

## Supplementary Information for Assessing the Design Rules of Electrides

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Table S1. The full list of 51 candidates is displayed in order of the value of the Materials Project materials ID number. The chemical formula, crystal type, symmetry, electrides type and average electronegative of materials are included in the table.

MP-ID	Formula	Crystal System	Space group	Symmetry number	Electrides type	Average electronegative
mp-1029640	Ba <sub>3</sub> OsN <sub>3</sub>	Hexagonal	P6 <sub>3</sub> /m	176	1D	1.998571429
mp-1029686	Sr <sub>3</sub> OsN <sub>3</sub>	Hexagonal	P6 <sub>3</sub> /m	176	1D	2.024285714
mp-1029741	Sr <sub>3</sub> IrN <sub>3</sub>	Hexagonal	P6 <sub>3</sub> /m	176	1D	2.024285714
mp-1029750	Sr <sub>3</sub> RuN <sub>3</sub>	Hexagonal	P6 <sub>3</sub> /m	176	1D	2.024285714
mp-1096	CeS	Cubic	Fm-3m	225	0D	1.85
mp-1103552	EuAl <sub>2</sub> Se <sub>4</sub>	Orthorhombic	Cccm	66	1D	2.088571429
mp-1103889	EuAl <sub>2</sub> S <sub>4</sub>	Orthorhombic	Cccm	66	1D	2.105714286
mp-1113208	Cs <sub>2</sub> EuCuCl <sub>6</sub>	Cubic	Fm-3m	225	0D	2.364
mp-1161	LaSe	Cubic	Fm-3m	225	0D	1.825
mp-1190820	Ba <sub>2</sub> FeGe <sub>2</sub> O <sub>7</sub>	Tetragonal	P-4 <sub>2</sub> 1m	113	0D	2.6425
mp-1197890	Li <sub>2</sub> Ti <sub>2</sub> P <sub>3</sub> O <sub>12</sub>	Orthorhombic	Pbcn	60	1D	2.783684211
mp-1199363	Ba <sub>3</sub> AlO <sub>4</sub>	Orthorhombic	Pnma	62	0D	2.255
mp-1219790	RbIr <sub>6</sub> O <sub>12</sub>	Tetragonal	I4/m	87	1D	2.910526316
mp-1226163	La <sub>2</sub> CeTe <sub>4</sub>	Tetragonal	I-42d	122	0D	1.674285714
mp-1044323	TiMoP <sub>3</sub> O <sub>12</sub>	Trigonal	R3c	161	1D	3.032352941
mp-1240	HoS	Cubic	Fm-3m	225	0D	1.905
mp-1044343	TiP <sub>3</sub> WO <sub>12</sub>	Trigonal	R3c	161	1D	3.044117647
mp-1245	Sr <sub>2</sub> N	Trigonal	R-3m	166	2D	1.646666667
mp-1610	TbS	Cubic	Fm-3m	225	0D	1.84
mp-1623	ErS	Cubic	Fm-3m	225	0D	1.91
mp-17242	Nb <sub>2</sub> P <sub>3</sub> O <sub>12</sub>	Trigonal	R-3c	167	1D	3.002941176
mp-1766	TmS	Cubic	Fm-3m	225	0D	1.915
mp-1892	Ba <sub>2</sub> N	Trigonal	R-3m	166	2D	1.606666667
mp-19165	BaFeSi <sub>4</sub> O <sub>10</sub>	Tetragonal	P4/ncc	130	1D	2.795
mp-19508	SrCrSi <sub>4</sub> O <sub>10</sub>	Tetragonal	P4/ncc	130	1D	2.788125
mp-19518	BaCrSi <sub>4</sub> O <sub>10</sub>	Tetragonal	P4/ncc	130	1D	2.784375
mp-22261	InCuTe <sub>2</sub>	Tetragonal	I-42d	122	1D	1.97
mp-22422	Ce <sub>3</sub> Te <sub>4</sub>	Cubic	I-43d	220	1D	1.68
mp-2350	LaS	Cubic	Fm-3m	225	0D	1.84
mp-2470	DyS	Cubic	Fm-3m	225	0D	1.9
mp-2563	CeSe	Cubic	Fm-3m	225	0D	1.835
mp-2686	Ca <sub>2</sub> N	Trigonal	R-3m	166	2D	1.68
mp-27334	Tl <sub>3</sub> FeCl <sub>5</sub>	Tetragonal	I4/mcm	140	0D	2.498888889
mp-37312	NaLa <sub>8</sub> Se <sub>12</sub>	Tetragonal	I-42d	122	0D	1.92047619

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<b>mp-3779</b>	CrSiTe <sub>3</sub>	Trigonal	R-3	148	2D	1.972
<b>mp-3787</b>	RbFe <sub>2</sub> S <sub>3</sub>	Orthorhombic	Cmcm	63	0D	2.036666667
<b>mp-510262</b>	Cs <sub>3</sub> O	Hexagonal	P6_3/mcm	193	1D	1.4525
<b>mp-510402</b>	GdS	Cubic	Fm-3m	225	0D	1.89
<b>mp-541318</b>	CsTi <sub>3</sub> Si <sub>2</sub> P <sub>6</sub> O <sub>25</sub>	Trigonal	P-31c	163	0D	2.928378378
<b>mp-541449</b>	CrGeTe <sub>3</sub>	Trigonal	R-3	148	2D	1.994
<b>mp-542475</b>	CsFe <sub>2</sub> S <sub>3</sub>	Orthorhombic	Cmcm	63	1D	2.031666667
<b>mp-569673</b>	PrI <sub>2</sub>	Cubic	F-43m	216	0D	2.15
<b>mp-573523</b>	Sr <sub>8</sub> Fe <sub>3</sub> N <sub>8</sub>	Monoclinic	C2/m	12	1D	1.968947368
<b>mp-574283</b>	GdTe	Cubic	Fm-3m	225	0D	1.65
<b>mp-656</b>	LuS	Cubic	Fm-3m	225	0D	1.925
<b>mp-662563</b>	CsFe <sub>2</sub> Se <sub>3</sub>	Orthorhombic	Cmcm	63	1D	2.016666667
<b>mp-672252</b>	LiEuPS <sub>4</sub>	Tetragonal	I4_1/acd	142	0D	2.098571429
<b>mp-675037</b>	Sm <sub>2</sub> EuS <sub>4</sub>	Tetragonal	I-42d	122	1D	1.98
<b>mp-721592</b>	Ca <sub>6</sub> Al <sub>7</sub> O <sub>16</sub>	Cubic	I-43d	220	0D	2.4713
<b>mp-867221</b>	Ce <sub>3</sub> Ta <sub>2</sub> N <sub>6</sub>	Tetragonal	I4/mmm	139	1D	2.236363636
<b>mp-867290</b>	TbTe	Hexagonal	P-6m2	187	0D	1.6

Table S2. The statistic on the composed elements of these 51 candidates.

Element	Cation							Anion		
	Lanthanide	Alkali metal	Alkali earth metal	Transition metal	III A	IV A	P	N	VI A	Halogen
Count	25	10	15	25	6	7	6	9	38	3
Percentage	26.6%	10.6%	16%	26.6%	6.4%	7.4%	6.4%	18%	76%	6%



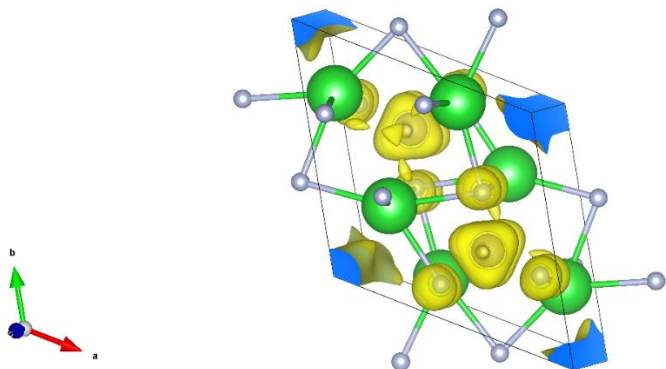


Figure S1:  $\text{Ba}_3\text{OsN}_3$ (mp-1029640). Symmetry: Hexagonal;  $P6_3/m$  (number 176).

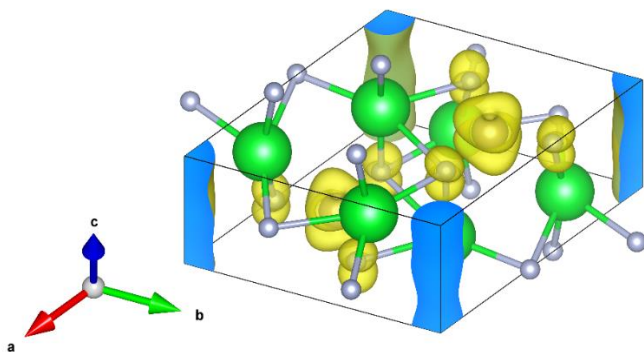


Figure S2:  $\text{Sr}_3\text{OSN}_3$ (mp-1029686). Symmetry: Hexagonal;  $P6_3/m$  (number 176).

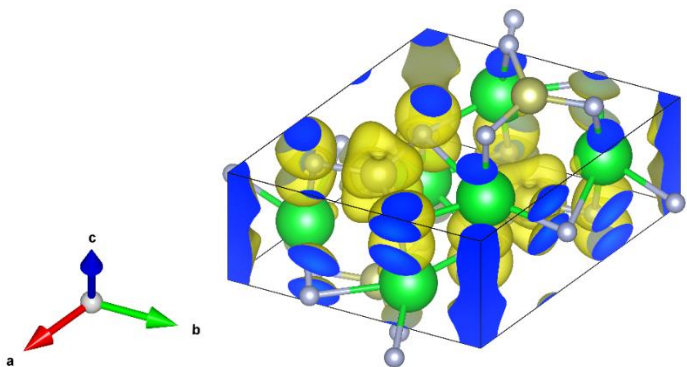


Figure S3:  $\text{Sr}_3\text{IrN}_3$ (mp-1029741). Symmetry: Hexagonal;  $P6_3/m$  (number 176).

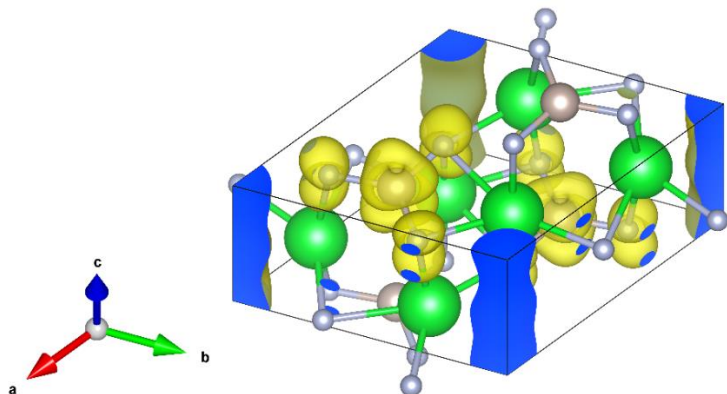


Figure S4:  $\text{Sr}_3\text{RuN}_3$ (mp-1029750). Symmetry: Hexagonal;  $P6_3/m$  (number 176).

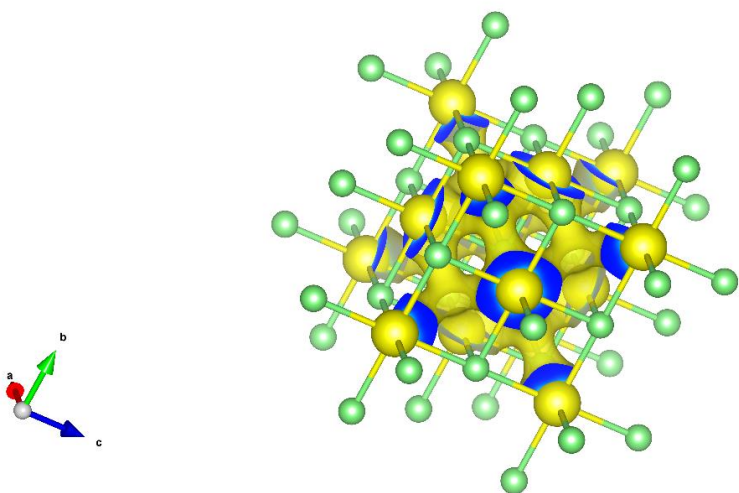


Figure S5: CeS(mp-1096), LaSe(mp-1161), HoS(mp-1240), TbS(mp-1610), ErS(mp-1623), TmS(mp-1766), LaS(mp-2350), DyS(mp-2470), CeSe(mp-2563), GdS(mp-510402), GdTe(mp-574283) and LuS(mp-656). Symmetry: Cubic; Fm-3m (number 225).

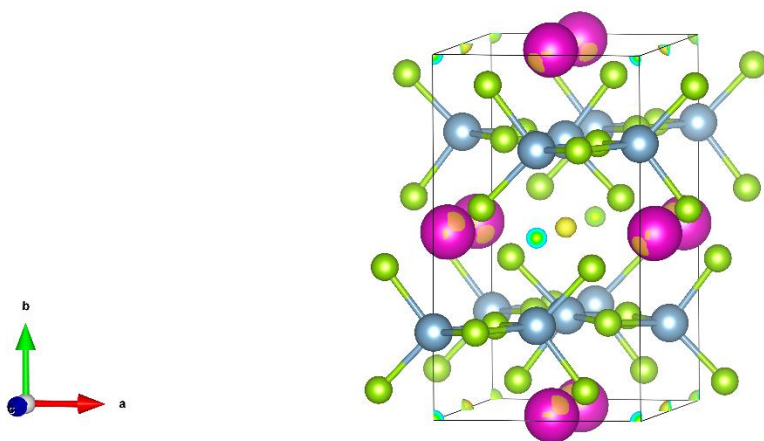


Figure S6:  $\text{EuAl}_2\text{Se}_4$ (mp-1103552). Symmetry: Orthorhombic; Cccm (number 66).

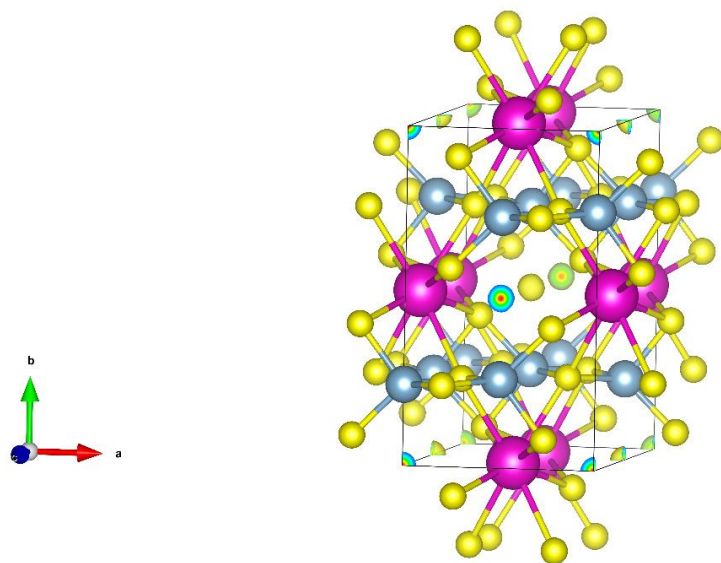


Figure S7:  $\text{EuAl}_2\text{S}_4$ (mp-1103889). Symmetry: Orthorhombic; Cccm (number 66).

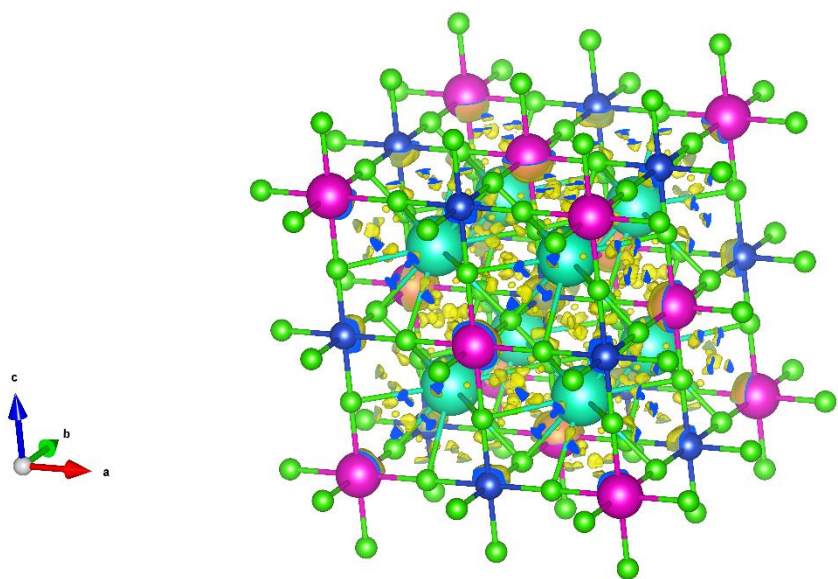


Figure S8:  $\text{Cs}_2\text{EuCuCl}_6$ (mp-1113208). Symmetry: Cubic; Fm-3m (number 225)..

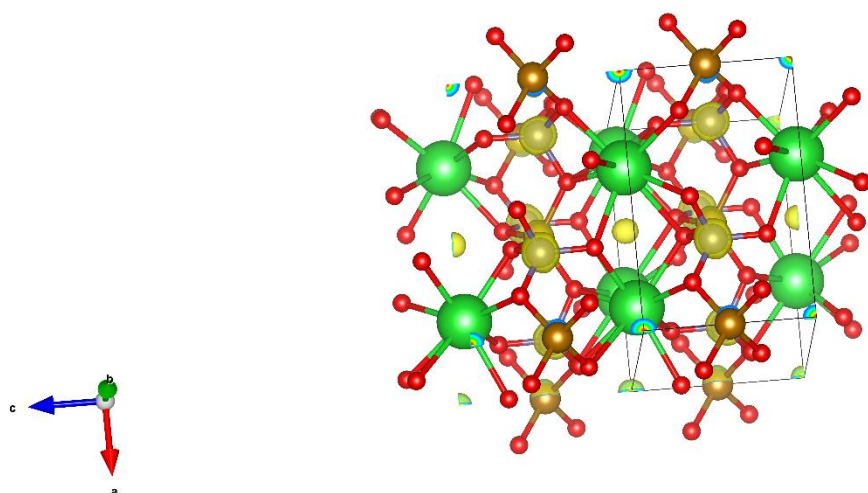


Figure S9:  $\text{Ba}_2\text{FeGe}_2\text{O}_7$ (mp-1190820). Symmetry: Tetragonal; P-42\_1m (number 113).

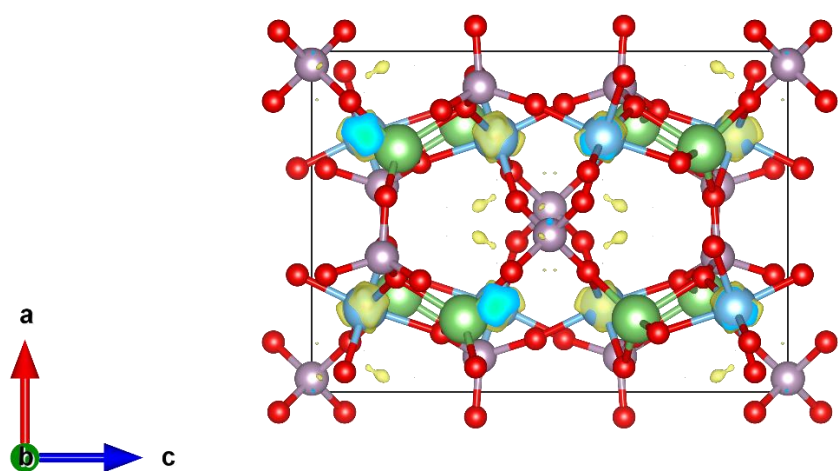


Figure S10:  $\text{Li}_2\text{Ti}_2\text{P}_3\text{O}_{12}$ (mp-1197890). Symmetry: Orthorhombic; Pbcn (number 60).

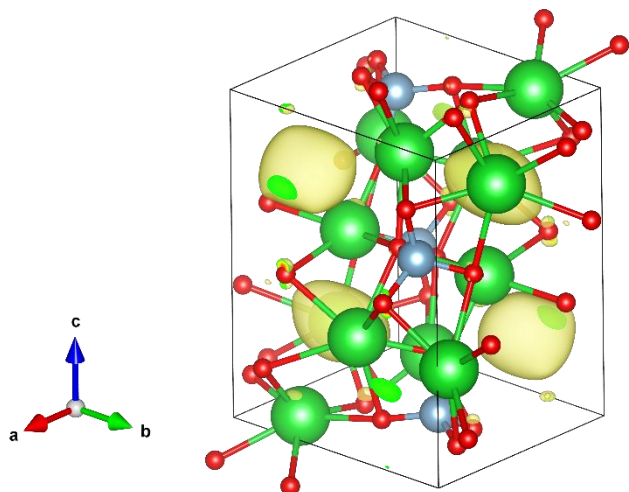


Figure S11: Ba<sub>3</sub>AlO<sub>4</sub>(mp-1199363). Symmetry: Orthorhombic; Pnma (number 62).

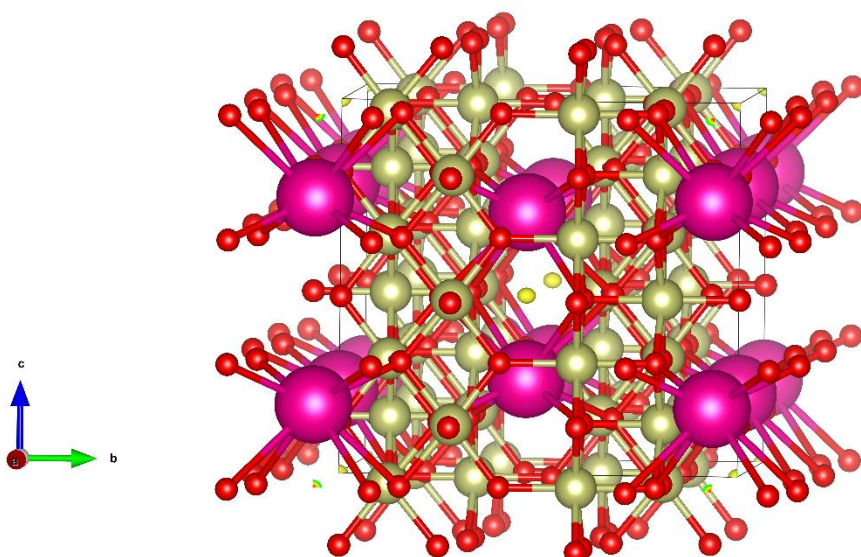


Figure S12: RbIr<sub>6</sub>O<sub>12</sub>(mp-1219790). Symmetry: Tetragonal; I4/m (number 87).

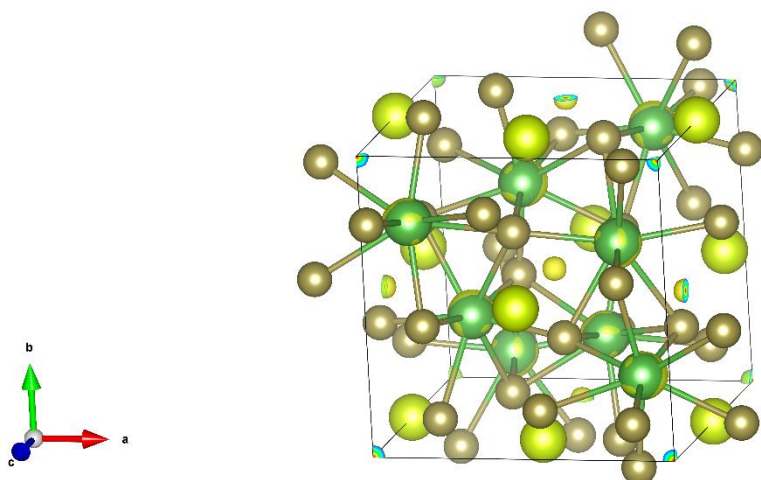


Figure S13: La<sub>2</sub>CeTe<sub>4</sub>(mp-1226163). Symmetry: Tetragonal; I-42d (number 122).

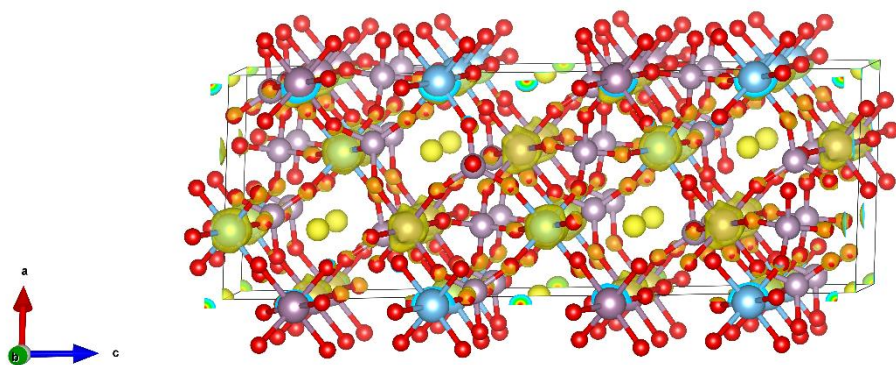


Figure S14: TiMoP<sub>3</sub>O<sub>12</sub>(mp-1044323). Symmetry: Trigonal; R3c (number 161).

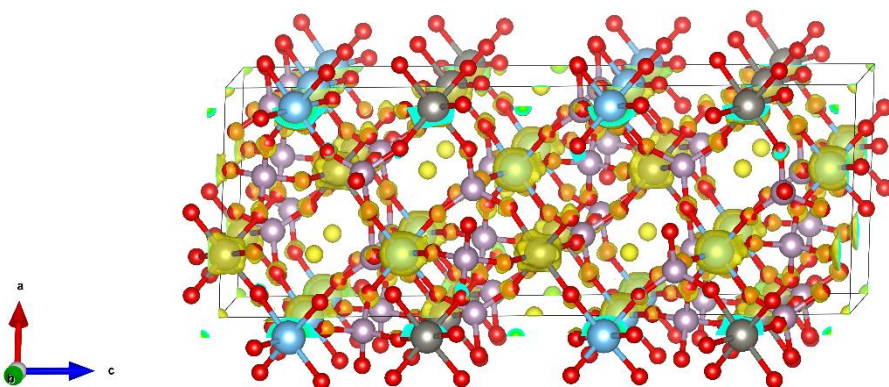


Figure S15: TiP<sub>3</sub>WO<sub>12</sub>(mp-1044343). Symmetry: Trigonal; R3c (number 161).

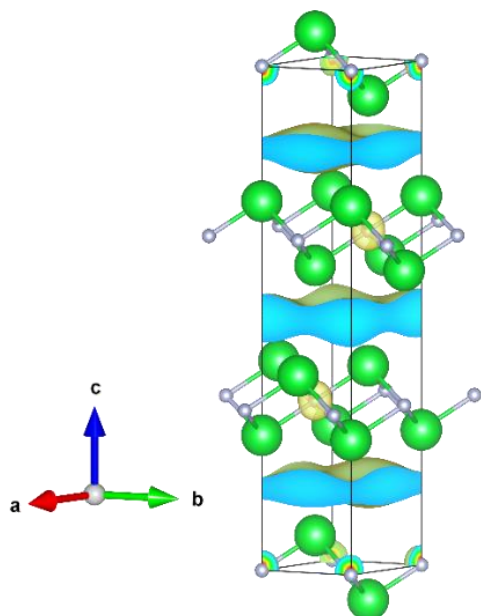


Figure S16: Sr<sub>2</sub>N(mp-1245). Symmetry: Trigonal; R-3m (number 166).



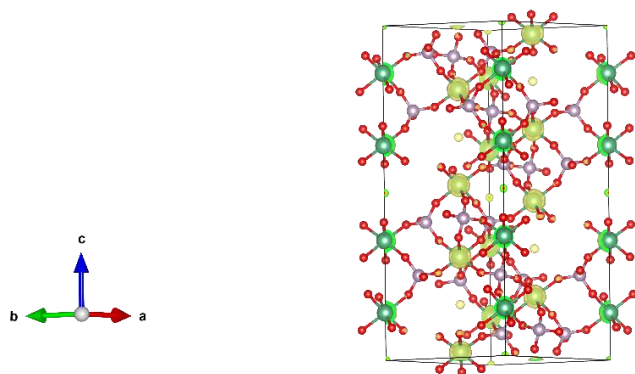


Figure S17: Nb<sub>2</sub>P<sub>3</sub>O<sub>12</sub>(mp-17242). Symmetry: Trigonal; R-3c (number 167).

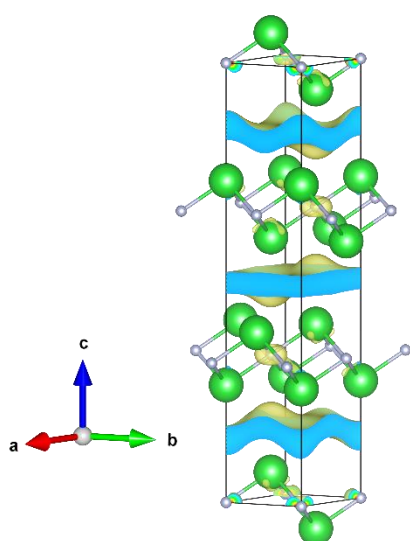


Figure S18: Ba<sub>2</sub>N(mp-1892). Symmetry: Trigonal; R-3m (number 166).

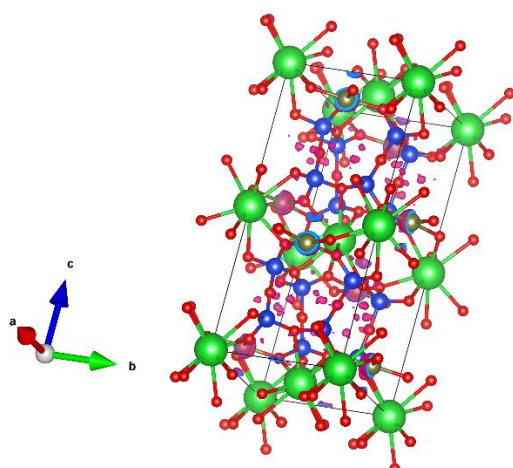


Figure S19: BaFeSi<sub>4</sub>O<sub>10</sub>(mp-19165). Symmetry: Tetragonal; P4/ncc (number 130).

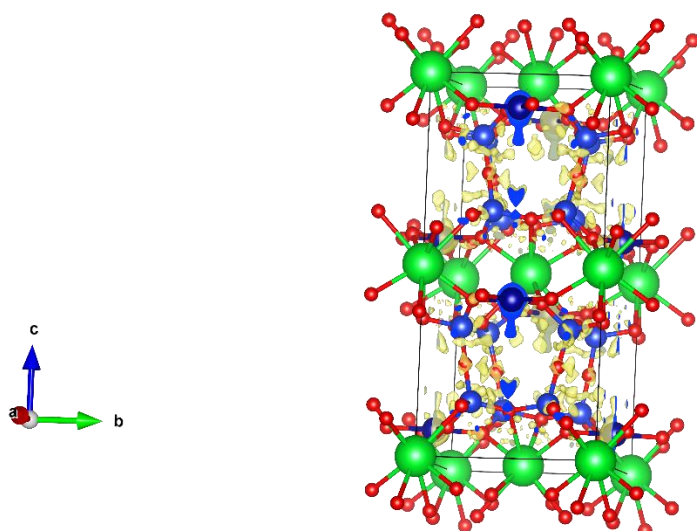


Figure S20:  $\text{SrCrSi}_4\text{O}_{10}$ (mp-19508). Symmetry: Tetragonal;  $P4/ncc$  (number 130).

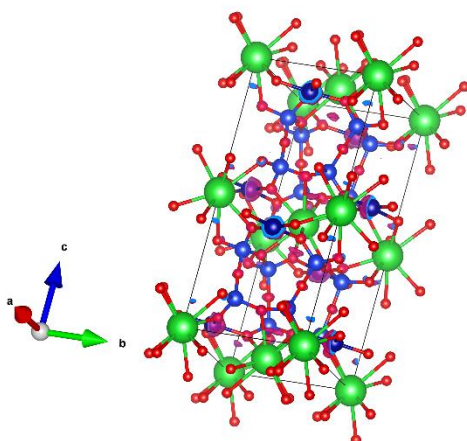


Figure S21:  $\text{BaCrSi}_4\text{O}_{10}$ (mp-19518). Symmetry: Tetragonal;  $P4/ncc$  (number 130).

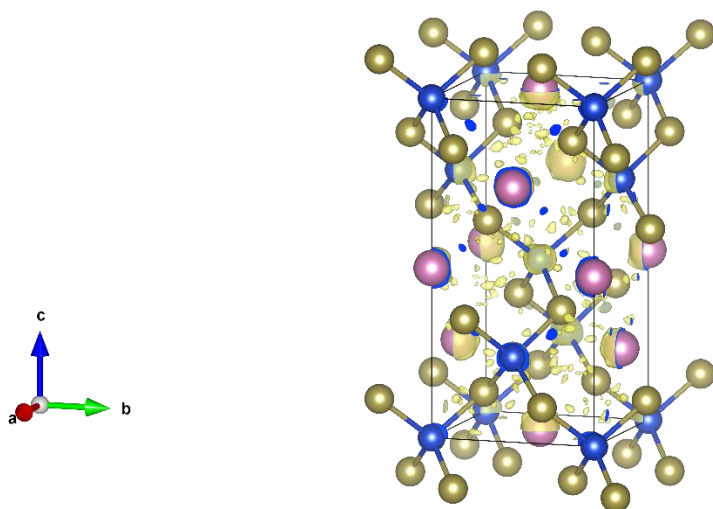


Figure S22:  $\text{InCuTe}_2$ (mp-22261). Symmetry: Tetragonal;  $I-42d$  (number 122).

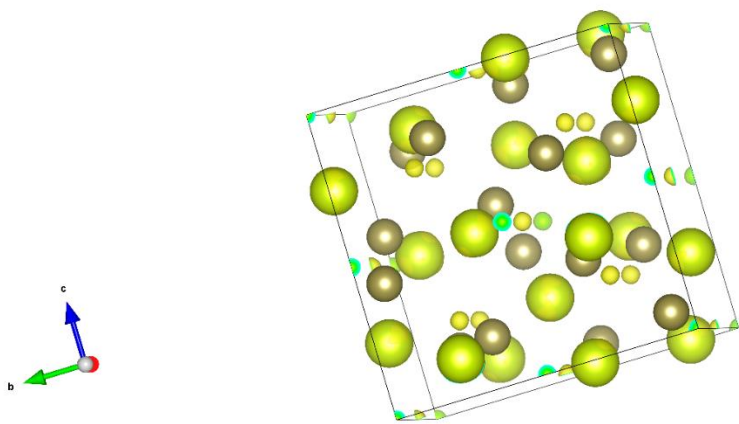


Figure S23: Ce<sub>3</sub>Te<sub>4</sub>(mp-22422). Symmetry: Cubic; I-43d (number 130).

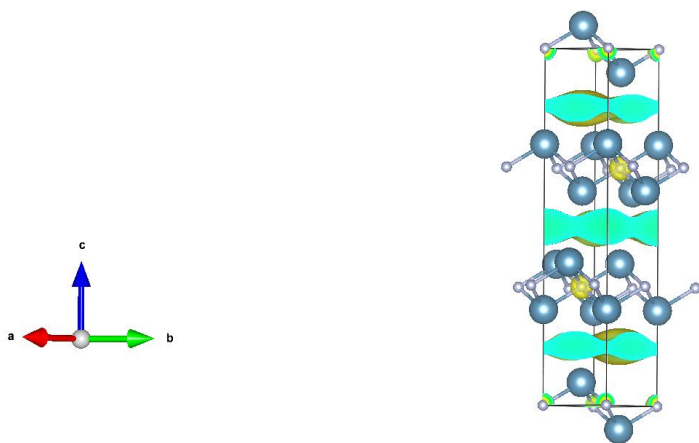


Figure S24: Ca<sub>2</sub>N(mp-2686). Symmetry: Trigonal; R-3m (number 166).

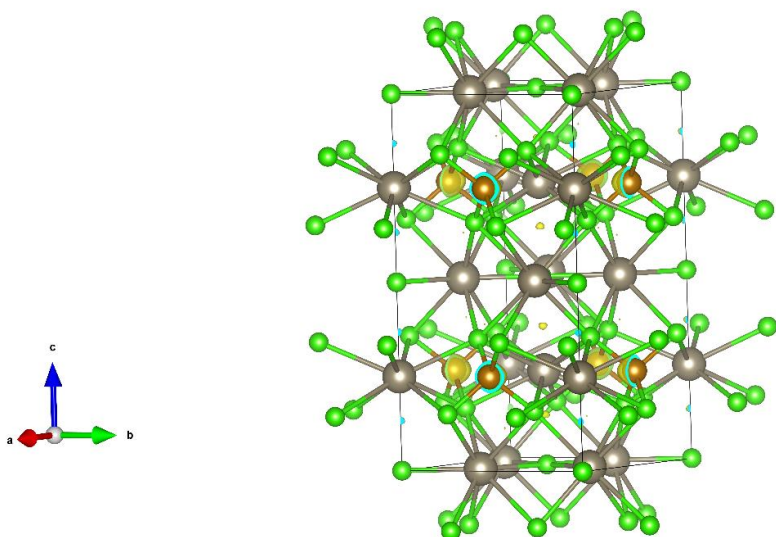


Figure S25: Tl<sub>3</sub>FeCl<sub>5</sub>(mp-27334). Symmetry: Tetragonal; I4/mcm (number 140).

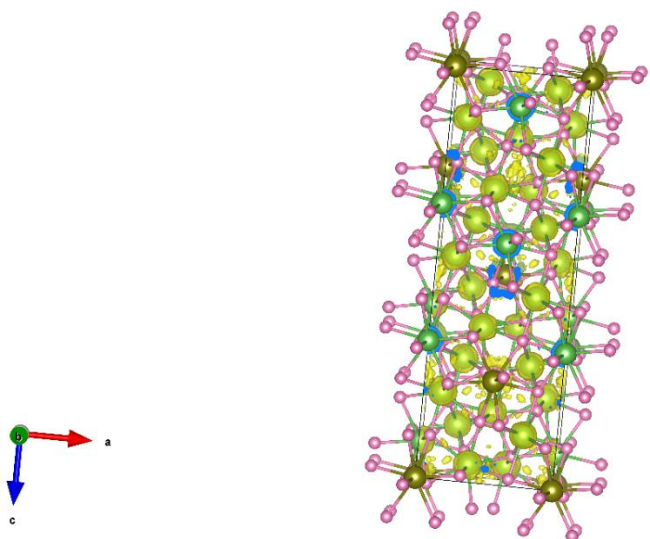


Figure S26: NaLa<sub>8</sub>Se<sub>12</sub>(mp-37312). Symmetry: Tetragonal; I-42d (number 122).

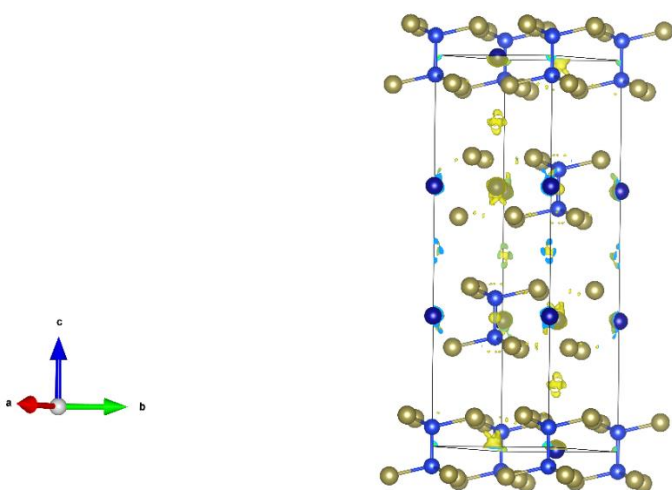


Figure S27: CrSiTe<sub>3</sub>(mp-3779). Symmetry: Trigonal; R-3 (number 148).

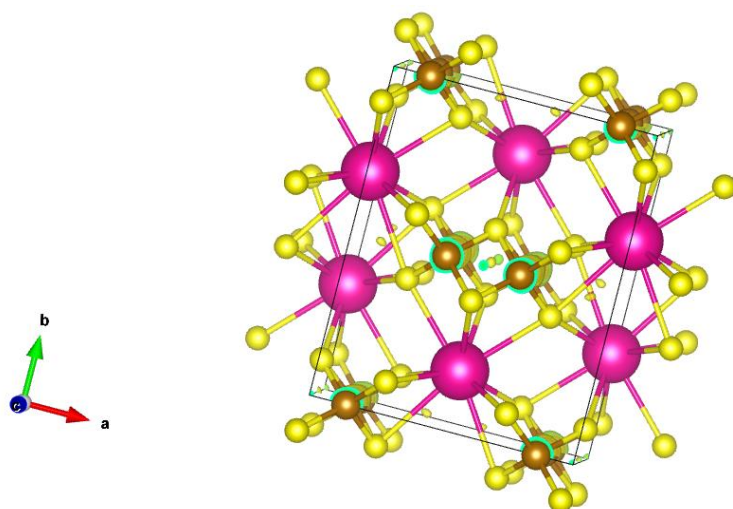


Figure S28: RbFe<sub>2</sub>S<sub>3</sub>(mp-3787). Symmetry: Orthorhombic; Cmcm (number 63)

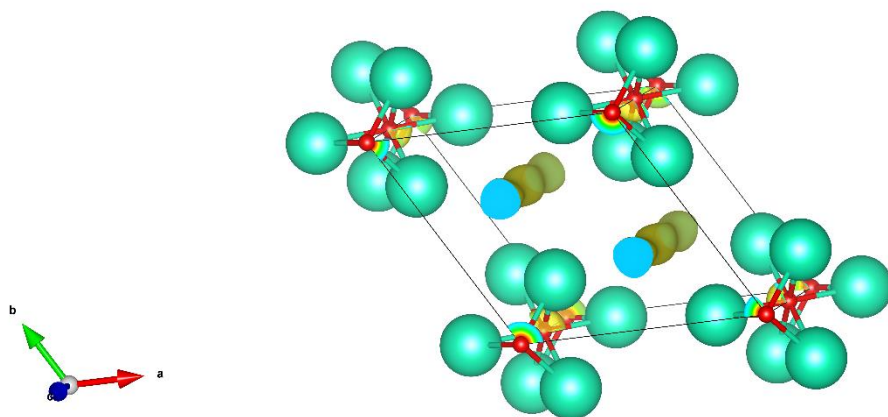


Figure S29: Cs<sub>3</sub>O(mp-510262). Symmetry: Hexagonal; P6<sub>3</sub>/mcm (number 193)

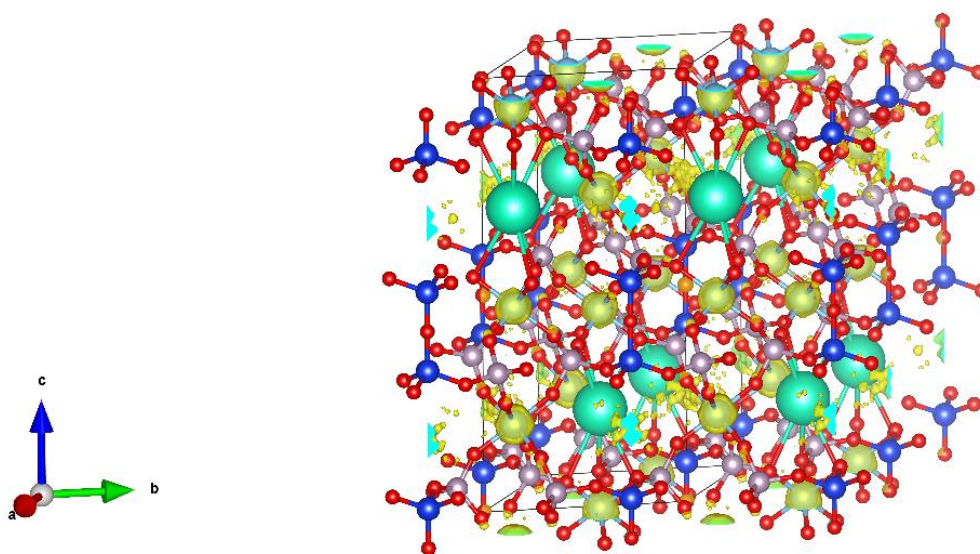


Figure S30: CsTi<sub>3</sub>Si<sub>2</sub>P<sub>6</sub>O<sub>25</sub>(mp-541318). Symmetry: Trigonal; P-31c (number 163)

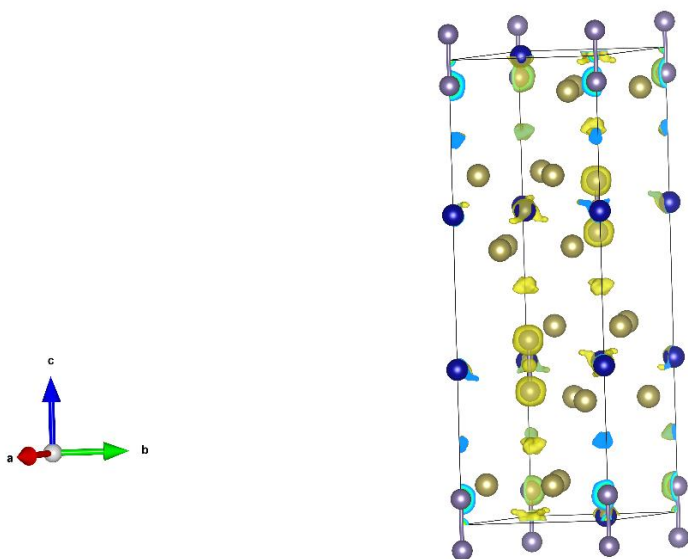


Figure S31: CrGeTe<sub>3</sub>(mp-541449). Symmetry: Trigonal; R-3 (number 148)

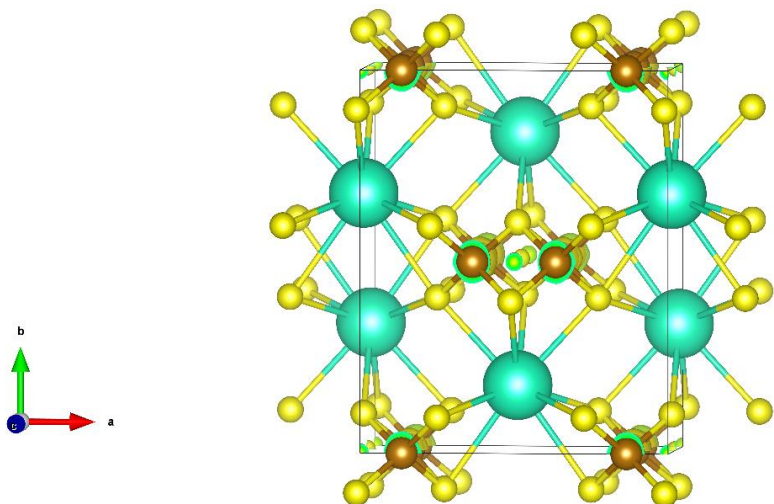


Figure S32: CsFe<sub>2</sub>S<sub>3</sub>(mp-542475). Symmetry: Orthorhombic; Cmc<sub>2</sub>m (number 63).

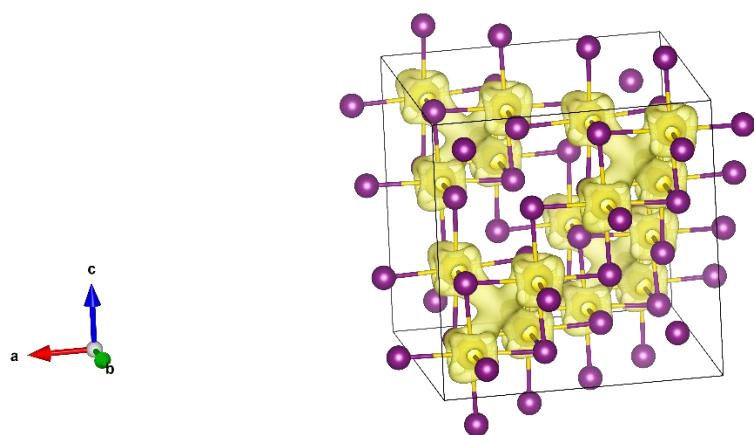


Figure S33: PrI<sub>2</sub>(mp-569673). Symmetry: Cubic; Fm $\bar{3}$ m (number 216)

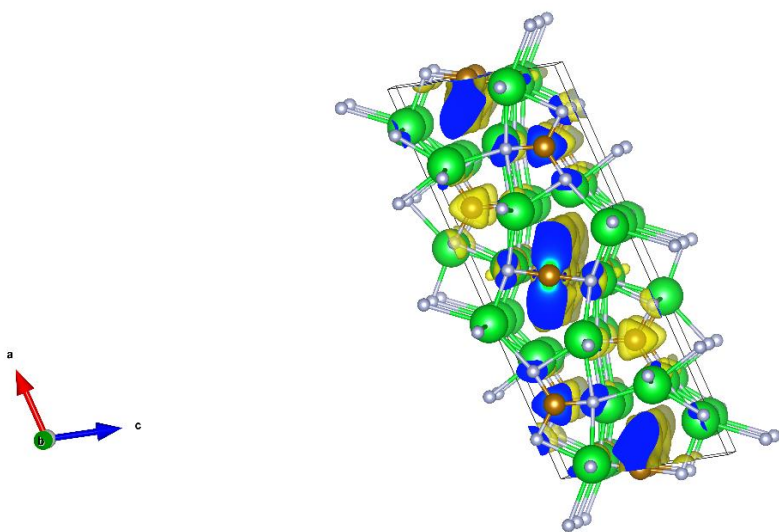


Figure S34: Sr<sub>8</sub>Fe<sub>3</sub>N<sub>8</sub>(mp-573523). Symmetry: Monoclinic; C2/m (number 12).

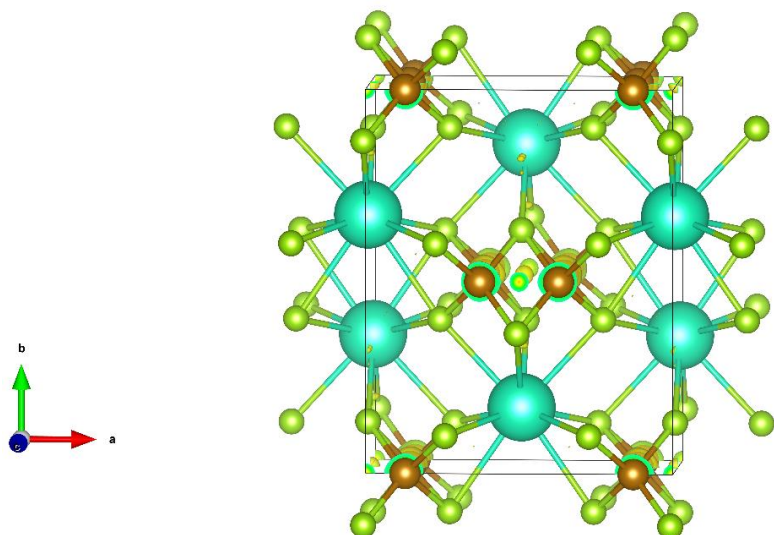


Figure S35: CsFe<sub>2</sub>Se<sub>3</sub>(mp-662563). Symmetry: Orthorhombic; Cmcm (number 63).

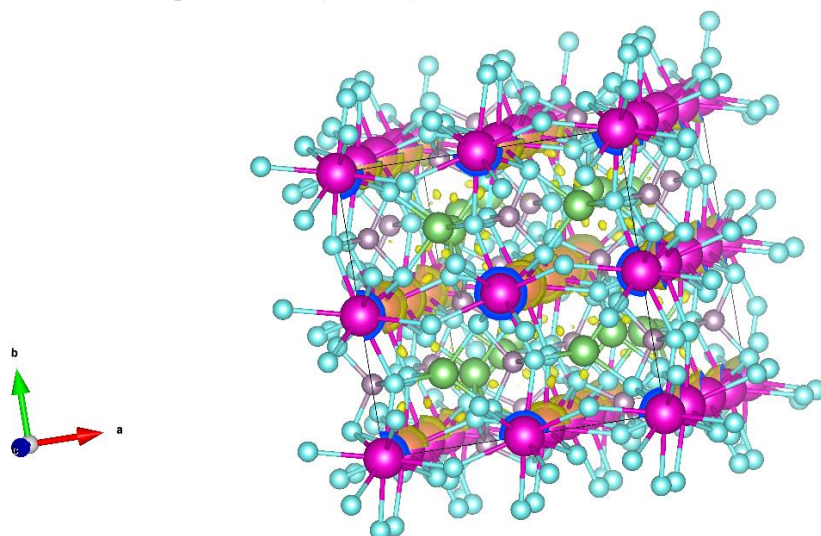


Figure S36: LiEuPS<sub>4</sub>(mp-672252). Symmetry: Tetragonal; I4<sub>1</sub>/acd (number 142).

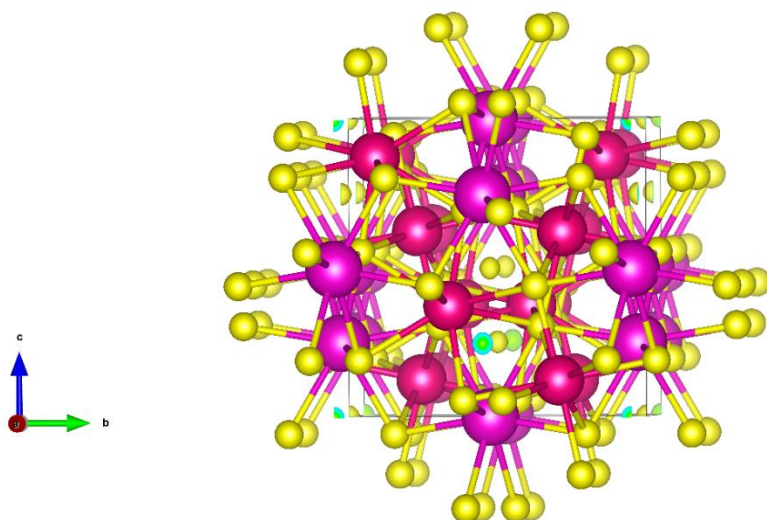


Figure S37: Sm<sub>2</sub>EuS<sub>4</sub>(mp-675037). Symmetry: Tetragonal; I-42d (number 122).

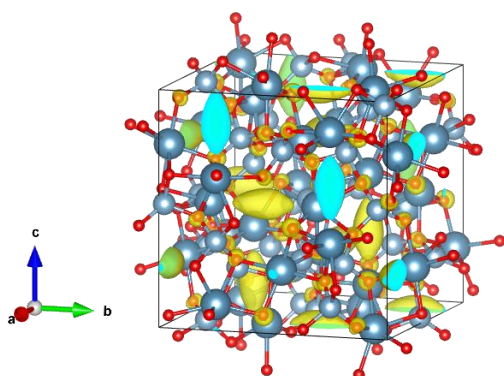


Figure S38: Ca<sub>6</sub>Al<sub>7</sub>O<sub>16</sub>(mp-721592). Symmetry: Cubic; I-43d (number 220).

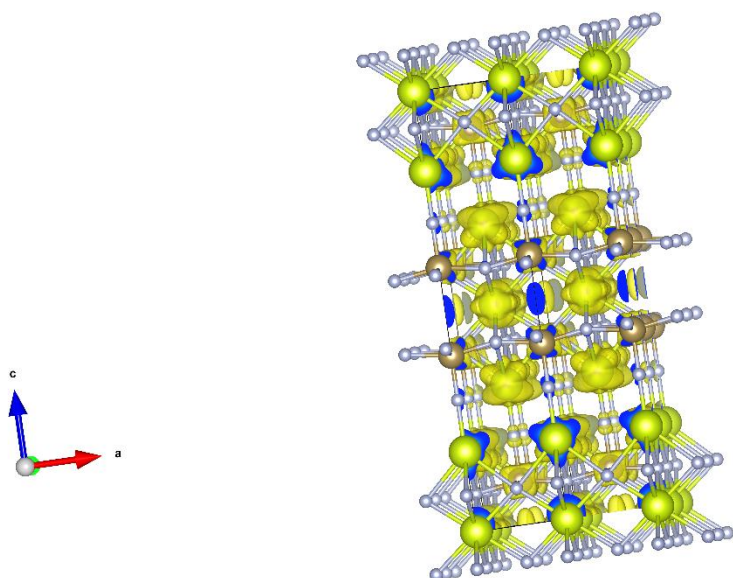


Figure S39: Ce<sub>3</sub>Ta<sub>2</sub>N<sub>6</sub>(mp-867221). Symmetry: Tetragonal; I4/mmm (number 139).

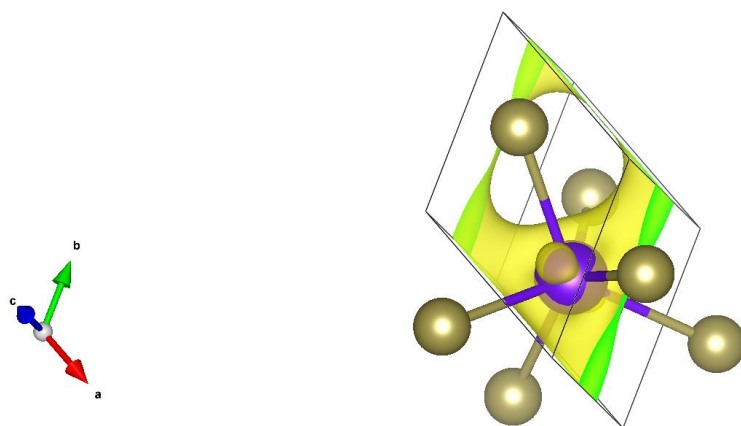


Figure S40: TbTe(mp-867290). Symmetry: Hexagonal; P-6m2 (number 187).