

High-Throughput Identification of Materials for Si Tandem Solar Cells – Supplementary Information

Yanzhen Zhao,^a Zhikun Yao,^a Chang Liu,^a Wei Ren,^{a,b} Geoffroy Hautier^c and Lee A. Burton^{*a,d}

Table S1. The band gap values (eV) of 881 candidates calculated by HSE.

Number	Materials Project ID	Material	Gap	Number	Materials Project ID	Material	Gap
1	mp-74	Rh	0.00	34	mp-1380	Zn ₃ Ru	0.00
2	mp-101	Ir	0.00	35	mp-1534	YS	0.00
3	mp-190	ReO ₃	0.00	36	mp-1540	HoTl	0.00
4	mp-246	TiF ₃	0.00	37	mp-1548	PrMg	0.00
5	mp-265	TaIr ₃	0.00	38	mp-1597	UO ₂	0.00
6	mp-429	ZnNi	0.00	39	mp-1610	TbS	0.00
7	mp-572	SmCd	0.00	40	mp-1623	ErS	0.00
8	mp-615	YMg	0.00	41	mp-1630	Zr ₃ Hg	0.00
9	mp-635	ScRh ₃	0.00	42	mp-1635	TbMg	0.00
10	mp-646	PrCd	0.00	43	mp-1766	TmS	0.00
11	mp-656	LuS	0.00	44	mp-1782	ScSe	0.00
12	mp-702	CeHg	0.00	45	mp-1842	NbAl ₃	0.00
13	mp-734	LaHg	0.00	46	mp-1857	YbCd	0.00
14	mp-771	MnAl	0.00	47	mp-1921	ThTe	0.00
15	mp-776	LaCd	0.00	48	mp-1948	LaAg	0.00
16	mp-869	TaAl ₃	0.00	49	mp-1959	PuO ₂	0.00
17	mp-873	VPd ₃	0.00	50	mp-1973	NbGa ₃	0.00
18	mp-922	CoPt ₃	0.00	51	mp-2011	UP	0.00
19	mp-945	NiPt	0.00	52	mp-2052	ScAs	0.00
20	mp-953	NbZn ₃	0.00	53	mp-2053	Nb ₃ Sb	0.00
21	mp-1020	TaRh ₃	0.00	54	mp-2070	CoS ₂	0.00
22	mp-1027	HfRh ₃	0.00	55	mp-2077	DyMg	0.00
23	mp-1059	NdCd	0.00	56	mp-2082	PIr ₂	0.00
24	mp-1073	CaCd	0.00	57	mp-2260	FePt	0.00
25	mp-1089	TiIr ₃	0.00	58	mp-2291	Si ₂ Ni	0.00
26	mp-1113	BW ₂	0.00	59	mp-2364	PaO ₂	0.00
27	mp-1144	ErP	0.00	60	mp-2367	LaC ₂	0.00
28	mp-1152	TiRh ₃	0.00	61	mp-2379	CoSi ₂	0.00
29	mp-1164	ThC	0.00	62	mp-2423	US	0.00
30	mp-1180	MnPt ₃	0.00	63	mp-2459	YbIn	0.00
31	mp-1240	HoS	0.00	64	mp-2470	DyS	0.00
32	mp-1326	Nb ₃ Sn	0.00	65	mp-2525	PrAg	0.00
33	mp-1327	NdMg	0.00	66	mp-2558	SmMg	0.00

67	mp-2616	NpO ₂	0.00	110	mp-4881	Er(SiNi) ₂	0.00
68	mp-2636	GdMg	0.00	111	mp-4883	Ba(FeP) ₂	0.00
69	mp-2678	VPt	0.00	112	mp-4903	Tm(CuSi) ₂	0.00
70	mp-2705	VPt ₃	0.00	113	mp-4973	CeSF	0.00
71	mp-2731	TiGa ₃	0.00	114	mp-4985	Dy(MnSi) ₂	0.00
72	mp-2732	PRh ₂	0.00	115	mp-4998	Sr ₂ IrO ₄	0.00
73	mp-2807	ScP	0.00	116	mp-5000	Tl(CuSe) ₂	0.00
74	mp-2861	CaTl	0.00	117	mp-5054	Pr(CoP) ₂	0.00
75	mp-2906	Ho(NiP) ₂	0.00	118	mp-5112	Pr(CoSi) ₂	0.00
76	mp-2924	Ho(SiNi) ₂	0.00	119	mp-5129	Y(CoSi) ₂	0.00
77	mp-2938	Tm(FeSi) ₂	0.00	120	mp-5150	HoSi ₂ Ni	0.00
78	mp-2958	Dy(BC) ₂	0.00	121	mp-5227	Dy(NiP) ₂	0.00
79	mp-3129	ScSi ₃ Ni	0.00	122	mp-5268	U ₂ SbN ₂	0.00
80	mp-3191	Ho(FeSi) ₂	0.00	123	mp-5326	Yb(CoSi) ₂	0.00
81	mp-3208	ZrGeTe	0.00	124	mp-5346	Lu(CuSi) ₂	0.00
82	mp-3210	Ca(CoP) ₂	0.00	125	mp-5451	Er(FeGe) ₂	0.00
83	mp-3239	Er(CoSi) ₂	0.00	126	mp-5497	Er(CoGe) ₂	0.00
84	mp-3262	Tm(CoSi) ₂	0.00	127	mp-5505	U ₂ TeN ₂	0.00
85	mp-3292	Tb(CoSi) ₂	0.00	128	mp-5517	Tb(NiP) ₂	0.00
86	mp-3299	Sr(FeP) ₂	0.00	129	mp-5529	MnFe ₂ Si	0.00
87	mp-3402	UTeN	0.00	130	mp-5597	Ca(FeP) ₂	0.00
88	mp-3437	Ce(CoSi) ₂	0.00	131	mp-5622	Nd(CoP) ₂	0.00
89	mp-3455	Er(NiP) ₂	0.00	132	mp-5666	Ho(MnGe) ₂	0.00
90	mp-3587	Sc(SiNi) ₂	0.00	133	mp-5671	Sr(CoP) ₂	0.00
91	mp-3758	Eu(NiP) ₂	0.00	134	mp-5677	Tb(MnSi) ₂	0.00
92	mp-3799	GdSF	0.00	135	mp-5688	Er(FeSi) ₂	0.00
93	mp-3854	Y(MnSi) ₂	0.00	136	mp-5765	Nd(BC) ₂	0.00
94	mp-4064	Ca(NiP) ₂	0.00	137	mp-5796	Ho(MnSi) ₂	0.00
95	mp-4105	Ho(CuSi) ₂	0.00	138	mp-5820	Ce(CoP) ₂	0.00
96	mp-4228	Nd(CoSi) ₂	0.00	139	mp-5835	Ho(CoSi) ₂	0.00
97	mp-4305	Er(CuSi) ₂	0.00	140	mp-5976	Dy(CoSi) ₂	0.00
98	mp-4374	UAsS	0.00	141	mp-5983	Tm(CoGe) ₂	0.00
99	mp-4415	Ho(CoGe) ₂	0.00	142	mp-5992	LaB ₂ Ir ₂ C	0.00
100	mp-4469	Tm(SiNi) ₂	0.00	143	mp-6191	CeB ₂ Rh ₂ C	0.00
101	mp-4487	Er(MnGe) ₂	0.00	144	mp-6205	Ba ₂ Ho(CuO ₂) ₄	0.00
102	mp-4492	MnCo ₂ Si	0.00	145	mp-6583	Ba ₂ Er(CuO ₂) ₄	0.00
103	mp-4574	YbTaO ₄	0.00	146	mp-6691	Ba ₂ Dy(CuO ₂) ₄	0.00
104	mp-4593	Mn ₃ AlC	0.00	147	mp-6710	Ba ₂ Tm(CuO ₂) ₄	0.00
105	mp-4595	VFe ₂ Si	0.00	148	mp-6779	Ba ₂ Pr(CuO ₂) ₄	0.00
106	mp-4596	Sr ₂ RuO ₄	0.00	149	mp-6790	Ba ₂ Y(CuO ₂) ₄	0.00
107	mp-4729	Er(MnSi) ₂	0.00	150	mp-6794	LaB ₂ Rh ₂ C	0.00
108	mp-4860	Gd ₂ CuO ₄	0.00	151	mp-6916	Sm(BC) ₂	0.00
109	mp-4875	GdTlO ₄	0.00	152	mp-6956	La(FeP) ₂	0.00

153	mp-6957	Ce(FeP) ₂	0.00	196	mp-11578	VZn ₃	0.00
154	mp-6969	Sc(CuSi) ₂	0.00	197	mp-12083	CrIr ₃	0.00
155	mp-7171	TmP	0.00	198	mp-12098	K(PRh) ₂	0.00
156	mp-7194	TbCuAs ₂	0.00	199	mp-12100	Lu(SiNi) ₂	0.00
157	mp-7298	Li(CuP) ₂	0.00	200	mp-12266	CaCuF ₄	0.00
158	mp-7349	Ba(BRh) ₂	0.00	201	mp-12382	ErSi ₂ Ni	0.00
159	mp-7818	Pd ₄ Se	0.00	202	mp-12585	CrRh ₃	0.00
160	mp-8137	NpSO	0.00	203	mp-12593	ScIr ₃	0.00
161	mp-8761	NdCoC ₂	0.00	204	mp-12599	PrTl	0.00
162	mp-9075	CdCuF ₄	0.00	205	mp-12625	U ₂ TeO ₂	0.00
163	mp-9463	ZrGeSb	0.00	206	mp-13473	Sm(MnSi) ₂	0.00
164	mp-9473	Ba(NiP) ₂	0.00	207	mp-13914	LiCo ₂ Ge	0.00
165	mp-9913	Fe ₃ B ₂ P	0.00	208	mp-13964	HfGeTe	0.00
166	mp-9930	UPSe	0.00	209	mp-15039	Ba ₂ Yb(CuO ₂) ₄	0.00
167	mp-10108	NpP	0.00	210	mp-15617	Cr ₃ B ₃	0.00
168	mp-10109	NpS	0.00	211	mp-15780	MgPPT ₅	0.00
169	mp-10181	LiSiNi ₂	0.00	212	mp-15805	Mn ₃ ZnN	0.00
170	mp-10192	LuP	0.00	213	mp-15968	Sm(CoSi) ₂	0.00
171	mp-10270	ScCo ₃ C	0.00	214	mp-16315	GePt ₃	0.00
172	mp-10350	BaNdCuBO ₅	0.00	215	mp-16334	Fe ₃ PdN	0.00
173	mp-10374	Cr ₃ PtN	0.00	216	mp-18331	GdCrO ₃	0.00
174	mp-10564	SrN ₂	0.00	217	mp-18725	YCrO ₃	0.00
175	mp-10852	La(BC) ₂	0.00	218	mp-19007	V ₂ PO ₅	0.00
176	mp-10853	Pr(BC) ₂	0.00	219	mp-19102	Sr ₂ FeO ₄	0.00
177	mp-10854	Tb(BC) ₂	0.00	220	mp-19269	NdCrO ₃	0.00
178	mp-10856	Er(BC) ₂	0.00	221	mp-19281	LaCrO ₃	0.00
179	mp-10964	CeB ₂ Ir ₂ C	0.00	222	mp-19722	MnCu ₂ SnS ₄	0.00
180	mp-10991	YCuAs ₂	0.00	223	mp-19756	GdB ₂ Rh ₂ C	0.00
181	mp-10992	DyCuAs ₂	0.00	224	mp-19815	Eu ₂ VO ₄	0.00
182	mp-10993	ErCuAs ₂	0.00	225	mp-19819	GdIn	0.00
183	mp-10994	TmCuAs ₂	0.00	226	mp-19966	GdTl	0.00
184	mp-11263	Zr ₃ Au	0.00	227	mp-20023	PrIn	0.00
185	mp-11286	CaHg	0.00	228	mp-20025	Mn(GaS ₂) ₂	0.00
186	mp-11374	DyTl	0.00	229	mp-20095	Eu(FeP) ₂	0.00
187	mp-11375	EuHg	0.00	230	mp-20188	GdCuAs ₂	0.00
188	mp-11387	HfGa ₃	0.00	231	mp-20263	CaIn	0.00
189	mp-11416	TaGa ₃	0.00	232	mp-20264	Tb(FeGe) ₂	0.00
190	mp-11467	NdHg	0.00	233	mp-20298	SmIn	0.00
191	mp-11469	PrHg	0.00	234	mp-20410	Ho(BC) ₂	0.00
192	mp-11504	MnZn ₃	0.00	235	mp-20422	KMnP	0.00
193	mp-11517	NbRu ₃	0.00	236	mp-20431	Ca ₂ FeSbO ₆	0.00
194	mp-11575	YTl	0.00	237	mp-20553	GdMnSi	0.00
195	mp-11576	YbTl	0.00	238	mp-20596	U(SiNi) ₂	0.00

239	mp-20614	EuMnO ₃	0.00	282	mp-29797	GdBrO	0.00
240	mp-20649	Y(MnGe) ₂	0.00	283	mp-30147	ZrTiAs	0.00
241	mp-20908	Ce(BC) ₂	0.00	284	mp-30682	ZrGa	0.00
242	mp-20913	UGeS	0.00	285	mp-30836	TaPd ₃	0.00
243	mp-20937	Cr ₃ C ₂	0.00	286	mp-30856	ZnPt ₃	0.00
244	mp-20947	CaRuO ₃	0.00	287	mp-30871	Ta ₃ Sn	0.00
245	mp-21000	Dy(MnGe) ₂	0.00	288	mp-30878	TbTl	0.00
246	mp-21289	TiZn ₃	0.00	289	mp-31054	La ₃ (VN ₃) ₂	0.00
247	mp-21298	NpSi ₂	0.00	290	mp-31138	MnPd ₃	0.00
248	mp-21302	Sr ₂ MnGaO ₅	0.00	291	mp-37014	GdPaO ₄	0.00
249	mp-21313	Mn ₃ GaC	0.00	292	mp-37297	U ₂ PS	0.00
250	mp-21364	HoCuAs ₂	0.00	293	mp-39159	CaLaTiCrO ₆	0.00
251	mp-21429	U(CoSi) ₂	0.00	294	mp-40630	CaPrMn ₂ O ₆	0.00
252	mp-21471	LiFeAs	0.00	295	mp-505820	NiPS	0.00
253	mp-21473	Gd(NiP) ₂	0.00	296	mp-510402	GdS	0.00
254	mp-21845	FePd ₃	0.00	297	mp-510624	SrFeO ₃	0.00
255	mp-22106	NdNiO ₃	0.00	298	mp-542915	TiAl ₃	0.00
256	mp-22152	NaFeAs	0.00	299	mp-542985	Gd(CoSi) ₂	0.00
257	mp-22159	UNiAs ₂	0.00	300	mp-545481	Ca ₂ Cu(BrO) ₂	0.00
258	mp-22280	PrNiO ₃	0.00	301	mp-545847	LuBi ₂ BrO ₄	0.00
259	mp-22306	Eu ₂ CuO ₄	0.00	302	mp-546295	Sr ₂ CuOsO ₆	0.00
260	mp-22374	U(CuSi) ₂	0.00	303	mp-549695	GdBi ₂ ClO ₄	0.00
261	mp-22486	Tb(MnGe) ₂	0.00	304	mp-550306	YCu ₂ Bi ₂ (SeO ₂) ₂	0.00
262	mp-22495	SmNiO ₃	0.00	305	mp-550566	EuBi ₂ ClO ₄	0.00
263	mp-23019	UNCl	0.00	306	mp-550805	LuBi ₂ ClO ₄	0.00
264	mp-23085	Ba ₂ Cu ₃ (ClO ₂) ₂	0.00	307	mp-551101	HoBi ₂ IO ₄	0.00
265	mp-23129	Ba ₂ Cu ₃ (BrO ₂) ₂	0.00	308	mp-551250	ErBi ₂ IO ₄	0.00
266	mp-23194	LaI ₂	0.00	309	mp-557018	Cs(CoS) ₂	0.00
267	mp-24092	GdH ₂	0.00	310	mp-557447	Ba ₂ Eu ₃ Mn ₂ (CuO ₆) ₂	0.00
268	mp-24095	PrH ₂	0.00	311	mp-562809	GdBi ₂ BrO ₄	0.00
269	mp-24096	NdH ₂	0.00	312	mp-567077	SmB ₂ Rh ₂ C	0.00
270	mp-24658	SmH ₂	0.00	313	mp-567341	PrCoC ₂	0.00
271	mp-24720	PuH ₂	0.00	314	mp-568902	Yb(CoGe) ₂	0.00
272	mp-27186	MgVO ₃	0.00	315	mp-568924	PrB ₂ Rh ₂ C	0.00
273	mp-27468	U ₂ BiN ₂	0.00	316	mp-568940	Y(NiP) ₂	0.00
274	mp-27496	YUO ₄	0.00	317	mp-569147	UP ₂	0.00
275	mp-27677	KCu ₄ S ₃	0.00	318	mp-569294	NdB ₂ Rh ₂ C	0.00
276	mp-27982	PuBrO	0.00	319	mp-569408	K(CoAs) ₂	0.00
277	mp-28614	NaBPT ₃	0.00	320	mp-569565	La ₃ (CrN ₃) ₂	0.00
278	mp-28753	NdI ₂	0.00	321	mp-569593	PmMg	0.00
279	mp-28884	Cs(FeAs) ₂	0.00	322	mp-569697	Ce(NiP) ₂	0.00
280	mp-29242	Ba ₃ PbO	0.00	323	mp-569974	Nd(NiP) ₂	0.00

281	mp-29243	Ba ₃ SnO	0.00	324	mp-570100	Tm(NiP) ₂	0.00
325	mp-570254	ThBC	0.00	368	mp-864943	MnBe ₂ Ir	0.00
326	mp-570412	Yb(NiP) ₂	0.00	369	mp-864944	MnBe ₂ Pt	0.00
327	mp-570456	Eu(CoAs) ₂	0.00	370	mp-864945	MnBe ₂ Rh	0.00
328	mp-570631	U(FeP) ₂	0.00	371	mp-865003	Be ₂ IrPd	0.00
329	mp-571098	Lu(FeSi) ₂	0.00	372	mp-865021	Be ₂ RuPt	0.00
330	mp-571342	TiGa ₂	0.00	373	mp-865181	EuGeO ₃	0.00
331	mp-571405	NdTl	0.00	374	mp-865229	Be ₂ NiIr	0.00
332	mp-571552	Lu(CoGe) ₂	0.00	375	mp-865308	Be ₂ CuRh	0.00
333	mp-573563	Sm(CoP) ₂	0.00	376	mp-865355	Zn ₃ Pt	0.00
334	mp-574199	Sm(NiP) ₂	0.00	377	mp-865786	CrPd ₃	0.00
335	mp-579496	Fe ₃ PtN	0.00	378	mp-865792	BeSiNi ₂	0.00
336	mp-580234	Fe ₃ RhN	0.00	379	mp-865869	Be ₂ CuPt	0.00
337	mp-601285	MnGaNi ₂	0.00	380	mp-865901	BeCo ₂ Si	0.00
338	mp-607111	AlPt ₃	0.00	381	mp-866115	Be ₂ PdRh	0.00
339	mp-611623	U(CoP) ₂	0.00	382	mp-866224	Be ₂ NiPt	0.00
340	mp-614981	Ba ₂ Nd(CuO ₂) ₃	0.00	383	mp-866288	BeVCo ₂	0.00
341	mp-639690	PuS ₂	0.00	384	mp-867270	Be ₂ CoPt	0.00
342	mp-644246	EuH ₃ Pd	0.00	385	mp-867273	Be ₂ CuIr	0.00
343	mp-654374	Ba ₂ YTlCu ₂ O ₇	0.00	386	mp-867274	Be ₂ CoIr	0.00
344	mp-672294	Eu(CoSi) ₂	0.00	387	mp-867293	LiCo ₂ Si	0.00
345	mp-675626	Cu ₃ AsSe ₄	0.00	388	mp-867304	BeVFe ₂	0.00
346	mp-677445	Y ₄ SiS ₃	0.00	389	mp-867816	TaRu ₃	0.00
347	mp-686050	CePaO ₄	0.00	390	mp-867878	AlFe ₂ Si	0.00
348	mp-691045	Na ₅ Ce ₃ Ti ₆ Nb ₂ O ₂₄	0.00	391	mp-867920	K ₂ Rh ₂ O ₅	0.00
349	mp-753398	WOF ₃	0.00	392	mp-972326	TcPt ₃	0.00
350	mp-754322	Sr ₂ CuO ₄	0.00	393	mp-973267	KTcO ₃	0.00
351	mp-754674	Lu(CuO ₂) ₂	0.00	394	mp-973633	LuSi ₂ Ni	0.00
352	mp-755713	Tb ₂ SbO ₂	0.00	395	mp-973908	PaFe ₃	0.00
353	mp-757102	Sr ₂ RhO ₄	0.00	396	mp-974358	Ir ₃ Ru	0.00
354	mp-861931	LiPt ₃	0.00	397	mp-974376	PtRh ₃	0.00
355	mp-861936	LiPd ₃	0.00	398	mp-974616	Pt ₃ Rh	0.00
356	mp-861939	Ac ₃ Sn	0.00	399	mp-976724	Hf(VH ₂) ₂	0.00
357	mp-862377	LiBe ₂ Ir	0.00	400	mp-977176	NaTcO ₃	0.00
358	mp-862600	Be ₂ PtRh	0.00	401	mp-978569	Sm(BRh) ₄	0.00
359	mp-862621	GaPt ₃	0.00	402	mp-989647	YReN ₃	0.00
360	mp-862669	BeFe ₂ Si	0.00	403	mp-998212	RbAgBr ₃	0.00
361	mp-862706	BeCo ₂ Ge	0.00	404	mp-998306	CsPdBr ₃	0.00
362	mp-862910	PmH ₃	0.00	405	mp-998344	CsAgBr ₃	0.00
363	mp-863709	Ir ₃ Rh	0.00	406	mp-1001836	MnGa	0.00
364	mp-864606	AcCuO ₃	0.00	407	mp-1006371	CePS	0.00
365	mp-864647	Hf ₂ N	0.00	408	mp-1008376	CeH ₃	0.00

366	mp-864655	PaCo ₃	0.00	409	mp-1014265	Zr ₂ N	0.00
367	mp-864895	Be ₂ NiRh	0.00	410	mp-1017554	CdNi ₃ N	0.00
411	mp-1018133	LiHPd	0.00	454	mp-1079403	Sr ₂ CoOsO ₆	0.00
412	mp-1018658	CaCoSi	0.00	455	mp-1079914	HfSb	0.00
413	mp-1018675	DyS ₂	0.00	456	mp-1079944	LuCuAs ₂	0.00
414	mp-1018709	Hf ₂ GaSb ₃	0.00	457	mp-1080176	Gd(BC) ₂	0.00
415	mp-1018727	HoS ₂	0.00	458	mp-1080399	ThB ₂ Rh ₂ C	0.00
416	mp-1018808	MgCoGe	0.00	459	mp-1080469	HfCuGe ₂	0.00
417	mp-1018828	NpSeO	0.00	460	mp-1087483	ThCuPO	0.00
418	mp-1019093	PaP ₂	0.00	461	mp-1095170	Sr ₂ FeOsO ₆	0.00
419	mp-1025200	Eu ₂ TiO ₄	0.00	462	mp-1095201	ZrCuGe ₂	0.00
420	mp-1025223	Hf ₄ Al ₃	0.00	463	mp-1095254	EuMoO ₄	0.00
421	mp-1025258	ZnPPd ₅	0.00	464	mp-1095614	ErAsS	0.00
422	mp-1025261	MgPPd ₅	0.00	465	mp-1095656	LuAsSe	0.00
423	mp-1025270	GaPPt ₅	0.00	466	mp-1095675	CeAsS	0.00
424	mp-1025271	AlPPt ₅	0.00	467	mp-1101828	TbAsS	0.00
425	mp-1025272	ZnPPt ₅	0.00	468	mp-1101897	GdAsS	0.00
426	mp-1025301	GaPPd ₅	0.00	469	mp-1102052	DyAsS	0.00
427	mp-1025393	TmSi ₂ Ni	0.00	470	mp-1102079	TmAsS	0.00
428	mp-1025519	RbCu ₄ S ₃	0.00	471	mp-1102733	HoAsS	0.00
429	mp-1058490	EuIn	0.00	472	mp-1102959	YAsS	0.00
430	mp-1063174	GdAu ₂	0.00	473	mp-1103398	TmAsSe	0.00
431	mp-1067935	Ho ₂ SbO ₂	0.00	474	mp-1103625	Np ₂ Se ₅	0.00
432	mp-1067937	Ho ₂ BiO ₂	0.00	475	mp-1103808	La ₄ H ₉	0.00
433	mp-1068300	Ca(FeAs) ₂	0.00	476	mp-1104116	La ₂ H ₅	0.00
434	mp-1068786	InCo ₃ N	0.00	477	mp-1104579	Ce ₂ H ₅	0.00
435	mp-1068954	Tb ₂ BiO ₂	0.00	478	mp-1105218	NaOsO ₃	0.00
436	mp-1069057	Sr(CoSi) ₂	0.00	479	mp-1106241	BaTbMn ₂ O ₅	0.00
437	mp-1069288	MnGa ₄	0.00	480	mp-1147653	CaCu ₃ O ₄	0.00
438	mp-1069561	Dy ₂ BiO ₂	0.00	481	mp-1178355	Er ₂ TeO ₂	0.00
439	mp-1069613	Er ₂ BiO ₂	0.00	482	mp-1178366	Dy ₂ SbO ₂	0.00
440	mp-1070152	Ca(CoSi) ₂	0.00	483	mp-1178924	Tm(BIr) ₄	0.00
441	mp-1070510	Y ₂ BiO ₂	0.00	484	mp-1183139	AcNiO ₃	0.00
442	mp-1070662	Gd ₂ BiO ₂	0.00	485	mp-1183419	Be ₂ IrRu	0.00
443	mp-1070713	InNi ₃ N	0.00	486	mp-1183998	Ga ₃ Tc	0.00
444	mp-1077133	GdCoSi	0.00	487	mp-1184119	CuPd ₃	0.00
445	mp-1077201	UAsP	0.00	488	mp-1184336	FeIr ₃	0.00
446	mp-1077374	ThSiS	0.00	489	mp-1185317	LiBe ₂ Pt	0.00
447	mp-1077453	HfCuGe	0.00	490	mp-1185616	Mn ₂ CrSi	0.00
448	mp-1077918	Sr ₂ TcO ₄	0.00	491	mp-1186117	NiPt ₃	0.00
449	mp-1078278	CrB ₄	0.00	492	mp-1186350	NiIr ₃	0.00
450	mp-1078518	Sr ₂ NiIrO ₆	0.00	493	mp-1186437	Pd ₃ W	0.00
451	mp-1078866	Y(BC) ₂	0.00	494	mp-1186902	Re ₃ Ir	0.00

452	mp-1078868	Sr ₂ MgReO ₆	0.00	495	mp-1187243	TaOs ₃	0.00
453	mp-1079111	EuTiO ₃	0.00	496	mp-1188853	CaTcO ₃	0.00
497	mp-1189046	Er(BIr) ₄	0.00	540	mp-1218352	Sr ₃ NdMn ₂ O ₈	0.00
498	mp-1189906	Ca ₂ CrSbO ₆	0.00	541	mp-1218450	Sr ₃ La(NiO ₄) ₂	0.00
499	mp-1190025	Ba ₂ US ₆	0.00	542	mp-1218451	Sr ₃ PrMn ₂ O ₈	0.00
500	mp-1206312	SmCr ₂ Si ₂ C	0.00	543	mp-1218464	Sr ₄ TlFe ₂ O ₉	0.00
501	mp-1206409	K(FeP) ₂	0.00	544	mp-1218503	Sr ₈ RuRh ₃ O ₁₆	0.00
502	mp-1206423	NdIn	0.00	545	mp-1218716	Sr ₂ Pr ₂ TlNi ₂ O ₉	0.00
503	mp-1206645	Sr ₂ TiMnO ₆	0.00	546	mp-1218769	Sr ₂ MnRuO ₆	0.00
504	mp-1206780	Ti ₂ Sb	0.00	547	mp-1218828	Sr ₂ FeO ₃ F	0.00
505	mp-1206830	Cs(CoAs) ₂	0.00	548	mp-1218849	Sr ₂ GdCu ₂ IrO ₈	0.00
506	mp-1207007	Tm(MnSi) ₂	0.00	549	mp-1219180	Sm ₂ SbO ₂	0.00
507	mp-1207079	SrH ₃ Pd	0.00	550	mp-1219319	Sm ₂ CoNiO ₆	0.00
508	mp-1207092	GdHSe	0.00	551	mp-1219665	PuPaO ₄	0.00
509	mp-1207112	Lu(MnSi) ₂	0.00	552	mp-1219797	Ni ₆ SnTe ₂	0.00
510	mp-1207117	Fe ₂ CoSi	0.00	553	mp-1219894	Pr ₂ InAg	0.00
511	mp-1207125	Cs(FeP) ₂	0.00	554	mp-1220715	Nb ₃ Fe(BiO ₃) ₆	0.00
512	mp-1207142	Rb(CoAs) ₂	0.00	555	mp-1221696	MnFePd ₆	0.00
513	mp-1207868	UAgF ₆	0.00	556	mp-1222266	Lu ₃ S ₄	0.00
514	mp-1209751	Pr ₂ MnNiO ₆	0.00	557	mp-1222329	LuAlCu	0.00
515	mp-1209940	NaSmCu ₂ F ₈	0.00	558	mp-1224337	HfScGe ₄	0.00
516	mp-1209951	NaYbCu ₂ F ₈	0.00	559	mp-1224680	Gd ₂ SbO ₂	0.00
517	mp-1210068	NaErCu ₂ F ₈	0.00	560	mp-1224823	GaGePt ₆	0.00
518	mp-1210079	NaGdCu ₂ F ₈	0.00	561	mp-1224947	FeNiPt ₆	0.00
519	mp-1210114	NaEu(MoO ₄) ₂	0.00	562	mp-1225447	ErPaO ₄	0.00
520	mp-1210555	Mn ₃ SnH	0.00	563	mp-1225518	Er ₂ SbO ₂	0.00
521	mp-1213889	Ce ₃ Cu ₄ (P ₂ O) ₂	0.00	564	mp-1225693	DyMn ₂ SiGe	0.00
522	mp-1214103	Ca ₂ TaCrO ₆	0.00	565	mp-1226070	CoCuS ₄	0.00
523	mp-1214115	Ca ₂ NbCrO ₆	0.00	566	mp-1226551	CePtRh	0.00
524	mp-1214577	Ba ₂ Sm(CuO ₂) ₄	0.00	567	mp-1226589	CeNdAl ₂ O ₆	0.00
525	mp-1214585	Ba ₂ Pr(CuO ₂) ₃	0.00	568	mp-1226653	CePt ₂ Au ₃	0.00
526	mp-1214720	Ba ₂ Gd(CuO ₂) ₄	0.00	569	mp-1226848	Ce ₄ Cu ₃ (SO) ₄	0.00
527	mp-1215169	ZrVW	0.00	570	mp-1226890	Ce ₄ H ₁₁	0.00
528	mp-1215378	Zr ₄ Ni ₃ As ₈	0.00	571	mp-1227161	CaPr ₃ (FeO ₃) ₄	0.00
529	mp-1215463	YbPaO ₄	0.00	572	mp-1227251	CaMnFeGe ₂	0.00
530	mp-1216092	YMn ₂ SiGe	0.00	573	mp-1227487	Ca ₂ MgReO ₆	0.00
531	mp-1216599	UCuSi ₂ Ni	0.00	574	mp-1227620	Ca ₃ YTi ₄ O ₁₂	0.00
532	mp-1216793	UNiP ₂	0.00	575	mp-1227698	Ca ₂ TlIn	0.00
533	mp-1217891	TaTiAl ₆	0.00	576	mp-1228257	Ba ₂ YCu ₃ PbO ₇	0.00
534	mp-1217893	TaNbAl ₆	0.00	577	mp-1228402	Ba ₂ NdTlCu ₂ O ₇	0.00
535	mp-1217981	SrNdNiO ₄	0.00	578	mp-1229131	Ba ₁₀ Pr ₄ Y(CuO ₂) ₂₀	0.00
536	mp-1218069	SrPr(FeO ₃) ₂	0.00	579	mp-1274387	La ₂ ZnCoO ₆	0.00
537	mp-1218104	SrPr ₃ (FeO ₃) ₄	0.00	580	mvc-10314	CaHo(FeO ₃) ₂	0.00

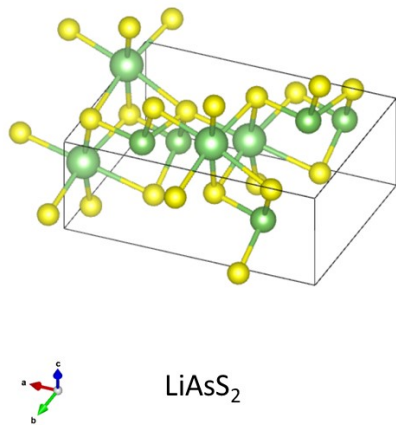
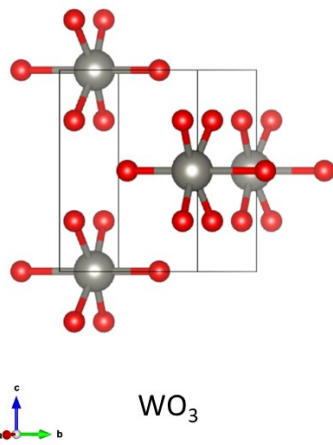
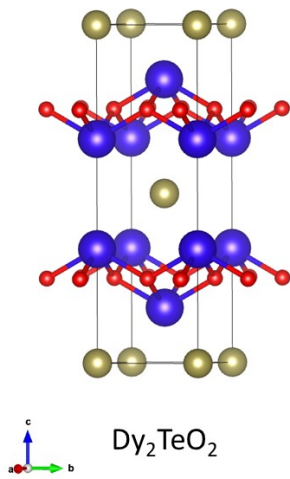
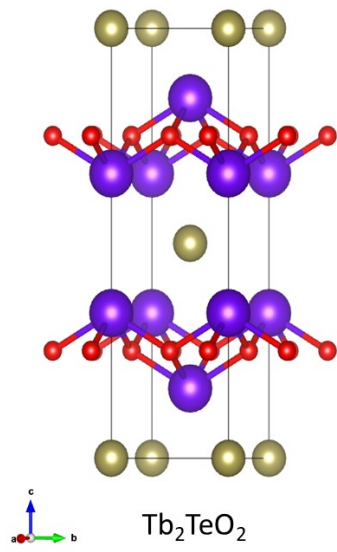
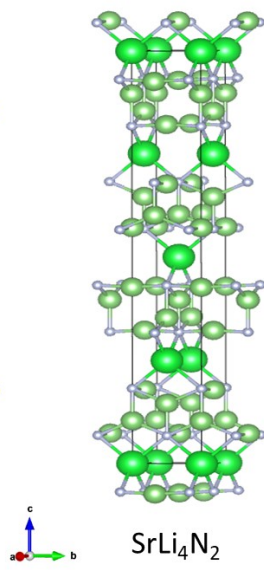
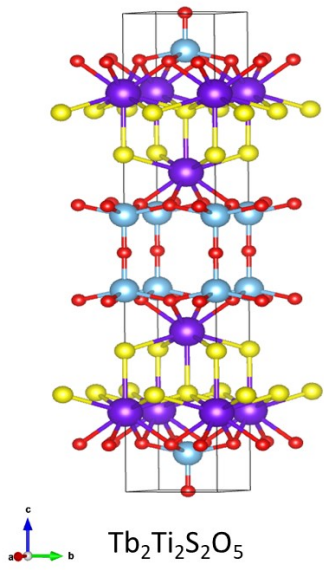
538	mp-1218155	SrLaNiO ₄	0.00	581	mvc-5785	Ca ₂ CrIrO ₆	0.00
539	mp-1218189	SrLaCrO ₄	0.00	582	mvc-9241	CaPrTi ₂ O ₆	0.00
583	mp-22619	NiP ₂	0.01	626	mp-4405	Rb ₃ AuO	1.09
584	mp-1078180	Sr ₂ MgOsO ₆	0.02	627	mp-22736	InCuS ₂	1.10
585	mp-1106184	MnB ₄	0.07	628	mp-10289	Ca(BC) ₂	1.10
586	mp-1101764	NdAsS	0.08	629	mp-35152	Sr ₂ H ₅ Rh	1.13
587	mp-1212091	HoAsSe	0.10	630	mp-1079541	ZnCu ₂ SnS ₄	1.15
588	mp-1102952	DyAsSe	0.10	631	mp-29754	SrLiN	1.15
589	mp-1102476	TbAsSe	0.10	632	mp-676409	EuPaO ₄	1.19
590	mp-1095603	YAsSe	0.10	633	mp-149	Si	1.20
591	mp-1213048	ErAsSe	0.10	634	mp-1101971	FePS	1.22
592	mp-22020	Ca ₂ NiOsO ₆	0.11	635	mp-9774	Ba ₄ Sb ₂ O	1.24
593	mp-1102762	SmAsS	0.13	636	mp-1079889	ZnAg ₂ SnS ₄	1.24
594	mp-505569	CeH ₂	0.16	637	mp-1013550	Ca ₃ SbP	1.24
595	mp-1189762	EuCrO ₃	0.23	638	mp-1009088	BeGeAs ₂	1.25
596	mp-1018144	LaH ₃	0.26	639	mp-773137	KCaBi	1.31
597	mp-19115	CaFeO ₃	0.26	640	mp-27763	UIN	1.35
598	mp-5702	Cu ₃ SbS ₄	0.29	641	mp-1575878	Ca ₃ Fe ₂ O ₇	1.38
599	mp-1078624	LaCoC ₂	0.29	642	mp-680339	Mn ₄ Si ₇	1.40
600	mp-1183416	BeCrFe ₂	0.30	643	mp-7623	MgAs ₄	1.40
601	mp-866152	TiBeCo ₂	0.36	644	mp-27762	UBrN	1.42
602	mp-1225890	Cu ₉ Sb(AsS ₆) ₂	0.38	645	mp-542187	Sr ₂ MnClO ₃	1.43
603	mp-18940	Sr ₂ NiMoO ₆	0.43	646	mp-6408	ZnCu ₂ GeS ₄	1.49
604	mp-1205944	Sr ₂ TaVO ₆	0.44	647	mp-1216153	Y ₂ CrFeO ₆	1.49
605	mp-1191365	GdPS	0.47	648	mp-1232352	Dy ₂ CrFeO ₆	1.49
606	mp-1013558	Ca ₃ BiP	0.53	649	mp-2199	Fe ₃ Si	1.50
607	mp-569001	Sr ₂ LiCoN ₂	0.56	650	mp-9200	K ₃ AuO	1.51
608	mp-1025467	Cu ₂ SnHgS ₄	0.61	651	mp-27891	Bi ₂ SO ₂	1.52
609	mp-18820	Sr ₃ Fe ₂ O ₇	0.65	652	mp-1218763	Sr ₂ MnSbO ₆	1.57
610	mp-14285	CoP ₂	0.72	653	mp-9306	Sr ₃ ZnN ₂	1.58
611	mp-1190998	PrPS	0.75	654	mp-1221609	MnGa(CuSe ₂) ₂	1.60
612	mp-1191667	NdPS	0.80	655	mp-13682	PdS ₂	1.63
613	mp-1219942	Sr ₂ YCu ₂ BiPbO ₈	0.80	656	mp-1178173	Ho ₂ TeO ₂	1.63
614	mp-1192185	DyPS	0.80	657	mp-19443	WO ₃	1.65
615	mp-1191026	YPS	0.88	658	mp-555874	LiAsS ₂	1.65
616	mp-1191565	SmPS	0.88	659	mp-1224851	GaCuGeSe ₄	1.67
617	mp-2097	SnO	0.88	660	mp-755756	Y ₂ TeO ₂	1.70
618	mp-1225836	Cu ₄ Bi ₃ Pb(SeO) ₄	0.89	661	mp-1009087	BeSiAs ₂	1.72
619	mp-1190952	TbPS	0.90	662	mp-16037	Dy ₂ TeO ₂	1.73
620	mp-1078292	CdCu ₂ SnS ₄	0.96	663	mp-1232332	ZnCu ₂ SiSe ₄	1.75
621	mp-10952	Cu ₂ HgGeS ₄	0.96	664	mp-10960	Tb ₂ Ti ₂ S ₂ O ₅	1.77
622	mp-552098	Bi ₂ SeO ₂	1.00	665	mp-1245502	Li ₂ TiN ₂	1.82
623	mp-23116	CuBiSeO	1.05	666	mp-16036	Tb ₂ TeO ₂	1.82

624	mp-1228030	Ba ₄ Bi ₂ O	1.08	667	mp-15845	SrLi ₄ N ₂	1.83
625	mp-865213	Ba ₈ Bi ₄ H ₂ O	1.09	668	mp-25305	Y ₂ Ti ₂ S ₂ O ₅	1.85
669	mp-5999	Sm ₂ Ti ₂ S ₂ O ₅	1.85	712	mp-1226996	CdBi ₁₂ (Cl ₇ O ₆) ₂	2.36
670	mp-20794	Sr ₂ NiWO ₆	1.86	713	mp-552008	DyBi ₂ ClO ₄	2.36
671	mp-9517	SrTiN ₂	1.90	714	mp-9158	LiCuO ₂	2.37
672	mp-552028	Nd ₂ Ti ₂ S ₂ O ₅	1.90	715	mp-549127	HoBi ₂ ClO ₄	2.38
673	mp-552963	Pr ₂ Ti ₂ S ₂ O ₅	1.90	716	mp-29091	Ti(CuS) ₄	2.38
674	mp-4524	ZnGeP ₂	1.96	717	mp-768368	K ₄ I ₂ O	2.39
675	mp-5238	GaCuS ₂	1.96	718	mp-549709	ErBi ₂ ClO ₄	2.39
676	mp-1226003	CoPS	1.98	719	mp-546082	TmBi ₂ ClO ₄	2.40
677	mp-3762	VCu ₃ S ₄	2.02	720	mp-22922	AgCl	2.43
678	mp-1025340	Cu ₂ WSe ₄	2.03	721	mp-23480	Bi ₂ WO ₆	2.43
679	mp-556560	MnF ₃	2.03	722	mp-23630	NbBi ₄ ClO ₈	2.46
680	mp-5760	NdSF	2.04	723	mp-1271282	CoF ₃	2.46
681	mp-4763	ZnSiP ₂	2.05	724	mp-551244	CsK ₂ CoO ₂	2.47
682	mp-3931	SmSF	2.07	725	mp-1274783	SrLaCoO ₄	2.49
683	mp-1522	FeS ₂	2.10	726	mp-1296711	LaCoO ₃	2.52
684	mp-10930	TbSF	2.10	727	mp-753353	Sr ₄ LiCu(CO ₅) ₂	2.54
685	mp-552857	TbBi ₂ IO ₄	2.12	728	mp-23602	TaBi ₄ ClO ₈	2.57
686	mp-9846	RbCaSb	2.12	729	mp-706	HgF	2.59
687	mp-29782	Bi ₂ W ₂ O ₉	2.13	730	mp-1211474	K ₂ Ti(CuS ₂) ₂	2.61
688	mp-546266	DyBi ₂ IO ₄	2.15	731	mp-5621	NbCu ₃ S ₄	2.61
689	mp-913	CdP ₂	2.16	732	mp-7129	Rb ₂ Ti(CuS ₂) ₂	2.63
690	mp-28171	K ₃ IO	2.18	733	mp-20090	PrCoO ₃	2.66
691	mp-551816	YBi ₂ IO ₄	2.18	734	mp-554207	TaBi ₄ BrO ₈	2.70
692	mp-10086	YSF	2.18	735	mp-22599	NdCoO ₃	2.72
693	mp-1105187	CuPS ₃	2.20	736	mp-5339	CsNaTe	2.73
694	mp-1541943	Zn(CuO ₂) ₂	2.21	737	mp-1212757	EuCoO ₃	2.87
695	mp-552738	TmBi ₂ IO ₄	2.22	738	mp-553310	CsCuO ₂	2.89
696	mp-550635	LuBi ₂ IO ₄	2.22	739	mp-10748	TaCu ₃ S ₄	2.94
697	mp-549475	TbBi ₂ BrO ₄	2.22	740	mp-7206	TcAgO ₄	2.99
698	mp-552992	DyBi ₂ BrO ₄	2.24	741	mp-11919	Sr(BeN) ₂	3.00
699	mp-1223929	InCuGeS ₄	2.25	742	mp-1080625	Sr ₂ LiReO ₆	3.03
700	mp-553243	YBi ₂ BrO ₄	2.26	743	mp-20652	PbF ₃	3.05
701	mp-546152	SmBi ₂ ClO ₄	2.26	744	mp-947	Au ₂ S	3.05
702	mp-546621	ErBi ₂ BrO ₄	2.28	745	mp-4979	AlCuS ₂	3.07
703	mp-19208	La ₂ MnCoO ₆	2.28	746	mp-20459	TiPbO ₃	3.07
704	mp-546625	HoBi ₂ BrO ₄	2.29	747	mp-7907	Al ₂ ZnSe ₄	3.14
705	mp-546350	TmBi ₂ BrO ₄	2.31	748	mp-23064	Bi ₂ MoO ₆	3.21
706	mp-2490	GaP	2.32	749	mp-23072	BiBrO	3.21
707	mp-27251	Bi ₂ TeO ₆	2.33	750	mp-20727	Sb ₂ PbO ₆	3.23
708	mp-1550	AlP	2.33	751	mp-13900	Sr(CuO) ₂	3.24
709	mp-547125	TbBi ₂ ClO ₄	2.34	752	mp-2352	Na ₂ O	3.27

710	mp-1189897	Ba ₂ ThS ₆	2.35	753	mp-4651	SrTiO ₃	3.27
711	mp-552604	YBi ₂ ClO ₄	2.35	754	mp-3349	Sr ₃ Ti ₂ O ₇	3.28
755	mp-1207386	ZrNF	3.29	798	mp-1216536	TmPaO ₄	4.17
756	mp-40830	NaSr ₃ LaTi ₅ O ₁₅	3.32	799	mp-973585	LuIO	4.17
757	mp-5532	Sr ₂ TiO ₄	3.35	800	mp-1222263	LuPaO ₄	4.22
758	mp-5350	Zn(GaS ₂) ₂	3.39	801	mp-1194523	Li ₂ CaTa ₂ O ₇	4.23
759	mp-1342	BaO	3.40	802	mp-27439	TmIO	4.34
760	mp-558917	LiMoIO ₆	3.43	803	mp-19426	CaWO ₄	4.37
761	mp-20194	CeO ₂	3.45	804	mp-1443	Sn ₃ F ₈	4.37
762	mp-694961	Na ₉ Sr ₂ Nd ₉ Ti ₂₀ O ₆₀	3.45	805	mp-28020	AlCuCl ₄	4.40
763	mp-643260	Na ₂ H ₄ Pd	3.47	806	mp-753173	HoIO	4.41
764	mp-1220820	NaBi ₃ (ClO ₂) ₂	3.48	807	mp-555560	CdTeMoO ₆	4.42
765	mp-560114	Er ₃ O ₂ F ₅	3.51	808	mp-2964	NaNO ₂	4.42
766	mp-1539317	Ta ₂ O ₅	3.51	809	mp-9126	Sr(SbO ₃) ₂	4.43
767	mp-1210016	NaNdMgWO ₆	3.51	810	mp-1173356	PrPaO ₄	4.44
768	mp-22939	BiClO	3.55	811	mp-1173377	NdPaO ₄	4.45
769	mp-556210	Bi ₂ CO ₅	3.57	812	mp-1173352	PmPaO ₄	4.46
770	mp-1539136	CaCu ₂ F ₈	3.60	813	mp-753712	YIO	4.46
771	mp-29362	GaCuCl ₄	3.61	814	mp-23730	NaMgH ₃	4.47
772	mp-11918	Ca(BeN) ₂	3.69	815	mp-1173297	SmPaO ₄	4.47
773	mp-1221380	Na ₃ EuTi ₂ Nb ₂ O ₁₂	3.70	816	mp-3338	NaGaO ₂	4.47
774	mp-1210188	Nd ₂ Ti ₃ (BiO ₆) ₂	3.70	817	mp-1173104	TbPaO ₄	4.49
775	mp-1210092	NaBi(MoO ₄) ₂	3.70	818	mp-1103472	Na ₂ UF ₈	4.51
776	mp-23089	SrTa ₂ Bi ₂ O ₉	3.70	819	mp-1100867	YPaO ₄	4.54
777	mp-7094	ReAgO ₄	3.72	820	mp-23360	Zn(IO ₃) ₂	4.60
778	mp-1173345	PaInO ₄	3.73	821	mp-557724	KBiF ₆	4.64
779	mp-1221219	Na ₃ SrTa ₄ O ₁₂	3.75	822	mp-19163	SrWO ₄	4.66
780	mp-1221182	NaCa ₂ Nb ₈ (BiO ₄) ₉	3.75	823	mp-1220980	NaNd(MoO ₄) ₂	4.72
781	mp-4019	CaTiO ₃	3.76	824	mp-19330	CaMoO ₄	4.80
782	mp-754225	YbTiO ₃	3.78	825	mp-38322	Mg(IO ₃) ₂	4.84
783	mp-562854	CsNb ₂ BiO ₇	3.78	826	mp-1220757	NaLa(MoO ₄) ₂	4.86
784	mp-22169	MoPbO ₄	3.82	827	mp-6391	Na ₂ ZnSiO ₄	4.90
785	mp-1221019	NaNb ₄ Bi ₅ O ₁₈	3.84	828	mp-16915	BaTiOF ₄	4.93
786	mp-1105	BaO ₂	3.84	829	mp-241	CdF ₂	4.96
787	mp-7801	CaGeN ₂	3.85	830	mp-5558	NaReO ₄	4.97
788	mp-23705	Na ₃ AlH ₆	3.89	831	mp-23859	CaHCl	5.09
789	mp-1222782	LaPaO ₄	3.93	832	mp-760762	NbOF ₃	5.12
790	mp-3858	NaTaO ₃	3.95	833	mp-1070852	YbHCl	5.17
791	mp-1211901	KLaTiO ₄	3.95	834	mp-18834	SrMoO ₄	5.18
792	mp-1223057	LaAg(MoO ₄) ₂	3.96	835	mp-24422	CaHBr	5.40
793	mp-1211538	KNdTiO ₄	3.96	836	mp-6406	Na ₂ MgSiO ₄	5.43

794	mp-1225510	DyPaO ₄	4.08	837	mp-5295	LaNbO ₄	5.46
795	mp-1223799	HoPaO ₄	4.09	838	mp-12931	SmTaO ₄	5.55
796	mp-9239	NaLaMgTeO ₆	4.09	839	mp-12427	Sr ₂ TaGaO ₆	5.57
797	mp-556697	CaTa ₂ Bi ₂ O ₉	4.10	840	mp-12932	TbTaO ₄	5.59
841	mp-1183115	AcAlO ₃	5.59	862	mp-1097916	CsCaCl ₃	6.65
842	mp-7703	DyTaO ₄	5.60	863	mp-1070599	CsYbCl ₃	6.73
843	mp-5985	HoTaO ₄	5.61	864	mp-7571	KNbF ₆	7.04
844	mp-3444	ErTaO ₄	5.62	865	mp-1213993	CaAs ₂ F ₁₂	7.16
845	mp-5377	YTaO ₄	5.64	866	mp-643759	GaH ₃ NF ₃	7.28
846	mp-754969	TmBrO	5.64	867	mp-5078	SrZnF ₄	7.34
847	mp-1206859	ErBrO	5.69	868	mp-632326	HCl	7.42
848	mp-29327	SmBrO	5.77	869	mp-557483	YbClF	7.45
849	mp-1178160	HoBrO	5.80	870	mp-463	KF	7.91
850	mp-643	ThO ₂	6.15	871	mp-8537	S(OH) ₂	7.94
851	mp-632229	HBr	6.25	872	mp-8416	BaCaGaF ₇	8.03
852	mp-28567	LiBiF ₄	6.27	873	mp-1540904	KTaF ₆	8.27
853	mp-7405	SmAlO ₃	6.29	874	mp-972825	SiH ₈	8.67
854	mp-1025185	Cs ₂ CaCl ₄	6.30	875	mp-674459	NaErF ₄	8.99
855	mp-34337	H ₄ NCl	6.33	876	mp-675798	NaHoF ₄	9.00
856	mp-1078265	Cs ₂ YbCl ₄	6.34	877	mp-2955	NaMgF ₃	9.02
857	mp-1213703	Cs ₃ Ca ₂ Cl ₇	6.39	878	mp-34081	NaYF ₄	9.04
858	mp-1207669	TmOF	6.53	879	mp-18065	BaCaAlF ₇	9.13
859	mp-1210775	LuOF	6.57	880	mp-2741	CaF ₂	9.18
860	mp-27478	Na ₃ PaF ₈	6.59	881	mp-1818	SiF ₄	10.04
861	mp-29731	HoClO	6.61				

Figure S1. The chemical structures for the 11 final-candidate made with VESTA.



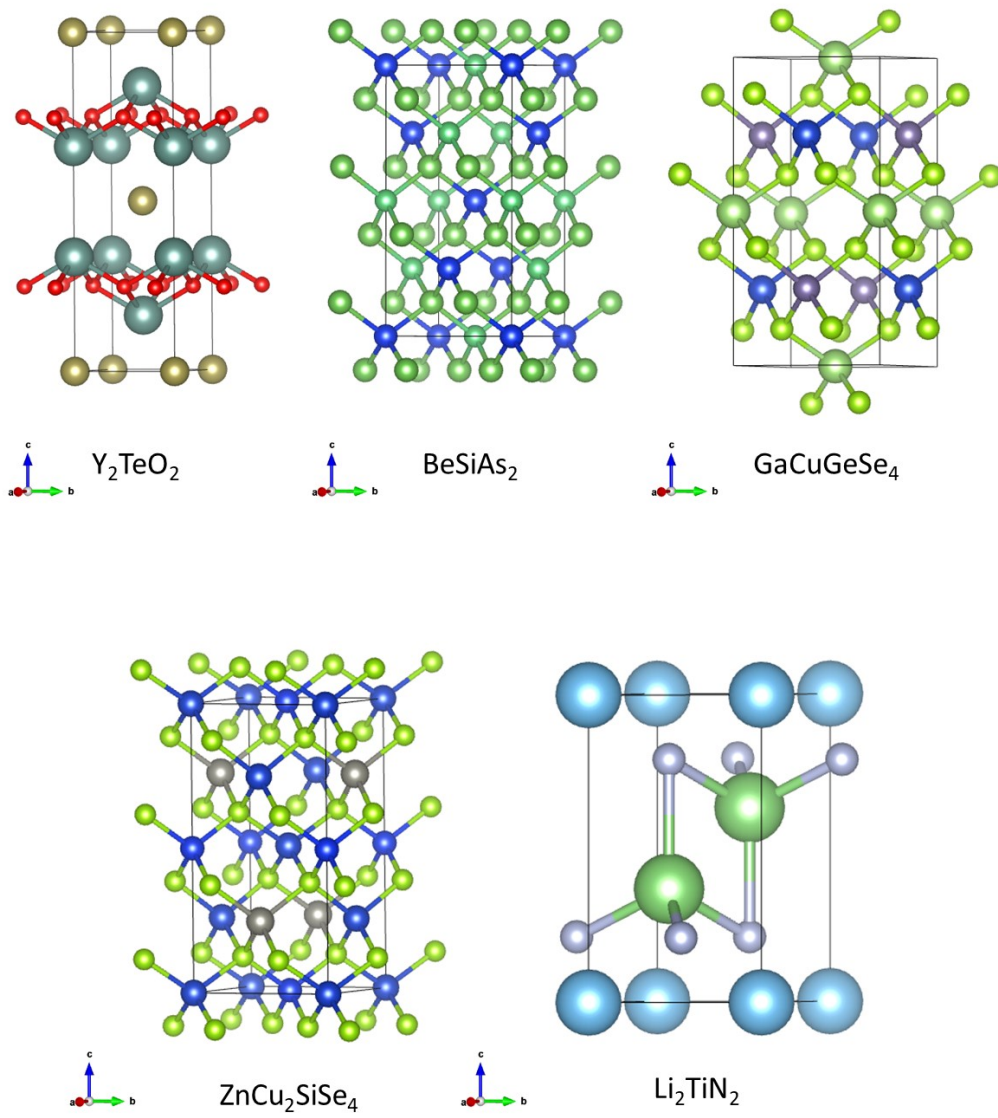
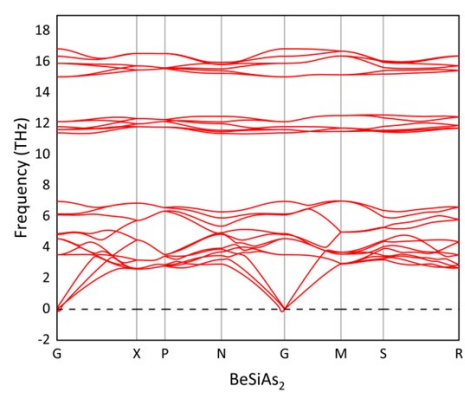
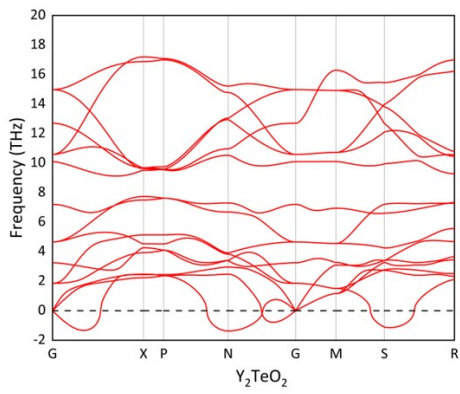
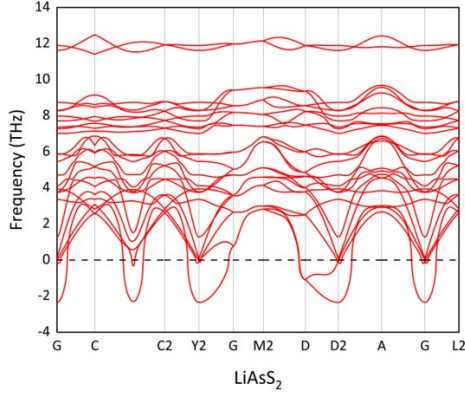
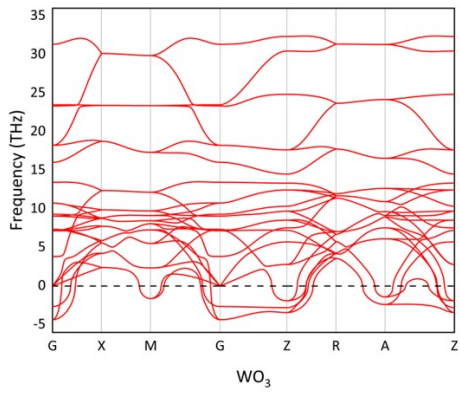
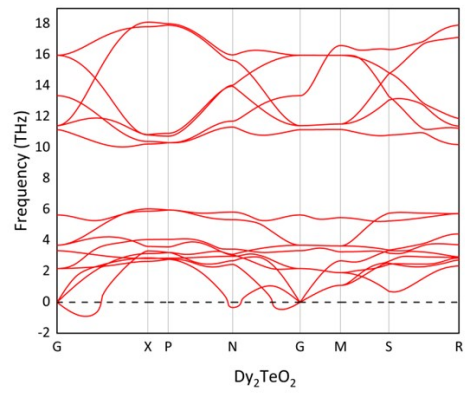
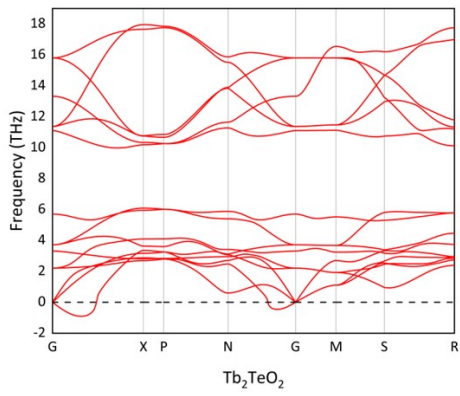
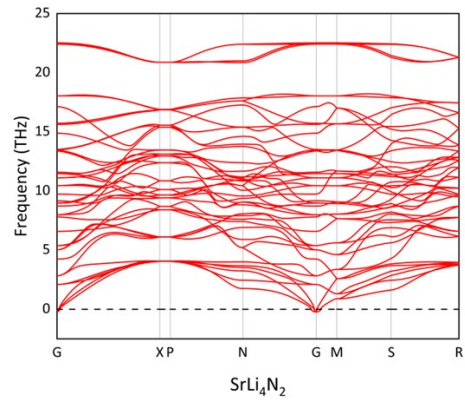
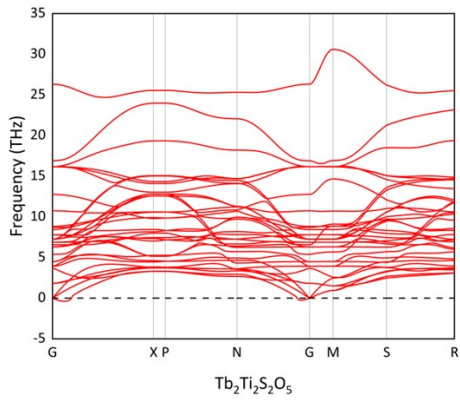


Figure S2. The phonon spectrums for the 11 final-candidate.



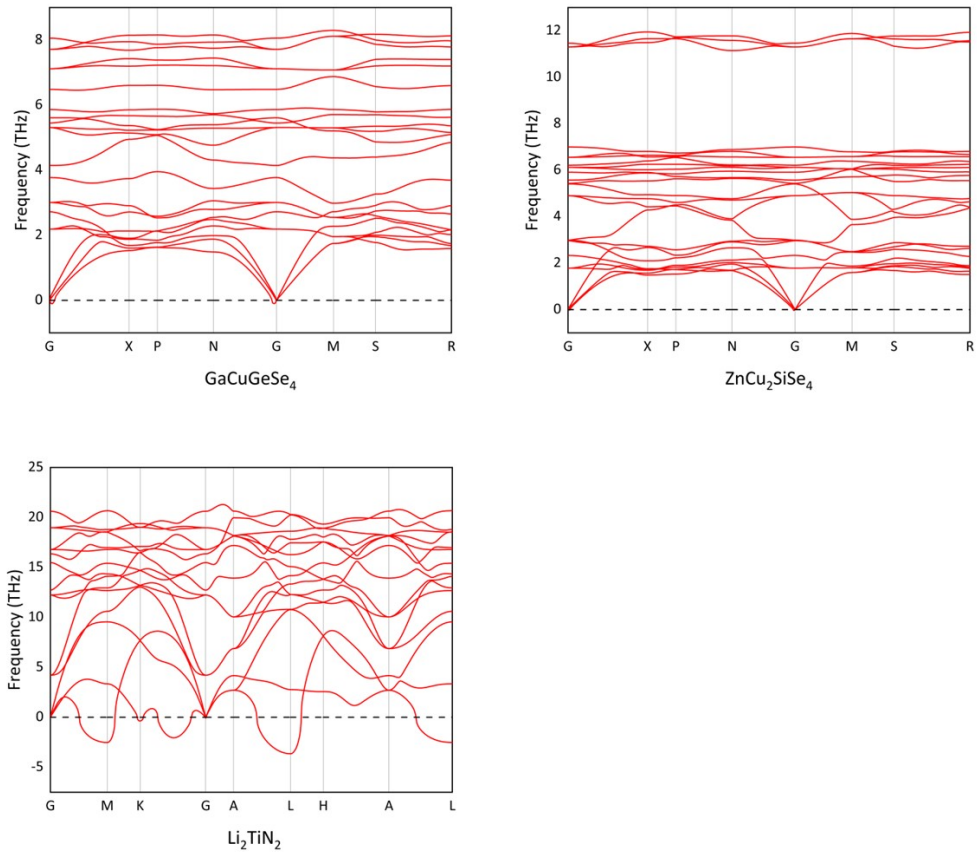
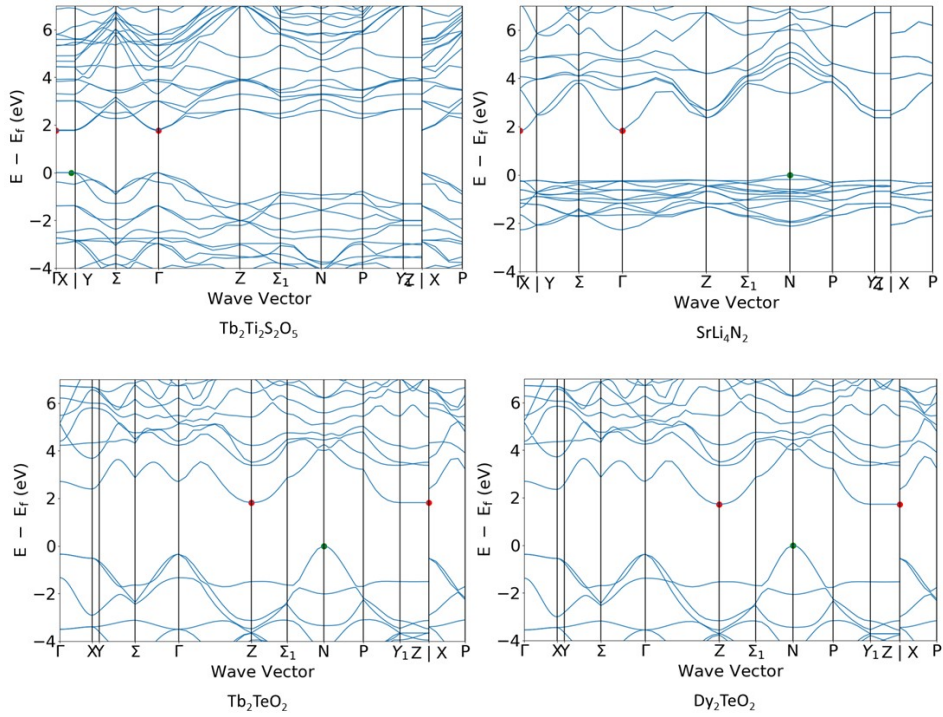


Figure S3. The band structures for the 11 final-candidate.



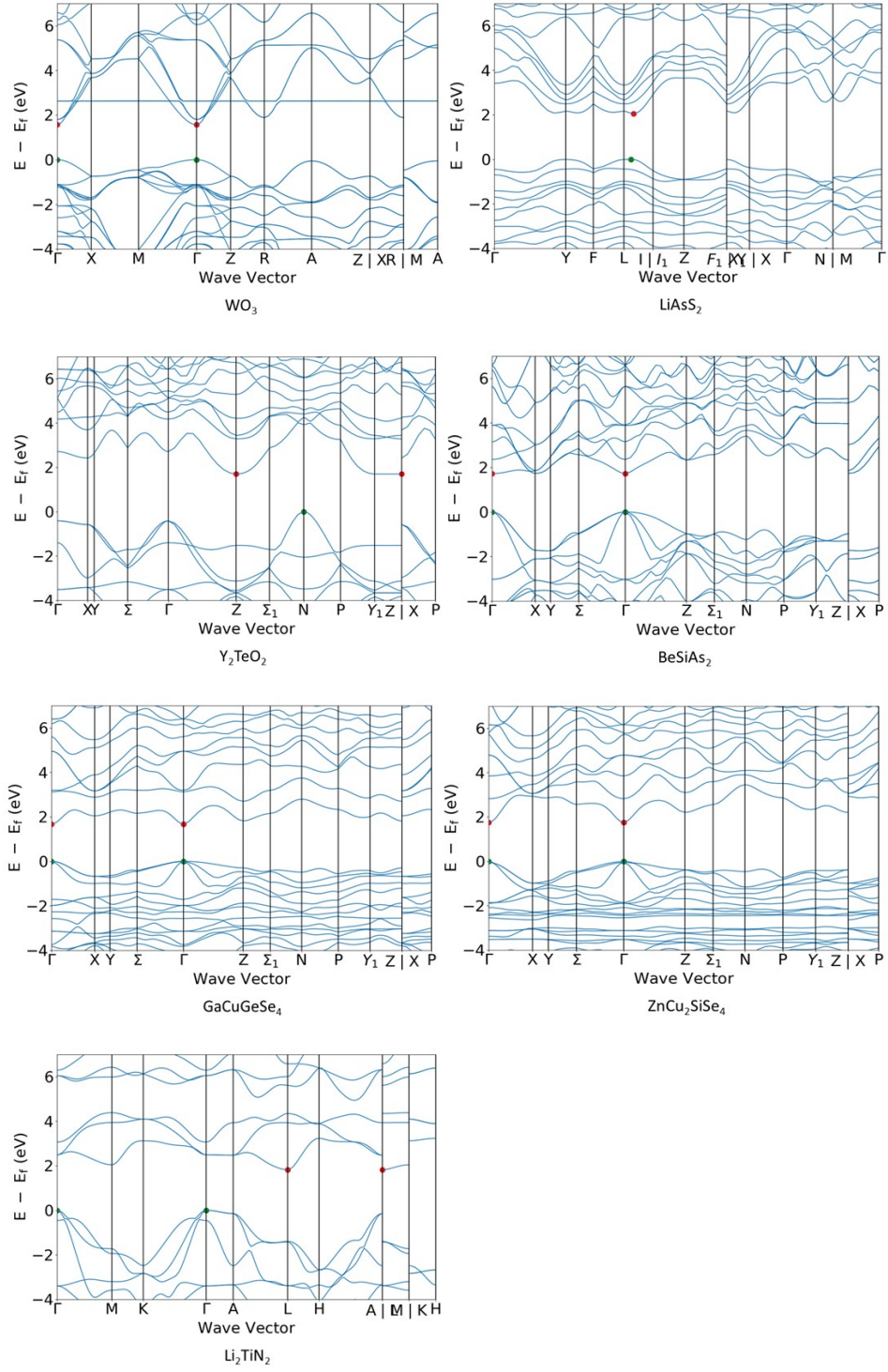


Figure S4. The light absorption coefficients calculated for the 11 final-candidate material as a function of energy. The HSE06 bandgap energy is indicated for each case.

