

**LIST OF ALL POTENTIAL TOPOLOGICAL MATERIALS PREDICTED**

Space Group	Formula	Space Group	Formula	Space Group	Formula
166	Pb <sub>2</sub> Pd <sub>3</sub> S <sub>2</sub>	109	Al <sub>1</sub> Ge <sub>1</sub> La <sub>1</sub>	194	Ca <sub>1</sub>
189	Re <sub>1</sub> Si <sub>1</sub> Ta <sub>1</sub>	160	Al <sub>4</sub> C <sub>6</sub> Zr <sub>3</sub>	229	Ca <sub>1</sub>
142	Ga <sub>2</sub> Pt <sub>1</sub>	109	As <sub>1</sub> Nb <sub>1</sub>	194	In <sub>1</sub> Mg <sub>3</sub>
180	Ge <sub>2</sub> Nb <sub>1</sub>	5	As <sub>2</sub> Ta <sub>1</sub>	194	Li <sub>1</sub> Tl <sub>1</sub>
198	Hg <sub>1</sub> Pd <sub>1</sub>	36	Bi <sub>1</sub> Pd <sub>1</sub>	216	N <sub>1</sub> Tl <sub>1</sub>
166	In <sub>1</sub> Mg <sub>3</sub>	4	Bi <sub>1</sub> Pd <sub>1</sub>	225	N <sub>1</sub> Tl <sub>1</sub>
216	In <sub>1</sub> Sb <sub>1</sub>	157	Bi <sub>2</sub> Pt <sub>1</sub>	225	Ga <sub>2</sub> Pt <sub>1</sub>
186	In <sub>1</sub> Sb <sub>1</sub>	129	Se <sub>1</sub> Ti <sub>1</sub>	123	Hg <sub>1</sub> Pd <sub>1</sub>
221	N <sub>1</sub> Ta <sub>1</sub>	194	Se <sub>1</sub> Ti <sub>1</sub>	193	Cl <sub>3</sub> Ti <sub>1</sub>
191	N <sub>1</sub> Ta <sub>1</sub> *	2	Se <sub>2</sub> Ta <sub>1</sub>	149	Cl <sub>3</sub> Ti <sub>1</sub> #
187	N <sub>1</sub> Ta <sub>1</sub>	166	Se <sub>2</sub> Ta <sub>1</sub>	12	Cl <sub>3</sub> Ti <sub>1</sub> #
225	N <sub>1</sub> Ta <sub>1</sub>	164	Se <sub>2</sub> Ta <sub>1</sub>	15	Cl <sub>3</sub> Ti <sub>1</sub> #
189	N <sub>1</sub> Ta <sub>1</sub>	194	Se <sub>2</sub> Ta <sub>1</sub> *	62	N <sub>3</sub> Ta <sub>1</sub> Th <sub>1</sub>
194	N <sub>1</sub> Ta <sub>1</sub>	160	Se <sub>2</sub> Ta <sub>1</sub>	189	Nb <sub>1</sub> Re <sub>1</sub> Si <sub>1</sub>
6	N <sub>2</sub> Re <sub>1</sub>	141	Sr <sub>1</sub>	229	Pb <sub>1</sub>
13	N <sub>2</sub> Re <sub>1</sub>	140	Sr <sub>1</sub>	194	Pb <sub>1</sub>
194	N <sub>2</sub> Re <sub>1</sub>	229	Sr <sub>1</sub>	186	N <sub>1</sub> Tl <sub>1</sub>
11	N <sub>2</sub> Re <sub>1</sub>	194	Sr <sub>1</sub>	46	Nb <sub>1</sub> Re <sub>1</sub> Si <sub>1</sub>
205	N <sub>2</sub> Re <sub>1</sub>	225	Ta <sub>1</sub>	109	P <sub>1</sub> Ta <sub>1</sub>
127	N <sub>2</sub> Re <sub>1</sub>	223	Ta <sub>1</sub>	86	P <sub>1</sub> Zr <sub>3</sub>
62	N <sub>2</sub> Re <sub>1</sub>	191	Ta <sub>1</sub>	199	Pb <sub>2</sub> Pd <sub>3</sub> S <sub>2</sub>
194	Nb <sub>1</sub> S <sub>2</sub>	229	Ta <sub>1</sub>	146	Pd <sub>8</sub> Sb <sub>3</sub> #
139	Nb <sub>1</sub> S <sub>2</sub>	194	Ta <sub>1</sub>	161	Pd <sub>8</sub> Sb <sub>3</sub> #
164	Nb <sub>1</sub> Se <sub>2</sub>	113	Ta <sub>1</sub>	46	Re <sub>1</sub> Si <sub>1</sub> Ta <sub>1</sub>
194	Nb <sub>1</sub> Se <sub>2</sub>	3	Ta <sub>1</sub>	92	Si <sub>4</sub> Zr <sub>5</sub>
187	Nb <sub>1</sub> Se <sub>2</sub> *	136	Ta <sub>1</sub>	167	Al <sub>5</sub> Mo <sub>1</sub>
74	P <sub>1</sub>	187	Te <sub>1</sub> Zr <sub>1</sub>	166	As <sub>2</sub> Sn <sub>2</sub> Sr <sub>1</sub>
139	S <sub>2</sub> Ti <sub>1</sub>	194	Te <sub>1</sub> Zr <sub>1</sub>	212	Ba <sub>1</sub> Si <sub>2</sub>
191	S <sub>2</sub> Ti <sub>1</sub>	129	Ag <sub>1</sub> Mg <sub>1</sub> Sb <sub>1</sub>	18	Be <sub>1</sub>
194	Sb <sub>1</sub>	206	Ge <sub>1</sub>	64	Bi <sub>1</sub>
186	Ca <sub>1</sub> Ge <sub>2</sub>	194	Ge <sub>1</sub> #		

**Table 1: High-confidence materials except Topogivity dataset predictions.** These potential topological materials are common predictions from Complete and Spaced datasets. Materials marked with an asterisk (\*) have already been identified in Topological Materials Database. Materials marked with a hash (#) have band structures similar to already identified TMs in Topological Materials Database.

Space Group	Formula	Space Group	Formula	Space Group	Formula
11	Bi <sub>1</sub> *	25	In <sub>1</sub> Sb <sub>1</sub>	164	S <sub>2</sub> Ti <sub>1</sub>
64	Ca <sub>1</sub> *	59	In <sub>1</sub> Sb <sub>1</sub>	194	S <sub>2</sub> Ti <sub>1</sub> *
92	Ca <sub>1</sub>	216	N <sub>1</sub> Ta <sub>1</sub>	62	S <sub>2</sub> Ti <sub>1</sub>
162	Cl <sub>3</sub> Ti <sub>1</sub> #	8	N <sub>2</sub> Re <sub>1</sub>	11	Sb <sub>1</sub>
229	Ge <sub>1</sub> #	64	P <sub>1</sub> *	160	Se <sub>2</sub> Ta <sub>1</sub>
148	Ge <sub>1</sub>	107	P <sub>2</sub> U <sub>1</sub> #	186	Se <sub>2</sub> Ta <sub>1</sub>
225	Ge <sub>1</sub>	5	Po <sub>1</sub>	74	Sr <sub>1</sub>
227	Ge <sub>1</sub>	160	S <sub>2</sub> Ta <sub>1</sub>	62	Te <sub>1</sub> Zr <sub>1</sub>
36	Ge <sub>6</sub> La <sub>4</sub> Mg <sub>5</sub>				

**Table 1: High-confidence materials common in all dataset predictions.** These potential topological materials are common predictions from all the datasets. Materials marked with an asterisk (\*) have already been identified in Topological Materials Database. Materials marked with a hash (#) have band structures similar to already identified TMs in Topological Materials Database.

Space Group	Formula
166	Ga <sub>1</sub> Mn <sub>1</sub> *
123	Ga <sub>1</sub> Mn <sub>1</sub> *
63	Pt <sub>2</sub> Ta <sub>1</sub>
62	Nb <sub>1</sub> Si <sub>1</sub>
221	Co <sub>1</sub> Ga <sub>1</sub>
180	Ge <sub>2</sub> Ta <sub>1</sub>
225	Bi <sub>1</sub> Ti <sub>1</sub>
194	Bi <sub>1</sub> Ti <sub>1</sub>
216	Bi <sub>1</sub> Ti <sub>1</sub>

**Table 3: Predicted Potential Topological Materials.** Materials which had ‘Unknown’ space groups. Materials marked with an asterisk (\*) have already been identified in Topological Materials Database.

Space Group	Formula
146	In <sub>1</sub> Mg <sub>3</sub>
216	Li <sub>21</sub> Si <sub>5</sub>
143	Al <sub>5</sub> Mo <sub>1</sub>
160	As <sub>2</sub> Sn <sub>2</sub> Sr <sub>1</sub>
194	Be <sub>1</sub>
151	Cl <sub>3</sub> Ti <sub>1</sub>
146	In <sub>1</sub> Mg <sub>3</sub>
43	In <sub>1</sub> Sr <sub>1</sub>
186	P <sub>3</sub> Sc <sub>7</sub>
156	Sb <sub>2</sub> Te <sub>3</sub>
62	Se <sub>1</sub> Ti <sub>1</sub>
81	Ta <sub>1</sub>
152	Ag <sub>1</sub> Pb <sub>4</sub> Pd <sub>6</sub>
80	As <sub>1</sub> Nb <sub>1</sub>

**Table 4: Predicted Potential Topological Materials.** Materials whose band structures were not found in Topological Materials Database.