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

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## Supplementary information

Table S1. Names, ICSD numbers, space groups, band gaps, dielectric tensors, and $\Delta E$ of binary carbides.

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | $\Delta E$ (meV/atom) |
|---|---|---|---|---|---|
| $(B_{12}C)C_2$ | 612562 | 166 | 2.49 | 8.3, 8.3, 10.7 | 0 |
| $Al_4C_3$ | 14397 | 160 | 2.16 | 15.8, 15.8, 18.0 | 0 |
| $Al_4C_3$ | 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 |
| $Be_2C$ | 616185 | 225 | 1.91 | 14.0, 14.0, 14.0 | 0 |
| $CSe_2$ | 60374 | 64 | 2.79 | 5.3, 7.3, 10.3 | 0 |
| $Cs_2C_2$ | 51534 | 62 | 4.31 | 7.4, 7.5, 8.9 | 0 |
| $K_2C_2$ | 89529 | 142 | 4.53 | 4.8, 5.0, 5.0 | 0 |
| $Li_2C_2$ | 89535 | 71 | 4.65 | 5.7, 5.8, 6.0 | 0 |
| $Mg_2C_3$ | 71941 | 58 | 2.42 | 6.0, 9.5, 14.3 | 0 |
| $Na_2C_2$ | 89527 | 142 | 4.65 | 5.0, 5.3, 5.3 | 0 |
| $Na_2C_2$ | 95835 | 71 | 4.76 | 5.1, 5.2, 5.3 | 1.8 |
| $Rb_2C_2$ | 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 |
| $Y_4C_7$ | 658826 | 14 | 1.19 | 29.3, 41.0, 41.1 | 0 |

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

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | Δ*E* (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 |
| $Be_3N_2$ | 616348 | 206 | 4.56 | 10.0, 10.0, 10.0 | 0 |
| $Be_3N_2$ | 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 |
| $Ca_3N_2$ | 169725 | 206 | 2.04 | 12.6, 12.6, 12.6 | 0 |
| $Ca_3N_2$ | 169726 | 12 | 2.39 | 17.0, 18.8, 22.6 | 50.68 |
| $Ca_3N_2$ | 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 |
| $Ge_3N_4$ | 637162 | 159 | 3.39 | 9.8, 9.8, 9.8 | 0 |
| $Ge_3N_4$ | 23672 | 176 | 3.26 | 10.0, 10.0, 10.1 | 0.41 |
| $Ge_3N_4$ | 87767 | 227 | 3.2 | 15.2, 15.2, 15.2 | 61.43 |
| $Hf_3N_4$ | 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 |
| $Li_3N$ | 156889 | 194 | 2.31 | 11.0, 11.0, 13.1 | 0 |
| $LiN_3$ | 34675 | 12 | 5.01 | 4.7, 5.3, 10.1 | 0 |
| $Mg_3N_2$ | 84917 | 206 | 2.69 | 9.8, 9.8, 9.8 | 0 |
| $N_4Se_4$ | 14325 | 15 | 2.58 | 10.8, 11.6, 11.9 | 0 |

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | $\Delta E$ (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 |
| $Se_4N_4$ | 74838 | 14 | 2.58 | 10.0, 12.1, 12.4 | 0 |
| $Si_3N_4$ | 170003 | 173 | 5.75 | 8.0, 8.0, 8.0 | 0 |
| $Si_3N_4$ | 164618 | 159 | 6.14 | 7.9, 8.1, 8.1 | 2.36 |
| $Si_3N_4$ | 67241 | 173 | 4.44 | 6.8, 6.8, 7.5 | 230.85 |
| $Sn_3N_4$ | 89525 | 227 | 1.46 | 15.0, 15.0, 15.0 | 0 |
| $Ta_3N_5$ | 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 |
| $Zn_3N_2$ | 84918 | 206 | 1.22 | 14.9, 14.9, 14.9 | 0 |
| $Zr_3N_4$ | 78944 | 62 | 1.97 | 46.3, 50.0, 59.7 | 0 |
| $Zr_3N_4$ | 97998 | 220 | 1.55 | 35.2, 35.2, 35.2 | 42.68 |

Table S3. Names, ICSD numbers, space groups, band gaps, dielectric tensors, and $\Delta E$ of binary fluorides

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | $\Delta E$ (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 | $\Delta E$ (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 |
| $B_2F_4$ | 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 |
| $Ge_3F_8$ | 427896 | 14 | 5.4 | 9.3, 16.0, 33.4 | 0 |
| $Ge_5F_{12}$ | 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 |
| $Hg_2F_2$ | 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 | $\Delta E$ (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 |
| $Nb_6F_{15}$ | 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 | $\Delta E$ (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 $\Delta E$ of binary phosphides.

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | $\Delta E$ (meV/atom) |
|---|---|---|---|---|---|
| $Ag_3P_{11}$ | 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 |
| $B_6P$ | 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 |
| $Ba_3P_{14}$ | 653664 | 14 | 2.42 | 13.2, 14.4, 18.6 | 0 |
| $Ba_3P_{14}$ | 23629 | 14 | 2.42 | 13.2, 13.4, 19.5 | 0.09 |
| $Ba_3P_4$ | 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 |
| $Be_3P_2$ | 616384 | 206 | 1.47 | 15.6, 15.6, 15.6 | 0 |
| $BeP_2$ | 2262 | 1 | 1.55 | 10.2, 10.5, 10.5 | 0 |
| $Ca_2P_2$ | 83352 | 189 | 1.01 | 10.6, 10.6, 17.7 | 0 |

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | $\Delta E$ (meV/atom) |
|---|---|---|---|---|---|
| $Ca_5P_8$ | 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 |
| $Cd_7P_{10}$ | 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 |
| $Cs_3P_7$ | 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 |
| $K_3P$ | 25550 | 194 | 0.75 | 12.9, 12.9, 23.9 | 0 |
| $K_4P_6$ | 33260 | 70 | 1.67 | 6.1, 8.9, 9.4 | 0 |
| $K_4P_6$ | 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 |
| $Li_3P$ | 240861 | 194 | 1.32 | 11.1, 11.1, 11.7 | 0 |
| $Li_3P_7$ | 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 |
| $Mg_3P_2$ | 642724 | 206 | 2.25 | 11.9, 11.9, 11.9 | 0 |
| $MgP_4$ | 42030 | 14 | 1.18 | 12.5, 14.1, 15.0 | 0 |
| $Na_3P$ | 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 |
| $P_2I_4$ | 203216 | 2 | 2.71 | 7.7, 9.9, 11.5 | 0 |

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | $\Delta E$ (meV/atom) |
|---|---|---|---|---|---|
| $P_4Se_4$ | 74878 | 14 | 3.08 | 8.0, 8.8, 12.8 | 0 |
| $P_4Se_5$ | 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 |
| $Rb_2P_3$ | 654296 | 69 | 1.36 | 6.2, 8.2, 8.4 | 0 |
| $Rb_4P_6$ | 65184 | 69 | 1.36 | 6.2, 8.2, 8.4 | 0 |
| $Re_2P_5$ | 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 |
| $Sr_3P_{14}$ | 42461 | 14 | 2.46 | 14.4, 14.6, 19.6 | 0 |
| $Sr_3P_{14}$ | 648173 | 14 | 2.5 | 13.9, 15.5, 17.3 | 6.96 |
| $Sr_3P_4$ | 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 |
| $Zn_3P_2$ | 603896 | 137 | 1.11 | 18.0, 22.4, 22.4 | 0 |
| $Zn_3P_2$ | 648310 | 206 | 1.04 | 22.2, 22.2, 22.2 | 17.58 |

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | $\Delta E$ (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 $\Delta E$ of binary sulfides.

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | $\Delta E$ (meV/atom) |
|---|---|---|---|---|---|
| $Al_2S_3$ | 609250 | 167 | 3.38 | 13.3, 13.3, 16.3 | 0 |
| $Al_2S_3$ | 609251 | 141 | 2.61 | 10.0, 10.0, 10.3 | 9.48 |
| $As_2S_3$ | 25792 | 14 | 2.66 | 10.8, 23.7, 25.3 | 0 |
| $As_2S_3$ | 655775 | 14 | 2.72 | 11.1, 22.4, 24.0 | 5.35 |
| $As_4S_3$ | 16145 | 62 | 2.86 | 10.2, 12.4, 12.7 | 0 |
| $As_4S_3$ | 16105 | 62 | 3.02 | 10.5, 11.1, 11.9 | 2.8 |
| $As_4S_4$ | 185032 | 14 | 2.41 | 11.3, 11.8, 14.5 | 0 |
| $As_4S_4$ | 80125 | 14 | 2.59 | 13.0, 13.3, 14.4 | 20.87 |
| $As_4S_4$ | 360 | 14 | 2.63 | 12.6, 14.0, 15.3 | 24.41 |
| $As_8S_9$ | 194921 | 13 | 2.34 | 12.0, 12.4, 13.6 | 0 |
| AsS | 24661 | 14 | 2.36 | 11.7, 13.0, 15.0 | 0 |
| $B_8S_{16}$ | 15268 | 14 | 3.65 | 3.8, 6.0, 6.3 | 0 |
| $Ba_2S_3$ | 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 |
| $Cs_2S$ | 183207 | 62 | 3.09 | 9.4, 9.7, 10.0 | 0 |

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | $\Delta E$ (meV/atom) |
|---|---|---|---|---|---|
| $Cs_2S$ | 183208 | 62 | 3.09 | 9.4, 9.7, 10.4 | 0.06 |
| $Cs_2S_2$ | 200474 | 71 | 2.77 | 5.1, 6.2, 6.5 | 0 |
| $Cs_2S_3$ | 14094 | 36 | 2.41 | 6.4, 6.8, 10.0 | 0 |
| $Cs_2S_5$ | 201073 | 19 | 2.76 | 6.5, 6.6, 7.5 | 0 |
| $Cs_2S_6$ | 428612 | 2 | 2.57 | 6.6, 6.8, 10.0 | 0 |
| $Ga_2S_3$ | 409550 | 9 | 2.72 | 9.2, 9.5, 12.6 | 0 |
| $Ga_2S_3$ | 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 |
| $K_2S$ | 183837 | 225 | 3.25 | 5.8, 5.8, 5.8 | 0 |
| $K_2S_2$ | 43406 | 189 | 2.55 | 4.7, 4.7, 6.0 | 0 |
| $K_2S_3$ | 1263 | 36 | 2.33 | 5.6, 7.5, 9.6 | 0 |
| $K_2S_5$ | 641320 | 19 | 2.71 | 7.6, 7.8, 8.5 | 0 |
| $K_2S_6$ | 247958 | 14 | 2.55 | 6.4, 7.0, 9.4 | 0 |
| $Li_2S$ | 642291 | 225 | 4.35 | 7.0, 7.0, 7.0 | 0 |
| $Li_2S$ | 91284 | 62 | 4.9 | 10.5, 11.0, 13.0 | 54.84 |
| $Li_2S$ | 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 |
| $Na_2S_2$ | 644955 | 194 | 2.33 | 5.8, 5.8, 10.0 | 0 |
| $Na_2S_4$ | 2586 | 122 | 3.06 | 8.2, 8.8, 8.8 | 0 |

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | $\Delta E$ (meV/atom) |
|---|---|---|---|---|---|
| $Na_2S_5$ | 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 |
| $Rb_2S$ | 29208 | 225 | 2.87 | 5.9, 5.9, 5.9 | 0 |
| $Rb_2S$ | 261444 | 62 | 2.9 | 8.1, 8.1, 8.8 | 27.53 |
| $Rb_2S$ | 261443 | 194 | 2.8 | 10.5, 10.5, 27.2 | 90.68 |
| $Rb_2S_2$ | 73176 | 189 | 2.64 | 4.8, 4.8, 6.9 | 0 |
| $Rb_2S_2$ | 73175 | 71 | 2.76 | 4.4, 4.8, 5.0 | 6.17 |
| $Rb_2S_3$ | 14092 | 36 | 2.36 | 5.0, 6.8, 8.9 | 0 |
| $Rb_2S_5$ | 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 |
| $Rh_2S_3$ | 15344 | 60 | 1.1 | 24.9, 25.6, 26.5 | 0 |
| $RuS_2$ | 56019 | 205 | 1.58 | 20.7, 20.7, 20.7 | 0 |
| $Sb_2S_3$ | 99799 | 62 | 1.87 | 20.8, 108.7, 110.3 | 0 |
| $Sb_2S_3$ | 85302 | 31 | 1.88 | 21.0, 108.5, 113.2 | 0.18 |
| $Sb_2S_3$ | 425648 | 62 | 1.88 | 20.9, 108.1, 110.7 | 0.93 |
| $Sb_2S_3$ | 26751 | 62 | 1.87 | 20.8, 108.8, 109.0 | 0.99 |
| $Sb_2S_3$ | 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 |
| $Sn_2S_3$ | 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 | $\Delta E$ (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 |
| $Tl_2S$ | 651245 | 146 | 1.25 | 32.9, 32.9, 35.8 | 0 |
| $Tl_2S_2$ | 78161 | 140 | 0.98 | 22.2, 22.2, 53.2 | 0 |
| $Tl_2S_5$ | 1911 | 19 | 2.4 | 18.4, 18.9, 19.7 | 0 |
| $Tl_4S_3$ | 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 |
| $Y_2S_3$ | 651408 | 11 | 2.4 | 14.2, 16.5, 16.6 | 0 |
| $Y_2S_3$ | 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 $\Delta E$ of binary chlorides

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | $\Delta E$ (meV/atom) |
|---|---|---|---|---|---|
| $(ICl_3)_2$ | 24714 | 2 | 2.81 | 8.0, 10.1, 10.1 | 0 |
| $(Si_5Cl_{12})(SiCl_4)$ | 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 | $\Delta E$ (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 |
| $Au_4Cl_8$ | 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 |
| $B_2Cl_4$ | 14213 | 61 | 4.13 | 3.8, 4.8, 5.0 | 0 |
| $B_4Cl_4$ | 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 |
| $Ga(Ga_2Cl_7)$ | 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 |
| $Hg_2Cl_2$ | 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 | $\Delta E$ (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 |
| $Nb_3Cl_8$ | 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 |
| $Re_3Cl_9$ | 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 | $\Delta E$ (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 |
| $Se_2Cl_2$ | 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 |
| $Te_3Cl_2$ | 105 | 14 | 1.94 | 15.1, 29.0, 30.1 | 0 |
| $TiCl_4$ | 280981 | 14 | 4.47 | 5.1, 5.8, 6.5 | 0 |
| TlCl | 61518 | 225 | 3.3 | 15.0, 15.0, 15.0 | 0 |
| TlCl | 109143 | 63 | 3.27 | 15.9, 16.9, 21.1 | 16.31 |
| TlCl | 29107 | 221 | 2.91 | 31.1, 31.1, 31.1 | 46.58 |
| $TlTlCl_4$ | 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 |
| $Y_2Cl_3$ | 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 Δ*E* of ternary fluorides.

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | Δ*E* (meV/atom) |
|---|---|---|---|---|---|
| $((Kr_2F_3)(SbF_6))(KrF_2)$ | 279628 | 2 | 3.27 | 4.4, 5.4, 6.4 | 0 |
| $(Ag_2C_2)(AgF)_8$ | 407646 | 81 | 3.29 | 15.9, 18.0, 18.3 | 0 |
| $(AsCl_4)(AsF_6)$ | 33884 | 85 | 4.75 | 5.0, 5.0, 5.2 | 0 |
| $(Br_3)(AsF_6)$ | 33811 | 2 | 2.94 | 5.7, 5.7, 8.4 | 0 |
| $(BrF_2)_2(GeF_6)$ | 321 | 14 | 4.68 | 4.5, 4.7, 7.0 | 0 |
| $(BrF_3)(AuF_3)$ | 93481 | 4 | 3.81 | 4.0, 4.3, 6.3 | 0 |
| $(C_6F_5)Se(C_6F_5)$ | 410720 | 4 | 4.09 | 3.0, 3.0, 3.4 | 0 |
| $(CF_2)_2Te_2$ | 73583 | 4 | 2.51 | 4.8, 8.7, 9.2 | 0 |
| $(CF_3)(IF_4)$ | 401706 | 14 | 6.25 | 4.1, 4.3, 4.9 | 0 |
| $(CF_3)_2O_3$ | 401780 | 2 | 6.96 | 2.0, 2.3, 2.6 | 0 |
| $(CF_3)TeTe(CF_3)$ | 401990 | 14 | 3.5 | 4.1, 4.6, 4.6 | 0 |
| $(ClF_2)(BiF_6)$ | 39555 | 2 | 3.88 | 5.0, 6.4, 8.9 | 0 |
| $(CsF)(Br_2)$ | 69124 | 123 | 3.03 | 4.2, 4.2, 66.4 | 0 |
| $(CsF)_2(Br_2)$ | 84021 | 139 | 3.82 | 5.1, 5.1, 13.4 | 0 |
| $(H_3O)F$ | 24382 | 62 | 8.84 | 3.5, 5.5, 6.9 | 0 |
| $(IF_4)(SbF_6)$ | 281154 | 73 | 6.17 | 3.8, 7.3, 7.3 | 0 |
| $(IOF_2)(IO_2F_4)$ | 201202 | 14 | 3.95 | 4.6, 5.6, 5.7 | 0 |
| $(InF_3)(SbF_5)_3$ | 421923 | 165 | 5.68 | 5.4, 5.8, 5.8 | 0 |
| $(KrF)(AsF_6)$ | 279624 | 14 | 4.68 | 4.3, 4.5, 5.2 | 0 |
| $(KrF)(BiF_6)$ | 279626 | 14 | 4.39 | 5.1, 5.3, 6.0 | 0 |
| $(KrF)(SbF_6)$ | 279625 | 14 | 4.55 | 4.5, 4.6, 5.0 | 0 |
| $(NH_4)(HF_2)$ | 415007 | 53 | 9.05 | 4.5, 5.9, 6.1 | 0 |
| $(NH_4)F$ | 23766 | 186 | 7.81 | 3.7, 3.7, 3.7 | 0 |
| $(NH_4)F(NH_3)$ | 419918 | 29 | 6.47 | 4.1, 4.4, 5.6 | 0 |
| $(NO)F$ | 411510 | 19 | 5.11 | 4.6, 5.9, 19.0 | 0 |
| $(PNF_2)_4$ | 31125 | 14 | 6.74 | 3.0, 3.3, 3.6 | 0 |
| $(ReF_5(NF))$ | 33543 | 14 | 3.76 | 4.0, 4.2, 4.5 | 0 |
| $(SeF_3)(NbF_6)$ | 9898 | 146 | 6.56 | 6.5, 6.5, 6.5 | 0 |
| $(SnF)(AsF_6)$ | 816 | 155 | 4.53 | 9.4, 9.4, 14.3 | 0 |
| $(TlF_3)(SbF_5)_3$ | 421924 | 147 | 3.92 | 4.7, 4.8, 4.8 | 0 |

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | $\Delta E$ (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 |
| $As_2F_7K$ | 36332 | 14 | 6.2 | 6.5, 9.8, 14.7 | 0 |
| $AsCl_2F_3$ | 25026 | 85 | 4.75 | 5.0, 5.0, 5.0 | 0 |
| $AsCsF_4$ | 413041 | 4 | 5.94 | 5.3, 5.7, 6.9 | 0 |
| $Au_3F_8(SbF_5)_2$ | 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 |
| $Ba_2NF$ | 262049 | 166 | 1.96 | 21.3, 185.4, 185.4 | 0 |
| $Ba_2PdF_6$ | 88802 | 64 | 3.93 | 6.4, 6.6, 6.6 | 0 |
| $Ba_2ZrF_8$ | 85717 | 62 | 8.29 | 8.6, 9.5, 10.2 | 0 |
| $Ba_3(In_2F_{12})$ | 48182 | 127 | 6.68 | 7.8, 10.3, 10.3 | 0 |
| $Ba_7F_{12}Cl_2$ | 410679 | 174 | 7.6 | 8.0, 8.0, 8.7 | 0 |
| $BaAlF_5$ | 37033 | 19 | 9.54 | 7.4, 7.7, 7.9 | 0 |
| $BaAu_2F_8$ | 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 | $\Delta E$ (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 |
| $Bi_3NF_6$ | 79395 | 57 | 3.9 | 18.5, 21.8, 27.1 | 0 |
| $Bi_7F_{11}O_5$ | 167074 | 5 | 5.15 | 15.3, 26.4, 40.6 | 0 |
| $BiLiF_4$ | 65404 | 88 | 6.26 | 10.6, 10.6, 17.8 | 0 |
| $CF_2Cl_2$ | 33946 | 43 | 7.45 | 2.7, 3.4, 3.6 | 0 |
| $CF_3Cl$ | 49696 | 36 | 8.43 | 2.5, 2.5, 3.0 | 0 |
| $CF_3I$ | 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 |
| $Ca_2AlF_7$ | 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 |
| $Cd_4F_6O$ | 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 |
| $Ce_2SeF_4$ | 21011 | 166 | 4.06 | 13.9, 13.9, 14.3 | 0 |
| $CeZrF_7$ | 39776 | 4 | 4.37 | 7.3, 7.7, 7.8 | 0 |
| $ClF_2BF_4$ | 202816 | 14 | 5.48 | 3.0, 4.2, 4.4 | 0 |

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | $\Delta E$ (meV/atom) |
|---|---|---|---|---|---|
| $ClF_2SbF_6$ | 9899 | 2 | 5.26 | 4.4, 5.0, 7.6 | 0 |
| $Cs(As_4F_{13})$ | 281641 | 82 | 6.78 | 8.6, 8.6, 12.2 | 0 |
| $Cs(AsF_6)$ | 408070 | 148 | 7.55 | 4.4, 4.4, 4.7 | 0 |
| $Cs(Au_2F_7)$ | 152057 | 15 | 3.77 | 4.3, 4.5, 5.3 | 0 |
| $Cs(AuF_4)$ | 152056 | 71 | 4.46 | 4.8, 5.0, 5.8 | 0 |
| $Cs(BF_4)$ | 21084 | 62 | 9.88 | 4.2, 4.4, 4.9 | 0 |
| $Cs(Br_2F_7)$ | 426291 | 14 | 4.33 | 5.4, 5.6, 7.5 | 0 |
| $Cs(BrF_4)$ | 426292 | 71 | 5.01 | 4.5, 7.2, 7.5 | 0 |
| $Cs(BrF_6)$ | 65712 | 148 | 5.17 | 5.7, 5.7, 5.8 | 0 |
| $Cs(HgF_3)$ | 15168 | 221 | 2.41 | 15.9, 15.9, 15.9 | 0 |
| $Cs(PbF_3)$ | 93438 | 161 | 4.49 | 10.0, 11.5, 11.5 | 0 |
| $Cs(Pd_2F_5)$ | 78777 | 74 | 2.42 | 13.0, 14.8, 146.6 | 0 |
| $Cs(Sb_2F_7)$ | 14119 | 15 | 5.53 | 9.3, 10.1, 11.8 | 0 |
| $Cs(SbF_6)$ | 201886 | 148 | 7.29 | 4.6, 4.6, 4.8 | 0 |
| $Cs_2(BeF_4)$ | 23152 | 33 | 8.78 | 6.1, 6.8, 6.9 | 0 |
| $Cs_2(GeF_6)$ | 35547 | 225 | 8.17 | 4.9, 4.9, 4.9 | 0 |
| $Cs_2(NbF_6)$ | 72832 | 164 | 2.28 | 47.3, 259.7, 260.8 | 0 |
| $Cs_2(PtF_6)$ | 78955 | 225 | 4.78 | 4.8, 4.8, 4.8 | 0 |
| $Cs_2(SiF_6)$ | 38548 | 225 | 9.13 | 4.8, 4.8, 4.8 | 0 |
| $Cs_2(TcF_6)$ | 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 |
| $Cs_3(GeF_7)$ | 202917 | 127 | 6.27 | 7.5, 7.5, 8.1 | 0 |
| $Cs_3(SiF_6)F$ | 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 |
| $Cs_4Mg_3F_{10}$ | 16084 | 64 | 8.31 | 6.1, 6.6, 10.2 | 0 |
| $Cs_4Zn_3F_{10}$ | 71589 | 64 | 7.14 | 6.0, 6.0, 8.6 | 0 |

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | $\Delta E$ (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 |
| $CsH_2F_3$ | 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 |
| $F_5N_3W$ | 201198 | 14 | 4.13 | 4.0, 4.7, 5.3 | 0 |
| $F_6O_4Os_2$ | 240331 | 14 | 2.11 | 5.0, 7.0, 7.5 | 0 |
| $F_6O_4Os_2$ | 240330 | 7 | 2.04 | 5.7, 7.5, 8.4 | 1.84 |
| $F_7O_3Os_2$ | 240329 | 14 | 1.51 | 4.7, 6.3, 6.4 | 0 |
| $H_2F_3P$ | 406359 | 36 | 8.42 | 3.2, 3.2, 7.0 | 0 |
| $H_3OH_3F_4$ | 32569 | 2 | 9.59 | 3.3, 4.2, 8.3 | 0 |
| $H_3OHF_2$ | 32568 | 14 | 9.21 | 3.8, 5.0, 8.8 | 0 |
| $HF_2N$ | 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 |
| $Hg_3S_2F_2$ | 16927 | 199 | 3.15 | 18.5, 18.5, 18.5 | 0 |
| $Hg_4OF_6$ | 99995 | 186 | 1.69 | 12.7, 367.7, 367.7 | 0 |
| $I_3AsF_6$ | 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 |
| $IO_2F$ | 280804 | 19 | 4.16 | 14.8, 24.1, 25.0 | 0 |

| Name | ICSD | Space group | $E_g$ (eV) | Dielectric tensor | $\Delta E$ (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 |
| $K(Sb_2F_7)$ | 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 |
| $K(Te_2F_9)$ | 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 | $\Delta E$ (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 | $\Delta E$ (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 |
| $Li(Sb_2F_7)$ | 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 |
| $Li_2F(BF_4)$ | 426821 | 141 | 9.79 | 4.8, 4.8, 4.9 | 0 |
| $Li_2HfF_6$ | 251074 | 162 | 9.64 | 7.4, 7.4, 9.4 | 0 |
| $Li_2SiF_6$ | 425923 | 150 | 10.54 | 5.3, 5.5, 5.5 | 0 |
| $Li_2TiF_6$ | 18313 | 136 | 6.19 | 6.8, 7.2, 7.2 | 0 |
| $Li_2ZrF_6$ | 155020 | 15 | 8.93 | 8.3, 9.4, 10.4 | 0 |
| $Li_2ZrF_6$ | 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 | $\Delta E$ (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 |
| $Mg_2NF$ | 262327 | 141 | 3.39 | 8.7, 8.7, 13.3 | 0 |
| $Mg_3NF_3$ | 262325 | 221 | 5.09 | 7.7, 7.7, 7.7 | 0 |
| $MgAu_2F_8$ | 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 |
| $N_3S_3F_3$ | 21015 | 148 | 5.56 | 4.7, 5.2, 5.2 | 0 |
| $N_4S_4F_4$ | 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 |
| $Na(Sb_3F_{10})$ | 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 |
| $Na_2AgF_4$ | 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 | $\Delta E$ (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 |
| $Na_5Hf_2F_{13}$ | 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 |
| $NbCl_4F$ | 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 |
| $OsO_3F_2$ | 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 |
| $Pb_2F_2O$ | 10416 | 137 | 3.88 | 14.8, 14.8, 18.0 | 0 |
| $Pb_2RhF_7$ | 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 | $\Delta E$ (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 |
| $Rb(Be_2F_5)$ | 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 |
| $Rb_2BeF_4$ | 61800 | 33 | 8.71 | 5.1, 6.0, 6.1 | 0 |
| $Rb_2GeF_6$ | 26633 | 164 | 7.99 | 5.2, 5.2, 5.9 | 9.65 |
| $Rb_2MgF_4$ | 69681 | 139 | 8.33 | 5.0, 5.6, 5.6 | 0 |
| $Rb_2PtF_6$ | 35108 | 164 | 4.68 | 4.8, 5.2, 5.2 | 0 |
| $Rb_2ZrF_6$ | 25597 | 164 | 9 | 7.2, 7.6, 7.6 | 0 |
| $Rb_3SiF_7$ | 9589 | 127 | 7.69 | 5.8, 6.7, 6.7 | 0 |
| $Rb_3TiF_7$ | 9595 | 127 | 4.6 | 7.5, 7.8, 7.8 | 0 |
| $Rb_6Mg_6F_{18}$ | 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 | $\Delta E$ (meV/atom) |
|---|---|---|---|---|---|
| $RbPbF_3$ | 161148 | 62 | 5.34 | 8.0, 9.0, 12.2 | 0 |
| $RbPd_2F_5$ | 72299 | 74 | 2.43 | 9.0, 13.4, 24.6 | 0 |
| $RbSb_2F_7$ | 200574 | 14 | 5.27 | 8.0, 11.3, 20.3 | 0 |
| $ReF_3O_2$ | 415424 | 64 | 4.86 | 4.3, 4.5, 5.3 | 0 |
| $ReF_3O_2$ | 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 |
| $S_4N_5F$ | 38254 | 2 | 3.57 | 6.0, 6.2, 7.3 | 0 |
| $SOF_2$ | 48148 | 14 | 6.99 | 2.8, 3.4, 4.7 | 0 |
| $SbCl_3F_2$ | 380014 | 82 | 3.07 | 4.1, 6.8, 6.8 | 0 |
| $SbCl_3F_2$ | 200039 | 79 | 2.97 | 3.8, 6.2, 6.2 | 4.23 |
| $SbCl_4F$ | 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 |
| $SiH_3F$ | 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 |
| $Sn_2ClF_3$ | 200032 | 19 | 4.57 | 26.0, 26.5, 26.5 | 0 |
| $Sn_2F_3BF_4$ | 15263 | 14 | 5.43 | 8.1, 8.7, 22.0 | 0 |
| $Sn_2F_3Cl$ | 2088 | 198 | 4.57 | 26.7, 26.7, 26.7 | 0.26 |
| $Sn_2F_3I$ | 2419 | 20 | 3.12 | 16.9, 17.6, 46.4 | 0.22 |
| $Sn_2IF_3$ | 38268 | 63 | 3.12 | 16.9, 17.6, 46.4 | 0 |
| $Sn_3BrF_5$ | 200031 | 14 | 3.95 | 43.0, 43.2, 69.7 | 0 |
| $Sn_4OF_6$ | 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 |
| $Sr_2InF_7$ | 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 | $\Delta E$ (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 |
| $TaCl_4F$ | 27413 | 82 | 4.24 | 5.2, 6.2, 6.2 | 0 |
| $TcO_3F$ | 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 |
| $Te_2O_3F_2$ | 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 |
| $Tl_2AlF_5$ | 25616 | 20 | 5.16 | 10.1, 10.5, 25.0 | 0.62 |
| $Tl_2BeF_4$ | 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 | $\Delta E$ (meV/atom) |
|---|---|---|---|---|---|
| $ZnSnF_6$ | 25012 | 148 | 5.85 | 6.2, 6.2, 6.9 | 0 |