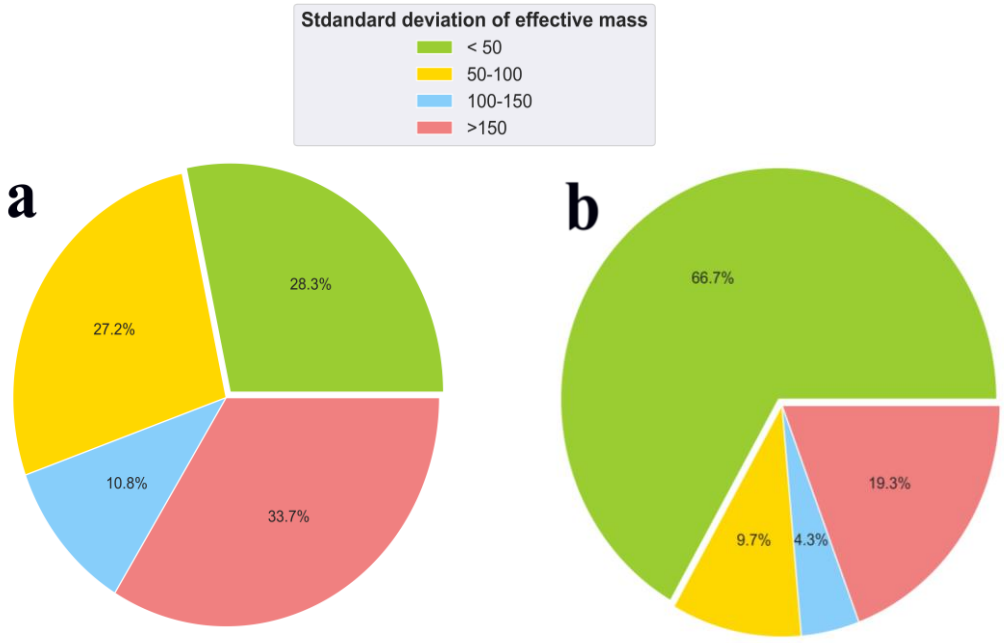


Figure S7: Interval distribution of conductivity effective mass standard deviation for (a) p-type and (b) n-type materials in Figure 5-d and -b of the main text.

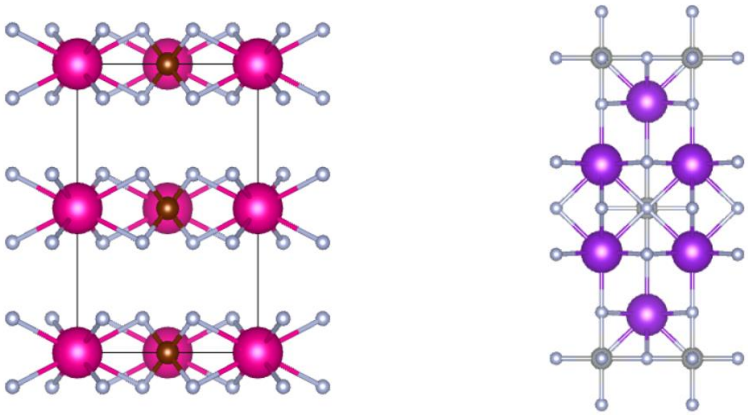


Figure S8: The schematic drawing of unit cell of the material with negative exfoliation. Left is mp-28577 with the chemical formula $RbBrF_4$, and the right is mp-556546, with the chemical formula K_2NiF_4.

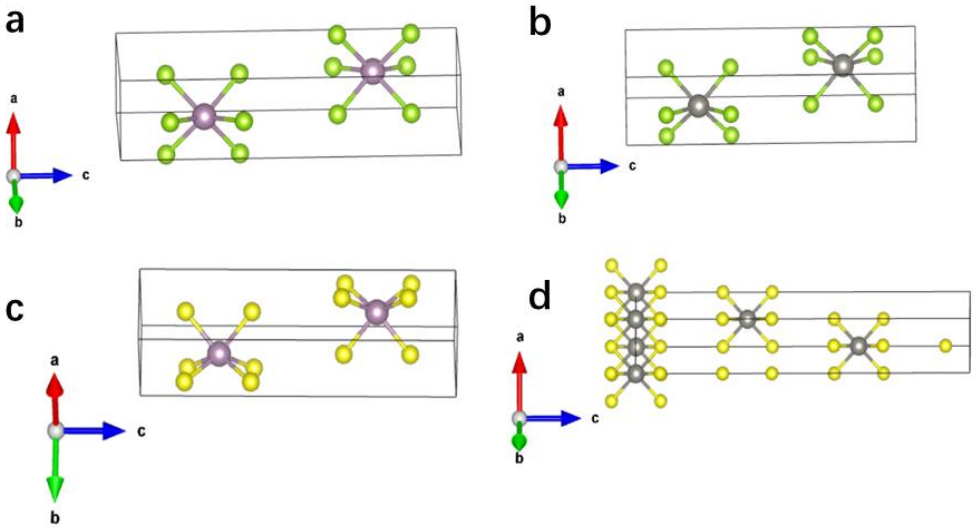


Figure S9 The atomic structure of a) $MoSe_2$ b) WSe_2 c) MoS_2 and d) WS_2.

Table S1 Data for the results shown in Figure 5-b (n-type doping) along with Material Project ID (MPID) and chemical formula.

MPID	Formula	Standard deviation of effective mass	E_f (eV/ Å^2)
mp-556546	K_2NiF_4	1000	0.004
mp-28479	Sc_2CCl_2	37.377	0.011
mp-567441	HfIN	164.028	0.011
mp-29966	NOF	7.637	0.008
mp-505727	NClO	45.887	0.007
mp-541911	HfNCl	47.249	0.016
mp-28233	$MnCl_2$	6.411	0.02
mp-552120	YClO	304.938	0.015
mp-27850	TiNCl	1000	0.015
mp-568592	ZrNCl	81.757	0.017
mp-546279	ScBrO	1000	0.014
mp-754031	YBrO	85.648	0.016
mp-27849	TiBrN	1000	0.016
mp-541912	ZrBrN	60.952	0.018
mp-30031	CaI_2	64.214	0.013
mp-643265	ReF_7	9.522	0.009
mp-568346	HfBrN	1000	0.015
mp-558928	KrF_2	8.825	0.011
mp-28306	$MnBr_2$	286.679	0.022
mp-23052	ZrIN	1000	0.017
mp-28257	SOF_2	9.03	0.007
mp-23184	BCl_3	5.267	0.009
mp-28013	MnI_2	84.792	0.024
mp-22987	BiIO	11.906	0.02
mp-554108	$LiRe(OF_2)_2$	309.02	0.014
mp-14653	$AgSb_2F_{12}$	104.41	0.013
mp-23072	BiBrO	6.077	0.022
mp-23309	$ScCl_3$	7.479	0.01
mp-23225	BBr_3	9.314	0.01
mp-23280	$AsCl_3$	12.579	0.011
mp-30103	AuF_5	90.227	0.009
mp-697133	Cs_2CaH_4	9.862	0.022
mp-28067	ThIN	24.438	0.027
mp-23189	BI_3	5.812	0.012
mp-573051	ReO_3F	7.545	0.012
mp-561317	Rb_2NiF_4	1000	0.03
mp-28099	SBr	12.025	0.017
mp-19167	Rb_2NiO_2	80.834	0.035

mp-29940	$SbClF_{10}$	1000	0.012
mp-22978	Rb_2MnCl_4	1000	0.029
mp-560851	$CsIOF_4$	30.547	0.017
mp-560449	$K_3Ni_2F_7$	543.866	0.045
mp-30943	$MgPSe_3$	55.675	0.021
mp-19252	K_2NiO_2	32.672	0.05
mp-8616	$ScAg(PS_3)_2$	11.061	0.023
mp-30295	W_6CCl_{18}	47.448	0.01
mp-28938	Nb_3TeCl_7	9.572	0.019
mp-558725	$Ba_5Ru_2Br_2O_9$	35.562	0.027
mp-642795	$PHSF_2$	5.391	0.021
mp-7148	$K_2SrTa_2O_7$	1000	0.051
mp-27358	Se_2O_5	12.301	0.026
mp-29422	$HfCl_4$	11.566	0.018
mp-23472	$Re(AgCl_3)_2$	12.521	0.025
mp-8192	Rb_2PtF_6	414.351	0.03
mp-561379	$GaRe(Cl_3O)_2$	25.821	0.01
mp-10402	$TiTl_2F_6$	15.446	0.029
mp-7979	K_2PdF_6	36.232	0.034
mp-3821	K_2PtF_6	25.801	0.036
mp-27501	Cs_2ThCl_6	84.576	0.021
mp-30984	$S(IO_3)_2$	5.617	0.015
mp-30977	B_5H_8Br	9.04	0.012
mp-27782	$XeIF_7$	66.555	0.019
mp-28601	$NbBr_5$	15.55	0.015
mp-29402	$KGaI_4$	7.274	0.019
mp-3970	K_2TiF_6	16.734	0.042
mp-7824	K_2ReF_6	13.822	0.039
mp-555805	$AlSCl_7$	26.41	0.031
mp-680059	$Re_3(SCl)_7$	389.736	0.016
mp-622197	$Cs_2PtS_6(O_3F)_6$	1000	0.017
mp-23076	Rb_2CoCl_4	384.623	0.02
mp-764233	Na_8CoO_6	26.061	0.039
mp-562569	$CsPPbS_4$	30.236	0.031
mp-561011	$Li_2Ta_2(OF_2)_3$	263.593	0.05
mp-624117	$Cs_3V_4Te_2ClO_{14}$	414.251	0.037
mp-29432	$NaScCl_4$	26.034	0.036
mp-8720	Rb_2MnTe_2	11.563	0.029
mp-638009	$RbPPbS_4$	15.74	0.035
mp-2865	K_2CuF_4	39.43	0.046
mp-9321	Ba_2HfS_4	52.806	0.063
mp-13985	Li_2PdF_6	302.332	0.07
mp-754128	$Ba_3Hf_2O_7$	13.48	0.089

mp-18003	$CsCuS_4$	40.912	0.034
mp-638150	$KPPbS_4$	25.154	0.038
mp-556741	$KNaThF_6$	145.108	0.046
mp-17095	$CsCuSe_4$	46.414	0.032
mp-10322	$BaHfN_2$	180.93	0.094
mp-8335	Ba_2ZrO_4	15.023	0.09
mp-3104	$BaZrN_2$	111.406	0.093
mp-755895	$Ba_3Zr_2O_7$	35.055	0.091
mp-9205	$KSeO_2F$	22.678	0.06
mp-27389	KSb_2F_7	62.235	0.025
mp-8719	K_2MnTe_2	15.405	0.037
mp-559068	$Na_2Pd(SeO_4)_2$	23.203	0.059
mp-540584	K_2PdO_2	42.654	0.089
mp-18365	$RbCuSe_4$	6.316	0.036
mp-5532	Sr_2TiO_4	1000	0.116
mp-3349	$Sr_3Ti_2O_7$	185.856	0.115
mp-6560	KSO_2F	45.937	0.066
mp-18996	TlV_3O_8	12.88	0.041
mp-9517	$SrTiN_2$	1000	0.121
mp-867570	$Rb_4Sb_2O_5$	29.446	0.034
mp-6384	$RbSO_2F$	52.814	0.063
mp-556645	$RbNbAsClO_5$	85.26	0.041
mp-29405	$RbSnI_3$	28.622	0.039
mp-19172	KV_3O_8	67.283	0.044
mp-3637	YOF	76	0.154
mp-757850	$K_4Sb_2O_5$	71.87	0.039
mp-567681	$CsPbBr_3$	5.531	0.043
mp-647813	Cs_2CrO_4	18.653	0.038
mp-559911	$V_4S_9Br_4$	22.272	0.018
mp-16915	$BaTiOF_4$	211.946	0.071
mp-29304	Y_2InCl_7	18.187	0.024
mp-572546	$CsRe(Cl_2O)_2$	125.655	0.029
mp-7928	K_2PtS_2	11.852	0.087
mp-8621	K_2PtSe_2	7.369	0.082
mp-8623	K_2Te_2Pt	5.966	0.073
mp-29300	Ga_2CuCl_8	912.276	0.045
mp-567776	$Cs_2AgAuCl_6$	144.263	0.045
mp-11924	$Rb_2TaCuSe_4$	5.247	0.029
mp-42190	$K_2NaTiOF_5$	759.456	0.069
mp-40143	Cs_2KZrOF_5	8.248	0.056
mp-8972	$K_2TaCuSe_4$	16.837	0.032
mp-555160	$CsYSeCl_2O_3$	178.754	0.053
mp-12047	$K_3Na(RuO_4)_2$	5.67	0.081

mp-27126	$Na_2Mn_3Cl_8$	22.402	0.06
mp-29817	GaP_2I_9	11.642	0.012
mp-8900	K_2VAgS_4	18.961	0.036
mp-866301	$BaBSbS_4$	8.359	0.046
mp-567928	$CsBi_3Se_5$	1000	0.054
mp-28453	$CsAuI_3$	29.869	0.041
mp-569548	$CsAuBr_3$	75.682	0.05
mp-8570	$Ba_3Zr_2S_7$	6.427	0.059
mp-23153	I	68.757	0.092
mp-765136	$LiMn_8F_{33}$	49.268	0.048
mp-6999	$ScPS_4$	12.448	0.077
mp-753546	Li_8TiS_6	8.148	0.077
mp-23484	$CsAuCl_3$	258.965	0.056
mp-8226	ThNF	75.174	0.224
mp-8725	$HfSnS_3$	13.635	0.092
mp-28046	AlP_2I_9	14.267	0.016
mp-766540	Li_4TiS_4	23.218	0.069
mp-28159	$As(BrF_2)_3$	24.029	0.074
mp-561259	Na_3NbOF_6	223.444	0.099
mp-7571	$KNbF_6$	37.49	0.117
mp-754712	$NClO_3$	5.328	0.116
mp-29526	$BrNO_3$	6.471	0.11
mp-29345	$LiGaI_3$	6.548	0.043
mp-600186	Cs_2MnBr_4	39.341	0.046
mp-770618	$MgMnO_3$	5.696	0.169
mp-28205	Na_3ReO_5	25.006	0.137
mp-8818	Ca_2ZnN_2	33.023	0.292
mp-29287	Cs_3CoBr_5	28.307	0.039
mp-23154	Br	41.875	0.126
mp-27445	$As(IF_2)_3$	11.694	0.078
mp-557772	$CsNiF_3$	26.27	0.112
mp-540760	$FePCl_8$	34.54	0.049
mp-641699	$CsNb_2PS_{10}$	6.859	0.039
mp-556244	$Xe_2NO_2F_{13}$	8.085	0.03
mp-14988	K_4SnO_3	6.088	0.053
mp-616439	Cs_2CuCl_4	18.102	0.052
mp-561710	$CsSnS_3$	5.572	0.083
mp-761057	$Sr_5Nb_4O_{15}$	6.653	0.142
mp-28178	$NaNbCl_6$	13.217	0.09
mp-560601	$K_2CuS(ClO_2)_2$	67.918	0.084
mp-769582	$Sr_5Ta_4O_{15}$	5.743	0.147
mp-19388	$BaNi_2(AsO_4)_2$	6.166	0.193
mp-569060	Cs_2PSe_5	6.238	0.075

mp-22876	CsI_3	6.657	0.061
mp-772813	$Ca_2Cu_2O_5$	7.715	0.116
mp-568244	$TlSn_2Br_5$	30.669	0.063
mp-17315	$Zr_3Tl_2OF_{12}$	66.292	0.083
mp-30106	$AsCl_5$	5.612	0.097
mp-27641	$CsBr_3$	12.17	0.07
mp-27750	$AsXeF_7$	9.36	0.106
mp-23515	K_2CoCl_4	122.478	0.052
mp-540572	NCl_3	9.496	0.063
mp-30164	$CsSn_2Cl_5$	74.504	0.071
mp-23541	KSn_2Br_5	60.07	0.068
mp-19660	$Sr_2V_2O_7$	41.456	0.091
mp-30011	$SbKrF_7$	6.025	0.079
mp-567780	$RbSn_2Br_5$	81.136	0.067
mp-554732	$RbSbS(O_2F)_2$	10.061	0.09
mp-30010	$AsKrF_7$	8.843	0.084
mp-760678	$Sb_2H_4AuF_{16}$	344.183	0.143
mp-23630	$NbBi_4ClO_8$	10.935	0.156
mp-510557	CsN_3	5.382	0.108
mp-17085	$Rb_2Zr_3OF_{12}$	1000	0.093
mp-7280	PPdS	8.968	0.153
mp-17256	$Rb_2Hf_3OF_{12}$	745.713	0.096
mp-672273	$AlBiCl_6$	7.566	0.054
mp-28163	K_2PdF_4	138.818	0.086
mp-17888	$K_2Zr_3OF_{12}$	693.092	0.1
mp-557451	$CsReOF_6$	226.783	0.088
mp-23539	KSn_2Cl_5	29.913	0.084
mp-13986	Li_2PtF_6	413.76	0.244
mp-622602	$NaMoAsO_6$	7.265	0.079
mp-621112	$Cs_5Nb_2S_4Cl_9$	395.289	0.07
mp-28211	IrS_3Cl_{11}	11.228	0.049
mp-607436	$ReCl_3O_2$	66.31	0.075
mp-540998	$FeTeBr_7$	7.435	0.091
mp-560578	$RbTeNO_3F_4$	12.553	0.084
mp-29541	$GaTeI_7$	11.113	0.108
mp-18997	$LiMnPO_4$	11.297	0.199
mp-560515	$K_4Ru_2Cl_{10}O$	13.197	0.11
mp-25305	$Y_2Ti_2S_2O_5$	1000	0.412
mp-554495	$CaZr(PO_4)_2$	5.573	0.139
mp-19123	Rb_2LiVO_4	9.373	0.085
mp-554643	$K_2SbSO_4F_3$	82.175	0.115
mp-570300	$MnTlCl_3$	236.563	0.188
mp-20459	$TiPbO_3$	793.901	0.405

mp-4829	Na_2ThF_6	39.647	0.192
mp-540997	$FeTeCl_7$	11.89	0.11
mp-556609	$KSb(PS_3)_2$	7.627	0.125
mp-557437	$KBi(PS_3)_2$	9.012	0.129
mp-560692	$K_4Nb_6O_{17}$	33.636	0.124
mp-9481	TcS_2	9.836	0.182
mp-30096	$Be_2Te_7Cl_6$	6.875	0.125
mp-644325	$CsFeSiO_4$	5.512	0.13
mp-18832	$K_2VO_2F_3$	13.439	0.157
mp-568396	$Ba(FeBr_4)_2$	79.162	0.047
mp-28232	$MgTi_2O_5$	25.173	0.184
mp-12885	$BaAl_2Sb_2O_7$	13.359	0.259
mp-505281	$CsSbS_6(O_3F)_6$	8.507	0.052
mp-571235	ZrI_4	6.252	0.096
mp-556637	$Ba_6Na_2Nb_2P_2O_{17}$	184.842	0.229
mp-27786	$SbAs_2Cl_{13}$	6.452	0.043
mp-555113	$Rb_3Cu_2(BiS_2)_5$	73.505	0.117
mp-555131	$CsCO_2$	7.292	0.095
mp-698206	$Ba_5Re_3O_{16}$	66.19	0.068
mp-1707	BaN_6	5.624	0.297
mp-706632	$H_{15}RhBr_3N_5$	5.962	0.095
mp-616597	$ReHgO_4$	14.447	0.24
mp-571035	$OsCl_4$	9.854	0.115
mp-27147	Rb_3BiBr_6	5.235	0.065
mp-17512	$Zn(AuF_4)_2$	9.485	0.227
mp-572597	$SbPS_4$	10.754	0.092
mp-644129	$KNiPH_2O_5$	167.451	0.276
mp-647366	$KICl_4$	45.375	0.118
mp-4758	K_2NbF_7	129.918	0.098
mp-3975	K_2TaF_7	15.668	0.1
mp-29144	KTe_2F_9	26.798	0.165
mp-8708	$Mg(AuF_4)_2$	70.156	0.234
mp-864954	$MgMoN_2$	186.497	1.046
mp-27774	$NClO_6$	270.388	0.115
mp-672248	$TaAsPCl_{13}$	32.549	0.049
mp-556631	$KZrSnF_7$	28.112	0.152
mp-19219	Li_3VO_4	15.426	0.294
mp-28719	$Ba(AuF_4)_2$	5.513	0.08
mp-23444	$AsCl_2F_3$	23.744	0.102
mp-21724	$ZnSiPbO_4$	96.555	0.189
mp-560675	$K_6Cu(SiO_4)_2$	175.722	0.207
mp-570962	$SbI_3(BrCl_3)_2$	5.358	0.15
mp-561153	XeF_3	10.884	0.165

mp-685281	$TiZnH_{12}(OF)_6$	17.145	0.1
mp-555741	$RbAu(SO_4)_2$	45.343	0.385
mp-560354	$SbCl(OF_3)_2$	42.049	0.198
mp-23576	$CsSbClF_3$	12.425	0.086
mp-8716	K_2MnSe_2	11.487	0.202
mp-505814	$CsBa_2Nb_3O_{10}$	1000	0.521
mp-556647	$Ba_5Re_3ClO_{15}$	6.71	0.079
mp-505034	Cs_2MnS_2	10.454	0.196
mp-3237	Na_2CuF_4	28.993	0.276
mp-644827	$TePCl_9$	47.914	0.057
mp-765493	$Ba_2Sb_2O_5$	5.199	0.165
mp-4002	Li_2ZrF_6	8.607	0.402
mp-554554	$K_9Bi(PS_4)_4$	46.437	0.102
mp-542332	$K_2Cu(CO_3)_2$	12.132	0.122
mp-541114	Sr_2RhF_7	15.675	0.134
mp-541134	$TeAuBr_8$	17.329	0.117
mp-27987	BrF_5	11.906	0.174
mp-15472	$Ba_4LiCu(CO_5)_2$	1000	0.264
mp-679927	$Rb_2Sc(NO_3)_5$	110.624	0.082
mp-27307	Na_2ZrF_6	38.877	0.29
mp-561523	$NbTlCl_4O$	15.49	0.085
mp-28575	$W(S_4Cl_3)_2$	1000	0.139
mp-6841	$Ba_4NaCu(CO_5)_2$	1000	0.264
mp-555546	$MgAs_2(XeF_5)_4$	6.311	0.068
mp-645272	$TlV_3(SeO_6)_2$	6.128	0.209
mp-8713	K_2MnS_2	6.876	0.241
mp-8714	Rb_2MnS_2	12.285	0.228
mp-866688	$Cs_4P_2PdSe_8$	6.072	0.092
mp-9639	$BaCu(SeO_3)_2$	30.499	0.211
mp-7181	$CsSr_2Ta_3O_{10}$	1000	0.589
mp-554805	$Sr_3Se_3(ClO_4)_2$	28.802	0.143
mp-504427	Ti_3PbO_7	472.968	0.367
mp-17559	Y_2TiO_5	217.449	0.244
mp-768915	Na_3AuO_3	25.938	0.105
mp-753353	$Sr_4LiCu(CO_5)_2$	1000	0.306
mp-18725	$YCrO_3$	8.167	0.323
mp-28175	$Pd(SeCl_3)_2$	14.895	0.065
mp-19443	WO_3	266.9	0.319
mp-9640	$SrCu(SeO_3)_2$	82.126	0.225
mp-560005	$TlRe_3(S_2Cl)_2$	42.675	0.163
mp-27921	Ti_2PCl_{13}	21.86	0.079
mp-19453	Te_2MoO_7	11.354	0.246
mp-23207	ClO_2	8.955	0.242

mp-680413	Rb_3As_7	8.375	0.047
mp-28179	$NaTaCl_6$	9.981	0.221
mp-573373	$PICl_8$	18.014	0.068
mp-560785	$K_2Y_4Sn_2S_{11}$	762.479	0.134
mp-17921	$NbSeOF_7$	112.453	0.167
mp-556518	$K_2Pd(NO_3)_4$	212.016	0.077
mp-680329	K_3As_7	12.073	0.051
mp-540628	$Al(TeCl_2)_2$	25.318	0.076
mp-28174	$Pd(SCl_3)_2$	6.364	0.34
mp-559309	$K_3ZnNCl_4O_3$	11.085	0.109
mp-767518	Na_2ScPCO_7	311.021	0.284
mp-559568	$K_2Se_2O_5$	17.689	0.096
mp-773432	$KMnPCO_7$	496.408	0.319
mp-505451	HS_9N	6.218	0.147
mp-767722	$VFe(P_2O_7)_2$	75.782	0.319
mp-570229	$ThBr_4$	11.808	0.226
mp-560715	$Sn_5(PO_5)_2$	17.242	0.223
mp-17035	$K_3Sc(PO_4)_2$	8.132	0.132
mp-554948	$NaI(OF)_2$	104.11	0.196
mp-27729	ICl_3	19.777	0.322
mp-554160	$K_2CuP_2O_7$	49.034	0.201
mp-27169	KTa_5O_{13}	5.207	0.167
mp-572149	$Cs_2Al(NO_3)_5$	1000	0.094
mp-679989	$Bi(Mo_2Cl_5)_3$	62.816	0.063
mp-28974	TiF_4	366.716	0.271
mp-27514	$NaFeCl_4$	179.897	0.172
mp-27322	$Nb_2Te_3O_{11}$	33.37	0.327
mp-9780	$RbHfAgTe_3$	18.509	0.279
mp-554523	$TeBrO_3F_5$	12.865	0.301
mp-696291	$ZnH_4(NO_4)_2$	6.801	0.295
mp-24030	$ZrP_2(HO_3)_2$	12.471	0.403
mp-556522	$K_3Cu_2(BiS_2)_5$	16.823	0.183
mp-29903	$TlTeF_5$	10.136	0.339
mp-622258	RbV_2SbO_8	18.412	0.214
mp-19496	KV_2SbO_8	16.962	0.219
mp-560794	$BaNbTePO_8$	1000	0.206
mp-29295	$Sr_3Sb_4S_9$	9.105	0.163
mp-769616	Na_2CrPCO_7	120.426	0.322
mp-558121	$K_4Ba(VS_4)_2$	34.669	0.121
mp-570186	$Ga_2Te_2Br_7$	694.027	0.096
mp-557059	$RbSnS_4$	5.294	0.079
mp-772763	K_2ScPCO_7	93.405	0.276
mp-28189	$FeSeCl_7$	9.3	0.206

mp-27664	$TiPCl_9$	12.168	0.175
mp-554432	$ReSbOF_{10}$	286.947	0.197
mp-29407	$AlTeI_7$	6.761	0.207
mp-775198	$Ti_3P_6WO_{24}$	1000	0.167
mp-557856	$BCl(OF_2)_2$	7.83	0.226
mp-753401	Sc_2TiO_5	22.5	0.278
mp-18815	KVO_3	8.549	0.359
mp-31012	$K_2(NbBr_3)_3$	43.286	0.058
mp-14864	$Cs_2Ti(PO_4)_2$	34.738	0.16
mp-8232	$BaZrF_6$	15.071	0.125
mp-23434	Al_2CuCl_8	186.94	0.228
mp-28387	$PAuCl_8$	54.932	0.074
mp-556705	$AsS(ClF_2)_3$	23.086	0.157
mp-672338	$Cs(Bi_2Te_3)_2$	5.915	0.178
mp-768140	Na_2BiPCO_7	347.916	0.307
mp-570857	$Y(AlCl_4)_3$	95.608	0.116
mp-581834	$CsNa_5(WN_3)_2$	12.479	0.118
mp-30938	$PAuS_4$	10.98	0.304
mp-622278	TlV_2SbO_8	5.802	0.233
mp-561328	$SbSe(BrF_2)_3$	10.342	0.146
mp-571324	$CNCl$	5.361	0.116
mp-772808	K_2BiPCO_7	10.175	0.277
mp-27859	SbI_5F_6	38.61	0.175
mp-27824	$PICl_6$	15.48	0.122
mp-769604	K_2MnPCO_7	343.232	0.318
mp-557260	$RbSb_2F_7$	240.128	0.204
mp-558309	$K_4SnSb_2F_{14}$	11.31	0.262
mp-16577	Li_2CaHfF_8	132.548	0.456
mp-720110	$KRe_3Os_3(Se_4Cl_3)_2$	1000	0.069
mp-650228	$KIn(MoO_4)_2$	8.478	0.231
mp-560591	$NaTi_2Al_5O_{12}$	36.473	0.453
mp-762082	$ThH_{10}N_4O_{17}$	11.524	0.102
mp-667283	$Sr_5Re_3ClO_{15}$	73.005	0.151
mp-629690	$Bi_2(PbS_2)_3$	24.657	0.22
mp-542289	$HgNO_3$	1000	0.22
mp-720586	CaH_4NClO_5	184.93	0.206
mp-680015	$Re_3(SeBr)_7$	148.261	0.156
mp-560120	$Na_2Pd(NO_3)_4$	41.464	0.216
mp-556552	$K_4VP_2S_9$	31.774	0.141
mp-6113	$LiTiAsO_5$	20.565	0.247
mp-7310	$ZrPbF_6$	43.492	0.144
mp-28536	$BaSe_2O_5$	10.981	0.228
mp-22694	$LiPPbO_4$	26.152	0.311

mp-19459	$K_2MgV_2O_7$	38.197	0.173
mp-569653	$SnPCl_9$	35.62	0.064
mp-556210	Bi_2CO_5	6.85	0.412
mp-23598	SIO_3F	10.375	0.182
mp-560016	$NaNb_2PO_8$	1000	0.334
mp-27472	$NbSbF_{10}$	296.273	0.292
mp-13792	$KTaP_4O_{13}$	105.003	0.206
mp-554129	$Br_3N(O_2F_5)_2$	87.93	0.164
mp-27017	$LiSnPO_4$	7.09	0.312
mp-17101	$CaNb_2O_6$	12.89	0.408
mp-667345	$NbTl_2PO_6$	785.295	0.186
mp-559151	$BaSrTa_2O_7$	1000	0.402
mp-642792	$BaBi_2(MoO_4)_4$	285.483	0.183
mp-15750	$TaAgP_4O_{13}$	10.954	0.212
mp-540921	$CsCuF_4$	5.731	0.322
mp-647102	$KNOF_2$	39.248	0.293
mp-29408	$AlSeBr_7$	9.956	0.299
mp-29048	$Sr(BiO_2)_2$	27.598	0.152
mp-17953	$MgNb_2O_6$	8.876	0.444
mp-679984	$Cs_4Ru_2Cl_{10}O$	215.367	0.089
mp-722900	CaH_3NO_5	73.369	0.104
mp-19474	$Ba_2V_2O_7$	43.321	0.239
mp-562977	$RbNbS_2O_9$	934.479	0.279
mp-27788	$TaPCl_{10}$	10.274	0.275
mp-558938	$Zn_4SiTePbO_{10}$	18.78	0.24
mp-29194	$Cs_2Au_2Se_3$	7.363	0.102
mp-638424	$Sb_2S_2O_9$	10.844	0.298
mp-683984	$Al(SeCl)_4$	123.78	0.094
mp-29264	$SICl_7$	6.002	0.124
mp-30003	$AuSO_4$	22.006	0.182
mp-768144	Na_2SbPCO_7	12.285	0.369
mp-559760	ScIO	31.994	0.175
mp-27780	$TcCl_4$	18.311	0.199
mp-555862	$CsZr(NO_3)_5$	83.51	0.148
mp-24656	$YH_3(SO_4)_3$	86.48	0.119
mp-541013	TiI_4	89.537	0.117
mp-29568	RuS_3Cl_8	6.11	0.23
mp-6764	$BaSi_2(NO)_2$	21.379	0.538
mp-555408	SbS_7IF_6	16.221	0.132
mp-28185	$TaClF_8$	132.977	0.233
mp-571313	$Hf(SeCl_6)_2$	15.143	0.094
mp-28330	$TeAuCl_7$	33.706	0.232
mp-5803	$NbPO_5$	17.831	0.386

mp-5900	Ba_2ZrF_8	87.531	0.255
mp-4325	$Zr(SO_4)_2$	15.019	0.302
mp-555490	$KRe_2O_4F_7$	27.503	0.48
mp-29129	$K_2Te_2O_5$	7.037	0.173
mp-649253	$NbClF_8$	24.122	0.246
mp-554147	$Rb_2Nb_2P_2S_{11}$	250.43	0.291
mp-18964	$K_3NaCr_2O_8$	15.89	0.245
mp-557132	$Os_2O_3F_7$	97.799	0.251
mp-28037	Mo_2SBr_2	50.8	0.126
mp-32311	Re_2NiO_8	389.368	0.536
mp-560208	$K_3NbAs_2O_9$	395.894	0.344
mp-558548	$Na_3B_6NO_{13}$	41.075	0.196
mp-531826	Li_2PtO_3	8.765	0.326
mp-554517	$NaMnF_4$	5.441	0.539
mp-30092	$TiCl_4$	34.442	0.235
mp-28870	$PRhO_4$	5.719	0.23
mp-743697	$MgZr_3Tl_{10}(MoO_4)_{12}$	66.332	0.154
mp-27452	Al_2PdCl_8	31.092	0.321
mp-27308	$SbBrF_8$	5.142	0.256
mp-581922	$CsMo_3Br_3Cl_4$	48.892	0.172
mp-24144	$Na_5ScH_4(C_2O_7)_2$	1000	0.278
mp-22869	ClO_3	8.408	0.302
mp-745150	$VZnHPbO_5$	6.671	0.338
mp-6539	$RbTiPO_5$	13.095	0.229
mp-555286	$CsNb(PO_4)_2$	18.872	0.341
mp-556047	K_2OsCBr_5O	73.933	0.202
mp-560732	$BaNaZrF_7$	36.255	0.312
mp-27735	$GaSbCl_6$	28.033	0.207
mp-23623	$B_5Pb_2BrO_9$	6.384	0.212
mp-680446	$Cu_3P_4Se_4Br_3$	6.146	0.133
mp-23396	$MoNCl_3$	7.436	0.267
mp-554412	$RbTa(PO_4)_2$	10.102	0.352
mp-6278	$Zn_2Cu(AsO_4)_2$	7.232	0.636
mp-5073	$RbNO_3$	7.47	0.166
mp-3247	Cs_2TiS_3	16.997	0.144
mp-23549	$Bi_3B_5O_{12}$	146.811	0.321
mp-9856	Cs_2ZrSe_3	6.837	0.13
mp-28431	$Sb(IF_3)_2$	90.746	0.33
mp-579086	$KSrNb_2O_6F$	1000	0.551
mp-562854	$CsNb_2BiO_7$	1000	0.558
mp-27935	$AlICl_6$	15.817	0.25
mp-686949	$ThCr(IO_5)_2$	20.08	0.245
mp-571412	$RbNa_5(WN_3)_2$	21.525	0.176

mp-23376	$GaSeBr_7$	37.737	0.371
mp-558521	$B_2Se_2O_7$	6.774	0.287
mp-28535	$Ca_2Se_3O_8$	9.24	0.38
mp-29114	$Re_3Te_4Cl_5$	83.855	0.117
mp-9172	Li_4TiO_4	11.561	0.306
mp-505113	$TiSn_6F_{16}$	300.755	0.121
mp-4674	BNF_8	6.725	0.179
mp-558114	Sr_4NbAlO_8	708.633	0.423
mp-28766	K_2TiS_3	12.61	0.187
mp-581217	$Cs_2Nb_4O_{11}$	27.075	0.22
mp-555512	$RbCO_2$	9.135	0.266
mp-672212	$NaNb_{13}O_{33}$	18.392	0.405
mp-28808	$TlReO_4$	5.645	0.227
mp-557108	$Ba_2Nb_2TeO_{10}$	9.696	0.245
mp-543046	$CsScP_2(HO_4)_2$	29.905	0.36
mp-559228	Rb_2HfS_4	7	0.278
mp-654447	$Ni(XeF_8)_2$	39.811	0.141
mp-706995	$ZnCoH_{18}N_6Cl_5$	10.752	0.294
mp-29419	$Hf(Te_2Cl_3)_2$	5.746	0.381
mp-757224	$Th_4P_6O_{23}$	1000	0.245
mp-6394	$RbTiAsO_5$	6.826	0.25
mp-541353	$K_2(TcS_2)_3$	294.556	0.116
mp-541740	$TaPO_5$	12.031	0.506
mp-541956	$CsTiAsO_5$	6.063	0.246
mp-6661	$BaTi(SiO_3)_3$	67.8	0.475
mp-30320	$RbHfF_5$	37.953	0.172
mp-30213	Sb_2BrF_{15}	30.305	0.234
mp-30946	Ga_2PdI_8	88.414	0.163
mp-554111	$Ti_3Tl_3(PO_4)_5$	16.901	0.196
mp-557163	$TaPbF_7$	6.702	0.513
mp-559519	$Na_4TiAs_2O_9$	246.875	0.162
mp-561062	$NaSb_3(PO_5)_2$	7.223	0.201
mp-640883	$VBi(PbO_3)_2$	8.868	0.422
mp-27802	$BaSn_2S_3$	7.677	0.231
mp-23809	$RbScBP_2HO_9$	83.277	0.423
mp-19276	$BaMoO_4$	6.726	0.604
mp-559516	$K_3Nb(SO_4)_4$	47.768	0.186
mp-21945	Ge_3Ru_2	8.495	0.359
mp-581864	$CsAsSe_2$	30.413	0.18
mp-9308	Li_4ZrF_8	6.425	0.356
mp-540629	$Al_2Te_2Cl_7$	955.423	0.188
mp-28358	$NbAlCl_8$	18.647	0.138
mp-570544	$Zr(SeCl_6)_2$	13.805	0.122

mp-560331	K_2ZrS_4	5.768	0.31
mp-560021	$AuS_3(O_3F)_3$	279.553	0.204
mp-28845	OsO_3F_2	17.789	0.669
mp-28933	Br_2O_3	8.73	0.266
mp-735504	$KVPHO_6$	1000	0.313
mp-743636	$NaNiP_2HO_7$	12.306	0.441
mp-555321	$BaNiF_4$	77.032	0.301
mp-556341	$Ti_4S_8Br_6O$	40.89	0.193
mp-19512	$BaV_2(PO_5)_2$	22.231	0.405
mp-558160	$NaYCO_3F_2$	13.614	0.447
mp-19048	$BaWO_4$	8.752	0.617
mp-27349	BSF_7	15.991	0.383
mp-30159	$AuBrF_6$	5.849	0.629
mp-6268	$KTiPO_5$	7.867	0.295
mp-19134	$CaCrP_2O_7$	172.673	0.534
mp-556418	$AlSCl_3O_2$	12.093	0.462
mp-504957	$RbReCl_4$	38.125	0.126
mp-555678	$Na_4Ti_5O_{12}$	14.804	0.836
mp-19057	$CaNiP_2O_7$	67.477	0.533
mp-582648	$RbRe_3Br_{10}$	52.746	0.122
mp-6651	$K_2Ta_2(OF_2)_3$	939.2	0.354
mp-683967	$Cd_7Te_7Cl_8O_{17}$	9.852	0.214
mp-8851	$BaCuP_2O_7$	13.388	0.537
mp-19487	$Ba_2Mn(PO_4)_2$	127.893	0.446
mp-753945	$ClOF_3$	11.59	0.533
mp-18953	$NaV(OF)_2$	286.651	0.921
mp-19450	$ScTl(MoO_4)_2$	7.219	0.718
mp-16831	$CaTi_4(PO_4)_6$	14.558	0.344
mp-647342	$SbP_3C(NCl_5)_3$	9.448	0.222
mp-559283	$TiSO_5$	439.127	0.373
mp-556017	$Th_2P_2O_9$	143.813	0.327
mp-680356	ZrN_6O_{17}	28.95	0.113
mp-555580	$SrZr_4(PO_4)_6$	16.932	0.328
mp-562434	$Cs_3Ta_5O_{14}$	12.357	0.393
mp-556091	$Cs_3Ta_2S_{11}$	56.443	0.226
mp-542662	$Ga_2Te_2Cl_7$	1000	0.21
mp-555119	$SrTaF_7$	34.287	0.61
mp-560843	$Na_4Zr_2Ti(CO_4)_4$	625.099	0.326
mp-28672	Zr_2TeBr_{12}	149.505	0.21
mp-558660	Mg_2BiPO_6	24.699	0.546
mp-30945	Ga_2PdBr_8	813.281	0.197
mp-867334	$KYGeS_4$	39.629	0.532
mp-554379	$AsXeF_{11}$	13.18	0.224

mp-6390	$Rb_3Ti_3(PO_4)_5$	37.59	0.242
mp-4200	$ScPO_4$	8.216	0.524
mp-505088	$NbTe_4I$	6.129	0.196
mp-770968	Na_3NiPCO_7	53.23	0.701
mp-569435	$KBi(PSe_3)_2$	12.93	0.25
mp-734042	$MgH_{12}(NO_6)_2$	15.861	0.293
mp-561392	$TcSO_6F$	21.307	0.391
mp-707060	$NbCl_4F$	51.804	0.313
mp-5403	Rb_2TiO_3	18.449	0.322
mp-679999	$Re_3(SeCl)_7$	1000	0.183
mp-758597	$K_2TiSi_3(HO_5)_2$	23.183	0.325
mp-652776	$Rb_2V(PO_4)_2$	33.758	0.343
mp-19075	$K_2SrV_4O_{12}$	27.846	0.192
mp-551826	$NbTlBr_4O$	128.59	0.429
mp-29555	$MoBr_2$	20.544	0.133
mp-735530	$Ba_2Fe_3P_6HO_{22}$	66.762	0.631
mp-29498	WBr_2	20.427	0.124
mp-12177	Te_2O_5	6.229	0.923
mp-23808	$KScBP_2HO_9$	33.476	0.541
mp-23398	$BClF_6$	30.661	0.452
mp-541299	$Zr_4Cd(PO_4)_6$	16.69	0.349
mp-40144	$SiNiH_{12}(OF)_6$	34.507	0.594
mp-558894	$Ba_4Ti_2PtO_{10}$	13.625	0.311
mp-734194	$BeH_8(IO_5)_2$	6.869	0.418
mp-18929	BaV_2O_6	7.669	0.22
mp-560742	$Ba_2TeP_2O_9$	26.278	0.485
mp-676448	$CsTiZnOF_5$	37.273	0.455
mp-505234	BaP_2PbO_7	15.311	0.474
mp-19165	$BaFe(Si_2O_5)_2$	231.838	0.44
mp-27854	$TaCl_4F$	84.639	0.145
mp-647385	$V_2Pb_4O_9$	16.72	0.284
mp-696940	$TiH_{12}C_2(NF)_6$	138.6	0.26
mp-558235	$CaTaF_7$	1000	0.214
mp-723109	$BeH_{14}(I_2O_9)_2$	6.214	0.369
mp-29085	$Sr_5Zr_3F_{22}$	1000	0.314
mp-18975	$Na_2SrV_4O_{12}$	8.662	0.22
mp-510018	$Rb_2CuH_{12}(SeO_7)_2$	170.716	0.31
mp-623854	$NaNb_3O_8$	50.175	0.749
mp-3368	$LiNb_3O_8$	6.256	0.668
mp-570531	NbP_2NCl_{12}	8.892	0.209
mp-696651	K_3NbHOF_7	1000	0.203
mp-561502	$Ba_8B_5N_{10}F$	28.191	0.295
mp-4609	$HfSiO_4$	6.179	0.602

mp-620029	$MoCl_2$	32.989	0.163
mp-573815	ReI_3	17.885	0.247
mp-541236	Na_5HfAs_3	11.99	0.428
mp-556442	$Tc_2O_5F_4$	69.656	0.318
mp-556587	$AuSCl_7$	54.996	0.301
mp-707276	$TeH_9SN_2O_5F_3$	36.057	0.526
mp-540946	$LiReO_4$	5.238	0.482
mp-17892	Ca_2VN_3	23.525	0.471
mp-541745	$Rb_3Nb_2S_{11}$	6.138	0.29
mp-645687	$CsTi(PS_4)_2$	25.612	0.182
mp-12185	$LiCu(PO_3)_3$	60.265	0.39
mp-559115	P_2RhClF_6	11.489	0.257
mp-567731	$Nb_3Se_{10}Br_3$	50.908	0.198
mp-683918	RbC_2N_3	30.391	0.553
mp-6488	$KTiAsO_5$	6.962	0.388
mp-556139	$BaZr(PO_4)_2$	9.963	0.606
mp-17407	Au_3F_8	21.838	0.467
mp-761037	$Hg(ClO_3)_2$	101.297	0.886
mp-559493	$TiPCl_7O$	242.735	0.168
mp-571011	CsI_4	20.275	0.31
mp-758103	$YH_2(CO_3)_2$	20.772	0.238
mp-706630	B_5H_7	35.634	0.404
mp-27213	$AuBr_3$	127.051	0.208
mp-24509	$CdH_4(BrO_4)_2$	6.006	0.466
mp-555122	$Rb_2Pd(NO_3)_4$	96.017	0.445
mp-676712	ReSeCl	9.598	0.173
mp-540876	$KTh_2(PO_4)_3$	13.684	0.237
mp-706386	$ZrH_6O_3F_4$	45.427	0.796
mp-554280	$RbTh_2(PO_4)_3$	12.969	0.235
mp-541975	$Rb_3Ta_2S_{11}$	39.477	0.308
mp-27556	$CsNbO_3$	11.536	0.348
mp-685352	Ca_2NF	1000	0.339
mp-570966	ZrP_2NCl_{11}	25.921	0.137
mp-867268	$K_4P_2PdS_8$	9.275	0.675
mp-23334	Bi_2TeO_5	20.322	0.324
mp-27245	BSBr	58.145	0.492
mp-556024	Na_2TiF_6	199.041	0.402
mp-557432	$GeClO_2F_5$	161.877	0.263
mp-5450	K_2ZrF_6	64.108	0.4
mp-28985	$SbSeCl_9$	6.182	0.301
mp-555272	$Na_5Zr_2F_{13}$	26.773	0.475
mp-567424	K_8NbAs_5Pb	8.334	0.107
mp-573429	$Cs_5Bi(MoO_4)_4$	28.052	0.376

mp-560407	$KNbSi_2O_7$	12.803	0.405
mp-559118	$CsTa(PO_4)_2$	13.579	0.7
mp-583297	$Ba_6Nb_4S_{13}O_3$	5.59	0.293
mp-530262	$Li_{15}Cr_2N_9$	9.747	0.36
mp-554605	$Rb_2SbCl_3F_2$	630.109	0.672
mp-29794	Ba_2PdF_6	111.318	0.305
mp-5996	$Na_2Ti_2Si_2O_9$	20.544	0.715
mp-19034	$Mg_3V_2O_8$	6.85	0.47
mp-6456	$LiNbGeO_5$	14.56	0.648
mp-570248	NaC_2N_3	107.041	0.393
mp-620652	$NaSr_2AlP_3$	48.767	0.28
mp-557599	$Rb_2Bi(ClO_4)_5$	18.993	0.402
mp-572864	$Rb_5Th(PS_4)_3$	5.663	0.258
mp-559530	$Ti_5(PO_5)_4$	10.715	0.347
mp-17803	$Nb_2Tl_4S_{11}$	6.075	0.462
mp-27998	KNb_3O_8	143.122	0.414
mp-505564	$Bi_2Se_4Cl_7$	150.112	0.303
mp-540668	BS_2	54.712	0.718
mp-3033	$RbTaO_3$	10.27	0.419
mp-556548	$Bi(BO_2)_3$	10.168	1.159
mp-677002	$SrZr_{12}B_2I_5Cl_{23}$	366.301	0.2
mp-27880	Nb_3Cl_7	25.236	0.195
mp-3488	$Na_2Ti_3O_7$	1000	1.075
mp-532604	$Na_2Zr_{12}B_2I_5Cl_{23}$	42.797	0.202
mp-707483	$TiP_2H_4O_9$	1000	0.801
mp-14873	$K_4Nb_8Si(P_2O_{17})_2$	5.79	0.306
mp-29282	P_2PtO_7	25.781	0.621
mp-560767	$KNaTiO_3$	14.556	0.559
mp-6228	Na_2TiGeO_5	8.632	0.804
mp-560977	$KTiPS_5$	18.466	0.295
mp-554195	$Sb_3As_2S_{14}(IF_8)_3$	306.889	0.482
mp-510036	$Fe_2Cu(P_2O_7)_2$	7.064	1.093
mp-29412	Ta_3Br_7	7.027	0.177
mp-29051	WS_9Cl_4	106.92	0.137
mp-559281	$Na_3Cr_2(PS_4)_3$	11.253	0.358
mp-561518	Mg_2BiAsO_6	27.563	0.39
mp-744625	$ZnCrH_{15}N_5Cl_4F$	24.275	0.275
mp-17499	$K_7Nb(SO_4)_6$	22.554	0.19
mp-28903	Zr_6FeCl_{14}	9.712	0.208
mp-769319	$LiNb(OF)_2$	14.717	1.044
mp-15004	$Ca_3ZrSi_2O_9$	13.591	0.516
mp-27212	Sb_2IF_{15}	15.954	0.302
mp-667426	$Bi_2Te_2O_7$	6.14	0.324

mp-28481	$Ti(ClO_4)_4$	997.878	0.381
mp-735541	$NiSn_2H_{12}(OF)_6$	11.028	0.901
mp-558244	$As(IF_3)_2$	288.427	0.307
mp-19179	$Ba_2V(SiO_4)_2$	579.592	0.548
mp-745159	$MoPH_3O_7$	12.897	0.927
mp-6138	Na_2TiSiO_5	9.441	0.953
mp-541947	$Rb_2Th(PSe_3)_3$	8.584	0.373
mp-745166	$Sr_2Fe_2H_2OF_{10}$	681.484	0.269
mp-18935	$K_2V(PO_4)_2$	85.85	0.583
mp-27697	ThI_4	6.776	0.654
mp-704408	$K_8V_2(S_2O_9)_3$	1000	0.214
mp-17455	$K_7Ta(SO_4)_6$	27.06	0.203
mp-16055	$KLi_3Zr_2(Si_2O_5)_6$	56.244	0.459
mp-28085	KAs_2F_7	23.872	0.645
mp-581868	$NaY(IO_3)_4$	12.684	0.242
mp-6081	$Ba_2Ti(SiO_4)_2$	461.582	0.576
mp-18687	NbF_5	128.531	0.287
mp-28346	$SrSe_2O_5$	5.266	0.884
mp-628908	$KICl_2$	5.281	0.455
mp-755663	$Ta_2Pb_2O_7$	5.708	0.395
mp-556615	$CaBi_6(PO_5)_4$	6.365	0.889
mp-23307	$NbCl_5$	32.447	0.119
mp-3180	$Ta_2Te_2O_9$	5.927	0.792
mp-559894	$Sb_2Te_2O_9$	27.64	0.615
mp-542148	$Sb_2N_5F_{11}$	663.868	0.308
mp-6708	$RbNb_2PS_{10}$	7.486	0.824
mp-560519	$Ba_3ScCO_3F_7$	23.06	0.287
mp-555305	$NaNb(OF)_2$	107.382	1.081
mp-745012	$Ni_2P_2O_7$	7.465	0.826
mp-677416	$Na_5Mg_5In_3(SO_4)_{12}$	39.732	0.666
mp-667305	$ReN(OF_2)_3$	832.88	0.423
mp-556902	KLi_4NbO_5	5.277	1.549
mp-7601	$NbGaO_4$	11.309	0.961
mp-680298	$Rb_3Ta_5O_{14}$	20.973	0.424
mp-778433	$Li_3Cr_2(PS_4)_3$	6.825	0.476
mp-558054	$SrLi_2Ta_2O_7$	811.809	0.459
mp-24196	$Tl_2CuH_{12}(SO_7)_2$	266.874	0.609
mp-557171	$Na_2Cu(PO_3)_4$	722.379	0.375
mp-765597	HS_2IO_8	45.397	0.775
mp-567414	$BiAuCl_6$	1000	0.715
mp-680756	$Na_4TiP_2O_9$	463.63	0.479
mp-654301	$Nb_5P_7O_{30}$	100.831	0.613
mp-561197	TaF_5	66.33	0.34

mp-752443	$Te(S_2O_7)_2$	5.521	1.043
mp-29426	$Y_5C_2I_9$	177.827	0.264
mp-570193	$NaAuCl_4$	5.481	0.391
mp-18914	K_2MoO_4	258.979	0.658
mp-557441	$KAu(IO_3)_4$	13.694	1.302
mp-18827	$AlVO_4$	15.685	1.001
mp-675651	$MgPS_3$	5.487	0.807
mp-18743	$CaMnP_2O_7$	44.716	1.217
mp-557628	$AsS(IF_3)_2$	62.65	0.407
mp-23403	$SbIF_5$	1000	0.364
mp-554572	$K_3NbP_2O_9$	635.167	0.545
mp-676801	$K_7Th_6F_{31}$	80.922	0.249
mp-27927	$NbAlO_4$	39.586	1.107
mp-29831	$TaCl_5$	32.357	0.155
mp-30142	$Be_4N_6O_{19}$	362.601	0.309
mp-28030	$Li_8Nb_2O_9$	15.153	1.089
mp-30097	$Bi_2Te_7Cl_8$	212.124	0.746
mp-28778	$KScF_4$	1000	0.818
mp-683955	$KTaPS_6$	12.234	0.226
mp-720104	$Na_4Al_3Ge_3NO_{14}$	95.99	0.331
mp-26949	$LiSn_2(PO_3)_5$	5.568	1.047
mp-555424	$CaNb_2(P_2O_7)_3$	1000	0.39
mp-14333	$TaAlO_4$	13.275	1.222
mp-569175	$ZrCl_4$	44.209	1.178
mp-13627	Y_3ReO_8	7.378	1.324
mp-648414	V_2PS_{10}	33.555	0.621
mp-555085	$KAu(NO_3)_4$	853.289	0.917
mp-572794	$ReP(Cl_2O)_3$	223.628	0.698
mp-768674	$Cs_4Zr_3Se_{14}$	19.411	0.3
mp-546285	NbI_3O	7.646	1.072
mp-10499	$LiZr_2(PO_4)_3$	13.468	0.752
mp-556719	$K_2Ti(SiO_3)_3$	7	0.689
mp-558692	$Sb_2ClO_2F_{11}$	278.963	0.755
mp-707219	$K_2Zr_2ZnH_{12}(OF_2)_6$	736.939	0.931
mp-542013	$Rb_4Zr_3Se_{14}$	16.964	0.328
mp-554376	$Y_4TiSi_2(O_3F_2)_3$	1000	0.397
mp-573751	$AlTeCl_7$	7.102	0.765
mp-23089	$SrTa_2Bi_2O_9$	102.905	0.447
mp-23614	$SrNb_2Bi_2O_9$	140.741	0.454
mp-559314	$Na_5TiP_2O_9F$	666.72	0.495
mp-540995	$Rb_5Nb_3OF_{18}$	1000	0.259
mp-707343	$ZrH_{12}C_2(NF)_6$	544.421	1.041
mp-27184	$B_{10}(Pb_2O_7)_3$	14.465	1.533

mp-23929	$ZnH_8(NO_5)_2$	1000	0.447
mp-707981	$Y_4H_9NO_{13}$	210.047	1.104
mp-541867	$CsRe_3(O_3F_5)_2$	286.69	0.892
mp-29040	$Li_3Zr_4F_{19}$	268.491	1.136
mp-6571	$BaCuAs_2O_7$	7.518	1.318
mp-549720	NbI_2O	48.468	1.077
mp-18271	$Na_5Ti_2Si_2PO_{13}$	831.071	1.732
mp-540675	$SeCl_4$	14.603	0.408
mp-559692	$Ta_2Cd(P_2O_7)_3$	6.393	0.597
mp-556697	$CaTa_2Bi_2O_9$	16.386	0.493
mp-541735	$K_4Ti_3S_{14}$	22.788	0.416
mp-5274	$ThTi_2O_6$	16.951	1.792
mp-561396	Li_3CrF_6	23.7	0.551
mp-723419	$Sb_2S_{19}F_{12}$	29.264	0.355
mp-672352	$Al(ICl_2)_3$	29.304	0.346
mp-542121	$Rb_4Nb_2Si_8O_{23}$	239.444	1.336
mp-559000	$SbSe_6IF_6$	7.999	1.079
mp-557256	RbP_3PbO_9	7.55	0.575
mp-680246	$Cs_4Zr_3S_{14}$	18.488	0.387
mp-752467	NbO_2F	18.971	1.412
mp-542067	$Rb_4Ti_3S_{14}$	24.197	0.429
mp-762295	$K_2Mn_3V_2(HO_5)_2$	8.655	0.875
mp-22583	$KInP_2S_7$	6.417	0.88
mp-558360	$AlAs_3S_8Cl_4$	16.729	1.25
mp-28774	$KSnF_3$	5.689	0.975
mp-560745	AuN_5O_{14}	91.854	1.168
mp-557786	$CaNb_2P_2O_{11}$	12.536	0.469
mp-680284	$Rb_6Ta_4S_{25}$	12.145	0.261
mp-31003	$B_{10}H_{13}I$	26.178	0.443
mp-707782	$K_6Zr_3H_8(OF)_{12}$	48.215	0.516
mp-571250	$TaP_2Se_2Cl_5$	54.341	0.907
mp-556728	$TaP_2S_2Cl_5$	110.898	0.936
mp-556834	$RuCl(OF_3)_2$	71.407	1.912
mp-505400	$BaZr_2F_{10}$	210.074	0.82
mp-559182	P_2IrClF_6	49.455	0.72
mp-554016	$K_4Ti_2PO_4F_9$	1000	1.229
mp-560322	$K_2RuN_3Cl_3O_5$	619.235	1.494
mp-530524	Zr_3TlF_{15}	41.929	1.293
mp-645364	$Sr(PN_2)_2$	13.411	0.333
mp-27994	$HgBrO_3$	6.458	0.948
mp-567515	$Rb_2Hg_2PdBr_8$	19.514	1.01
mp-560297	$LiTaSiO_5$	7.34	1.526
mp-8796	$Sr_2LiSc(B_2O_5)_2$	9.845	1.371

mp-680410	$K_3Nb_2S_{11}$	5.78	0.333
mp-557470	$K_2Sb_2S(O_2F_3)_2$	10.262	1.773
mp-557301	$K_2Ti(Si_2O_5)_3$	515.602	1.043
mp-542863	$Ca_7NbSi_4O_{17}F$	752.817	1.229
mp-569561	$TeCl_4$	8.249	0.513
mp-561454	$KAu(SO_4)_2$	85.428	1.149
mp-19440	$LiVO_3$	28.172	0.844
mp-769404	$YSeO_3$	77.611	1.308
mp-30996	$RbAuBr_4$	15.044	2.149
mp-24522	CuH_2SO_5	10.268	3.727
mp-560032	$NaNb_2AsO_8$	5.251	2.276
mp-30930	AlI_3	8.877	1.683
mp-27926	$AsClF_8$	21.765	1.509
mp-676501	$K_3Sn_2S_3BrO_{12}$	961.711	1.289
mp-16691	$SrLi_2Ti_6O_{14}$	5.899	0.535
mp-640341	$Mo_3S_7Cl_4$	8.736	0.908
mp-27300	$RbAuBr_3$	197.527	1.113
mp-27678	Y_2Cl_3	22.792	1.798
mp-756570	Rb_4SnO_3	27.911	0.791
mp-849433	$SrTiH_4(OF_3)_2$	42.834	1.816
mp-13361	$Cd_2Cu(PO_4)_2$	72.015	4.315
mp-532315	$Sr_{17}(Ta_5S_{21})_2$	31.146	0.787
mp-667369	$Ca_2Zr_5Ti_2O_{16}$	7.519	0.741
mp-23569	$AsSe_6IF_6$	5.224	1.813
mp-541240	$Sb_3O_2F_5$	19.142	2.039
mp-626799	ReH_3O_5	5.39	3.158
mp-15543	$NaLiZr(Si_2O_5)_3$	36.614	0.466
mp-19432	$KNaV_2O_6$	13.294	1.097
mp-3283	$RbNbO_3$	15.27	2.752
mp-24215	ScH_3Br_3N	13.604	1.784
mp-29704	$Cs(SO_2)_2$	282.641	1.001
mp-554737	$CsAu_2F_7$	29.952	0.995
mp-505260	$Te_{10}Mo_3I_{10}$	5.745	1.187
mp-21533	CuP_2PbO_7	50.136	2.834
mp-568252	$Rb_2Hg_2PdCl_8$	48.555	1.637
mp-572526	$SbBr(OF_3)_2$	296.203	2.967
mp-6245	$K_5Nb_4O_{12}F$	1000	2.081
mp-684010	$K_8Ti_5P_2(O_4F_{11})_2$	644.604	1.197
mp-707811	ZrH_6NOF_5	120.473	2.653
mp-18957	$NaMnO_2$	10.029	2.203
mp-543042	$ScP(H_2O_3)_2$	6.227	2.472
mp-554706	$AsSe(ClF_2)_3$	25.016	1.919
mp-555059	$TcSb(OF_4)_2$	563.916	1.831

mp-30325	$In_2(Se_2O_5)_3$	11.794	1.105
mp-2650	P_4S_7	7.169	1.284
mp-679987	$NbP_2S_2Cl_5$	392.618	1.718
mp-568666	$RbAuI_3$	73.873	1.423
mp-554704	$TiPHO_5$	6.718	2.874
mp-569675	$Tl_2Hg_2PdCl_8$	44.225	1.907
mp-30998	$Ti(NO_3)_4$	82.762	1.392
mp-561065	$MgTi_2(PO_5)_2$	6.649	2.879
mp-707735	$MgH_{12}(I_4O_3)_2$	18.207	2.471
mp-28885	PSe	7.678	2.073
mp-556006	$OsCl_4O$	5.215	2.826
mp-28017	$Na_8Ti_5O_{14}$	114.356	2.574
mp-30309	$Y_2Au_5F_{21}$	9.798	2.312
mp-557792	$HfSCl_6O$	53.127	1.161
mp-560146	$Ba_{17}Y_{16}Zn_8Pt_4O_{57}$	20.123	0.339
mp-27297	$ReCl_4O$	52.846	2.328
mp-556689	$KZrF_5$	157.295	3.105
mp-581967	Nb_2O_5	175.162	2.406
mp-505794	$ScH_6N_2Cl_3$	68.959	2.91
mp-643570	NiH_2SO_5	28.218	3.828
mp-759651	$ScH_6Br_3N_2$	72.12	2.943
mp-867371	$K_2Y_4Cu_4Se_9$	27.094	3.531
mp-29602	K_2ZrTe_3	22.201	2.229
mp-30989	$Sn(NO_3)_4$	5.38	1.874
mp-28261	Na_4SnO_3	45.119	2.309
mp-559790	$K_2Nb_3Cl_7O_5$	10.044	1.485
mp-559150	$Na_9ZrP_4ClO_{16}$	117.255	4.688
mp-573581	Na_2TeSe_3	8.173	1.894
mp-23635	$TlRe_6Se_8Cl_3$	17.558	2.945
mp-542931	$Bi_2B_8O_{15}$	13.966	2.505
mp-561190	$NaAu(SO_4)_2$	67.572	6.162
mp-24741	ScH_3NCl_3	13.94	3.925
mp-40575	$LiNi_2P_4H_3O_{14}$	30.278	1.919
mp-638749	$Te_3(PdBr)_4$	8.304	3.696
mp-607454	$AlC_3(NCl_2)_3$	617.323	3.606
mp-28372	$AuSeCl_7$	87.366	3.042
mp-29027	TaI_2O	9.064	4.227
mp-29603	Rb_2ZrTe_3	10.878	2.961
mp-6118	$Ca_3Cu_3(PO_4)_4$	9.157	6.581
mp-579058	$Cs_4Tc_6S_{13}$	331.553	1.715
mp-19080	$Na_2Mn_3O_7$	40.891	7.179
mp-696078	$K_3ZrH_2S(OF)_5$	977.22	2.646
mp-756748	$ScH_3(ClO_5)_2$	16.106	4.379

mp-18582	$Rb_2Ti(Si_2O_5)_3$	115.967	3.292
mp-583581	W_2NCl_9	29.183	2.243
mp-757840	$Ba_4(PtO_3)_3$	8.272	3.692
mp-637112	AsS_7IF_6	67.595	2.478
mp-5449	$Na_2Ti_6O_{13}$	24.507	5.759
mp-504934	Sc_2CI_3	83.524	3.307
mp-555207	$BN(OF_2)_2$	616.756	7.495
mp-680168	$K_2Re_3C_2Se_5N_2$	11.488	2.694
mp-867823	$RbTaGeS_5$	195.612	7.264
mp-558153	$Ba_4Nb_2(OF_4)_3$	1000	1.192
mp-8065	$K_2Ti_6O_{13}$	5.952	6.088
mp-6698	$Th_2Cu(PO_4)_3$	94.794	2.523
mp-6748	$Cs_2Ti(Si_2O_5)_3$	97.322	3.767
mp-560348	$K_6Nb_4S_{25}$	7.345	1.887
mp-31034	ThF_4	7.683	2.633
mp-865606	$CsTaGeS_5$	342.591	7.844
mp-573340	$Nb_2Se_{17}Cl_{12}$	7.8	2.662
mp-583762	$Na_3W_3Cl_{13}$	167.611	1.927
mp-541155	VS_4	73.238	3.387
mp-30954	GaI_3	5.604	6.746
mp-554657	$Na_2Tl_2B_{10}O_{17}$	10.285	3.111
mp-541758	$Ta_2Se_{17}Br_{12}$	7.18	3.077
mp-567734	$AlAs_3(SeCl)_4$	11.968	1.935
mp-581963	$K_4Hf_3Te_{17}$	8.674	1.714
mp-28684	$Sb_7Se_8F_{35}$	110.513	3.438
mp-758985	$RbTiPS_5$	276.494	4.444
mp-554702	$NaZr_2NiF_{11}$	1000	9.393
mp-557289	$TiP_2Cl_8O_3$	21.72	4.185
mp-15141	$NaZr_2ZnF_{11}$	174.022	9.722
mp-680498	$RbTaPS_6$	18.91	2.623
mp-6903	$Na_2Ca_4ZrNbSi_4O_{17}F$	1000	8.669
mp-559292	$P_6Pb_3Xe_{11}F_{58}$	19.078	4.657
mp-4351	$K_2B_2S_7$	5.326	7.665
mp-559602	$AgSb(S_8F_3)_2$	5.425	5.965
mp-542630	P_4S_9	13.52	7.557
mp-744764	$Mn_7P_6(HO_6)_4$	24.557	18.046
mp-556837	$AgAs(S_8F_3)_2$	7.251	6.588
mp-559968	Na_2NbAsO_6	43.798	5.883
mp-698567	$Cr(Bi_7O_{12})_2$	29.149	12.56
mp-14651	Zr_2AgPdF_{11}	151.913	15.531
mp-581877	$Cs_2Zr(Si_2O_5)_3$	5.575	5.288
mp-4649	$PdSe_2O_5$	15.388	15.828
mp-582483	$Na_2Th(PO_4)_2$	707.888	8.262

mp-680048	RbW_3Br_7	5.237	3.851
mp-28075	$K_2Ti_2O_5$	108.599	29.567
mp-28079	$Na_2Mn_2S_3$	13.111	7.235
mp-557863	$K_2Ag_4Pt_3(NO_2)_{12}$	1000	7.542
mp-505392	$Ba_3V_4O_{13}$	21.692	9.037
mp-554626	$Ba(BrO_3)_2$	10.039	13.071
mp-640389	$Cs_2Th(PS_3)_3$	29.473	8.789
mp-685928	$Rb_5Tc_3S_7$	1000	7.251
mp-555231	$Ba_3Bi_2(PO_4)_4$	37.493	7.803
mp-770948	Na_3CoPCO_7	18.044	21.714
mp-28368	$TlAuCl_4$	31.851	20.874
mp-559336	$NaNb_3(TeO_4)_4$	421.234	31.033
mp-676313	$RbMo_3Br_7$	9.011	4.937
mp-677246	$Ba_6Ti_2Nb_{10}Si_8O_{51}$	19.041	16.78
mp-18664	$K_4Ta_2S_{11}$	7.005	20.739
mp-14935	P_3RhO_9	9.056	7.341
mp-554686	$MgAs_2(XeF_9)_2$	1000	16.96
mp-721471	$CuPH_4O_5F$	321.263	34.64
mp-569442	$RbAuCl_4$	45.825	29.085
mp-761870	$H_7C_3N_6Cl$	6.42	9.915
mp-28501	$K_2(NbCl_3)_3$	21.383	16.066
mp-674338	$K_{16}Zr_{12}Se_{61}$	28.124	16.372
mp-505798	Na_4TiSe_4	11.083	14.4
mp-698655	$KMgIn(MoO_4)_3$	13.333	20.776
mp-755492	$NaCuP_2O_7$	6.842	63.362
mp-862605	$Rb_4Zr_6CCl_{18}$	18.411	28.79
mp-8989	$Na_2P_2PdO_7$	36.655	66.25
mp-6467	$Na_2CuP_2O_7$	20.11	102.782
mp-680237	$K_{10}Th_3(P_5S_{18})_2$	8.846	29.878

Table S2 Data for the results shown in Figure 5-d (p-type doping) along with Material Project ID (MPID) and chemical formula.

MPID	Formula	Standard deviation of effective mass	E_f (eV/ Å^2)
mp-10070	$BaAg(PO_3)_3$	41.465	0.355
mp-10408	K_2CN_2	76.387	2.298
mp-10419	Na_4ReN_3	48.202	0.591
mp-10919	Rb_2PtC_2	41.749	0.15
mp-11923	Rb_2TaCuS_4	143.032	0.033
mp-11924	$Rb_2TaCuSe_4$	39.98	0.029
mp-12444	SrCuSF	96.916	0.455
mp-13445	Rb_2As_2Pt	375.636	0.113
mp-13738	$CsCd(PO_3)_3$	37.395	0.313
mp-13743	K_3GaO_3	52.059	0.191
mp-13792	$KTaP_4O_{13}$	31.553	0.205
mp-13985	Li_2PdF_6	91.644	0.07
mp-13998	Na_5AlO_4	56.541	0.214
mp-14128	K_2HfF_6	32.977	0.201
mp-14364	Cs_2LiAsO_4	223.612	0.292
mp-14368	$SbAsO_5$	38.927	0.227
mp-14401	$NaCaPO_4$	106.408	0.257
mp-14484	$KNaLi_2(SO_4)_2$	156.301	0.349
mp-14488	$Li_3In_2(PO_4)_3$	1000	5.59
mp-14511	$NaAlGeO_4$	43.467	8.086
mp-14651	Zr_2AgPdF_{11}	306.05	15.951
mp-14653	$AgSb_2F_{12}$	207.196	0.013
mp-14734	$CsCOF_3$	51.255	0.094
mp-14873	$K_4Nb_8Si(P_2O_{17})_2$	90.699	0.314
mp-14972	$Ba_3Sc(BO_3)_3$	1000	0.13
mp-15107	$KSnAsO_5$	132.049	0.226
mp-15108	$RbSnAsO_5$	198.784	0.237
mp-15141	$NaZr_2ZnF_{11}$	1000	9.722
mp-15254	Li_3AlF_6	420.613	0.487
mp-15395	$CsBePO_4$	715.706	0.354
mp-15433	$K_2Ga_2Sb_3$	34.195	0.065
mp-15437	MgP_4O_{11}	79.608	3.451
mp-15472	$Ba_4LiCu(CO_5)_2$	1000	0.264
mp-15558	Li_3GaF_6	67.025	0.424
mp-15750	$TaAgP_4O_{13}$	72.872	0.212
mp-15845	$SrLi_4N_2$	223.471	0.274
mp-15865	$RbScAsO_4F$	36.393	0.189

mp-15919	$BeAgPO_4$	37.5	11.375
mp-1602	SiS_2	42.316	0.017
mp-16194	Rb_2SiO_3	52.123	2.358
mp-16543	$Cs_3Cu_5O_4$	59.506	0.351
mp-16828	$Li_3B_7O_{12}$	39.151	0.272
mp-16980	$Rb_2B_4O_7$	99.406	1.125
mp-17015	K_4GeO_4	38.661	0.721
mp-1707	BaN_6	119.849	0.297
mp-17077	K_2YF_5	38.215	0.354
mp-17085	$Rb_2Zr_3OF_{12}$	51.089	0.092
mp-17166	$K_2B_4O_7$	123.576	1.34
mp-17229	$RbBe_3ZnF_9$	64.722	0.242
mp-17256	$Rb_2Hf_3OF_{12}$	54.403	0.096
mp-17297	Na_2GeF_6	58.04	0.277
mp-17315	$Zr_3Tl_2OF_{12}$	120.774	0.083
mp-17337	$RbAsOF_4$	1000	3.077
mp-17394	$NaYGeO_4$	57.394	0.549
mp-17401	Rb_3Sn_4Au	162.327	0.063
mp-17447	$Sr_{10}P_6SO_{24}$	63.346	0.191
mp-17512	$Zn(AuF_4)_2$	36.972	0.227
mp-17516	$Ca_{10}P_6SeO_{24}$	142.124	0.216
mp-17539	$KAsOF_4$	1000	2.789
mp-17650	$KGaS_2$	38.93	0.081
mp-17693	$SrCdP_2O_7$	59.739	1.885
mp-17730	K_2SnO_3	47.597	0.283
mp-17761	$CaGeO_3$	35.803	1.113
mp-17771	$NaMg_4(AsO_4)_3$	65.098	0.377
mp-17850	$K_3NaTh_2O_6$	38.186	0.516
mp-17886	$K_2Al_2Sb_3$	31.445	0.068
mp-17888	$K_2Zr_3OF_{12}$	297.491	0.057
mp-17941	$Na_2B_4O_7$	852.73	0.536
mp-17951	$Cs_4Zn_3F_{10}$	47.488	0.142
mp-18003	$CsCuS_4$	55.095	0.034
mp-18065	$BaCaAlF_7$	355.368	0.537
mp-18183	$YSnF_7$	266.442	0.957
mp-18253	$SrGa_4O_7$	74.4	0.82
mp-18271	$Na_5Ti_2Si_2PO_{13}$	1000	1.809
mp-18343	$BaMgP_2O_7$	60.512	1.427
mp-18347	$KAlTe_2$	44.584	0.055
mp-18429	$KAg(NO_3)_2$	146.466	0.08
mp-18460	$K_2Si_6GeO_{15}$	47.19	0.858
mp-18463	$RbZnPO_4$	814.522	0.306

mp-18464	Rb_4GeO_4	82.165	0.4
mp-18500	K_3Sn_4Au	63.539	0.068
mp-18582	$Rb_2Ti(Si_2O_5)_3$	56.681	3.293
mp-18687	NbF_5	80.099	0.289
mp-18702	$AgPO_3$	35.846	3.348
mp-18809	Li_2VGeO_5	41.355	0.468
mp-18832	$K_2VO_2F_3$	41.004	0.157
mp-18860	Li_2VSiO_5	77.685	0.658
mp-18935	$K_2V(PO_4)_2$	1000	0.637
mp-18953	$NaV(OF)_2$	54.461	0.92
mp-18997	$LiMnPO_4$	48.838	0.181
mp-19026	Na_4FeO_3	97.224	0.706
mp-19037	$K_2W_2O_7$	677.551	0.298
mp-19167	Rb_2NiO_2	1000	0.039
mp-19252	K_2NiO_2	1000	0.05
mp-19261	Na_3MnPCO_7	52.405	0.377
mp-19334	Na_4WO_5	48.527	8.514
mp-19388	$BaNi_2(AsO_4)_2$	51.825	0.199
mp-19443	WO_3	541.643	0.328
mp-19488	$Rb_2MnSO_4F_3$	128.85	0.279
mp-19508	$SrCr(Si_2O_5)_2$	1000	0.314
mp-19512	$BaV_2(PO_5)_2$	321.495	0.405
mp-19514	Sr_2CrO_4	33.178	0.116
mp-19518	$BaCr(Si_2O_5)_2$	316.448	0.353
mp-19660	$Sr_2V_2O_7$	75.99	0.091
mp-19893	$PbCO_3$	33.228	0.257
mp-19956	Ba_2InO_3F	1000	0.098
mp-20352	$Ba_3In_2O_6$	756.838	0.095
mp-20546	$Ba_2In_2O_5$	1000	0.184
mp-2131	SrN_6	54.119	0.154
mp-21760	$Rb_2In_2Sb_3$	34.439	0.057
mp-21835	$Cs_2In_2Sb_3$	38.878	0.053
mp-22216	In_2S_3	111.485	0.065
mp-22661	$InAg(PS_3)_2$	35.454	0.023
mp-22935	$CsBrF$	42.677	0.141
mp-22977	$CsVCl_3$	941.685	0.114
mp-22978	Rb_2MnCl_4	1000	0.029
mp-22991	$CsVI_3$	123.316	0.085
mp-23038	$CsVBr_3$	370.219	0.096
mp-23162	$ZrCl_2$	164.1	0.018
mp-23174	$ReCl_3$	107.61	0.136
mp-23184	BCl_3	406.905	0.009

mp-23189	BI_3	257.1	0.012
mp-23225	BBr_3	397.264	0.01
mp-23267	$BeCl_2$	124.691	0.013
mp-23403	$SbIF_5$	1000	0.34
mp-23434	Al_2CuCl_8	33.103	0.241
mp-23515	K_2CoCl_4	45.879	0.069
mp-23550	$KBrF_4$	40.266	0.289
mp-23568	$XeN_2(OF_4)_2$	112.556	0.065
mp-23576	$CsSbClF_3$	60.886	0.086
mp-23598	SIO_3F	59.668	0.159
mp-23634	$KSbClF_3$	54.807	0.059
mp-23660	$KNa_{22}C_2S_9ClO_{42}$	1000	0.15
mp-23701	$CaB_8H_4O_{15}$	268.138	2.556
mp-23702	LiH_2N	148.954	0.527
mp-23748	$MgBHO_3$	33.791	0.642
mp-23776	$BeH_8(ClO_2)_2$	34.684	0.392
mp-23780	$Na_3H(SO_4)_2$	60.694	0.684
mp-23800	$KHSO_4$	182.417	0.255
mp-23846	KHF_2	40.637	0.228
mp-23904	BaH_4O_3	37.764	0.109
mp-24007	Rb_2HBrO	118.278	0.432
mp-24022	$RbH_3(SeO_3)_2$	319.111	0.055
mp-24030	$ZrP_2(HO_3)_2$	34.289	0.403
mp-24058	$AgBH_2OF_4$	94.627	0.034
mp-24072	$AgH_5S_2O_9$	192.166	0.501
mp-24097	$Mg_3Si_2H_4O_9$	874.274	0.072
mp-24112	$Rb_2ZnH_{12}(SO_7)_2$	45.946	0.97
mp-24118	$H_{10}SO_8$	64.247	0.253
mp-2414	SO_3	46.657	0.009
mp-24141	$CsHSeO_4$	63.503	0.052
mp-24144	$Na_5ScH_4(C_2O_7)_2$	43.771	0.279
mp-2416	YF_3	38.522	0.092
mp-24160	BH_3NF_3	43.809	0.415
mp-24193	NaH_3O_2	233.038	0.037
mp-24196	$Tl_2CuH_{12}(SO_7)_2$	287.037	0.596
mp-24230	$HCNO$	106.142	1.843
mp-24302	$CdAs_2HF_{13}$	169.244	0.165
mp-24308	$AlSiH_9C_3Cl_2O$	38.546	0.557
mp-24340	$K_3GeH_3S_3O_2$	41.239	0.045
mp-24428	KH_2N	227.471	0.066
mp-24460	$MgH_6(SO_4)_4$	31.603	0.505
mp-2452	P_2O_5	276.733	0.248

mp-24656	$YH_3(SO_4)_3$	88.053	0.118
mp-24683	$RbZn_2P_2HO_8$	269.408	0.544
mp-24747	Na_3H_6Rh	50.151	0.247
mp-24757	$AlBP_2H_5NO_9$	89.354	0.473
mp-24761	$RbGaBP_2HO_9$	48.344	0.51
mp-24822	$Na_5Al_3H_{14}$	45.009	0.167
mp-25305	$Y_2Ti_2S_2O_5$	104.897	0.394
mp-2632	TlF_3	32.158	0.045
mp-27094	$LiSn_2(PO_4)_3$	39.449	6.108
mp-27169	KTa_5O_{13}	93.502	0.177
mp-27212	Sb_2IF_{15}	516.296	0.293
mp-27213	$AuBr_3$	184.201	0.208
mp-27256	$Sb_2(S_2O_7)_3$	34.965	1.047
mp-27288	$RuXeF_7$	889.614	3.571
mp-27297	$ReCl_4O$	48.064	2.425
mp-27307	Na_2ZrF_6	609.02	0.29
mp-27308	$SbBrF_8$	42.724	0.251
mp-27322	$Nb_2Te_3O_{11}$	143.941	0.327
mp-27344	$Be(BH_4)_2$	52.712	0.116
mp-27345	Na_3BiO_4	38.823	11.373
mp-27349	BSF_7	383.077	0.399
mp-27353	$SbCl_2F_3$	1000	3.807
mp-27376	$Rb_6Si_{10}O_{23}$	72.924	0.226
mp-27384	$AgIO_3$	59.98	0.044
mp-27389	KSb_2F_7	98.386	0.025
mp-27396	$NiCl_2$	114.004	0.029
mp-27399	$SbBr_3$	32.221	0.012
mp-27425	$Sr(HO)_2$	45.673	0.106
mp-27452	Al_2PdCl_8	116.934	0.319
mp-27472	$NbSbF_{10}$	102.484	0.292
mp-27473	Sb_2TeF_{14}	1000	0.193
mp-27556	$CsNbO_3$	82.062	0.351
mp-27579	$Na_4P_2O_7$	257.254	0.27
mp-27648	Te_2Br	48.04	0.098
mp-27664	$TiPCl_9$	55.331	0.177
mp-27674	$K_5As_3O_{10}$	121.894	0.521
mp-27692	BaB_4O_7	60.276	1.135
mp-27697	ThI_4	66.134	0.658
mp-27702	$InClO$	38.623	0.011
mp-27786	$SbAs_2Cl_{13}$	41.19	0.042
mp-27792	$K_2S_5O_{16}$	1000	0.403
mp-27849	$TiBrN$	1000	0.016

mp-27850	TiNCl	1000	0.015
mp-27863	AlClO	38.261	0.012
mp-27866	MoS_2Cl_3	68.11	2.035
mp-27915	K_2BeO_2	1000	1.496
mp-27921	Ti_2PCl_{13}	68.51	0.08
mp-27988	IF_7	252.788	0.004
mp-27998	KNb_3O_8	134.539	0.415
mp-28037	Mo_2SBr_2	73.71	0.126
mp-28064	SbS_8Cl_3	57.507	5.73
mp-28065	ThNCl	56.654	0.063
mp-28066	ThBrN	65.802	0.044
mp-28085	KAs_2F_7	56.973	0.645
mp-28125	$H_{11}NF_8$	299.72	0.32
mp-28163	K_2PdF_4	39.728	0.086
mp-28174	$Pd(SCl_3)_2$	93.732	0.34
mp-28185	$TaClF_8$	70.05	0.243
mp-28202	K_3NO_4	37.314	0.092
mp-28204	CsH_7O_4	49.284	0.402
mp-28211	IrS_3Cl_{11}	123.291	0.049
mp-28233	$MnCl_2$	41.814	0.019
mp-28257	SOF_2	47.62	0.007
mp-28270	KCuS	1000	0.039
mp-28273	K_3CuO_2	45.875	0.12
mp-28306	$MnBr_2$	39.541	0.022
mp-28330	$TeAuCl_7$	1000	0.211
mp-28375	Ta_2AgF_{12}	361.697	0.553
mp-28387	$PAuCl_8$	206.169	0.075
mp-28428	$K_3Nb_2Se_{11}$	407.069	0.265
mp-28479	Sc_2CCl_2	1000	0.011
mp-28541	$Bi_2P_4O_{13}$	780.371	0.963
mp-28575	$W(S_4Cl_3)_2$	86.047	0.137
mp-28577	$RbBrF_4$	87.135	0.006
mp-28627	K_4Br_2O	152.929	0.024
mp-28634	KI_3F_{16}	569.98	0.164
mp-2865	K_2CuF_4	193.04	0.046
mp-28676	$S_2O_5F_2$	42.764	0.289
mp-28683	$Ta(ICl)_2$	118.127	0.022
mp-28684	$Sb_7Se_8F_{35}$	178.307	3.438
mp-28726	KYF_4	231.912	0.086
mp-28744	Y_4OsBr_4	63.002	0.133
mp-28778	$KScF_4$	42.74	0.826
mp-28788	$Ba_9(AuO_6)_2$	56.272	0.264

mp-28804	TcO_2F_3	80.725	0.385
mp-28859	K_2HgS_2	493.024	0.037
mp-28883	GeP_2O_7	51.775	0.258
mp-28913	Ti_6CCl_{14}	96.222	0.203
mp-28974	TiF_4	137.524	0.237
mp-28985	$SbSeCl_9$	98.748	0.298
mp-29030	$ThTl_3F_7$	48.71	0.085
mp-29040	$Li_3Zr_4F_{19}$	872.779	1.138
mp-29085	$Sr_5Zr_3F_{22}$	81.824	0.302
mp-29095	H_4SO_5	32.859	1.46
mp-29114	$Re_3Te_4Cl_5$	54.136	0.117
mp-29144	KTe_2F_9	34.814	0.165
mp-29149	Li_4NCl	64.134	0.239
mp-29193	$Nb_2Se_4O_{13}$	44.935	0.347
mp-29226	$Ca_3Ga_4O_9$	38.803	0.399
mp-29264	$SICl_7$	33.727	0.124
mp-29274	P_2PdO_6	248.025	0.251
mp-29276	$Cd_2P_6O_{17}$	94.408	3.713
mp-29300	Ga_2CuCl_8	258.235	0.231
mp-29330	$K_2H_5F_7$	409.557	0.686
mp-29363	Rb_3GaP_2	33.943	0.091
mp-29369	Sb_7F_{29}	65.329	0.233
mp-29386	$K_6Sn_2Se_7$	44.03	0.212
mp-29391	$SbCl_3F_2$	298.863	0.117
mp-29411	$Na_2B_2S_5$	254.298	0.15
mp-29449	$Rb_4Cu_5Cl_9$	720.388	2.207
mp-29568	RuS_3Cl_8	97.974	0.229
mp-29693	Rb_2AgCl_3	45.127	0.038
mp-29694	$KAuBr_4$	63.043	0.126
mp-29704	$Cs(SO_2)_2$	166.096	1.002
mp-29794	Ba_2PdF_6	786.129	0.312
mp-29871	Na_4SeO_5	65.976	0.993
mp-29877	K_2ReH_9	44.463	0.323
mp-29878	Re_2PCl_{13}	49.037	0.122
mp-29940	$SbClF_{10}$	129.999	0.012
mp-29966	NOF	38.936	0.008
mp-29970	$Cs_3Sb_5O_{14}$	79.605	0.21
mp-30003	$AuSO_4$	42.77	0.19
mp-30005	Rb_6Br_4O	56.333	0.06
mp-30010	$AsKrF_7$	520.887	0.085
mp-30011	$SbKrF_7$	236.739	0.079
mp-30012	$BiKrF_7$	98.53	0.107

mp-30023	$Ba(AlCl_4)_2$	54.072	0.178
mp-30103	AuF_5	49.4	0.009
mp-30120	K_3BiO_4	51.776	0.672
mp-30130	$Bi_4I_2O_5$	51.695	0.618
mp-30139	$BeBr_2$	89.954	0.013
mp-30142	$Be_4N_6O_{19}$	1000	0.309
mp-30213	Sb_2BrF_{15}	98.469	0.226
mp-30315	Ca_3BN_3	71.811	0.199
mp-30320	$RbHfF_5$	43.961	0.178
mp-30325	$In_2(Se_2O_5)_3$	34.521	1.105
mp-30934	$As(S_8I)_3$	40.519	0.035
mp-30943	$MgPSe_3$	607.328	0.021
mp-30979	$GaPS_4$	42.264	2.158
mp-30983	CaP_4O_{11}	40.226	1.849
mp-30989	$Sn(NO_3)_4$	102.293	1.874
mp-31040	$NbCl_4$	311.268	1.383
mp-31050	Cl_2O_7	50.657	0.008
mp-31060	$Rb_4(BS)_9$	31.243	0.323
mp-31073	$Na_3B_7O_{12}$	58.367	0.501
mp-3125	$K_3Zn_2F_7$	212.99	0.042
mp-31373	$H_{18}SO_{12}$	1000	1.694
mp-3247	Cs_2TiS_3	38.701	0.144
mp-3281	Al_5BO_9	58.979	0.53
mp-3283	$RbNbO_3$	37.601	2.779
mp-3318	Na_2BeF_4	32.236	0.241
mp-34022	Mg_2SnO_4	57.419	0.264
mp-3416	Na_3AlF_6	62.631	0.896
mp-3637	YOF	75.031	0.154
mp-36381	$Sn(PS_3)_2$	48.48	0.142
mp-3765	$Sr(PO_3)_2$	434.796	0.299
mp-3775	Na_2SiF_6	42.421	0.405
mp-3779	$CrSiTe_3$	92.944	0.039
mp-3788	$SrAl_4O_7$	88.266	1.765
mp-3848	$BaGe_4O_9$	31.846	0.439
mp-3870	$Sr_2Nb_2O_7$	84.024	0.35
mp-3881	$BaZnF_4$	45.195	0.277
mp-39140	$Na_4Al_3Si_3HO_{13}$	481.206	0.487
mp-3928	$Na_5P_3O_{10}$	59.727	0.407
mp-3963	K_2CO_3	53.555	0.124
mp-3975	K_2TaF_7	71.01	0.114
mp-39823	$Na_8Al_6Si_6CO_{27}$	1000	0.288
mp-4009	$BaPdS_2$	43.652	0.135

mp-40144	$SiNiH_{12}(OF)_6$	36.413	0.335
mp-40575	$LiNi_2P_4H_3O_{14}$	33.208	1.102
mp-4138	Rb_2CO_3	43.842	0.112
mp-41473	$CsTiNiOF_5$	43.314	0.45
mp-4185	Na_3ScF_6	42.774	6.116
mp-43068	$Na_3Al_3Si_3AgBrO_{12}$	330.145	0.315
mp-4531	$NaNO_3$	233.466	0.127
mp-4649	$PdSe_2O_5$	97.616	15.793
mp-4661	ScOF	113.203	1.87
mp-4691	Ag_2CO_3	36.994	0.276
mp-4758	K_2NbF_7	95.126	0.097
mp-5039	KPO_3	62.174	0.483
mp-504427	Ti_3PbO_7	241.862	0.364
mp-504894	$MgH_{12}SeO_9$	63.329	0.12
mp-505234	BaP_2PbO_7	84.65	0.465
mp-505260	$Te_{10}Mo_3I_{10}$	31.917	1.187
mp-505368	$As_2Pb_3O_8$	37.497	8.354
mp-505392	$Ba_3V_4O_{13}$	69.252	9.036
mp-505400	$BaZr_2F_{10}$	45.541	0.82
mp-505727	NClO	49.827	0.007
mp-505771	$K_2NaH_5(CO_4)_2$	110.91	0.08
mp-505794	$ScH_6N_2Cl_3$	79.274	2.902
mp-505798	Na_4TiSe_4	50.041	14.416
mp-505814	$CsBa_2Nb_3O_{10}$	1000	0.521
mp-5073	$RbNO_3$	151.791	0.183
mp-510018	$Rb_2CuH_{12}(SeO_7)_2$	1000	0.312
mp-510075	$Cs_7Au_5O_2$	1000	0.04
mp-510076	$Rb_7Au_5O_2$	1000	0.047
mp-530449	$Ca_3(AsO_4)_2$	159.639	0.247
mp-530524	Zr_3TlF_{15}	1000	1.293
mp-531826	Li_2PtO_3	34.665	0.326
mp-532315	$Sr_{17}(Ta_5S_{21})_2$	38.198	0.787
mp-5348	$MgCO_3$	35.699	0.328
mp-5401	$Sr_2B_2O_5$	39.374	0.334
mp-540584	K_2PdO_2	68.439	0.089
mp-540629	$Al_2Te_2Cl_7$	57.275	0.187
mp-540656	$Sb(S_8I)_3$	42.345	0.03
mp-540668	BS_2	488.003	0.718
mp-540760	$FePCl_8$	51.436	0.065
mp-540862	$Ba_2CaMgAl_2F_{14}$	126.218	0.165
mp-540868	$Ca_3Si(ClO_2)_2$	1000	0.34
mp-540995	$Rb_5Nb_3OF_{18}$	106.425	0.27

mp-541114	Sr_2RhF_7	67.681	0.134
mp-541134	$TeAuBr_8$	41.207	0.117
mp-541240	$Sb_3O_2F_5$	31.821	2.039
mp-541393	$K_3NaRe_2O_9$	68.739	0.101
mp-541415	$KH_5S_2O_9$	294.862	0.281
mp-541459	$KSnPO_5$	40.672	0.241
mp-541656	$AuCl_2$	32.778	0.169
mp-541682	K_3AlAs_2	174.942	3.335
mp-541684	K_3AlP_2	282.448	2.887
mp-541747	$MgGeH_{12}(OF)_6$	64.462	1.824
mp-541758	$Ta_2Se_{17}Br_{12}$	97.06	3.078
mp-541766	Rb_3InP_2	32.043	3.071
mp-541771	Bi_4RuI_2	173.3	0.107
mp-541772	Bi_4RuBr_2	136.43	9.824
mp-541867	$CsRe_3(O_3F_5)_2$	1000	0.878
mp-541932	$H_{13}S_2N_3O_8$	136.189	0.383
mp-542085	Sr_2GeO_4	47.668	1.8
mp-542129	$CsAlBP_2HO_9$	32.003	0.683
mp-542130	$RbAlBP_2HO_9$	49.159	0.649
mp-542148	$Sb_2N_5F_{11}$	177.176	0.308
mp-542168	Cs_2CoSiO_4	1000	0.27
mp-542417	$Cs_2MgH_{12}(SO_7)_2$	44.707	0.99
mp-542451	$Rb_2NaAl_3F_{12}$	317.444	0.247
mp-542662	$Ga_2Te_2Cl_7$	49.858	0.211
mp-542863	$Ca_7NbSi_4O_{17}F$	209.533	1.229
mp-542931	$Bi_2B_8O_{15}$	1000	2.505
mp-546279	ScBrO	49.938	0.014
mp-546285	NbI_3O	172.674	1.072
mp-547244	$SrBiClO_2$	153.051	0.262
mp-5476	$Cs_4Mg_3F_{10}$	34.135	0.178
mp-5504	$BaCO_3$	74.578	0.283
mp-551456	Ba_2CuClO_2	63.313	0.228
mp-552234	$SrBiBrO_2$	49.199	0.251
mp-552537	Sr_2CuBrO_2	235.363	0.252
mp-552934	Ba_2CuBrO_2	49.444	0.226
mp-554012	$SClO_2F$	33.774	0.116
mp-554016	$K_4Ti_2PO_4F_9$	643.841	1.237
mp-554111	$Ti_3Tl_3(PO_4)_5$	678.824	0.196
mp-554129	$Br_3N(O_2F_5)_2$	1000	0.168
mp-554146	$K_{14}In_4O_{13}$	419.086	5.769
mp-554147	$Rb_2Nb_2P_2S_{11}$	1000	0.291
mp-554157	$KNaZnP_2O_7$	56.566	2.005

mp-554160	$K_2CuP_2O_7$	37.275	0.197
mp-554195	$Sb_3As_2S_{14}(IF_8)_3$	31.132	0.482
mp-554259	$SrAgB_7O_{12}$	1000	0.31
mp-554359	$Cs_2Si_3SnO_9$	38.868	0.203
mp-554379	$AsXeF_{11}$	1000	0.227
mp-554432	$ReSbOF_{10}$	463.54	0.16
mp-554572	$K_3NbP_2O_9$	69.404	0.543
mp-554605	$Rb_2SbCl_3F_2$	1000	0.667
mp-554673	$KZnB(PO_4)_2$	88.009	0.285
mp-554686	$MgAs_2(XeF_9)_2$	223.001	16.951
mp-554701	$SbP(OF_3)_2$	64.341	0.393
mp-554702	$NaZr_2NiF_{11}$	420.641	9.413
mp-554754	$Na_2Zn(SO_4)_2$	53.055	0.816
mp-554805	$Sr_3Se_3(ClO_4)_2$	153.954	0.127
mp-554808	$SnH_{22}(Cl_3O_5)_2$	935.584	0.536
mp-554819	$MgP_4(Cl_5O_3)_2$	1000	0.531
mp-554842	$Cs_5Si_3AgO_9$	47.377	0.178
mp-554948	$NaI(OF)_2$	40.447	0.222
mp-555005	$Na_3Mg_2P_5O_{16}$	116.266	0.371
mp-555059	$TcSb(OF_4)_2$	359.496	1.834
mp-555076	$KNaSnF_6$	159.092	0.229
mp-555082	$CsLi_5(BO_3)_2$	40.755	5.418
mp-555113	$Rb_3Cu_2(BiS_2)_5$	141.766	0.117
mp-555118	$NaPO_3$	57.932	0.275
mp-555122	$Rb_2Pd(NO_3)_4$	101.129	0.446
mp-555155	$KNa_2Y(Si_2O_5)_3$	60.384	0.371
mp-555203	$Sr_5B_3ClO_9$	234.009	0.184
mp-555207	$BN(OF_2)_2$	34.134	7.495
mp-555212	Ba_2InBrO_3	1000	0.028
mp-555230	$Rb_2YGa(SiO_3)_4$	1000	4.847
mp-555231	$Ba_3Bi_2(PO_4)_4$	53.688	7.79
mp-555300	$Na_2Zn_3(SiO_4)_2$	69.291	1.275
mp-555305	$NaNb(OF)_2$	403.768	1.078
mp-555321	$BaNiF_4$	169.746	0.304
mp-555376	$CsAu(SO_4)_2$	66.199	0.271
mp-555392	$K_6NaAu_2IO_8$	652.967	4.334
mp-555424	$CaNb_2(P_2O_7)_3$	44.872	0.4
mp-555467	$Sr_2AlCO_3F_5$	159.373	0.642
mp-555488	$Na_5AlP_2(O_4F)_2$	66.696	0.202
mp-555490	$KRe_2O_4F_7$	96.279	0.355
mp-555526	$RbAg(NO_3)_2$	232.719	0.066
mp-555546	$MgAs_2(XeF_5)_4$	108.784	0.062

mp-555609	$Sr_2Zn_4(CuO_7)_2$	801.71	0.487
mp-555629	$SbTe(ClF_2)_3$	69.559	0.011
mp-555652	$K_2Zn(SO_4)_2$	37.364	0.536
mp-555661	$Ca_9In(PO_4)_7$	33.99	0.365
mp-555805	$AlSCl_7$	36.463	0.031
mp-555825	$Na_4Sc_2Si_4O_{13}$	36.896	0.341
mp-555862	$CsZr(NO_3)_5$	77.688	0.147
mp-555866	$K_6Be_4C_6O_{19}$	44.85	0.263
mp-555958	$Ba_2Li_3(PO_3)_7$	106.159	0.804
mp-555980	$Ba_2Zn_3(PO_3)_{10}$	34.474	99.99
mp-556024	Na_2TiF_6	47.52	0.409
mp-556061	$CsSb_2F_{11}$	123.704	0.285
mp-556078	$MgAs_2(XeF_8)_2$	64.55	0.041
mp-556117	$Ga_3Pb_5F_{19}$	69.078	0.11
mp-556122	$BaCa(PO_3)_4$	42.051	2.278
mp-556171	$CdP_2Xe_5F_{22}$	477.201	0.104
mp-556234	$Rb_3Sb_5O_{14}$	39.634	0.224
mp-556244	$Xe_2NO_2F_{13}$	44.916	0.055
mp-556258	$Na_3BeAl(SiO_4)_2$	246.29	0.324
mp-556282	Ba_2AlInO_5	1000	0.179
mp-556325	$TeAs(ClF_2)_3$	39.371	0.543
mp-556341	$Ti_4S_8Br_6O$	32.997	0.193
mp-556442	$Tc_2O_5F_4$	1000	0.318
mp-556463	KGe_2BO_6	83.005	0.232
mp-556518	$K_2Pd(NO_3)_4$	633.723	0.077
mp-556521	$KNa_7Pb_2O_7$	91.752	0.183
mp-556522	$K_3Cu_2(BiS_2)_5$	497.895	0.183
mp-556539	$BaSb_2Xe_5F_{22}$	236.767	0.314
mp-556546	K_2NiF_4	1000	0.004
mp-556577	$Na_3Sb_3(AsO_7)_2$	63.609	0.931
mp-556637	$Ba_6Na_2Nb_2P_2O_{17}$	721.98	0.23
mp-556653	Cd_2BiAsO_6	217.158	0.35
mp-556655	Li_2AlBO_4	78.779	0.681
mp-556676	$Na_3Al_2(AsO_4)_3$	42.72	1.396
mp-556689	$KZrF_5$	176.068	3.14
mp-556709	Na_2ZrSiO_5	1000	4.371
mp-556756	KSb_2PO_8	50.906	0.372
mp-556785	$RbTeF_5$	133.757	0.072
mp-556801	$Na_3B_6PO_{13}$	793.714	0.299
mp-556834	$RuCl(OF_3)_2$	46.212	1.787
mp-556996	K_2LiAlF_6	36.08	0.416
mp-557022	$Sb_8Cl_2O_{11}$	40.821	1.939

mp-557090	$Bi_2Au_5F_{21}$	35.306	0.11
mp-557132	$Os_2O_3F_7$	88.335	0.42
mp-557171	$Na_2Cu(PO_3)_4$	87.342	0.376
mp-557180	$CaAs_2(XeF_5)_4$	59.884	0.298
mp-557237	$K_5In_3(SiO_3)_7$	133.558	0.27
mp-557250	$HgINO_3$	146.947	0.013
mp-557256	RbP_3PbO_9	90.734	0.574
mp-557260	$RbSb_2F_7$	159.701	0.205
mp-557289	$TiP_2Cl_8O_3$	93.903	4.195
mp-557301	$K_2Ti(Si_2O_5)_3$	37.215	1.043
mp-557352	$CaP_2Xe_5F_{22}$	682.362	0.103
mp-557355	$Rb_2SiP_4O_{13}$	193.087	0.236
mp-557359	$Cs_2Al_2Sb_2O_7$	33.44	0.242
mp-557417	$As_2Cl_3OF_5$	129.94	0.329
mp-557432	$GeClO_2F_5$	495.14	0.269
mp-557451	$CsReOF_6$	955.691	0.089
mp-557470	$K_2Sb_2S(O_2F_3)_2$	68.153	1.772
mp-557531	$Pb_2S(O_2F)_2$	48.772	3.899
mp-557577	$K_3ScSi_2O_7$	167.742	0.2
mp-557628	$AsS(IF_3)_2$	236.93	0.406
mp-557650	$Sr_3P_6(N_4O_3)_2$	170.919	0.535
mp-557662	$Ca_2Mg_5Si_8(O_{11}F)_2$	95.257	1.43
mp-557772	$CsNiF_3$	1000	0.11
mp-557778	$RbNbSiO_5$	34.827	0.273
mp-557792	$HfSCl_6O$	247.825	1.161
mp-557809	$SbSCl_9$	153.663	6.751
mp-557856	$BCl(OF_2)_2$	98.556	0.226
mp-557874	$KAg(PO_3)_2$	32.8	1.462
mp-557926	$CdAs_2(XeF_5)_4$	601.337	0.069
mp-558063	$KCu(BiS_2)_2$	92.807	0.153
mp-558114	Sr_4NbAlO_8	61.155	0.422
mp-558149	BF_3	53.123	0.141
mp-558153	$Ba_4Nb_2(OF_4)_3$	698.417	1.204
mp-558160	$NaYCO_3F_2$	1000	0.451
mp-558162	$RbP(OF)_2$	35.392	0.146
mp-558208	$RbInAs_2O_7$	66.426	0.369
mp-558227	$K_2RbMn_2F_7$	1000	0.049
mp-558235	$CaTaF_7$	1000	0.19
mp-558240	$K_3Al_4P_2O_8F_9$	739.267	1.139
mp-558243	Ba_2InClO_3	1000	0.099
mp-558330	$IClOF$	424.422	0.011
mp-558383	Na_2CrF_4	69.802	0.547

mp-558396	$Rb_2Te(H_6O_5)_2$	44.763	0.649
mp-558430	BaB_2F_8	41.133	13.549
mp-558480	$K_2P_2O_5F_2$	46.674	0.1
mp-558514	$RbZrCdF_7$	184.495	0.136
mp-558523	$PAuClF_3$	271.612	0.213
mp-558603	$K_2Si_4O_9$	42.575	0.685
mp-558607	$K_3BSb_4O_{13}$	39.33	0.646
mp-558660	Mg_2BiPO_6	112.279	0.546
mp-558692	$Sb_2ClO_2F_{11}$	1000	0.751
mp-558725	$Ba_5Ru_2Br_2O_9$	132.837	0.027
mp-558861	$KI(OF)_2$	124.981	0.052
mp-558924	$Na_5Ga_3F_{14}$	59.738	7.488
mp-558938	$Zn_4SiTePbO_{10}$	38.742	0.24
mp-558967	$K_3Ta_2S_{11}$	489.795	0.274
mp-559062	$KP(OF)_2$	38.438	0.223
mp-559064	$SnP_2(Cl_5O)_2$	559.659	0.207
mp-559068	$Na_2Pd(SeO_4)_2$	121.657	0.059
mp-559115	P_2RhClF_6	573.669	0.257
mp-559150	$Na_9ZrP_4ClO_{16}$	198.398	4.687
mp-559151	$BaSrTa_2O_7$	66.558	0.423
mp-559182	P_2IrClF_6	855.904	0.708
mp-559228	Rb_2HfS_4	52.628	0.3
mp-559281	$Na_3Cr_2(PS_4)_3$	39.881	0.086
mp-559292	$P_6Pb_3Xe_{11}F_{58}$	1000	4.657
mp-559309	$K_3ZnNCl_4O_3$	1000	0.112
mp-559314	$Na_5TiP_2O_9F$	70.316	0.501
mp-559378	$Ba_5Ta_2Cl_2O_9$	1000	0.031
mp-559493	$TiPCl_7O$	43.309	0.14
mp-559516	$K_3Nb(SO_4)_4$	43.967	0.193
mp-559533	$NaLiCO_3$	33.938	0.103
mp-559537	$Ca_4P_6O_{19}$	132.46	1.134
mp-559568	$K_2Se_2O_5$	86.791	0.096
mp-559610	$Rb_2NaAl_2(PO_4)_3$	1000	0.239
mp-559710	$NaInAs_2O_7$	62.737	0.873
mp-559724	$Ta_4S_9Br_8$	124.45	0.197
mp-559759	$CaAlBO_4$	143.977	0.577
mp-559783	$Na_3B(PO_4)_2$	78.997	0.27
mp-559786	$NaAs_4BrO_6$	46.229	0.207
mp-559790	$K_2Nb_3Cl_7O_5$	127.361	1.499
mp-559894	$Sb_2Te_2O_9$	122.821	0.616
mp-559923	$Nb(PS_4)_2$	194.05	0.231
mp-559984	$Rb_8AlAu_3O_4$	50.458	0.07

mp-560005	$TlRe_3(S_2Cl)_2$	107.313	0.163
mp-560008	PNF_2	120.224	0.266
mp-560032	$NaNb_2AsO_8$	42.964	2.277
mp-560120	$Na_2Pd(NO_3)_4$	94.265	0.22
mp-560121	H_5CNO_3	58.023	0.253
mp-560144	K_2RuBr_5NO	49.182	0.101
mp-560146	$Ba_{17}Y_{16}Zn_8Pt_4O_{57}$	394.031	0.335
mp-560208	$K_3NbAs_2O_9$	200.748	0.344
mp-560216	$Cs_2GeP_4O_{13}$	73.782	0.213
mp-560222	Na_3SO_4F	227.406	38.747
mp-560310	$SbPOF_8$	298.406	0.562
mp-560314	$In_2H_{10}S_3O_{17}$	57.164	0.302
mp-560320	$KBa_2(PO_3)_5$	50.167	25.678
mp-560322	$K_2RuN_3Cl_3O_5$	159.586	1.463
mp-560324	$Rb_3Hg_2S_3ClO_{12}$	82.828	1.793
mp-560348	$K_6Nb_4S_{25}$	97.358	1.886
mp-560352	$SrP_2(XeF_6)_3$	1000	1.472
mp-560423	$KBS_4(ClO_3)_4$	395.706	0.601
mp-560449	$K_3Ni_2F_7$	481.564	0.043
mp-560459	$Rb_3Al_2(PO_4)_3$	1000	0.144
mp-560515	$K_4Ru_2Cl_{10}O$	1000	0.11
mp-560535	$K_4Sr(SiO_3)_3$	86.342	0.434
mp-560555	$Li_8Bi_2PdO_{10}$	71.588	0.306
mp-560578	$RbTeNO_3F_4$	108.544	0.076
mp-560585	P_3IrO_9	48.227	2.831
mp-560587	$Rb_2Sb_8O_{13}$	517.656	0.284
mp-560595	Ca_2AsClO_4	115.857	0.193
mp-560601	$K_2CuS(ClO_2)_2$	139.292	0.084
mp-560629	$K_3Al_2(PO_4)_3$	1000	0.187
mp-560632	$NaGaSiO_4$	34.954	0.335
mp-560666	$K_4Nb_2Se_{11}O$	47.26	0.07
mp-560675	$K_6Cu(SiO_4)_2$	426.588	0.206
mp-560692	$K_4Nb_6O_{17}$	1000	0.167
mp-560732	$BaNaZrF_7$	35.021	0.312
mp-560739	$K_3Li_3TeO_6$	45.633	0.224
mp-560745	AuN_5O_{14}	67.498	1.168
mp-560884	$TaSCl_7O$	62.597	0.088
mp-560891	$SnP_2Cl_8O_3$	359.885	0.76
mp-560919	$Na_5Y(CO_3)_4$	1000	0.429
mp-560921	$NaAlAs_2O_7$	51.672	1.582
mp-560928	$Sb_2IBr_2F_{11}$	306.673	0.142
mp-560966	K_2RuNCl_5O	57.542	0.182

mp-561011	$Li_2Ta_2(OF_2)_3$	1000	0.05
mp-561058	$Na_3Ga(PO_4)_2$	48.779	0.936
mp-561153	XeF_3	97.709	0.132
mp-561176	Sb_2POF_{13}	1000	0.514
mp-561179	Ba_2CuIO_2	31.932	0.073
mp-561197	TaF_5	60.467	0.302
mp-561222	$K_2HgBr_2(NO_6)_2$	859.12	0.083
mp-561226	$BTe_3(OF_5)_3$	122.966	0.008
mp-561243	Sr_2CuClO_2	971.78	0.254
mp-561259	Na_3NbOF_6	79.154	0.099
mp-561283	$CdGaH_{14}O_7F_5$	116.834	0.832
mp-561317	Rb_2NiF_4	960.056	0.03
mp-561369	$K_3Bi_2(AsO_4)_3$	47.834	1.006
mp-561396	Li_3CrF_6	304.38	0.357
mp-561407	$RbGaS_2$	92.366	0.046
mp-561424	$KAlF_4$	34.914	2.419
mp-561441	Y_2GeO_5	44.372	3.241
mp-561486	$Na_2Mg_5(PO_4)_4$	54.112	4.281
mp-561491	$KNaMg_2Si_4(O_5F)_2$	37.27	1.192
mp-5616	$Sr_2P_2O_7$	126.608	0.459
mp-561647	Cs_2TeOF_4	110.542	0.223
mp-561827	Cs_3TlF_6	283.259	0.045
mp-562102	$K_2S_2O_7$	102.082	0.347
mp-562441	Cs_3AlO_3	65.532	0.629
mp-562442	Cs_2SeO_4	35.192	0.04
mp-562569	$CsPPbS_4$	62.471	0.031
mp-562854	$CsNb_2BiO_7$	48.85	0.555
mp-562977	$RbNbS_2O_9$	165.859	0.29
mp-567441	HfIN	391.693	0.011
mp-567558	$CsAgCl_2$	1000	0.021
mp-567734	$AlAs_3(SeCl)_4$	33.796	1.937
mp-567743	$AlSb_2(TeCl_2)_2$	200.512	1.652
mp-5680	$Ca(PO_3)_2$	59.073	0.485
mp-568136	$RbVBr_3$	309.137	0.096
mp-568252	$Rb_2Hg_2PdCl_8$	42.372	1.636
mp-568346	HfBrN	51.766	0.015
mp-568350	Rb_2ZnCl_4	46.968	0.048
mp-568540	$Ag_5Hg_4P_8Cl_5$	78.325	0.549
mp-568644	K_9InSe_7	84.025	0.066
mp-569050	NaW_6NCl_{18}	58.582	0.033
mp-569386	P_3NCl_{12}	185.278	2.406
mp-569442	$RbAuCl_4$	35.445	29.085

mp-569787	$Al(BH_4)_3$	40.979	0.235
mp-569984	$Cs_3Au_2Br_{11}$	45.806	0.086
mp-570021	$Ti_6Tl_5AgSe_{27}$	31.805	0.119
mp-570193	$NaAuCl_4$	96.231	0.397
mp-570248	NaC_2N_3	732.874	0.396
mp-570315	PBr_2N	138.051	0.103
mp-570411	$K_{12}In_2Se_9$	35.569	0.937
mp-570453	$Ba_4W(N_2Cl)_2$	117.175	0.04
mp-570530	$Cs(BCl)_6$	209.746	0.184
mp-570531	NbP_2NCl_{12}	63.028	0.209
mp-570703	$Ca(AlCl_4)_2$	35.737	0.091
mp-570873	$Nb(Te_2I_3)_2$	160.347	1.471
mp-570966	ZrP_2NCl_{11}	551.611	0.137
mp-571250	$TaP_2Se_2Cl_5$	154.827	0.906
mp-571324	CNCl	139.842	0.116
mp-571464	$RbPSe_3$	254.303	0.061
mp-572149	$Cs_2Al(NO_3)_5$	61.184	0.094
mp-572634	Al_2AgCl_5O	125.095	0.128
mp-572794	$ReP(Cl_2O)_3$	341.005	0.7
mp-573373	$PICl_8$	115.338	0.069
mp-573429	$Cs_5Bi(MoO_4)_4$	557.382	0.357
mp-573751	$AlTeCl_7$	153.106	0.754
mp-574571	Rb_3YCl_6	40.556	0.243
mp-579086	$KSrNb_2O_6F$	1000	0.551
mp-581644	$Y_2Si_2O_7$	1000	0.449
mp-581862	$Cs_2NaAl(PO_4)_2$	332.558	0.139
mp-581868	$NaY(IO_3)_4$	359.643	0.242
mp-581877	$Cs_2Zr(Si_2O_5)_3$	57.396	5.294
mp-581887	$Ca_2As_4Xe_5F_{34}$	63.033	5.635
mp-581955	$CsSi_2SbO_7$	197.604	0.25
mp-581967	Nb_2O_5	1000	2.407
mp-582185	$Cs_{12}Nb(In_2As_3)_3$	67.481	0.081
mp-5824	Hg_2NO_4	83.125	0.135
mp-5860	K_2HgO_2	265.232	0.245
mp-6032	$SrSi_2(BO_4)_2$	53.015	0.656
mp-6044	$Sr_6B(PO_4)_5$	43.039	0.478
mp-607454	$AlC_3(NCl_2)_3$	1000	3.602
mp-607931	$Cs_3NaLi_2(BO_3)_2$	49.754	0.263
mp-607987	$CsInI_4$	67.231	0.209
mp-6138	Na_2TiSiO_5	79.548	0.954
mp-619575	ClF_3	35.294	0.256
mp-619651	Cs_3AlP_2	38.807	0.132

mp-620652	$NaSr_2AlP_3$	36.89	0.28
mp-621112	$Cs_5Nb_2S_4Cl_9$	272.652	0.07
mp-622018	$BAs_5(Pb_3O_{10})_2$	70.951	0.321
mp-622195	$CsSO_3F$	88.405	0.213
mp-622197	$Cs_2PtS_6(O_3F)_6$	131.553	0.017
mp-6228	Na_2TiGeO_5	85.596	0.804
mp-6238	$Ba_2Ta_6Te_2O_{21}$	44.8	0.792
mp-624117	$Cs_3V_4Te_2ClO_{14}$	1000	0.036
mp-6245	$K_5Nb_4O_{12}F$	129.922	2.068
mp-625054	$AlHO_2$	1000	0.259
mp-625475	H_2SO_4	40.897	1.399
mp-625661	H_9BrO_4	1000	0.478
mp-625801	$Sr(H_8O_5)_2$	95.192	0.342
mp-626256	H_3NO_4	55.31	0.265
mp-626785	KHO	114.588	0.405
mp-6289	$Ba_2Ti(GeO_4)_2$	121.385	0.453
mp-628908	$KICl_2$	46.662	0.455
mp-6310	$Ba_3Y(BO_3)_3$	976.503	0.128
mp-634378	$NaHSO_4$	49.087	1.167
mp-638009	$RbPPbS_4$	39.253	0.035
mp-6390	$Rb_3Ti_3(PO_4)_5$	1000	0.242
mp-640389	$Cs_2Th(PS_3)_3$	302.791	8.789
mp-642795	$PHSF_2$	73.515	0.021
mp-642834	BaH_5ClO_3	72.881	0.041
mp-643253	Ba_2H_6Pt	31.36	0.211
mp-643265	ReF_7	422.213	0.008
mp-643586	$CsHS_2(O_3F)_2$	76.692	1.675
mp-643902	$SnH_4(NF)_2$	78.116	0.705
mp-6441	K_2PO_3F	50.092	0.079
mp-644129	$KNiPH_2O_5$	938.959	0.277
mp-644828	$AuXe_2F_{17}$	1000	0.14
mp-645272	$TlV_3(SeO_6)_2$	455.777	0.204
mp-6459	$CaMg(CO_3)_2$	119.968	0.309
mp-6467	$Na_2CuP_2O_7$	50.354	102.781
mp-647342	$SbP_3C(NCl_5)_3$	751.922	0.221
mp-647385	$V_2Pb_4O_9$	154.813	0.285
mp-6481	$Na_2ZnSi_3O_8$	112.155	1.269
mp-648414	V_2PS_{10}	111.788	0.621
mp-648932	Nb_2PS_{10}	80.488	0.037
mp-649253	$NbClF_8$	45.933	0.245
mp-649616	$Pd(XeF_8)_2$	1000	0.082
mp-6500	KRb_2ScF_6	35.602	4.966

mp-651786	$Ca_5MnSi_6(Pb_3O_{11})_3$	37.442	0.225
mp-652776	$Rb_2V(PO_4)_2$	350.147	0.364
mp-653633	K_2ZnCl_4	87.449	0.098
mp-653973	$KZnPO_4$	134.445	0.194
mp-654447	$Ni(XeF_8)_2$	41.006	0.147
mp-6648	$KLiB_4O_7$	36.928	0.518
mp-6651	$K_2Ta_2(OF_2)_3$	475.867	0.356
mp-667283	$Sr_5Re_3ClO_{15}$	37.373	0.158
mp-667292	$K_2MgSi_5O_{12}$	206.73	0.298
mp-667305	$ReN(OF_2)_3$	391.443	0.587
mp-667326	K_5InO_4	184.588	10.983
mp-667360	$CsSbOF_4$	629.926	0.162
mp-667379	$Ba_7Al_{64}O_{103}$	109.608	0.203
mp-6675	$Na_2Zn(SiO_3)_2$	96.215	0.326
mp-669455	$Ga_4Hg_{11}(AsBr_4)_4$	102.079	0.099
mp-669508	TaP_2NCl_{12}	75.83	0.182
mp-6698	$Th_2Cu(PO_4)_3$	1000	2.524
mp-672212	$NaNb_{13}O_{33}$	1000	0.405
mp-672248	$TaAsPCl_{13}$	48.458	0.049
mp-6748	$Cs_2Ti(Si_2O_5)_3$	82.248	3.768
mp-6759	$BaGa_2(SiO_4)_2$	56.289	2.6
mp-676130	$TlSnF_3$	144.508	7.066
mp-676501	$K_3Sn_2S_3BrO_{12}$	295.104	1.289
mp-676801	$K_7Th_6F_{31}$	698.275	0.254
mp-677192	$K_4PH_5S_3O_{16}$	815.19	0.795
mp-677248	$Ca_2AlH_{10}IO_8$	53.719	16.91
mp-677416	$Na_5Mg_5In_3(SO_4)_{12}$	1000	0.702
mp-677520	$KBa_6Zn_4(GaO_3)_7$	52.738	0.308
mp-677638	$Na_{27}Ca_3Al_5(P_2O_7)_{12}$	1000	8.195
mp-679989	$Bi(Mo_2Cl_5)_3$	218.163	0.062
mp-679997	$CsAg_2(B_5O_8)_3$	356.693	0.33
mp-680198	$Cs_4Th_2P_5Se_{17}$	82.617	0.143
mp-680240	$Sb_2Cl_5F_4$	33.179	0.219
mp-680284	$Rb_6Ta_4S_{25}$	186.505	0.261
mp-680374	$KAlSiO_4$	138.265	0.203
mp-680410	$K_3Nb_2S_{11}$	61.395	0.332
mp-680498	$RbTaPS_6$	80.361	2.623
mp-680683	CsB_9O_{14}	34.013	0.282
mp-683918	RbC_2N_3	177.231	0.553
mp-683925	$CsSb_3F_{16}$	1000	0.107
mp-683949	$AlP_3(NCl_3)_3$	69.515	0.152
mp-683955	$KTaPS_6$	52.34	0.226

mp-684010	$K_8Ti_5P_2(O_4F_{11})_2$	1000	1.179
mp-684018	SrB_8O_{13}	263.004	0.967
mp-6841	$Ba_4NaCu(CO_5)_2$	1000	0.264
mp-685352	Ca_2NF	1000	0.344
mp-685478	Na_2PdO_3	98.993	0.155
mp-685810	AsN_2F_7	162.828	0.393
mp-686464	$Ca_{10}P_6SO_{24}$	43.127	0.311
mp-6867	$KCaCO_3F$	1000	0.07
mp-6870	$KBe_2BO_3F_2$	109.536	0.207
mp-6903	$Na_2Ca_4ZrNbSi_4O_{17}F$	36.766	8.604
mp-693620	$KCa_2Be_2Al(Si_2O_5)_6$	100.95	0.435
mp-693753	$BaNa_5Ca_7P_6(O_8F)_3$	1000	1.963
mp-695043	$K_4PH_5Se_3O_{16}$	478.105	0.747
mp-695963	$K_2NaH_{10}IO_{10}$	48.679	0.261
mp-696078	$K_3ZrH_2S(OF)_5$	439.921	2.645
mp-696189	$TlH_6(NO_4)_3$	99.081	0.152
mp-696379	BH_3OF_4	37.357	3.303
mp-696396	$NaHCO_3$	31.92	2.498
mp-696497	$Mg_3Si_4(HO_6)_2$	58.268	0.557
mp-696528	KPH_3NO_3	44.836	4.123
mp-696656	$BH_4O_2F_3$	37.681	0.218
mp-696683	K_3SnHF_8	752.93	0.156
mp-696940	$TiH_{12}C_2(NF)_6$	137.98	0.26
mp-697078	$Cs_2SiP_4(HO_7)_2$	401.69	20.004
mp-697253	$SiH_{12}C_2(NF)_6$	263.583	0.386
mp-698063	$Na_2P_2H_2O_7$	106.778	0.494
mp-698479	$RbTeHOF_4$	939.074	0.462
mp-699453	$RbAs_2H_5O_8$	36.257	0.152
mp-7012	KRb_2YF_6	31.408	21.638
mp-703476	$P_2H_{16}N_4O_7$	132.497	0.194
mp-704408	$K_8V_2(S_2O_9)_3$	1000	0.212
mp-7049	$ZrTlCuS_3$	35.098	0.119
mp-705134	$In_2(MoO_4)_3$	42.359	0.916
mp-705514	$SbHC_3(NCl_3)_3$	44.952	0.879
mp-705900	$Hf_3Tl_{10}Mo_{12}PbO_{48}$	39.2	0.133
mp-706239	$NaCa_2Mg_2V_3O_{12}$	42.547	0.262
mp-706243	$Al_2Si_3H_8(NO_5)_2$	1000	0.359
mp-706386	$ZrH_6O_3F_4$	63.275	0.796
mp-706631	$Na_2B_3HO_6$	63.635	0.59
mp-706976	$PH_4N(OF)_2$	66.979	0.313
mp-706986	PH_4NO_3	44.736	0.167
mp-706995	$ZnCoH_{18}N_6Cl_5$	361.971	0.28

mp-707195	$KSiHO_3$	65.447	0.264
mp-707219	$K_2Zr_2ZnH_{12}(OF_2)_6$	1000	0.892
mp-707343	$ZrH_{12}C_2(NF)_6$	73.812	1.041
mp-707443	$Na_7AlH_2C_4(O_3F)_4$	131.212	0.387
mp-707453	$K_5NaP_3(HO_4)_3$	1000	0.157
mp-707536	$KHSeO_4$	132.704	0.192
mp-707782	$K_6Zr_3H_8(OF)_{12}$	1000	0.193
mp-707960	$ZnH_{12}C_2(N_3Cl_2)_2$	112.254	0.046
mp-7089	KMgSb	36.129	0.033
mp-708961	BeH_8SeO_8	33.064	0.274
mp-709350	$Sr_5As_5HO_{18}$	1000	0.253
mp-720104	$Na_4Al_3Ge_3NO_{14}$	53.887	0.331
mp-720294	$AsH_{18}N_3O_7$	337.227	0.666
mp-720583	$Na_3B_3H_2O_7$	145.069	0.527
mp-720586	CaH_4NClO_5	34.626	0.206
mp-720642	$NaB_3H_4O_7$	49.166	1.45
mp-721182	$PH_{11}(NO_2)_2$	44.086	0.182
mp-721471	$CuPH_4O_5F$	269.346	34.574
mp-722246	$SiH_{10}(O_2F_3)_2$	38.043	2.323
mp-722272	$Li_2H_{12}C_3SN_6O_7$	115.551	0.586
mp-722832	PH_3NF_5	64.284	0.278
mp-722900	CaH_3NO_5	32.128	0.104
mp-723109	$BeH_{14}(I_2O_9)_2$	1000	0.369
mp-730154	$NaAs_3H_2O_9$	35.605	5.748
mp-730460	$Na_5H_3(CO_3)_4$	195.525	0.056
mp-7323	$RbBe_2BO_3F_2$	117.107	0.206
mp-733468	K_2PHO_4	739.107	0.15
mp-733637	NaH_8O_5	67.917	1.355
mp-733655	$KH_3(SO_4)_2$	151.232	12.43
mp-734042	$MgH_{12}(NO_6)_2$	108.906	0.289
mp-735541	$NiSn_2H_{12}(OF)_6$	212.651	0.901
mp-7404	Na_3SbO_4	55.058	15.818
mp-740714	$LiB_5H_2O_9$	44.43	0.343
mp-741045	$Na_4AlP_2HO_9$	186.599	0.606
mp-743538	$CrH_{18}(O_3F)_3$	48.72	0.118
mp-744205	$K_2Cr_2AsHO_{10}$	1000	0.299
mp-744625	$ZnCrH_{15}N_5Cl_4F$	271.211	0.273
mp-744751	$NaMn_6Al_3H_{42}(SO_{19})_2$	1000	0.155
mp-745159	$MoPH_3O_7$	87.865	0.928
mp-745166	$Sr_2Fe_2H_2OF_{10}$	38.365	0.295
mp-7470	RbCuO	57.385	0.057
mp-752709	$InBP_2H_5NO_9$	31.437	0.513

mp-753353	$Sr_4LiCu(CO_5)_2$	1000	0.306
mp-753798	Rb_2SnO_3	33.412	0.183
mp-753854	$Rb_2PH_3SeO_8$	39.743	5.369
mp-754370	Ba_3GeO_5	52.945	0.209
mp-755428	Rb_3ClO	55.311	0.053
mp-755663	$Ta_2Pb_2O_7$	99.902	0.396
mp-756748	$ScH_3(ClO_5)_2$	835.572	4.337
mp-756769	Na_2TlPCO_7	83.096	0.272
mp-756981	K_2SbPCO_7	551.023	0.353
mp-757218	$K_4Na_2H_{18}Pd(IO_{10})_2$	1000	0.481
mp-757594	$Os(OF_2)_2$	112.018	0.01
mp-757723	$SrH_4(SO_4)_3$	140.54	0.49
mp-757840	$Ba_4(PtO_3)_3$	31.053	3.692
mp-757850	$K_4Sb_2O_5$	57.992	0.039
mp-757878	$Na_5Cu(HO_2)_2$	75.359	0.175
mp-757963	$K_2MgH_8(CO_5)_2$	36.138	0.647
mp-757981	$Na_2SnGe_2(HO_4)_2$	32.916	0.647
mp-758007	$Ba_2CaP_4(H_3O_8)_2$	50.442	1.053
mp-758103	$YH_2(CO_3)_2$	146.8	0.238
mp-758337	$Ca_2P_6O_{17}$	50.269	1.052
mp-758814	$CaAs_2H_6F_{18}$	128.146	0.415
mp-758948	$Cs_2H_6CO_6$	64.982	0.166
mp-758957	As_2HPbF_{13}	77.247	0.128
mp-759223	$Sn(SO_4)_2$	31.634	0.326
mp-759344	$P_3H_{30}N_7O_{12}$	617.373	1.643
mp-7594	$CsLiF_2$	69.014	0.23
mp-759651	$ScH_6Br_3N_2$	71.267	2.943
mp-759900	K_2LiNbO_4	150.376	0.332
mp-760046	$LiPH_{21}S_3N_7$	54.395	0.713
mp-760417	Rb_4I_2O	266.004	0.017
mp-760678	$Sb_2H_4AuF_{16}$	155.061	0.163
mp-760762	$NbOF_3$	92.699	0.374
mp-761252	$RbPH_3O_4F$	48.893	0.73
mp-762082	$ThH_{10}N_4O_{17}$	78.29	0.097
mp-762295	$K_2Mn_3V_2(HO_5)_2$	147.196	0.871
mp-764233	Na_8CoO_6	154.44	0.084
mp-765136	$LiMn_8F_{33}$	385.197	0.256
mp-765597	HS_2IO_8	48.891	0.774
mp-766175	$RbInBP_2HO_9$	32.36	0.629
mp-767430	Na_3CdPCO_7	36.525	0.397
mp-767521	Na_2InPCO_7	84.543	0.284
mp-767722	$VFe(P_2O_7)_2$	36.389	0.319

mp-768144	Na_2SbPCO_7	115.289	0.367
mp-768368	K_4I_2O	119.281	0.02
mp-768670	K_3MgPCO_7	64.208	0.387
mp-769604	K_2MnPCO_7	1000	0.249
mp-769616	Na_2CrPCO_7	97.502	0.324
mp-769971	$BaGa_4O_7$	226.992	0.688
mp-770773	$Rb_2S_2O_7$	119.558	3.982
mp-770839	$LiCr(CO_3)_2$	76.429	0.182
mp-770968	Na_3NiPCO_7	314.864	0.702
mp-771127	Rb_4TiO_4	63.485	0.462
mp-771139	Cs_4HfO_4	46.969	1.76
mp-771185	$K_2Ge_2O_5$	55.224	2.356
mp-771255	Cs_4SiO_4	76.117	2.087
mp-772228	CdP_4O_{11}	102.459	3.327
mp-772808	K_2BiPCO_7	77.839	0.276
mp-773432	$KMnPCO_7$	98.931	0.32
mp-774848	$H_{10}SeO_8$	72.129	0.19
mp-775198	$Ti_3P_6WO_{24}$	171.429	0.204
mp-775430	$LiBi_3(IO_2)_2$	44.344	0.196
mp-775466	$K_2InSi_4HO_{11}$	69.994	0.366
mp-778977	$CaAs_2HF_{13}$	231.203	0.229
mp-8065	$K_2Ti_6O_{13}$	33.153	6.088
mp-8201	Rb_3PdF_5	66.954	0.283
mp-8226	ThNF	1000	0.224
mp-8333	$RbNaSnF_6$	165.123	0.156
mp-8416	$BaCaGaF_7$	139.816	0.425
mp-8449	$Rb_2Li_2SiO_4$	34.593	0.643
mp-8450	$Rb_2Li_2GeO_4$	41.311	0.822
mp-849311	$MgSb_2H_2F_{14}$	34.571	0.166
mp-849433	$SrTiH_4(OF_3)_2$	307.592	1.802
mp-849805	$B_{12}H_{21}C_4S_2I$	163.805	0.749
mp-8570	$Ba_3Zr_2S_7$	46.359	0.059
mp-8603	RbAgO	116.333	0.048
mp-863420	$Rb_4H_4C_3O_{10}$	274.258	0.339
mp-865427	$KSrCO_3F$	1000	0.06
mp-865500	$Na_2Hf_2O_5$	1000	0.164
mp-866311	Bi_3BrO_4	950.861	0.386
mp-866620	$Cs_2MgP_4(HO_2)_8$	78.205	0.036
mp-866638	$KSc(BH_4)_4$	44.707	0.141
mp-867261	$RbSrCO_3F$	1000	0.057
mp-867300	$Rb_2Hf_2O_5$	449.153	0.141
mp-867975	$CsB_2H_5O_6$	43.616	0.124

mp-8708	$Mg(AuF_4)_2$	49.625	0.241
mp-8796	$Sr_2LiSc(B_2O_5)_2$	1000	1.371
mp-8810	$SrZn_2(PO_4)_2$	36.547	0.439
mp-8892	$LiInF_4$	46.764	0.275
mp-8962	Rb_2HgF_4	1000	0.036
mp-8963	Cs_2HgF_4	841.758	0.027
mp-8985	$Ba_2YC_2(O_2F)_3$	120.528	0.116
mp-8989	$Na_2P_2PdO_7$	378.386	66.238
mp-9029	Ca_3VN_3	128.975	0.155
mp-9068	K_2NaAlP_2	55.037	0.04
mp-9069	$K_2NaAlAs_2$	41.286	0.038
mp-9107	$NaZrCuS_3$	32.33	0.137
mp-9195	BaCuSeF	118.965	0.376
mp-9306	Sr_2ZnN_2	86.26	0.108
mp-9396	$HfTlCuS_3$	78.058	0.121
mp-9486	K_2AlF_5	76.328	0.136
mp-9511	K_2AsAuS_4	50.963	0.102
mp-9583	K_2ZnF_4	978.704	0.042
mp-96	S	74.632	0.205
mp-9640	$SrCu(SeO_3)_2$	46.448	0.196
mp-9672	K_2NiP_2	188.085	0.136
mp-9726	$SrBeF_4$	45.242	1.029
mp-9986	CsAuO	383.093	0.044

The Python code for automatically creating the slab structures is made availabl e on Github at the following address (https://github.com/bmd-lab/mss_auto) and

is also included below as plain text to facilitate long-term reproducibility.

```
from pymatgen.core import Structure
import numpy as np
from os.path import isfile, join,isdir
from os import listdir,remove,rename,mkdir,getcwd,rmdir
import re
from shutil import copy
import  sys
import  getopt
pattern_id = r'[m][p][-]\d+'
opts,args =
getopt.getopt(sys.argv[1:],'hl:d:n:',["help","length=",'direction=','
name='])

def make_supercell(path_unit_cell, path_super_cell,direction):
    """
    Function:
    Make supercell according to the length
    of unit cell along with z direction,and
    the length of final supercell is at least
    15 anstrom.

    Parameters:
    path_poscar_cart: string
    The path of unit cell structure
    super_cell_dir: string
    The path of supercell structure
    """
    dic_line={'x':2,'y':3,'z':4}

dic_supercell={'x':[[1,1,1],[2,1,1],[3,1,1],[4,1,1],[5,1,1],[6,1,1]],

'y':[[1,1,1],[1,2,1],[1,3,1],[1,4,1],[1,5,1],[1,6,1]],

'z':[[1,1,1],[1,1,2],[1,1,3],[1,1,4],[1,1,5],[1,1,6]]}
    files = [f for f in listdir(path_unit_cell)
                         if isfile(join(path_unit_cell, f))]
    # print("There have {} files of unit cell
files".format(len(files)))
    for i in range(len(files)):
        file_read = open(path_unit_cell + '\\' + files[i], 'r')
        lines = file_read.readlines()
        l = np.array([float(lines[dic_line[direction]].split()[0]),
```

```
                    float(lines[dic_line[direction]].split()[1]),
                    float(lines[dic_line[direction]].split()[2])])
        ll = l * l
        L = np.sqrt(ll[0] + ll[1] + ll[2])
        if L >= 15:
            id = re.search(pattern_id, files[i]).group()
            struc = Structure.from_file(path_unit_cell
                                        + '\\' + files[i])
            struc.make_supercell(dic_supercell[direction][0])
            struc.to(filename=path_super_cell + '\\' + id +
str("POSCAR"))
            print(id, ' has make supercell
',dic_supercell[direction][0])
        elif 7.5 <= L < 15:
            id = re.search(pattern_id, files[i]).group()
            struc = Structure.from_file(path_unit_cell + '\\'
                                        + files[i])
            struc.make_supercell(dic_supercell[direction][1])
            struc.to(filename=path_super_cell + '\\' + id +
str("POSCAR"))
            print(id, ' has make supercell
',dic_supercell[direction][1])
        elif 5 <= L < 7.5:
            id = re.search(pattern_id, files[i]).group()
            struc = Structure.from_file(path_unit_cell + '\\'
                                        + files[i])
            struc.make_supercell(dic_supercell[direction][2])
            struc.to(filename=path_super_cell + '\\' + id +
str("POSCAR"))
            print(id, ' has make supercell
',dic_supercell[direction][2])
        elif 3.75 <= L < 5:
            id = re.search(pattern_id, files[i]).group()
            # print(id)
            struc = Structure.from_file(path_unit_cell + '\\'
                                        + files[i])
            struc.make_supercell(dic_supercell[direction][3])
            struc.to(filename=path_super_cell + '\\' + id +
str("POSCAR"))
            print(id, ' has make supercell
',dic_supercell[direction][3])
        elif 3 <= L < 3.75:
            id = re.search(pattern_id, files[i]).group()
            struc = Structure.from_file(path_unit_cell + '\\'
```

```
                                    + files[i])
            struc.make_supercell(dic_supercell[direction][4])
            struc.to(filename=path_super_cell + '\\' + id +
str("POSCAR"))
            print(id, ' has make supercell
',dic_supercell[direction][4])
        elif 2.5 <= L < 3:
            id = re.search(pattern_id, files[i]).group()
            struc = Structure.from_file(path_unit_cell + '\\'
                                    + files[i])
            struc.make_supercell(dic_supercell[direction][5])
            struc.to(filename=path_super_cell + '\\' + id +
str("POSCAR"))
            print(id, ' has make supercell
',dic_supercell[direction][5])

def add_atom(path_1, path_2,direction):
    """
    Function:
    Produce 1600 different supercell files that the fake
    atom in different position of box for every supercell

    Parameters:
    path_1: string
    The path of POSCAR(super cell),and it must be direction
coordinate
    path_2: string
    The path of POSCAR files that contain a fake atom,
    and it will include 1600 different cases.

    """
    for i in range(100):  # i is the z coordinate of fake atom
        with open(path_1, 'r') as f:
            lines = f.readlines()
            lines[6] = (lines[6].strip('\n')) + ' 1' + '\n'  # add
one for  atom number
            lines[5] = (lines[5].strip('\n')) + ' X' + '\n'  #
suppose the fake atom is X
        for m in np.arange(0.05, 0.95, 0.25):  # m is the x
coordinate of fake atom
            for n in np.arange(0.05, 0.95, 0.25):  # m is the y
coordinate of fake atom
                with open(path_2 + '//' + 'POSCAR'
                          + '_' + str(m) + '_'
```

```
                        + str(n) + '_' + str(i), 'w+') as l:
                    for j in range(len(lines)):
                        l.write(lines[j])
                    if direction == 'x':
                        l.write(str(i * 0.01 + 0.005) + ' ' +
                                str(m) + ' ' +
                                str(n) + ' X')
                    elif direction == 'y':
                        l.write(str(m) + ' ' +
                                str(i * 0.01 + 0.005) + ' ' +
                                str(n) + ' X')
                    elif direction == 'z':
                        l.write(str(m) + ' ' +
                                str(n) + ' ' +
                                str(i * 0.01 + 0.005) + ' X')

def delet_file(Dir, File):
    # delet files in Dir except File
    files = [f for f in listdir(Dir) if isfile(join(Dir, f))]
    for i in files:
        if i == File:
            pass
        else:
            remove(Dir + '//' + i)

def get_nearest_distance(path):
    """
    Return the list of minimum distance to fake atom of all
supercells
    and the corresponding structures.

    Parameters
    path:  string
    The path to the folder containing supercells files,and the
supercell
    must be already added with fake atom.
    """
    files = [f for f in listdir(path) if isfile(join(path, f))]
    distance, structure = [], []
    for i in range(len(files)):
        s = Structure.from_file(path + '//' + files[i])
        d = s.distance_matrix
        t = d[:, -1]
        tt = np.delete(t, [-1])
```

```
            min_d = np.min(tt)
            distance.append(min_d)
            structure.append(files[i])
    return distance, structure

def dir_trans_cart(dir_path, cart_path):
    """
    Function:
    Transform the coordinate of POSCAR from direction
    to cartesian in batch.

    Parameters
    dir_path: string
    The path of POSCAR files with direction coordinate
    cart_path: string
    The path of POSCAR files that after convert into
    cartesian coordinate
    """
    onlyfiles = [f for f in listdir(dir_path) if
isfile(join(dir_path, f))]
    for i in range(len(onlyfiles)):
        try:
            file_read = open(dir_path + "\\" + onlyfiles[i], 'r')
            line = file_read.readlines()
            file_read.close()
            a1 = float(line[2].split()[0])
            a2 = float(line[3].split()[0])
            a3 = float(line[4].split()[0])
            b1 = float(line[2].split()[1])
            b2 = float(line[3].split()[1])
            b3 = float(line[4].split()[1])
            c1 = float(line[2].split()[2])
            c2 = float(line[3].split()[2])
            c3 = float(line[4].split()[2])
            num_atoms = sum([int(x) for x in line[6].split()])
            x_cartesian = []
            y_cartesian = []
            z_cartesian = []
            start_num = 8
            for k in range(start_num, num_atoms + start_num):
                x_cartesian.append(
                    float(line[k].split()[0]) * a1
                    + float(line[k].split()[1])* a2
                    + float(line[k].split()[2]) * a3)
```

```
                y_cartesian.append(
                    float(line[k].split()[0]) * b1
                    + float(line[k].split()[1]) * b2
                    + float(line[k].split()[2]) * b3)
                z_cartesian.append(
                    float(line[k].split()[0]) * c1
                    + float(line[k].split()[1]) * c2
                    + float(line[k].split()[2]) * c3)
            with open(cart_path + "\\" + onlyfiles[i], "w",
encoding="utf-8") as f:
                for j in range(7):
                    f.write(line[j])
                f.write("Cartesian\n")
                for l in range(num_atoms):
                    string = str(x_cartesian[l]) \
                             + "  " + str(y_cartesian[l]) \
                             + "  " + str(z_cartesian[l]) + "\n"
                    f.write(string)
        except:
            print(onlyfiles[i])

def Get_num_of_atom(path, file):
    # get the number of atoms in POSCAR
    # return a data of int type
    with open(path + '//' + file, 'r') as f:
        line = f.readlines()
        num_atoms = sum([int(x) for x in line[6].split()])
    return num_atoms

def insert_empty(dir1, dir2, distance, file,direction):
    """
    Function:
    Introduce an empty layer in the end of POSCAR
    along with z direction

   Parameters:
   dir1: string
   The path of origin POSCAR files and the coordinate of POSCAR
   can be direction or cartesian
   dir_2: string
   The path of POSCAR files that have introduced empty layer
   space
   distance: int
   The length of empty layer
```

```
    file: string
    Name of structure,such as :POSCAR,id+POSCAR
    """
     dic_line = {'x': 2, 'y': 3, 'z': 4}
     with open(dir1 + '//' + file, 'r') as f:
         lines = f.readlines()
         # print(len(lines))
         a, b, c = float(lines[dic_line[direction]].split()[0]), \
                   float(lines[dic_line[direction]].split()[1]), \
                   float(lines[dic_line[direction]].split()[2])
         # print(a,b,c)
         vector = np.array([a, b, c])
         length = np.sum(np.square(vector)) ** 0.5
         L = length + distance
         ratio = L / length
         new_vector = vector * ratio
         with open(dir2 + '//' + file, 'w') as f:
             lines[dic_line[direction]] = str(new_vector[0]) \
                       + ' ' + str(new_vector[1])\
                       + ' ' + str(new_vector[2]) + '\n'
             for i in lines:
                 f.write(i)

def move_atom(dir1, atom_num, dir2, file, length,direction):
    """
    Function:
    Move atoms that higher than fake atom,
    equivalent to the effect of moving the
    vacuum layer.

    Parameters:
    dir1:  string
    The path of supercell files that
    contain vacuum layer,and the atoms haven't
    moved
    atom_num: int
    The number of atoms in POSCAR file
    dir2: string
    The path of supercell files that
    contain vacuum layer,and the atoms have
    moved according to the position of atoms
    file: string
    Name of structure,such as :POSCAR,id+POSCAR
    length: int
```

```
The distance of atom need to be moved,
it should stay the same with the
length of vacuum layer
"""
dic_num={'x':0, 'y':1,'z':2}
with open(dir1 + '//' + file, 'r') as f:
    lines = f.readlines()
    high = float(lines[-1].split()[dic_num[direction]])
    #         print(z_fake)
    for i in range(atom_num - 1):
        x, y, z = float(lines[8 + i].split()[0]), \
                  float(lines[8 + i].split()[1]), \
                  float(lines[8 + i].split()[2])
        if direction == 'x':
            if high < 0 and x < high:
                x_new = x - length
                lines[8 + i] = str(x_new) + ' ' \
                               + str(y) + ' ' \
                               + str(z) + '\n'
            elif high > 0 and x > high:
                x_new = x + length
                lines[8 + i] = str(x_new) + ' ' \
                               + str(y) + ' ' \
                               + str(z) + '\n'
        elif direction == 'y':
            if high < 0 and y < high:
                y_new = y - length
                lines[8 + i] = str(x) + ' ' \
                               + str(y_new) + ' ' \
                               + str(z) + '\n'
            elif high > 0 and y > high:
                y_new = y + length
                lines[8 + i] = str(x) + ' ' \
                               + str(y_new) + ' ' \
                               + str(z) + '\n'
        elif direction == 'z':
            if high < 0 and z < high:
                z_new = z - length
                lines[8 + i] = str(x) + ' ' \
                               + str(y) + ' ' \
                               + str(z_new) + '\n'
            elif high > 0 and z > high:
                z_new = z + length
                lines[8 + i] = str(x) + ' ' \
```

```
                                    + str(y) + ' ' \
                                    + str(z_new) + '\n'
        with open(dir2 + '//' + file, 'w+') as f:
            for i in lines:
                f.write(i)

def delet_fake_atom(dir1, dir2, file):
    """
    Function:
    Delet the fake atom of slab structure

    Parameters:
    dir1: string
    The path of slab structure contained
    with fake atom
    dir2: string
    The path of slab structure that
    have deleted fake atom
    file: string
    Name of structure,such as :POSCAR,id+POSCAR
    """
    with open(dir1 + '//' + file, 'r') as f:
        lines = f.readlines()
        s = lines[5].split()
        s2 = lines[6].split()
        n_s, n_s2 = s[:-1], s2[:-1]
        line5, line6 = '', ''
        for i in range(len(n_s)):
            line5 += n_s[i] + ' '
            line6 += n_s2[i] + ' '
        new_line5 = line5 + '\n'
        new_line6 = line6 + '\n'
        #         print(new_line5,new_line6)
        lines[5], lines[6] = new_line5, new_line6
        with open(dir2 + '//' + file, 'w+') as f:
            for i in lines:
                f.write(i)

def main(length,direction,unit_cell_dir):
    name=unit_cell_dir.split('//')[-1]
    supercell_dir=unit_cell_dir[:-len(name)]+'super'
    slab_dir=unit_cell_dir[:-len(name)]+'slab'
    mkdir(supercell_dir)
    mkdir(slab_dir)
```

```
    make_supercell(unit_cell_dir, supercell_dir,direction)
    files=[f for f in listdir(supercell_dir) if isfile
(join(supercell_dir,f))]
    mkdir(slab_dir+'//Final_slab')
    for file in files:
        mkdir(slab_dir + '//' + file)
        mkdir(slab_dir + '//' + file + '/add')
        mkdir(slab_dir + '//' + file + '/cartesian')
        mkdir(slab_dir + '//' + file + '/add_empty')
        mkdir(slab_dir + '//' + file + '/move_atom')
        mkdir(slab_dir + '//' + file + '/final_slab')

        poscar_dir= slab_dir+'//'+file+"/add"
        cart_dir = slab_dir+'//'+file+"/cartesian"
        insert_empty_dir = slab_dir+'//'+file+'/add_empty'
        move_atom_dir = slab_dir+'//'+file+'/move_atom'
        final_slab_dir = slab_dir+'//'+file+'/final_slab'

        s = Structure.from_file(supercell_dir + '//' + file)
        s.to(filename=slab_dir + '//' + file + '//' + 'POSCAR')
        path_1 = slab_dir + '//' + file + '//' + 'POSCAR'
        path_2 = slab_dir + '//' + file + '//' + 'add'
        try:
            max_dis=[]
            add_atom(path_1, path_2, direction)
            d, stru = get_nearest_distance(path_2)
            max_dis.append(max(d))
            delet_file(path_2, stru[d.index(max(d))])
            rename(path_2 + '//' + stru[d.index(max(d))], path_2 +
'//' + file)
            print(file, 'is OK!!!')
        except:
            print(file, 'Happen something wrong')
        dir_trans_cart(poscar_dir,cart_dir)
        num = Get_num_of_atom(cart_dir, file)
        insert_empty(cart_dir,insert_empty_dir,length,file,direction)
        move_atom(insert_empty_dir, num, move_atom_dir,
file,length,direction)
        delet_fake_atom(move_atom_dir, final_slab_dir, file)
        copy(final_slab_dir+'//'+file,slab_dir+'//Final_slab//'+file)
dir=getcwd()
unit_name='unit_cell'
length,direction='',''
```

```
try:
    for k, v in opts:
        if k in ('-n', '--name'):
            unit_name = v
        elif k in ('-l', '--length'):
            length = int(v)
        elif k in ('-d','--direction'):
            direction = v
        elif k in ('-h','--help'):
            print('Hello!! ','\n',
                  'Before running this script' \
                  ' you are expect to creat a new folder named','\n',
                  'unit_cell for storing the unit cell files' \
                  ' and fill the following three options','\n',
                  'with right information','\n'
                  'Options:','\n',
                  '-n,  --name   the name of '\
                  'unit cell folder','\n',
                  '-l,  --length   the length of '\
                  'empty layer','\n',
                  '-d,  --direction   the direction of ' \
                  'makeing supercell','\n'
                  )
    unit_dir=dir+'\\'+ unit_name
    main(length,direction,unit_dir)
except:
    rmdir(dir+'\\'+'slab')
    rmdir(dir+'\\'+'super')
```