

High-throughput *ab initio* calculations on dielectric constants and band gap of non-oxide dielectrics

Miso Lee¹, Yong Youn¹, Kanghoon Yim^{2*} & Seungwu Han^{1*}

¹Department of Materials Science and Engineering and Research Institute of Advanced Materials, Seoul National University, Seoul 08826, Korea

²Korea Institute of Energy Research, Daejeon 34129, Korea

Supplementary information

Table S1. Names, ICSD numbers, space groups, band gaps, dielectric tensors, and ΔE of binary carbides.

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
(B ₁₂ C)C ₂	612562	166	2.49	8.3, 8.3, 10.7	0
Al ₄ C ₃	14397	160	2.16	15.8, 15.8, 18.0	0
Al ₄ C ₃	654940	166	2.16	15.0, 15.0, 18.1	0.01
BaC ₂	88101	139	2.81	9.0, 11.5, 11.5	0
BaC ₂	186576	166	2.56	15.1, 15.1, 16.1	80.68
Be ₂ C	616185	225	1.91	14.0, 14.0, 14.0	0
CSe ₂	60374	64	2.79	5.3, 7.3, 10.3	0
Cs ₂ C ₂	51534	62	4.31	7.4, 7.5, 8.9	0
K ₂ C ₂	89529	142	4.53	4.8, 5.0, 5.0	0
Li ₂ C ₂	89535	71	4.65	5.7, 5.8, 6.0	0
Mg ₂ C ₃	71941	58	2.42	6.0, 9.5, 14.3	0
Na ₂ C ₂	89527	142	4.65	5.0, 5.3, 5.3	0
Na ₂ C ₂	95835	71	4.76	5.1, 5.2, 5.3	1.8
Rb ₂ C ₂	51532	62	4.84	6.0, 6.5, 7.2	0
SiC	603798	216	2.26	10.2, 10.2, 10.2	0
SiC	164429	186	2.94	10.2, 10.2, 10.7	7.85
SiC	107204	156	2.66	10.2, 10.2, 10.7	9.12
SrC ₂	91051	15	3.47	8.0, 8.2, 8.8	0
SrC ₂	91050	139	2.93	7.0, 10.2, 10.2	11.43
Y ₄ C ₇	658826	14	1.19	29.3, 41.0, 41.1	0

Table S2. Names, ICSD numbers, space groups, band gaps, dielectric tensors, and ΔE of binary nitrides.

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
AgN ₃	183201	140	2.71	11.0, 11.5, 11.5	0
AlN	183638	186	5.58	7.7, 7.7, 9.2	0
AlN	105522	225	5.96	16.3, 16.3, 16.3	159.77
As(N ₃) ₃	413360	14	3.68	9.0, 9.5, 12.5	0
BN	240996	187	5.48	4.6, 7.1, 7.1	0
BN	24644	194	5.47	4.8, 7.1, 7.1	1.21
BN	77374	186	4.69	3.8, 7.5, 7.5	2.72
BN	27879	216	5.76	6.6, 6.6, 6.6	52.65
BN	20946	42	3.71	4.0, 7.1, 7.1	84.44
BN	27986	164	0.51	6.6, 6.6, 6.6	2035.87
Ba(N ₃) ₂	26202	11	5	4.5, 6.5, 7.1	0
Ba(N ₃) ₂	412253	11	5.01	4.5, 6.5, 7.2	1.63
Be ₃ N ₂	616348	206	4.56	10.0, 10.0, 10.0	0
Be ₃ N ₂	25656	194	4.65	10.8, 10.8, 36.5	30.63
BrN ₃	423741	110	3.23	6.0, 10.5, 10.5	0
Ca ₃ N ₂	169725	206	2.04	12.6, 12.6, 12.6	0
Ca ₃ N ₂	169726	12	2.39	17.0, 18.8, 22.6	50.68
Ca ₃ N ₂	169727	164	2.91	20.4, 20.6, 26.3	102.51
CsN ₃	627047	140	5.32	4.5, 5.3, 5.3	0
GaN	157398	186	2.94	9.2, 9.2, 10.1	0
GaN	41500	225	1.67	34.4, 34.4, 34.4	404.25
Ge ₃ N ₄	637162	159	3.39	9.8, 9.8, 9.8	0
Ge ₃ N ₄	23672	176	3.26	10.0, 10.0, 10.1	0.41
Ge ₃ N ₄	87767	227	3.2	15.2, 15.2, 15.2	61.43
Hf ₃ N ₄	97997	220	1.98	30.1, 30.1, 30.1	0
Hg(N ₃) ₂	426343	45	3.52	6.0, 12.7, 13.6	0
KN ₃	34269	140	5.53	3.6, 5.0, 5.0	0
Li ₃ N	156889	194	2.31	11.0, 11.0, 13.1	0
LiN ₃	34675	12	5.01	4.7, 5.3, 10.1	0
Mg ₃ N ₂	84917	206	2.69	9.8, 9.8, 9.8	0
N ₄ Se ₄	14325	15	2.58	10.8, 11.6, 11.9	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
NaN ₃	34267	166	5.06	2.9, 2.9, 5.5	0
NaN ₃	644523	160	5.04	3.0, 3.2, 5.1	2.2
RbN ₃	34272	140	5.45	3.9, 5.4, 5.4	0
RbN ₃	16963	123	4.96	3.8, 3.8, 6.0	19.43
Sb(N ₃) ₃	422405	2	3.44	12.4, 17.6, 19.3	0
Sb(N ₃) ₃	413359	148	3.01	12.9, 22.0, 23.8	7.74
Se ₄ N ₄	74838	14	2.58	10.0, 12.1, 12.4	0
Si ₃ N ₄	170003	173	5.75	8.0, 8.0, 8.0	0
Si ₃ N ₄	164618	159	6.14	7.9, 8.1, 8.1	2.36
Si ₃ N ₄	67241	173	4.44	6.8, 6.8, 7.5	230.85
Sn ₃ N ₄	89525	227	1.46	15.0, 15.0, 15.0	0
Ta ₃ N ₅	66533	63	2.1	34.8, 36.5, 48.1	0
W(N ₃) ₆	413860	147	2.38	6.9, 6.9, 7.5	0
YN	76528	225	1.1	111.2, 111.2, 111.2	0
Zn(N ₃) ₂	430430	5	4.4	6.9, 7.0, 7.5	0
Zn ₃ N ₂	84918	206	1.22	14.9, 14.9, 14.9	0
Zr ₃ N ₄	78944	62	1.97	46.3, 50.0, 59.7	0
Zr ₃ N ₄	97998	220	1.55	35.2, 35.2, 35.2	42.68

Table S3. Names, ICSD numbers, space groups, band gaps, dielectric tensors, and ΔE of binary fluorides

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
(SbF ₃) ₃ (SbF ₅)	35709	11	5.11	7.0, 14.4, 31.2	0
(SnF) ₂ (SnF ₆)	32592	14	4.32	8.4, 14.5, 22.2	0
(XeF ₂)(XeF ₄)	18128	14	4.09	4.6, 5.0, 5.3	0
AlF ₃	29131	150	9.8	4.5, 4.5, 4.5	0
AlF ₃	130021	221	9.7	4.5, 4.5, 4.5	0.23
AlF ₃	202681	63	9.87	4.0, 4.1, 4.3	0.55
AlF ₃	30274	155	10.02	4.7, 4.7, 4.8	1.95
AlF ₃	79816	127	9.75	4.3, 4.3, 4.4	3.46
AsF ₃	35132	33	6.77	5.4, 5.5, 7.0	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
Au(AuF ₄) ₂	89620	14	2.67	5.2, 7.1, 9.9	0
AuF ₅	411877	62	2.75	4.8, 5.0, 8.3	0
B ₁₀ F ₁₂	412618	88	4.53	3.7, 3.7, 4.1	0
B ₂ F ₄	27867	14	6.78	3.0, 3.3, 3.5	0
BaF ₂	41649	225	8.97	6.1, 6.1, 6.1	0
BaF ₂	41651	62	7.74	10.3, 10.3, 14.2	146.77
BeF ₂	261194	152	10.63	3.5, 3.5, 3.6	0
BiF ₃	9015	62	6.07	24.6, 28.9, 32.9	0
BiF ₅	25023	87	3.47	8.8, 8.8, 25.6	0
CaF ₂	60371	225	9.23	7.3, 7.3, 7.3	0
CaF ₂	656449	62	9.7	9.7, 9.9, 10.9	55
CdF ₂	183500	225	4.96	7.6, 7.6, 7.6	0
CeF ₃	81674	165	4.64	12.1, 12.2, 12.5	0
CsF	53832	225	7.08	8.3, 8.3, 8.3	0
CsF	61563	221	7.86	13.9, 13.9, 13.9	108.82
GaF ₃	409507	167	6.97	5.7, 5.7, 6.6	0
Ge ₃ F ₈	427896	14	5.4	9.3, 16.0, 33.4	0
Ge ₅ F ₁₂	10295	14	5.66	19.7, 23.1, 23.5	0
GeF ₂	18030	19	5.18	15.7, 24.4, 28.0	0
GeF ₄	202558	217	7.47	3.9, 3.9, 3.9	0
Hg ₂ F ₂	27700	139	2.55	11.0, 16.0, 16.0	0
HgF ₂	33614	225	2.86	9.7, 9.7, 9.7	0
IF ₃	411036	62	3.61	4.1, 7.7, 22.0	0
InF ₃	38306	167	5.99	7.1, 7.1, 7.4	0
IrF ₃	77619	167	2.99	7.2, 7.2, 7.9	0
IrF ₆	171654	62	2.85	4.0, 4.1, 4.1	0
KF	64686	225	7.83	5.0, 5.0, 5.0	0
KF	61558	221	8.17	7.5, 7.5, 7.5	102.64
KrF ₂	23534	136	4.71	2.5, 4.5, 4.5	0
KrF ₂	279623	139	4.84	2.8, 2.8, 7.2	7
LaF ₃	246323	185	10.21	10.7, 12.2, 12.2	0
LaF ₃	34108	194	9.9	11.7, 11.7, 14.9	14.08

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
LaF ₃	167553	59	8.84	15.4, 15.5, 18.0	201.8
LiF	41409	225	12.5	5.6, 5.6, 5.6	0
MgF ₂	8120	136	9.18	4.3, 5.3, 5.3	0
MgF ₂	422263	58	9.17	4.3, 5.3, 5.4	0.18
MgF ₂	94282	205	9.04	9.3, 9.3, 9.3	66.96
MoF ₃	68527	167	3.44	5.7, 5.7, 6.7	0
MoF ₃	30612	221	2.59	137.8, 137.8, 137.8	45.76
MoF ₆	36219	62	5.33	4.3, 4.3, 4.3	0
NaF	262837	225	8.45	4.3, 4.3, 4.3	0
Nb ₆ F ₁₅	415950	229	0.93	6.6, 6.6, 6.6	0
OsF ₅	27227	14	2.94	4.0, 4.4, 4.6	0
PbF ₂	76420	225	5.77	21.6, 21.6, 21.6	0
PbF ₄	78895	139	3.45	6.0, 16.0, 16.0	0
PdF ₄	1555	43	2.75	4.8, 7.0, 7.2	0
PtF ₄	71579	43	3.14	4.2, 6.1, 6.4	0
RbF	53828	225	7.34	5.7, 5.7, 5.7	0
RbF	61562	221	8.62	6.7, 6.7, 6.7	124.67
ReF ₇	78311	2	3.56	3.8, 4.0, 4.3	0
RhF ₃	62262	167	2.98	8.6, 8.6, 9.7	0
RhF ₃	29134	150	1.41	15.0, 15.0, 18.0	95.35
RuF ₄	165398	14	2.58	6.7, 11.2, 12.2	0
RuF ₅	27226	14	2.86	5.6, 6.1, 6.3	0
SbF ₃	16142	40	5.61	13.8, 14.7, 25.2	0
SiF ₄	24500	217	10.04	2.7, 2.7, 2.7	0
SnF ₂	14195	92	4.21	17.7, 17.7, 22.8	0
SnF ₂	14194	19	4.21	16.4, 22.0, 23.2	0.45
SnF ₂	308	15	3.19	19.4, 25.1, 43.7	82.8
SnF ₄	78894	139	5.24	4.7, 12.2, 12.2	0
SrF ₂	40414	225	9.34	5.5, 5.5, 5.5	0
SrF ₂	262349	62	9.88	6.7, 6.8, 7.2	60.02
SrF ₂	262350	194	8.71	9.2, 9.2, 17.0	190.34
TeF ₄	85452	19	5.2	5.9, 12.4, 19.6	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
TeF ₆	67609	62	6.52	3.2, 3.2, 3.2	0
TlF	90994	57	3.87	10.6, 21.5, 21.7	0
TlF	90993	129	3.99	9.0, 19.3, 19.3	6.29
TlF	9873	28	4	10.7, 20.7, 20.8	8.67
TlF	9893	139	3.1	25.9, 28.6, 28.6	38.03
TlF	30268	69	3.12	27.4, 27.6, 28.5	42.72
TlF ₃	18029	62	2.32	8.9, 11.1, 17.0	0
WF ₆	81854	62	6.59	4.2, 4.2, 4.2	0
XeF ₂	260950	139	4.34	3.7, 3.7, 6.5	0
XeF ₄	27467	14	4.56	4.2, 5.4, 5.4	0
YF ₃	26595	62	9.92	8.8, 9.0, 12.3	0
ZnF ₂	20364	60	6.51	6.0, 6.0, 7.0	0
ZrF ₄	35100	84	7.31	9.7, 10.0, 10.0	0

Table S4. Names, ICSD numbers, space groups, band gaps, dielectric tensors, and ΔE of binary phosphides.

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
Ag ₃ P ₁₁	26563	8	1.43	13.0, 13.2, 14.2	0
AlP	24490	216	2.33	10.4, 10.4, 10.4	0
B ₁₂ P ₂	62748	166	3.44	7.0, 7.0, 8.0	0
B ₆ P	615157	166	3.45	7.0, 7.0, 8.0	0
BP	615154	216	1.97	9.3, 9.3, 9.3	0
BP	615155	186	1.73	9.1, 9.1, 9.6	12.48
Ba ₃ P ₁₄	653664	14	2.42	13.2, 14.4, 18.6	0
Ba ₃ P ₁₄	23629	14	2.42	13.2, 13.4, 19.5	0.09
Ba ₃ P ₄	38322	43	1.1	16.9, 20.0, 23.5	0
BaP ₁₀	35295	36	1.89	13.2, 16.9, 17.2	0
BaP ₃	23618	12	1.15	15.0, 15.4, 18.0	0
BaP ₈	96544	2	1.42	14.7, 16.0, 17.0	0
Be ₃ P ₂	616384	206	1.47	15.6, 15.6, 15.6	0
BeP ₂	2262	1	1.55	10.2, 10.5, 10.5	0
Ca ₂ P ₂	83352	189	1.01	10.6, 10.6, 17.7	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
Ca ₅ P ₈	74854	12	1.89	15.7, 17.0, 19.6	0
CaP	26261	189	0.98	10.4, 10.4, 16.8	0
CaP ₃	74479	2	0.49	20.8, 24.0, 28.8	0
Cd ₇ P ₁₀	200596	43	1.73	18.6, 20.1, 20.4	0
CdP ₂	620214	33	2.16	10.9, 11.0, 12.7	0
CdP ₂	620210	92	2.17	11.3, 11.8, 11.8	4.12
CdP ₂	16500	96	2.17	11.5, 11.6, 11.6	5.02
CdP ₄	620212	14	0.99	20.3, 35.5, 63.7	0
Cs ₃ P ₇	62259	76	3.08	7.2, 7.6, 7.6	0
CsP ₇	428141	57	1.96	8.0, 8.9, 12.0	0
GaP	77087	216	2.43	12.4, 12.4, 12.4	0
GeP	637492	12	1.11	24.1, 24.5, 28.0	0
InP	53105	216	1.12	14.2, 14.2, 14.2	0
IrP ₂	174229	14	1.17	21.6, 21.9, 22.4	0
IrP ₃	640899	204	0.73	17.7, 17.7, 17.7	0
K ₃ P	25550	194	0.75	12.9, 12.9, 23.9	0
K ₄ P ₆	33260	70	1.67	6.1, 8.9, 9.4	0
K ₄ P ₆	33259	69	1.32	6.1, 8.0, 8.9	0.53
KP	14010	19	1.7	8.0, 10.1, 13.5	0
LaP ₂	42015	9	1	24.4, 25.1, 28.0	0
Li ₃ P	240861	194	1.32	11.1, 11.1, 11.7	0
Li ₃ P ₇	60774	19	2.47	10.0, 10.5, 10.8	0
LiP	642222	14	1.39	16.6, 19.5, 20.0	0
LiP ₅	88710	33	1.88	14.2, 14.6, 18.0	0
LiP ₅	23620	33	1.88	14.0, 14.7, 18.8	0.05
Mg ₃ P ₂	642724	206	2.25	11.9, 11.9, 11.9	0
MgP ₄	42030	14	1.18	12.5, 14.1, 15.0	0
Na ₃ P	171012	194	1.05	13.5, 15.0, 15.0	0
NaP	14009	19	1.57	11.7, 13.4, 16.7	0
OsP ₂	238252	58	1.44	28.0, 28.2, 31.3	0
OsP ₄	647710	2	2.07	19.6, 21.8, 22.0	0
P ₂ I ₄	203216	2	2.71	7.7, 9.9, 11.5	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
P ₄ Se ₄	74878	14	3.08	8.0, 8.8, 12.8	0
P ₄ Se ₅	16140	33	2.31	13.6, 13.7, 17.3	0
PBr ₃	8052	62	4.25	4.9, 6.0, 14.0	0
PBr ₅	15559	57	2.65	9.4, 12.2, 13.1	0
PBr ₇	26025	62	2.35	9.4, 13.5, 17.5	0
PI ₃	311	173	3.1	9.1, 11.4, 11.4	0
PbP ₇	427804	14	1.36	25.0, 25.9, 36.8	0
PdP ₂	48163	15	1.01	24.6, 29.4, 38.5	0
PtP ₂	71029	205	1.61	22.7, 22.7, 22.7	0
Rb ₂ P ₃	654296	69	1.36	6.2, 8.2, 8.4	0
Rb ₄ P ₆	65184	69	1.36	6.2, 8.2, 8.4	0
Re ₂ P ₅	24808	2	1.11	23.9, 24.5, 25.8	0
ReP ₃	647985	62	0.63	29.7, 33.9, 34.9	0
ReP ₄	8197	61	1.47	22.8, 24.5, 25.6	0
RhP ₂	174223	14	0.86	26.7, 27.0, 27.5	0
RuP ₂	42607	58	1.05	29.0, 29.5, 33.0	0
RuP ₃	62420	2	2.03	22.2, 23.2, 23.4	0
RuP ₄	2492	2	2.06	20.3, 22.0, 22.3	0
RuP ₄	648018	14	1.5	21.3, 23.4, 24.3	19.33
SiP	23724	36	2.08	11.1, 13.0, 13.4	0
SiP ₂	43098	55	1.98	14.4, 14.9, 16.0	0
Sr ₃ P ₁₄	42461	14	2.46	14.4, 14.6, 19.6	0
Sr ₃ P ₁₄	648173	14	2.5	13.9, 15.5, 17.3	6.96
Sr ₃ P ₄	38321	43	1.52	14.0, 16.5, 18.2	0
SrP	26262	189	1.15	10.3, 10.3, 17.9	0
SrP ₃	23628	12	0.86	14.8, 16.2, 17.8	0
TcP ₃	35200	62	1.04	28.2, 31.0, 33.5	0
TcP ₄	35117	61	1.62	22.9, 24.0, 25.4	0
TlP ₅	15021	26	1.74	20.0, 20.5, 56.2	0
YP ₅	409188	11	0.68	16.0, 16.2, 18.5	0
Zn ₃ P ₂	603896	137	1.11	18.0, 22.4, 22.4	0
Zn ₃ P ₂	648310	206	1.04	22.2, 22.2, 22.2	17.58

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
ZnP ₂	250014	96	2.18	10.5, 11.1, 11.1	0
ZnP ₂	601257	92	2.19	10.5, 11.1, 11.1	0.03
ZnP ₄	40428	92	1.46	19.3, 27.0, 27.0	0

Table S5. Names, ICSD numbers, space groups, band gaps, dielectric tensors, and ΔE of binary sulfides.

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
Al ₂ S ₃	609250	167	3.38	13.3, 13.3, 16.3	0
Al ₂ S ₃	609251	141	2.61	10.0, 10.0, 10.3	9.48
As ₂ S ₃	25792	14	2.66	10.8, 23.7, 25.3	0
As ₂ S ₃	655775	14	2.72	11.1, 22.4, 24.0	5.35
As ₄ S ₃	16145	62	2.86	10.2, 12.4, 12.7	0
As ₄ S ₃	16105	62	3.02	10.5, 11.1, 11.9	2.8
As ₄ S ₄	185032	14	2.41	11.3, 11.8, 14.5	0
As ₄ S ₄	80125	14	2.59	13.0, 13.3, 14.4	20.87
As ₄ S ₄	360	14	2.63	12.6, 14.0, 15.3	24.41
As ₈ S ₉	194921	13	2.34	12.0, 12.4, 13.6	0
AsS	24661	14	2.36	11.7, 13.0, 15.0	0
B ₈ S ₁₆	15268	14	3.65	3.8, 6.0, 6.3	0
Ba ₂ S ₃	70058	109	2.61	10.2, 14.4, 14.4	0
BaS	616053	225	3.08	13.8, 13.8, 13.8	0
BaS ₂	2004	15	2.67	8.4, 10.2, 11.0	0
BaS ₃	70059	113	2.43	10.9, 13.1, 13.1	0
BaS ₃	26765	18	1.94	9.8, 11.0, 17.0	23.32
BeS	44724	216	4.1	7.0, 7.0, 7.0	0
CaS	619529	225	3.42	11.7, 11.7, 11.7	0
CdS	192569	216	2.1	10.8, 10.8, 10.8	0
CdS	154186	186	2.38	8.7, 8.7, 9.1	48.62
CdS	600773	59	1.21	25.1, 25.1, 25.9	130.19
CdS	52825	225	1.22	25.7, 25.7, 25.7	131.52
CdS ₂	620305	205	2.22	13.7, 13.7, 13.7	0
Cs ₂ S	183207	62	3.09	9.4, 9.7, 10.0	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
Cs ₂ S	183208	62	3.09	9.4, 9.7, 10.4	0.06
Cs ₂ S ₂	200474	71	2.77	5.1, 6.2, 6.5	0
Cs ₂ S ₃	14094	36	2.41	6.4, 6.8, 10.0	0
Cs ₂ S ₅	201073	19	2.76	6.5, 6.6, 7.5	0
Cs ₂ S ₆	428612	2	2.57	6.6, 6.8, 10.0	0
Ga ₂ S ₃	409550	9	2.72	9.2, 9.5, 12.6	0
Ga ₂ S ₃	488	9	3.09	9.0, 9.1, 11.7	8.91
GaS	40824	166	2.46	6.8, 10.2, 10.2	0
GeS	1256	62	1.77	27.6, 41.3, 50.1	0
GeS	653896	62	1.74	27.9, 41.6, 56.6	0.34
GeS ₂	1947	14	3.33	6.0, 8.9, 10.0	0
GeS ₂	44	7	3.37	6.9, 9.2, 10.1	8.31
GeS ₂	31685	43	3.38	6.9, 9.2, 10.1	9.65
GeS ₂	167194	122	3.46	10.1, 10.1, 11.5	14.4
GeS ₂	85527	142	3.31	8.4, 8.4, 9.2	15.5
HfS ₂	601164	164	1.92	8.2, 46.4, 46.4	0
HfS ₃	638846	11	1.86	7.3, 12.2, 17.2	0
HgS	81923	152	2.49	24.0, 24.4, 32.6	0
HgS	639165	154	2.48	23.8, 23.9, 32.7	0.39
K ₂ S	183837	225	3.25	5.8, 5.8, 5.8	0
K ₂ S ₂	43406	189	2.55	4.7, 4.7, 6.0	0
K ₂ S ₃	1263	36	2.33	5.6, 7.5, 9.6	0
K ₂ S ₅	641320	19	2.71	7.6, 7.8, 8.5	0
K ₂ S ₆	247958	14	2.55	6.4, 7.0, 9.4	0
Li ₂ S	642291	225	4.35	7.0, 7.0, 7.0	0
Li ₂ S	91284	62	4.9	10.5, 11.0, 13.0	54.84
Li ₂ S	91283	33	4.08	7.2, 7.3, 7.5	173.98
MgS	41234	225	3.78	13.3, 13.3, 13.3	0
MoS ₂	644250	194	1.73	7.7, 15.5, 15.5	0
MoS ₂	38401	160	1.66	8.8, 16.3, 16.3	0.04
Na ₂ S ₂	644955	194	2.33	5.8, 5.8, 10.0	0
Na ₂ S ₄	2586	122	3.06	8.2, 8.8, 8.8	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
Na ₂ S ₅	644956	62	2.75	5.0, 7.8, 8.3	0
NaS	644958	194	2.32	5.8, 5.8, 10.0	0
PbS	68712	5	0.62	82.1, 82.9, 103.7	0
PbS	62190	225	0.92	98.9, 98.9, 98.9	22.94
PbS	648438	62	0.93	94.7, 106.0, 108.4	26.43
PbS	250761	63	1.67	25.0, 112.6, 156.6	75.32
PtS	649539	84	1.17	19.9, 19.9, 20.4	0
PtS ₂	649534	164	1.38	23.5, 35.3, 35.4	0
Rb ₂ S	29208	225	2.87	5.9, 5.9, 5.9	0
Rb ₂ S	261444	62	2.9	8.1, 8.1, 8.8	27.53
Rb ₂ S	261443	194	2.8	10.5, 10.5, 27.2	90.68
Rb ₂ S ₂	73176	189	2.64	4.8, 4.8, 6.9	0
Rb ₂ S ₂	73175	71	2.76	4.4, 4.8, 5.0	6.17
Rb ₂ S ₃	14092	36	2.36	5.0, 6.8, 8.9	0
Rb ₂ S ₅	100321	19	2.75	6.7, 7.0, 7.7	0
ReS ₂	650077	2	1.88	7.0, 16.1, 16.4	0
ReS ₂	81814	2	1.88	8.4, 15.9, 16.1	1.3
Rh ₂ S ₃	15344	60	1.1	24.9, 25.6, 26.5	0
RuS ₂	56019	205	1.58	20.7, 20.7, 20.7	0
Sb ₂ S ₃	99799	62	1.87	20.8, 108.7, 110.3	0
Sb ₂ S ₃	85302	31	1.88	21.0, 108.5, 113.2	0.18
Sb ₂ S ₃	425648	62	1.88	20.9, 108.1, 110.7	0.93
Sb ₂ S ₃	26751	62	1.87	20.8, 108.8, 109.0	0.99
Sb ₂ S ₃	95558	62	1.88	20.9, 108.9, 111.0	1.08
SiS ₂	26858	72	3.92	4.8, 5.2, 9.4	0
SiS ₂	291212	14	4.17	5.5, 7.5, 8.1	13.12
SiS ₂	291213	14	3.76	7.3, 7.5, 7.7	27.64
SiS ₂	291214	122	4.05	8.0, 8.0, 9.1	31.46
Sn ₂ S ₃	653956	62	1.23	24.1, 29.2, 31.9	0
SnS	651018	62	1.26	40.5, 50.1, 64.0	0
SnS	30271	62	1.25	40.7, 50.3, 65.0	0.23
SnS	52108	62	1.24	40.6, 51.2, 64.6	0.29

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
SnS	52110	62	1.24	41.1, 49.2, 65.9	0.3
SnS	43409	216	0.53	20.2, 20.2, 20.2	281.24
SnS ₂	100611	164	2.32	9.0, 19.4, 19.4	0
SnS ₂	43003	186	2.15	9.0, 18.8, 18.8	0.73
SnS ₂	193391	227	1.96	14.4, 14.4, 14.4	4.38
SrS	651054	225	3.46	11.0, 11.0, 11.0	0
SrS	52111	221	2.72	23.2, 23.2, 23.2	299.74
SrS ₂	642	140	2.35	9.0, 9.9, 9.9	0
TcS ₂	81816	2	1.68	20.0, 22.0, 28.3	0
TiS ₃	651177	11	0.98	11.1, 17.0, 20.2	0
Tl ₂ S	651245	146	1.25	32.9, 32.9, 35.8	0
Tl ₂ S ₂	78161	140	0.98	22.2, 22.2, 53.2	0
Tl ₂ S ₅	1911	19	2.4	18.4, 18.9, 19.7	0
Tl ₄ S ₃	2647	14	1.25	35.8, 40.0, 40.4	0
TlS	651242	140	1	22.4, 22.4, 54.9	0
WS ₂	202367	160	1.8	7.7, 14.0, 14.0	0
WS ₂	651387	194	1.83	7.1, 14.0, 14.0	0.34
Y ₂ S ₃	651408	11	2.4	14.2, 16.5, 16.6	0
Y ₂ S ₃	651407	62	1.47	17.1, 17.3, 18.3	1.95
Zn(S ₂)	651447	205	2.5	14.9, 14.9, 14.9	0
ZnS	291064	216	3.46	8.0, 8.0, 8.0	0
ZnS	107611	160	3.47	8.0, 8.0, 8.0	4.97
ZnS	291066	186	3.55	7.9, 7.9, 8.2	12.87
ZrS ₂	601166	164	1.82	9.2, 50.8, 50.9	0
ZrS ₃	604573	11	1.88	7.6, 11.2, 16.4	0

Table S6. Names, ICSD numbers, space groups, band gaps, dielectric tensors, and ΔE of binary chlorides

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
(ICl ₃) ₂	24714	2	2.81	8.0, 10.1, 10.1	0
(Si ₅ Cl ₁₂)(SiCl ₄)	2767	219	5.91	3.9, 3.9, 3.9	0
AgCl	56541	11	2.41	10.5, 10.6, 11.5	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
AgCl	56539	225	2.41	11.0, 11.0, 11.0	1.84
AlCl ₃	39566	12	6.73	3.7, 6.5, 6.5	0
AsCl ₃	280796	19	4.89	5.0, 5.2, 29.0	0
Au ₄ Cl ₈	201436	2	1.63	5.0, 13.3, 14.5	0
AuCl	6052	141	3.03	7.0, 7.0, 9.5	0
AuCl ₃	22146	14	2.52	6.8, 7.4, 9.2	0
B ₂ Cl ₄	14213	61	4.13	3.8, 4.8, 5.0	0
B ₄ Cl ₄	27872	137	4.2	3.7, 4.0, 4.0	0
BCl ₃	24526	176	6.22	2.6, 3.6, 3.6	0
BaCl ₂	2191	225	6.72	6.8, 6.8, 6.8	0
BaCl ₂	79891	14	6.45	8.3, 8.8, 8.9	26.06
BaCl ₂	262674	62	6.37	7.8, 8.4, 8.7	32.83
BaCl ₂	2190	189	5.82	8.6, 8.6, 9.9	34.79
BeCl ₂	92583	72	7.81	3.0, 3.3, 5.0	0
BeCl ₂	92586	142	7.89	4.0, 4.0, 4.2	6.23
BiCl ₃	2866	33	4.46	18.7, 25.7, 114.2	0
BrCl	424850	36	3.04	3.0, 5.9, 58.1	0
CaCl ₂	246416	58	7.05	6.1, 6.7, 7.9	0
CaCl ₂	56769	60	7.06	6.5, 6.7, 7.5	8.49
CaCl ₂	86209	62	7.06	4.8, 6.0, 6.5	17.71
CdCl ₂	86440	166	4.87	4.3, 7.9, 7.9	0
CeCl ₃	31575	176	3.88	7.5, 7.5, 9.6	0
CsCl	61515	225	6.11	5.3, 5.3, 5.3	0
CsCl	622366	221	6.35	7.1, 7.1, 7.1	49.66
Ga(Ga ₂ Cl ₇)	67279	33	4.93	8.5, 11.2, 11.9	0
Ga(GaCl ₄)	62664	52	4.78	11.0, 12.5, 14.2	0
GeCl ₄	280880	14	5.46	3.9, 4.0, 4.1	0
HfCl ₄	402054	13	5.38	4.6, 5.1, 9.1	0
Hg ₂ Cl ₂	31173	139	3.59	11.6, 16.6, 16.6	0
HgCl ₂	23277	62	4.22	9.8, 10.2, 16.0	0
ICl	411014	14	2.79	9.6, 11.6, 16.1	0
InCl	425449	63	1.89	25.3, 26.8, 54.6	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
InCl	2432	36	1.89	25.2, 27.3, 59.5	0.1
IrCl ₃	25716	70	3.38	5.0, 5.8, 6.7	0
IrCl ₃	23171	12	3.27	4.9, 6.9, 6.9	14.24
KCl	165593	225	6.35	4.7, 4.7, 4.7	0
KCl	60402	221	6.27	6.0, 6.0, 6.0	83.7
LaCl ₃	23146	176	5.77	7.1, 7.2, 9.0	0
LiCl	26909	225	7.73	9.9, 9.9, 9.9	0
MgCl ₂	17063	164	6.98	3.0, 6.1, 6.1	0
MgCl ₂	26157	166	6.92	3.7, 6.1, 6.1	0.65
MoCl ₃	26108	12	1.54	9.1, 17.9, 139.1	0
MoCl ₃	26109	15	2.13	5.0, 8.1, 9.0	28.08
MoCl ₅	84620	2	0.87	16.4, 32.9, 33.0	0
NaCl	165592	225	6.43	5.1, 5.1, 5.1	0
NaCl	622368	221	5.34	11.2, 11.2, 11.2	162.8
Nb ₃ Cl ₈	408645	164	1.07	4.9, 9.8, 9.8	0
NbCl ₄	1010	12	2.02	5.3, 7.0, 13.2	0
NbCl ₅	66537	14	3.43	6.7, 7.0, 7.0	0
OsCl ₄	1165	65	2.1	21.9, 35.4, 63.3	0
PbCl ₂	81976	62	4.83	24.6, 28.5, 30.9	0
PbCl ₂	81978	14	4.82	24.8, 28.1, 31.4	0.24
PbCl ₄	280975	15	2.74	8.2, 10.1, 12.4	0
PdCl ₂	404624	148	2.85	9.1, 9.7, 9.9	0
PdCl ₂	421221	14	2.28	5.9, 6.4, 9.9	8.78
PdCl ₂	421220	10	2.46	4.0, 8.2, 10.4	26.17
PdCl ₂	421213	58	2.52	4.6, 8.3, 10.4	27.23
PtCl ₂	44512	58	2.46	5.0, 6.0, 9.6	0
PtCl ₃	413423	148	1.91	10.3, 10.3, 11.2	0
RbCl	18016	225	6.12	4.7, 4.7, 4.7	0
RbCl	26877	221	6.08	6.5, 6.5, 6.5	59.84
Re ₃ Cl ₉	14209	166	1.57	5.1, 5.7, 5.7	0
ReCl ₃	62222	166	1.58	5.1, 5.7, 5.7	0
ReCl ₄	10293	13	1.95	8.0, 16.0, 44.0	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
RhCl ₃	25764	12	3.07	5.7, 7.9, 7.9	0
SbCl ₃	22191	62	4.68	7.8, 9.1, 73.3	0
SbCl ₅	412110	14	2.9	5.4, 6.0, 8.0	0
Se ₂ Cl ₂	37018	14	2.91	9.1, 15.9, 17.7	0
SiCl ₂	85526	19	2.88	3.9, 4.1, 6.6	0
SiCl ₄	62279	14	7.05	3.5, 3.5, 3.6	0
SnCl ₂	81977	62	3.96	17.3, 53.1, 55.1	0
SnCl ₂	81979	14	3.97	17.0, 52.9, 55.2	0.02
SnCl ₄	411242	14	4.88	4.7, 4.9, 5.3	0
SrCl ₂	28964	225	6.56	7.0, 7.0, 7.0	0
TaCl ₄	402406	12	2.1	5.5, 6.1, 11.4	0
TcCl ₃	261105	166	1.94	5.6, 6.4, 6.4	0
TcCl ₃	262639	12	0.54	13.1, 27.3, 31.7	114.69
TcCl ₄	26055	61	2.56	7.8, 8.1, 162.6	0
Te ₃ Cl ₂	105	14	1.94	15.1, 29.0, 30.1	0
TiCl ₄	280981	14	4.47	5.1, 5.8, 6.5	0
TiCl	61518	225	3.3	15.0, 15.0, 15.0	0
TiCl	109143	63	3.27	15.9, 16.9, 21.1	16.31
TiCl	29107	221	2.91	31.1, 31.1, 31.1	46.58
TiTiCl ₄	4031	88	2.75	15.2, 15.7, 15.8	0
WCl ₄	165263	12	1	11.6, 14.8, 18.7	0
WCl ₆	425147	148	2.64	10.3, 10.3, 10.4	0
WCl ₆	425148	164	2.54	8.6, 8.6, 12.8	0.03
Y ₂ Cl ₃	23337	12	1.3	9.8, 9.8, 13.0	0
YCl ₃	15684	12	5.96	5.0, 7.1, 7.1	0
ZnCl ₂	27673	122	5.79	4.7, 4.7, 5.7	0
ZnCl ₂	26152	137	5.57	3.8, 6.5, 6.5	7.57
ZnCl ₂	26153	14	5.63	5.7, 12.3, 24.2	30.7
ZrCl ₂	30052	160	1.48	4.4, 12.5, 12.5	0
ZrCl ₃	43292	162	1.38	4.9, 11.2, 13.7	0
ZrCl ₄	26049	13	4.97	5.0, 5.0, 10.2	0

Table S7. Names, ICSD numbers, space groups, band gaps, dielectric tensors, and ΔE of ternary fluorides.

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
$((\text{Kr}_2\text{F}_3)(\text{SbF}_6))(\text{KrF}_2)$	279628	2	3.27	4.4, 5.4, 6.4	0
$(\text{Ag}_2\text{C}_2)(\text{AgF})_8$	407646	81	3.29	15.9, 18.0, 18.3	0
$(\text{AsCl}_4)(\text{AsF}_6)$	33884	85	4.75	5.0, 5.0, 5.2	0
$(\text{Br}_3)(\text{AsF}_6)$	33811	2	2.94	5.7, 5.7, 8.4	0
$(\text{BrF}_2)_2(\text{GeF}_6)$	321	14	4.68	4.5, 4.7, 7.0	0
$(\text{BrF}_3)(\text{AuF}_3)$	93481	4	3.81	4.0, 4.3, 6.3	0
$(\text{C}_6\text{F}_5)\text{Se}(\text{C}_6\text{F}_5)$	410720	4	4.09	3.0, 3.0, 3.4	0
$(\text{CF}_2)_2\text{Te}_2$	73583	4	2.51	4.8, 8.7, 9.2	0
$(\text{CF}_3)(\text{IF}_4)$	401706	14	6.25	4.1, 4.3, 4.9	0
$(\text{CF}_3)_2\text{O}_3$	401780	2	6.96	2.0, 2.3, 2.6	0
$(\text{CF}_3)\text{TeTe}(\text{CF}_3)$	401990	14	3.5	4.1, 4.6, 4.6	0
$(\text{ClF}_2)(\text{BiF}_6)$	39555	2	3.88	5.0, 6.4, 8.9	0
$(\text{CsF})(\text{Br}_2)$	69124	123	3.03	4.2, 4.2, 66.4	0
$(\text{CsF})_2(\text{Br}_2)$	84021	139	3.82	5.1, 5.1, 13.4	0
$(\text{H}_3\text{O})\text{F}$	24382	62	8.84	3.5, 5.5, 6.9	0
$(\text{IF}_4)(\text{SbF}_6)$	281154	73	6.17	3.8, 7.3, 7.3	0
$(\text{IOF}_2)(\text{IO}_2\text{F}_4)$	201202	14	3.95	4.6, 5.6, 5.7	0
$(\text{InF}_3)(\text{SbF}_5)_3$	421923	165	5.68	5.4, 5.8, 5.8	0
$(\text{KrF})(\text{AsF}_6)$	279624	14	4.68	4.3, 4.5, 5.2	0
$(\text{KrF})(\text{BiF}_6)$	279626	14	4.39	5.1, 5.3, 6.0	0
$(\text{KrF})(\text{SbF}_6)$	279625	14	4.55	4.5, 4.6, 5.0	0
$(\text{NH}_4)(\text{HF}_2)$	415007	53	9.05	4.5, 5.9, 6.1	0
$(\text{NH}_4)\text{F}$	23766	186	7.81	3.7, 3.7, 3.7	0
$(\text{NH}_4)\text{F}(\text{NH}_3)$	419918	29	6.47	4.1, 4.4, 5.6	0
$(\text{NO})\text{F}$	411510	19	5.11	4.6, 5.9, 19.0	0
$(\text{PNF}_2)_4$	31125	14	6.74	3.0, 3.3, 3.6	0
$(\text{ReF}_5(\text{NF}))$	33543	14	3.76	4.0, 4.2, 4.5	0
$(\text{SeF}_3)(\text{NbF}_6)$	9898	146	6.56	6.5, 6.5, 6.5	0
$(\text{SnF})(\text{AsF}_6)$	816	155	4.53	9.4, 9.4, 14.3	0
$(\text{TlF}_3)(\text{SbF}_5)_3$	421924	147	3.92	4.7, 4.8, 4.8	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
Ag(AuF ₄) ₂	85416	14	2.06	6.4, 11.2, 14.3	0
Ag(BF ₄)	415320	62	5.3	5.5, 6.4, 19.7	0
Ag(BiF ₆) ₂	79879	2	2.45	9.0, 14.7, 16.0	0
Ag(SbF ₆) ₂	65186	2	2.81	5.2, 5.9, 6.1	0
Ag(SnF ₆)	51505	2	2.66	6.6, 7.6, 9.4	0
Ag(TaF ₆) ₂	62543	2	3.19	6.1, 6.6, 7.1	0
Ag(TiF ₆)	51506	2	2.32	20.7, 21.7, 23.1	0
AgZnF ₃	28950	221	3.58	15.1, 15.1, 15.1	0
As ₂ F ₇ K	36332	14	6.2	6.5, 9.8, 14.7	0
AsCl ₂ F ₃	25026	85	4.75	5.0, 5.0, 5.0	0
AsCsF ₄	413041	4	5.94	5.3, 5.7, 6.9	0
Au ₃ F ₈ (SbF ₅) ₂	412235	14	2.11	5.0, 7.4, 7.8	0
Ba(AlF ₅)	80565	4	9.47	9.5, 9.7, 10.0	13.53
Ba(BF ₄) ₂	240991	12	10.38	5.8, 6.2, 6.7	0
Ba(BrF ₄) ₂	428086	82	5.03	6.4, 8.9, 8.9	0
Ba(SbF ₅)	68455	57	6.11	6.0, 6.2, 9.2	0
Ba(SbF ₆) ₂	39346	1	6.48	5.1, 5.5, 5.7	0
Ba(ZnF ₄)	402926	36	7.02	9.7, 11.2, 13.0	0
Ba(ZrF ₆)	1697	14	8.69	9.8, 11.9, 12.7	0
Ba ₁₂ F ₁₉ Cl ₅	78943	189	7.46	7.1, 7.1, 8.0	0
Ba ₂ (ZnF ₆)	21054	139	7.32	9.0, 10.7, 10.7	0
Ba ₂ NF	262049	166	1.96	21.3, 185.4, 185.4	0
Ba ₂ PdF ₆	88802	64	3.93	6.4, 6.6, 6.6	0
Ba ₂ ZrF ₈	85717	62	8.29	8.6, 9.5, 10.2	0
Ba ₃ (In ₂ F ₁₂)	48182	127	6.68	7.8, 10.3, 10.3	0
Ba ₇ F ₁₂ Cl ₂	410679	174	7.6	8.0, 8.0, 8.7	0
BaAlF ₅	37033	19	9.54	7.4, 7.7, 7.9	0
BaAu ₂ F ₈	65289	82	4.52	5.3, 6.3, 6.3	0
BaBeF ₄	414412	62	9.72	6.7, 6.7, 37.4	0
BaFBr	35393	129	6.11	7.6, 7.6, 8.0	0
BaFI	1128	129	5.02	8.0, 8.0, 9.5	0
BaGaF ₅	200316	19	7.87	8.0, 8.1, 8.2	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
BaMgF ₄	182596	36	8.97	7.5, 8.0, 12.7	0
BaPdF ₄	108991	140	3.62	6.0, 6.0, 6.0	0
BaSnF ₄	166207	129	4.67	7.4, 23.9, 23.9	0
BaSnF ₆	33788	148	7.27	7.9, 8.1, 8.1	0
BaTeF ₆	88416	43	6.61	11.0, 11.1, 15.2	0
Bi ₃ NF ₆	79395	57	3.9	18.5, 21.8, 27.1	0
Bi ₇ F ₁₁ O ₅	167074	5	5.15	15.3, 26.4, 40.6	0
BiLiF ₄	65404	88	6.26	10.6, 10.6, 17.8	0
CF ₂ Cl ₂	33946	43	7.45	2.7, 3.4, 3.6	0
CF ₃ Cl	49696	36	8.43	2.5, 2.5, 3.0	0
CF ₃ I	73268	64	4.93	2.9, 3.8, 3.8	0
CFCl ₃	74766	61	6.46	3.1, 3.1, 3.7	0
Ca(AlF ₅)	69563	15	9.65	4.8, 6.0, 6.1	0.18
Ca(HF ₂) ₂	419144	70	9.9	4.0, 6.2, 8.3	0
Ca(PdF ₆)	26164	148	4.28	5.2, 5.2, 5.9	0
Ca(SiF ₆)	183914	148	9.81	4.8, 4.8, 5.2	0
Ca(SnF ₆)	35723	148	7.7	5.7, 5.7, 6.0	0
Ca ₂ AlF ₇	100308	62	9.36	6.1, 6.1, 8.1	0
CaAlF ₅	171399	14	9.47	5.3, 6.2, 6.7	0
CaClF	1130	129	7.27	9.1, 9.1, 9.2	0
CaPdF ₄	32674	140	3.29	6.0, 6.0, 6.7	0
CaPtF ₆	37443	148	4.7	4.8, 4.8, 5.3	0
CaZnF ₄	31366	88	7.77	10.6, 13.2, 13.2	0
Cd(AuF ₄) ₂	85413	124	3.72	4.6, 4.6, 5.2	0
Cd(PdF ₆)	26166	148	3.86	5.7, 5.7, 6.6	0
Cd(PtF ₆)	78906	148	4.2	5.1, 5.1, 5.8	0
Cd ₄ F ₆ O	74031	137	3.56	7.5, 8.3, 8.3	0
CdSnF ₆	25017	148	6	6.5, 6.5, 6.9	0
CdTiF ₆	16233	148	6.1	8.2, 8.2, 10.3	0
Ce ₂ SeF ₄	21011	166	4.06	13.9, 13.9, 14.3	0
CeZrF ₇	39776	4	4.37	7.3, 7.7, 7.8	0
ClF ₂ BF ₄	202816	14	5.48	3.0, 4.2, 4.4	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
ClF_2SbF_6	9899	2	5.26	4.4, 5.0, 7.6	0
$\text{Cs}(\text{As}_4\text{F}_{13})$	281641	82	6.78	8.6, 8.6, 12.2	0
$\text{Cs}(\text{AsF}_6)$	408070	148	7.55	4.4, 4.4, 4.7	0
$\text{Cs}(\text{Au}_2\text{F}_7)$	152057	15	3.77	4.3, 4.5, 5.3	0
$\text{Cs}(\text{AuF}_4)$	152056	71	4.46	4.8, 5.0, 5.8	0
$\text{Cs}(\text{BF}_4)$	21084	62	9.88	4.2, 4.4, 4.9	0
$\text{Cs}(\text{Br}_2\text{F}_7)$	426291	14	4.33	5.4, 5.6, 7.5	0
$\text{Cs}(\text{BrF}_4)$	426292	71	5.01	4.5, 7.2, 7.5	0
$\text{Cs}(\text{BrF}_6)$	65712	148	5.17	5.7, 5.7, 5.8	0
$\text{Cs}(\text{HgF}_3)$	15168	221	2.41	15.9, 15.9, 15.9	0
$\text{Cs}(\text{PbF}_3)$	93438	161	4.49	10.0, 11.5, 11.5	0
$\text{Cs}(\text{Pd}_2\text{F}_5)$	78777	74	2.42	13.0, 14.8, 146.6	0
$\text{Cs}(\text{Sb}_2\text{F}_7)$	14119	15	5.53	9.3, 10.1, 11.8	0
$\text{Cs}(\text{SbF}_6)$	201886	148	7.29	4.6, 4.6, 4.8	0
$\text{Cs}_2(\text{BeF}_4)$	23152	33	8.78	6.1, 6.8, 6.9	0
$\text{Cs}_2(\text{GeF}_6)$	35547	225	8.17	4.9, 4.9, 4.9	0
$\text{Cs}_2(\text{NbF}_6)$	72832	164	2.28	47.3, 259.7, 260.8	0
$\text{Cs}_2(\text{PtF}_6)$	78955	225	4.78	4.8, 4.8, 4.8	0
$\text{Cs}_2(\text{SiF}_6)$	38548	225	9.13	4.8, 4.8, 4.8	0
$\text{Cs}_2(\text{TcF}_6)$	425912	164	4.45	6.0, 6.0, 6.0	0
Cs_2CaF_4	82616	139	8.01	6.6, 9.5, 9.5	0
Cs_2HfF_6	25600	164	9.32	7.1, 7.2, 7.2	0
Cs_2HgF_4	72353	139	3.8	6.3, 17.2, 17.2	0
Cs_2PdF_6	28674	225	4.37	4.7, 4.7, 4.7	0
Cs_2PtF_6	35107	164	4.7	5.4, 5.5, 5.5	13
Cs_2SnF_6	291386	164	7.57	6.2, 6.2, 6.4	0
Cs_2ZrF_6	25598	164	9.06	7.3, 7.6, 7.6	0
$\text{Cs}_3(\text{GeF}_7)$	202917	127	6.27	7.5, 7.5, 8.1	0
$\text{Cs}_3(\text{SiF}_6)\text{F}$	9588	127	7.57	6.9, 6.9, 7.6	0
Cs_3TiF_7	9594	127	4.52	8.1, 8.1, 8.9	0
$\text{Cs}_4\text{Mg}_3\text{F}_{10}$	16084	64	8.31	6.1, 6.6, 10.2	0
$\text{Cs}_4\text{Zn}_3\text{F}_{10}$	71589	64	7.14	6.0, 6.0, 8.6	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
CsAlF ₄	10012	189	9.13	5.7, 5.7, 6.0	0
CsBeF ₃	9870	62	8.73	4.6, 4.8, 5.6	0
CsBiF ₆	15122	148	4.91	5.2, 5.2, 5.3	0
CsCaF ₃	45309	221	9.15	8.6, 8.6, 8.6	0
CsCdF ₃	49582	221	5.27	9.2, 9.2, 9.2	0
CsH ₂ F ₃	415005	19	9.04	4.9, 5.0, 5.5	0
CsHF ₂	45858	140	8.53	5.5, 6.0, 6.0	0
CsLiF ₂	18020	15	8.5	6.6, 6.8, 8.1	0
CsMgF ₃	49584	221	8.93	6.4, 6.4, 6.4	0
CsNbF ₆	183851	148	7.12	5.9, 5.9, 6.5	0
CsSbF ₄	201405	55	5.61	6.9, 7.1, 11.7	0
CsSnF ₃	236903	14	4.7	7.1, 8.7, 21.3	0
CsTeF ₅	200252	62	6.11	5.0, 6.3, 8.1	0
F ₂ (OPOPO)F ₂	248122	54	7.53	2.0, 3.9, 4.2	0
F ₅ N ₃ W	201198	14	4.13	4.0, 4.7, 5.3	0
F ₆ O ₄ Os ₂	240331	14	2.11	5.0, 7.0, 7.5	0
F ₆ O ₄ Os ₂	240330	7	2.04	5.7, 7.5, 8.4	1.84
F ₇ O ₃ Os ₂	240329	14	1.51	4.7, 6.3, 6.4	0
H ₂ F ₃ P	406359	36	8.42	3.2, 3.2, 7.0	0
H ₃ OH ₃ F ₄	32569	2	9.59	3.3, 4.2, 8.3	0
H ₃ OHF ₂	32568	14	9.21	3.8, 5.0, 8.8	0
HF ₂ N	404200	29	6.87	2.8, 3.0, 3.0	0
HOF	63681	19	5.97	3.1, 3.7, 5.7	0
Hg((CF)(CF ₂)) ₂	165635	2	4.94	3.1, 3.5, 3.7	0
Hg(AuF ₄) ₂	85414	124	3.41	5.0, 5.0, 6.1	0
Hg ₃ (AsF ₆) ₂	9323	14	3.51	7.2, 7.5, 11.1	0
Hg ₃ S ₂ F ₂	16927	199	3.15	18.5, 18.5, 18.5	0
Hg ₄ OF ₆	99995	186	1.69	12.7, 367.7, 367.7	0
I ₃ AsF ₆	15527	2	2.39	6.6, 8.6, 14.1	0
I ₄ (SbF ₆) ₂	63301	2	1.3	5.6, 9.0, 12.3	0
I ₅ (AsF ₆)	59115	15	2.29	4.7, 8.2, 16.9	0
IO ₂ F	280804	19	4.16	14.8, 24.1, 25.0	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
IOF ₃	4076	19	4.76	6.9, 10.5, 12.0	0
In(AsF ₆)	417952	148	4.46	13.3, 21.5, 21.5	0
In(BF ₄)	50218	62	5.54	14.0, 14.3, 15.0	0
K(AlF ₄)	166825	62	9.1	4.3, 4.7, 5.0	0
K(AlF ₄)	60525	11	9.06	4.5, 4.7, 4.7	6.81
K(AlF ₄)	285	123	9	8.0, 8.0, 8.8	14.39
K(AsF ₆)	59413	148	7.27	4.5, 4.6, 4.6	0
K(BF ₄)	21081	62	10.25	4.1, 4.3, 6.7	0
K(BiF ₄)	63166	227	4.97	22.0, 22.0, 22.0	0
K(BrF ₄)	10326	140	4.91	4.7, 4.7, 5.7	0
K(CdF ₃)	201329	62	5.32	7.4, 7.5, 9.9	0
K(CeF ₄)	23229	62	4.52	6.1, 6.6, 8.8	0
K(GaF ₄)	203108	62	7.5	4.8, 5.2, 5.3	0
K(HF ₂)	9345	140	9.15	4.1, 5.4, 5.4	0
K(OsF ₆)	27664	148	3.6	5.2, 5.2, 5.2	0
K(PF ₆)	25576	205	9.7	5.0, 5.0, 5.0	0
K(Sb ₂ F ₇)	14118	14	5.31	6.7, 10.9, 25.6	0
K(SbF ₄)	200572	59	5.67	6.5, 8.0, 8.7	0
K(SnF ₃)	72472	2	4.39	7.0, 11.1, 13.0	0
K(Te ₂ F ₉)	84364	2	5.94	6.0, 7.0, 9.8	0
K(TeF ₅)	16155	57	6.73	4.0, 4.2, 5.2	0
K(ZrF ₅)	83584	2	7.94	8.2, 8.8, 9.2	0
K ₂ (AgF ₄)	421461	14	2.9	5.0, 5.5, 6.0	0
K ₂ (AlF ₅)	81864	123	8.45	4.5, 4.5, 5.7	0
K ₂ (BeF ₄)	50337	33	8.92	4.8, 6.8, 7.8	0
K ₂ (BeF ₄)	153081	62	8.94	4.8, 6.7, 7.0	0.04
K ₂ (BiF ₅)	418777	62	6.25	6.2, 6.4, 10.2	0
K ₂ (GeF ₆)	24026	164	8	5.5, 5.5, 6.2	3.24
K ₂ (HfF ₆)	47246	189	9	5.0, 5.0, 9.0	46.36
K ₂ (PdF ₄)	33888	12	4.13	4.0, 4.7, 4.9	0
K ₂ (ReF ₆)	1528	164	4.06	5.2, 6.3, 6.3	0
K ₂ (SbF ₅)	39634	14	5.97	6.0, 7.0, 8.0	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
$K_2(SiF_6)$	158483	186	9.51	5.0, 5.0, 5.3	0
$K_2(TcF_6)$	425914	164	4.34	5.5, 6.2, 6.2	0
$K_2(TiF_6)$	280318	164	6.51	6.1, 6.6, 6.6	0
$K_2(ZrF_6)$	865	15	7.88	5.7, 8.0, 9.0	0
K_2GeF_6	30310	186	8.08	5.4, 5.4, 5.4	0
K_2HfF_6	29514	15	8.52	5.5, 7.8, 8.1	0
K_2MgF_4	33519	139	8.53	4.0, 5.9, 5.9	0
K_2PdF_6	27486	164	4.2	5.2, 5.6, 5.6	0
K_2PtF_6	16892	164	4.61	4.8, 5.6, 5.6	0
K_2ReF_8	20029	62	3.26	4.8, 4.8, 5.5	0
K_2SiF_6	29407	225	9.43	4.6, 4.6, 4.6	5.44
K_2TaF_7	19067	14	7.54	4.9, 5.0, 5.4	0
K_2YF_5	20692	33	8.97	5.7, 5.9, 6.3	0
K_2ZnF_4	100298	139	6.59	4.7, 6.0, 6.0	0
$K_3(SiF_6)F$	23875	127	8.02	5.7, 7.2, 7.2	0
$K_3(Zn_2F_7)$	100299	139	6.5	5.1, 6.1, 6.1	0
K_3BeF_5	14114	130	8.27	5.4, 6.0, 6.0	0
K_3TaF_8	248063	186	5.52	5.4, 5.4, 5.5	0
K_3YF_6	416296	14	8.44	6.9, 7.4, 11.9	0
$KAuF_4$	10327	140	4.39	4.0, 4.0, 4.0	0
$KCaF_3$	153628	62	8.74	6.7, 6.9, 9.0	0
KH_3F_4	202107	167	9.52	4.6, 4.6, 11.4	0
$KMgF_3$	40477	221	9.15	5.8, 5.8, 5.8	0
KSb_4F_{13}	4049	82	5.96	14.6, 17.0, 17.0	0
$KTlF_4$	4046	144	4.08	6.8, 6.8, 9.1	0
KY_3F_{10}	427142	225	9.1	9.1, 9.1, 9.1	0
$KZnF_3$	44787	221	6.29	6.4, 6.4, 6.4	0
$La(Zr_2F_{11})$	424908	72	8.16	7.8, 8.4, 8.5	0
$LaOF$	76427	129	6.28	9.0, 13.6, 13.6	0
$LaOF$	30622	166	5.8	11.4, 12.4, 12.5	0.45
$LaRbF_4$	262425	62	8.85	6.0, 6.7, 8.2	0
$LaSF$	31938	129	2.45	13.0, 14.0, 14.0	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
LaSeF	21010	194	2.66	15.1, 15.1, 17.6	0
LaSnF ₇	78896	14	7.31	6.0, 6.8, 7.0	0
Li(AsF ₆)	74831	148	7.52	4.6, 4.6, 5.1	0
Li(AuF ₄)	33953	13	4.14	4.4, 4.8, 5.1	0
Li(AuF ₆)	165209	148	3.96	4.8, 4.8, 5.5	0
Li(HF ₂)	23883	166	10.38	4.6, 4.9, 8.6	0
Li(InF ₄)	66693	60	6.23	7.4, 7.9, 11.7	0
Li(NbF ₆)	165202	148	7.04	6.8, 6.8, 6.8	0
Li(OsF ₆)	165214	148	3.51	5.2, 5.2, 5.6	0
Li(PF ₆)	74830	148	10.13	4.5, 4.5, 4.8	0
Li(RuF ₆)	165203	148	3.5	5.7, 5.7, 6.2	0
Li(Sb ₂ F ₇)	428176	62	5.96	6.9, 23.7, 37.9	0
Li(SbF ₆)	23924	148	7.16	4.8, 4.8, 5.0	0
Li(TaF ₆)	165205	148	8.17	6.2, 6.2, 6.2	0
Li ₂ (BeF ₄)	72422	148	9.9	3.9, 3.9, 4.2	0
Li ₂ (GeF ₆)	69622	150	8.27	5.6, 5.8, 5.8	0
Li ₂ (GeF ₆)	23406	136	7.97	5.2, 5.9, 5.9	3.38
Li ₂ (NbF ₆)	201755	162	2.06	15.6, 126.7, 199.0	0
Li ₂ (PdF ₆)	165212	136	4.04	5.5, 6.0, 6.0	0
Li ₂ (PtF ₆)	165216	136	4.55	5.0, 5.4, 5.4	0
Li ₂ (RuF ₆)	165210	136	2.48	30.9, 257.4, 257.4	0
Li ₂ (ZrF ₆)	409667	14	8.54	7.3, 7.4, 10.0	10.53
Li ₂ F(BF ₄)	426821	141	9.79	4.8, 4.8, 4.9	0
Li ₂ HfF ₆	251074	162	9.64	7.4, 7.4, 9.4	0
Li ₂ SiF ₆	425923	150	10.54	5.3, 5.5, 5.5	0
Li ₂ TiF ₆	18313	136	6.19	6.8, 7.2, 7.2	0
Li ₂ ZrF ₆	155020	15	8.93	8.3, 9.4, 10.4	0
Li ₂ ZrF ₆	2644	162	8.93	7.8, 7.8, 10.0	0.69
Li ₃ (AlF ₆)	34672	33	10.31	6.3, 6.7, 7.1	0
LiAuF ₄	9908	15	4.18	4.3, 4.5, 5.1	3.06
LiBF ₄	171375	152	10.61	3.6, 4.9, 5.0	0
LiBaF ₃	45310	221	8.63	11.3, 11.3, 11.3	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
LiBiF ₆	15119	148	4.5	6.0, 6.1, 6.1	0
LiSbF ₄	428177	198	6.58	21.9, 21.9, 21.9	0
LiYF ₄	73709	88	10.13	7.6, 7.7, 7.7	0.53
Mg(PdF ₆)	26163	148	3.95	4.8, 4.8, 5.5	0
Mg ₂ NF	262327	141	3.39	8.7, 8.7, 13.3	0
Mg ₃ NF ₃	262325	221	5.09	7.7, 7.7, 7.7	0
MgAu ₂ F ₈	65287	14	3.94	4.0, 4.2, 5.0	0
MgPbF ₆	15106	148	5.05	6.7, 6.7, 7.0	0
MoOF ₄	16867	14	5.17	3.9, 4.5, 6.2	0
N ₃ S ₃ F ₃	21015	148	5.56	4.7, 5.2, 5.2	0
N ₄ S ₄ F ₄	71039	114	4.87	3.8, 5.1, 5.1	0
NH ₄ (F(HF) ₃)	38337	161	9.51	4.9, 4.9, 7.0	0
NH ₄ (F(HF) ₄)	38338	88	9.63	3.0, 4.2, 4.2	0
NPF ₂	9684	36	7.24	2.8, 3.3, 5.5	0
Na(AlF ₄)	248088	63	8.96	4.4, 4.8, 8.7	0
Na(AsF ₆)	184562	148	7.53	3.0, 3.5, 3.5	0
Na(BF ₄)	161160	63	10.19	3.3, 4.0, 4.1	0
Na(HF ₂)	415006	166	9.14	2.8, 2.8, 5.5	0
Na(MgF ₃)	158931	62	9.03	5.3, 5.3, 9.5	0
Na(Sb ₃ F ₁₀)	1968	173	6.32	6.5, 17.4, 17.4	0
Na(SbF ₄)	24750	14	5.64	6.5, 7.6, 8.0	0
Na(TiF ₄)	389	60	2.95	8.6, 67.7, 230.0	0
Na ₂ (BeF ₄)	12101	62	9.02	3.5, 3.7, 3.7	0
Na ₂ (BeF ₄)	28105	14	9.06	3.8, 4.0, 4.4	6.82
Na ₂ (GeF ₆)	69623	150	8.02	4.4, 4.4, 5.4	0
Na ₂ (PtF ₆)	428575	150	4.77	4.2, 4.2, 5.3	0
Na ₂ (SbF ₅)	28061	19	6.21	5.4, 5.8, 7.0	0
Na ₂ (SiF ₆)	40917	1	9.46	4.2, 4.2, 5.5	0
Na ₂ (SiF ₆)	61274	150	9.31	4.2, 4.2, 5.4	20.23
Na ₂ (TiF ₆)	40916	1	6.6	5.2, 5.2, 8.6	0
Na ₂ AgF ₄	425149	14	2.85	5.1, 5.2, 5.8	0
Na ₃ (AlF ₆)	74200	14	9.14	4.0, 4.9, 8.4	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
Na ₃ (TaF ₈)	260875	15	6.82	4.7, 8.0, 10.0	0
Na ₅ (F(ZrF ₆) ₂)	155759	12	8.44	5.7, 6.5, 6.8	0
Na ₅ Hf ₂ F ₁₃	251075	12	8.87	5.4, 6.1, 6.4	0
NaAgF ₄	9903	140	3.34	5.1, 5.1, 5.3	0
NaAuF ₄	9905	140	4.05	4.7, 4.7, 5.1	0
NaBiF ₆	15120	148	4.89	4.5, 5.0, 5.0	0
NaMgF ₃	156157	63	8.88	4.0, 4.7, 7.5	33.07
NaZnF ₃	72320	62	6.36	5.8, 5.9, 8.9	0
NbCl ₄ F	26155	2	3.63	6.0, 7.0, 7.1	0
NbSbF ₁₀	16095	2	6.44	5.3, 7.4, 7.7	0
O ₂ (AuF ₆)	411864	2	1.39	14.8, 17.3, 21.4	0
OsO ₃ F ₂	73732	14	3.49	4.3, 6.2, 9.4	0
OsOF ₄	417246	14	2.45	5.9, 6.1, 6.8	0
OsOF ₄	417245	19	2.39	5.7, 6.9, 7.9	4.1
OsOF ₅	16872	62	2.71	5.0, 5.1, 5.7	0
OsOF ₅	240332	33	2.81	5.0, 5.0, 5.3	0.34
PHF ₂	406360	19	4.6	6.2, 7.6, 15.2	0
PHF ₄	406358	14	9.58	3.0, 3.0, 3.1	0
POF ₃	250498	164	7.73	2.4, 3.5, 3.5	0
Pb ₂ F ₂ O	10416	137	3.88	14.8, 14.8, 18.0	0
Pb ₂ RhF ₇	37141	14	3.85	12.5, 14.8, 16.3	0
PbBrF	30288	129	3.59	21.1, 33.0, 33.0	0
PbClF	30287	129	4.64	19.0, 28.3, 28.3	0
PbF(AsF ₆)	411788	2	5.69	11.1, 11.7, 20.1	0
PbF(SbF ₆)	429016	2	5.12	10.6, 13.3, 25.6	0
PbIF	56667	129	2.28	25.0, 38.5, 38.5	0
PbPdF ₄	108992	140	3.01	8.2, 11.3, 11.3	0
Pd(AuF ₄) ₂	50213	14	2.95	5.2, 10.6, 12.0	0
Pd(ZrF ₆)	73133	148	3.99	7.1, 7.1, 7.9	0
PdPtF ₆	64661	148	3.06	8.6, 8.6, 10.4	0
Pt(PF ₃) ₄	418726	217	6.28	3.7, 3.7, 3.7	0
Rb(AlF ₄)	54120	127	9.16	5.8, 5.8, 6.2	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
Rb(AlF ₄)	54123	59	9.2	5.7, 6.0, 6.1	1.03
Rb(AlF ₄)	54119	123	9.08	6.2, 6.2, 6.9	2.22
Rb(AsF ₆)	408069	148	7.38	4.2, 4.2, 4.3	0
Rb(BF ₄)	21083	62	10.05	3.9, 4.0, 5.8	0
Rb(Be ₂ F ₅)	28541	1	9.15	4.2, 4.2, 4.5	0
Rb(BrF ₄)	65713	140	5.05	5.6, 5.6, 12.4	0
Rb(HF ₂)	45859	140	8.87	4.4, 5.5, 5.5	0
Rb(SF ₅)	65221	62	6.33	4.1, 6.7, 7.6	0
Rb(SbF ₆)	408071	148	7.15	4.6, 4.6, 4.8	0
Rb(ZnF ₃)	41618	194	6.72	5.9, 5.9, 6.4	0
Rb ₂ (GeF ₆)	68982	225	8.15	4.7, 4.7, 4.7	0
Rb ₂ (GeF ₆)	25662	186	8.07	5.2, 5.2, 5.3	3.36
Rb ₂ (HfF ₆)	25599	164	9.25	6.9, 7.1, 7.1	0
Rb ₂ (NbF ₆)	72831	164	2.27	103.6, 175.7, 199.7	0
Rb ₂ (PdF ₆)	28675	225	4.41	4.6, 4.6, 4.6	0
Rb ₂ (SiF ₆)	38547	225	9.25	4.4, 4.4, 4.4	0
Rb ₂ (TcF ₆)	425918	164	4.41	5.0, 5.0, 5.4	0
Rb ₂ BeF ₄	61800	33	8.71	5.1, 6.0, 6.1	0
Rb ₂ GeF ₆	26633	164	7.99	5.2, 5.2, 5.9	9.65
Rb ₂ MgF ₄	69681	139	8.33	5.0, 5.6, 5.6	0
Rb ₂ PtF ₆	35108	164	4.68	4.8, 5.2, 5.2	0
Rb ₂ ZrF ₆	25597	164	9	7.2, 7.6, 7.6	0
Rb ₃ SiF ₇	9589	127	7.69	5.8, 6.7, 6.7	0
Rb ₃ TiF ₇	9595	127	4.6	7.5, 7.8, 7.8	0
Rb ₆ Mg ₆ F ₁₈	410385	194	8.93	5.5, 5.5, 5.8	0
RbAuF ₄	9907	140	4.49	4.0, 4.3, 4.3	0
RbBiF ₆	15121	148	4.78	5.0, 5.0, 5.3	0
RbCaF ₃	201252	221	8.46	13.8, 13.8, 13.8	0
RbCdF ₃	49587	221	5.14	16.3, 16.3, 16.3	0
RbHfF ₅	95846	14	8.82	6.6, 7.6, 8.3	0
RbMgF ₃	49585	221	9.18	5.6, 5.6, 5.6	0
RbMgF ₃	33689	194	8.85	5.5, 5.5, 5.8	1.32

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
RbPbF ₃	161148	62	5.34	8.0, 9.0, 12.2	0
RbPd ₂ F ₅	72299	74	2.43	9.0, 13.4, 24.6	0
RbSb ₂ F ₇	200574	14	5.27	8.0, 11.3, 20.3	0
ReF ₃ O ₂	415424	64	4.86	4.3, 4.5, 5.3	0
ReF ₃ O ₂	415421	14	4.86	4.0, 4.9, 8.2	3.27
ReFO ₃	415418	13	4.37	4.0, 4.6, 12.1	0
RuOF ₄	417249	14	2.94	17.8, 23.5, 23.8	0
RuOF ₄	417248	19	2.35	7.2, 9.9, 13.2	0.17
S ₄ N ₅ F	38254	2	3.57	6.0, 6.2, 7.3	0
SOF ₂	48148	14	6.99	2.8, 3.4, 4.7	0
SbCl ₃ F ₂	380014	82	3.07	4.1, 6.8, 6.8	0
SbCl ₃ F ₂	200039	79	2.97	3.8, 6.2, 6.2	4.23
SbCl ₄ F	74783	82	2.65	5.6, 5.8, 5.8	0
SbOF	21099	61	4.45	12.9, 14.2, 21.1	0
SbOF	19019	62	4.32	9.1, 9.7, 32.1	4.28
SeOF ₂	12110	29	5.4	4.4, 6.8, 7.9	0
SiH ₃ F	60065	14	7.36	4.1, 4.6, 6.4	0
Sn(SnOF ₅)	409393	12	2.94	9.6, 12.4, 14.2	0
Sn ₂ (SnOF ₂) ₂	948	12	3.48	16.2, 18.3, 22.0	0
Sn ₂ ClF ₃	200032	19	4.57	26.0, 26.5, 26.5	0
Sn ₂ F ₃ BF ₄	15263	14	5.43	8.1, 8.7, 22.0	0
Sn ₂ F ₃ Cl	2088	198	4.57	26.7, 26.7, 26.7	0.26
Sn ₂ F ₃ I	2419	20	3.12	16.9, 17.6, 46.4	0.22
Sn ₂ IF ₃	38268	63	3.12	16.9, 17.6, 46.4	0
Sn ₃ BrF ₅	200031	14	3.95	43.0, 43.2, 69.7	0
Sn ₄ OF ₆	78356	19	4.2	13.7, 14.2, 17.9	0
SnClF	647	62	4.34	14.1, 18.6, 48.6	0
Sr(BeF ₄)	404396	14	9.78	5.9, 6.0, 6.9	0
Sr(SbF ₅)	68454	57	6.14	6.0, 6.6, 12.6	0
Sr(TaF ₇)	417254	11	7.49	7.6, 8.0, 8.2	0
Sr ₂ InF ₇	38307	14	6.99	7.0, 7.2, 8.8	0
SrClF	68373	129	7.36	7.4, 7.6, 7.6	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
SrFBr	35392	129	6.32	7.6, 7.6, 7.9	0
SrMgF ₄	193584	36	8.85	6.4, 7.3, 15.3	0
SrPdF ₄	108990	140	3.45	5.7, 5.7, 6.0	0
SrZnF ₄	31367	88	7.97	7.4, 13.1, 13.1	0
TaCl ₄ F	27413	82	4.24	5.2, 6.2, 6.2	0
TcO ₃ F	249509	14	3.89	4.8, 7.2, 11.2	0
Te(OTeF ₅) ₆	2174	148	4.03	4.2, 4.3, 4.3	0
Te ₂ O ₃ F ₂	82162	2	4.62	15.6, 22.8, 31.5	0
TeOF ₂	88415	4	5.63	12.8, 19.0, 20.4	0
Tl(AlF ₄)	202458	15	5.76	9.0, 10.9, 62.1	0
Tl(AsF ₆)	417954	148	5.91	8.0, 8.0, 8.4	0
Tl(BF ₄)	300222	62	7	7.5, 7.7, 10.4	0
Tl ₂ (AlF ₅)	109365	63	5.11	10.6, 10.9, 29.2	0
Tl ₂ (SiF ₆)	38549	225	6.25	11.1, 11.1, 11.1	0
Tl ₂ (SnF ₆)	410801	164	5.57	16.3, 23.9, 23.9	0
Tl ₂ (TiF ₆)	410802	164	4.54	14.9, 17.6, 17.6	0
Tl ₂ AlF ₅	25616	20	5.16	10.1, 10.5, 25.0	0.62
Tl ₂ BeF ₄	171183	62	5.65	15.7, 19.7, 20.0	0
TlPF ₆	28899	205	7.65	8.0, 8.0, 8.0	0
TlSbF ₄	201084	14	5.14	14.0, 16.9, 22.9	0
TlSnF ₇	78899	14	3.4	6.3, 7.7, 8.4	0
TlTeF ₅	90619	62	5.77	9.6, 10.3, 13.8	0
WSF ₄	249977	29	4.22	4.0, 5.0, 6.1	0
YFS	250885	129	2.24	12.0, 15.5, 15.5	0
YFSe	2635	62	2.53	10.6, 13.1, 21.9	0
YLiF ₄	96728	15	10.13	7.0, 7.7, 7.7	0
YOF	184004	166	6.62	11.3, 12.0, 12.0	0
YOF	76426	129	6.57	9.0, 14.7, 14.7	6.61
YSnF ₇	74963	14	7.16	6.0, 6.7, 6.9	0
Zn(PdF ₆)	26165	148	3.66	5.8, 5.8, 6.7	0
ZnPbF ₆	15107	148	3.46	7.9, 7.9, 8.7	0
ZnPtF ₆	37444	148	4.18	5.1, 5.1, 5.8	0

Name	ICSD	Space group	E_g (eV)	Dielectric tensor	ΔE (meV/atom)
ZnSnF ₆	25012	148	5.85	6.2, 6.2, 6.9	0