

Supporting Information for

Machine Learning Assisted Predictions of Intrinsic Dielectric Breakdown Strength of ABX_3 Perovskites

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S1: Dataset used for prediction of intrinsic dielectric breakdown field

S1: DATASET USED FOR PREDICTION OF INTRINSIC DIELECTRIC BREAKDOWN FIELD

Table S1. List of 209 dynamically stable insulating perovskites with predicted intrinsic dielectric breakdown field (F_b), DFT-calculated band gap (E_g), maximum phonon frequency at the Γ point (ω_{\max}), and structural information (6 lattice parameters $\{a, b, c, \alpha, \beta$ and $\gamma\}$ and space group). The following data can also be found at <http://khazana.uconn.edu>.

| Name | F_b (MV/m) | E_g (eV) | ω_{\max} (THz) | a (Å) | b (Å) | c (Å) | α (°) | β (°) | γ (°) | Space group |
|----------------------|--------------|------------|-----------------------|---------|---------|---------|--------------|-------------|--------------|---------------|
| AlBeO ₂ F | 772.07 | 4.36 | 27.56 | 3.45 | 4.20 | 3.45 | 89.95 | 90.00 | 89.98 | <i>P4mm</i> |
| AlBO ₃ | 1986.75 | 4.96 | 39.30 | 3.91 | 3.92 | 3.92 | 82.17 | 82.16 | 82.16 | <i>R3m</i> |
| AlTaON ₂ | 276.76 | 2.42 | 24.55 | 4.65 | 3.81 | 3.81 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| AlZrO ₂ F | 114.25 | 1.21 | 19.78 | 3.61 | 3.61 | 4.67 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| AsAlO ₃ | 820.28 | 5.30 | 23.48 | 3.78 | 3.78 | 3.78 | 87.90 | 87.90 | 87.90 | <i>R3m</i> |
| AsGaO ₃ | 693.43 | 4.82 | 23.38 | 3.92 | 3.92 | 3.92 | 87.24 | 87.24 | 87.24 | <i>R3m</i> |
| AsGeO ₂ N | 507.29 | 3.59 | 25.79 | 4.48 | 3.28 | 4.48 | 87.76 | 76.73 | 87.76 | <i>Cm</i> |
| AsInO ₃ | 607.55 | 4.50 | 23.12 | 4.25 | 4.25 | 4.25 | 86.00 | 86.04 | 86.04 | <i>R3m</i> |
| AsNbON ₂ | 245.77 | 2.16 | 24.91 | 4.20 | 3.98 | 3.98 | 89.76 | 87.12 | 87.12 | <i>Cm</i> |
| AsSiO ₂ N | 896.98 | 4.85 | 26.94 | 4.41 | 3.08 | 4.41 | 88.41 | 77.07 | 88.41 | <i>Cm</i> |
| AsYO ₃ | 821.79 | 5.51 | 22.62 | 4.37 | 4.37 | 4.37 | 87.73 | 87.74 | 87.74 | <i>R3m</i> |
| BaAlO ₂ F | 447.98 | 4.99 | 17.10 | 3.82 | 4.00 | 3.82 | 90.00 | 90.00 | 90.00 | <i>P4/mmm</i> |
| BaBO ₂ F | 5038.93 | 6.49 | 44.07 | 4.24 | 3.82 | 4.24 | 83.62 | 82.56 | 83.64 | <i>Cm</i> |
| BaGaO ₂ F | 238.82 | 2.95 | 17.73 | 3.91 | 4.08 | 3.91 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| BaHfO ₃ | 437.22 | 5.10 | 16.44 | 4.12 | 4.12 | 4.12 | 90.00 | 90.00 | 90.00 | <i>Pm-3m</i> |
| BaNbO ₂ N | 205.23 | 2.08 | 21.97 | 4.03 | 4.27 | 4.03 | 89.99 | 90.00 | 89.99 | <i>P4mm</i> |
| BaScO ₂ F | 401.97 | 4.92 | 16.06 | 4.11 | 4.11 | 4.09 | 90.00 | 90.00 | 90.00 | <i>P4/mmm</i> |
| BaSiO ₃ | 403.97 | 3.01 | 26.30 | 4.87 | 3.52 | 3.52 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| BaSnO ₃ | 231.62 | 2.67 | 19.06 | 4.10 | 4.10 | 4.10 | 90.00 | 90.00 | 90.00 | <i>Pm-3m</i> |
| BaTaO ₂ N | 178.83 | 2.00 | 19.95 | 4.03 | 4.19 | 4.03 | 89.99 | 90.00 | 89.99 | <i>P4mm</i> |
| BaTeO ₃ | 144.03 | 2.19 | 14.48 | 4.31 | 4.31 | 4.31 | 91.38 | 91.42 | 91.42 | <i>R3m</i> |
| BaTiO ₂ S | 252.64 | 2.84 | 19.39 | 4.20 | 4.77 | 4.16 | 91.16 | 89.45 | 91.21 | <i>P1</i> |
| BaTiO ₃ | 212.89 | 3.16 | 14.95 | 3.96 | 3.96 | 3.96 | 89.97 | 89.97 | 89.97 | <i>R3m</i> |
| BaTiONF | 238.06 | 2.20 | 23.75 | 3.93 | 4.03 | 4.24 | 89.99 | 90.00 | 90.00 | <i>Pmm2</i> |
| BaZrO ₃ | 380.29 | 4.65 | 16.31 | 4.17 | 4.17 | 4.17 | 90.00 | 90.00 | 90.00 | <i>Pm-3m</i> |
| BeHfO ₂ S | 410.44 | 4.01 | 20.00 | 3.40 | 5.10 | 3.40 | 89.96 | 90.00 | 89.97 | <i>P4mm</i> |
| BeSiO ₃ | 735.13 | 4.02 | 29.05 | 3.54 | 3.55 | 3.55 | 87.33 | 87.38 | 87.38 | <i>Cm</i> |
| BiAlO ₂ S | 231.03 | 2.85 | 17.85 | 3.69 | 3.69 | 5.41 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |

| Name | F_b (MV/m) | E_g (eV) | ω_{\max} (THz) | a (Å) | b (Å) | c (Å) | α (°) | β (°) | γ (°) | Space group |
|----------------------|--------------|------------|-----------------------|---------|---------|---------|--------------|-------------|--------------|--------------|
| BiAlO ₃ | 319.58 | 3.08 | 21.63 | 4.25 | 3.62 | 3.62 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| BiBeO ₂ F | 564.06 | 4.01 | 24.77 | 3.69 | 4.19 | 3.69 | 87.88 | 89.12 | 87.89 | <i>Cm</i> |
| BiBO ₂ S | 474.41 | 2.44 | 36.35 | 3.83 | 4.97 | 3.83 | 86.54 | 85.80 | 86.55 | <i>Cm</i> |
| BiBO ₃ | 1284.21 | 4.27 | 37.05 | 3.87 | 3.87 | 3.87 | 81.68 | 81.70 | 81.70 | <i>R3m</i> |
| BiBONF | 676.02 | 2.86 | 38.79 | 3.56 | 3.89 | 4.49 | 84.98 | 83.11 | 85.27 | <i>P1</i> |
| BiGaO ₂ S | 164.70 | 2.21 | 16.64 | 3.76 | 5.49 | 3.76 | 89.85 | 90.00 | 89.88 | <i>Cm</i> |
| BiGaONF | 207.00 | 2.21 | 20.77 | 3.77 | 3.85 | 4.59 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| BiGeO ₂ N | 191.02 | 1.97 | 21.63 | 4.62 | 3.73 | 3.60 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| BiHfO ₂ N | 282.23 | 2.97 | 20.29 | 4.10 | 4.23 | 4.10 | 89.71 | 86.52 | 89.71 | <i>Cm</i> |
| BiInONF | 173.98 | 1.86 | 20.89 | 3.88 | 4.87 | 4.12 | 89.92 | 90.00 | 90.12 | <i>P1</i> |
| BiMgO ₂ F | 298.66 | 3.38 | 18.68 | 3.82 | 3.82 | 4.44 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| BiNbON ₂ | 147.63 | 1.47 | 22.15 | 4.53 | 3.91 | 3.91 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| BiScO ₂ S | 189.68 | 2.52 | 16.82 | 3.84 | 5.74 | 3.84 | 89.32 | 89.99 | 89.32 | <i>Cm</i> |
| BiSnO ₂ N | 276.29 | 2.46 | 24.09 | 4.18 | 4.02 | 4.18 | 89.86 | 86.92 | 89.86 | <i>Cm</i> |
| BiTaON ₂ | 168.16 | 1.80 | 20.80 | 4.23 | 3.99 | 3.99 | 90.00 | 89.96 | 89.96 | <i>P4mm</i> |
| BiTiO ₂ N | 244.47 | 2.32 | 23.01 | 3.69 | 4.46 | 3.90 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| BiWN ₃ | 49.18 | 0.18 | 27.05 | 3.82 | 3.82 | 4.63 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| BiYO ₃ | 419.58 | 4.30 | 18.94 | 4.39 | 4.39 | 4.39 | 88.91 | 88.95 | 88.95 | <i>R3m</i> |
| BiZnO ₂ F | 172.86 | 2.30 | 16.80 | 3.78 | 3.78 | 4.72 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| BSiO ₂ F | 2497.34 | 5.39 | 40.03 | 4.56 | 4.24 | 4.10 | 103.21 | 57.45 | 84.66 | <i>P1</i> |
| CaGeO ₃ | 303.32 | 2.84 | 22.50 | 3.72 | 3.72 | 3.72 | 90.00 | 90.00 | 90.00 | <i>Pm-3m</i> |
| CaHfO ₃ | 602.60 | 5.32 | 19.46 | 4.16 | 3.99 | 3.99 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| CaHfONF | 248.34 | 3.03 | 17.89 | 3.98 | 4.14 | 4.23 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| CaSiO ₃ | 1062.70 | 6.22 | 23.07 | 3.54 | 3.54 | 3.54 | 90.00 | 90.00 | 90.00 | <i>Pm-3m</i> |
| CaSnO ₂ S | 159.65 | 1.93 | 18.43 | 3.81 | 3.81 | 5.64 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| CaTaO ₂ N | 267.63 | 2.51 | 22.99 | 3.86 | 4.25 | 3.86 | 89.83 | 89.99 | 89.84 | <i>Cm</i> |
| CaTiO ₃ | 358.14 | 3.48 | 20.88 | 3.95 | 3.79 | 3.79 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| CaZrONF | 231.15 | 2.92 | 17.42 | 4.02 | 4.14 | 4.37 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| CdHfO ₂ S | 224.46 | 2.73 | 18.12 | 3.92 | 5.41 | 3.86 | 90.01 | 90.01 | 85.04 | <i>P1</i> |
| CdHfONF | 216.56 | 2.54 | 18.88 | 4.02 | 4.17 | 4.16 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| CdSiO ₃ | 240.11 | 2.32 | 22.70 | 3.55 | 3.55 | 3.55 | 90.00 | 90.00 | 90.00 | <i>Pm-3m</i> |
| CdSiONF | 315.36 | 2.36 | 27.98 | 5.02 | 2.95 | 3.55 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| CsIrN ₃ | 27.58 | 0.01 | 28.32 | 3.36 | 4.97 | 4.97 | 89.01 | 89.74 | 89.74 | <i>Cm</i> |

| Name | F_b (MV/m) | E_g (eV) | ω_{\max} (THz) | a (Å) | b (Å) | c (Å) | α (°) | β (°) | γ (°) | Space group |
|---------------------------------|--------------|------------|-----------------------|---------|---------|---------|--------------|-------------|--------------|--------------|
| CsMnN ₃ | 35.36 | 0.05 | 26.42 | 4.15 | 4.16 | 4.16 | 89.95 | 89.97 | 89.97 | <i>R3m</i> |
| CsTaO ₃ | 263.11 | 3.70 | 15.38 | 4.09 | 4.09 | 4.09 | 89.94 | 89.94 | 89.94 | <i>R3m</i> |
| GaHfO ₂ F | 272.01 | 3.48 | 16.82 | 3.96 | 3.96 | 4.22 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| GaTaO ₂ S | 34.65 | 0.08 | 16.35 | 3.90 | 4.91 | 3.90 | 89.95 | 90.00 | 89.98 | <i>Cm</i> |
| GaTaONF | 55.20 | 0.38 | 17.76 | 3.86 | 4.30 | 3.84 | 90.14 | 90.00 | 89.72 | <i>P1</i> |
| Ge ₂ O ₃ | 124.29 | 1.27 | 21.03 | 3.78 | 3.78 | 3.78 | 89.53 | 89.53 | 89.53 | <i>R3m</i> |
| GeAlO ₂ F | 425.07 | 3.82 | 21.54 | 3.57 | 3.57 | 4.37 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| GeBO ₂ F | 1265.12 | 4.00 | 39.23 | 3.82 | 3.96 | 3.84 | 85.83 | 82.34 | 85.85 | <i>P1</i> |
| GeGaO ₂ F | 338.56 | 3.39 | 20.55 | 3.66 | 3.66 | 4.51 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| GeInO ₂ F | 386.84 | 3.73 | 20.60 | 4.11 | 4.40 | 4.11 | 88.56 | 89.42 | 88.63 | <i>Cm</i> |
| GePbO ₃ | 39.09 | 0.12 | 19.05 | 4.27 | 4.27 | 4.27 | 87.69 | 87.73 | 87.73 | <i>R3m</i> |
| GeSiO ₂ S | 86.11 | 0.79 | 20.25 | 3.45 | 3.45 | 5.21 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| GeSnO ₃ | 221.55 | 2.32 | 21.13 | 4.05 | 4.05 | 4.05 | 89.02 | 89.02 | 89.02 | <i>R3m</i> |
| GeSnONF | 179.88 | 1.68 | 23.85 | 3.84 | 3.87 | 4.62 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| GeTiO ₃ | 284.73 | 2.93 | 20.76 | 3.88 | 3.88 | 3.88 | 89.22 | 89.22 | 89.22 | <i>R3m</i> |
| GeTiONF | 120.72 | 1.32 | 19.49 | 3.63 | 3.76 | 4.61 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| Hf ₂ ON ₂ | 376.25 | 3.04 | 24.80 | 5.76 | 3.93 | 3.93 | 90.31 | 74.46 | 74.46 | <i>Cm</i> |
| HfAlO ₂ N | 529.52 | 3.73 | 25.57 | 3.30 | 3.30 | 4.73 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| HfBeO ₃ | 652.62 | 4.65 | 23.36 | 4.22 | 3.27 | 3.27 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| HfCdONF | 245.10 | 2.70 | 19.80 | 3.34 | 3.68 | 5.28 | 89.98 | 89.76 | 90.00 | <i>Pm</i> |
| HfMgO ₂ S | 368.69 | 3.68 | 20.17 | 3.54 | 3.54 | 5.66 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| HfSnON ₂ | 236.55 | 2.07 | 25.09 | 5.69 | 3.96 | 3.96 | 90.44 | 75.28 | 75.28 | <i>Cm</i> |
| HfTiON ₂ | 229.62 | 1.93 | 26.25 | 5.55 | 3.84 | 3.84 | 90.30 | 74.03 | 74.03 | <i>Cm</i> |
| HfZrON ₂ | 334.11 | 2.81 | 24.49 | 5.76 | 3.95 | 3.95 | 90.34 | 75.43 | 75.43 | <i>Cm</i> |
| HgHfONF | 236.68 | 2.76 | 18.79 | 3.95 | 4.24 | 4.15 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| InReON ₂ | 32.15 | 0.03 | 28.77 | 3.83 | 4.59 | 3.70 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| InTeO ₂ F | 139.58 | 1.98 | 15.43 | 3.90 | 4.87 | 3.90 | 90.37 | 89.99 | 89.96 | <i>P1</i> |
| KSbO ₃ | 89.33 | 0.79 | 21.34 | 3.94 | 3.94 | 3.94 | 90.00 | 90.00 | 90.00 | <i>Pm-3m</i> |
| KSiO ₂ F | 440.83 | 3.40 | 24.80 | 3.40 | 3.40 | 4.69 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| KSnO ₂ F | 169.99 | 1.74 | 21.77 | 3.96 | 4.25 | 3.96 | 89.98 | 90.00 | 89.99 | <i>P4mm</i> |
| KWO ₂ N | 139.01 | 1.17 | 26.01 | 3.87 | 4.15 | 3.87 | 89.99 | 90.00 | 89.99 | <i>P4mm</i> |
| LaAlO ₂ S | 329.03 | 4.21 | 16.18 | 3.74 | 3.74 | 5.44 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| LaAlO ₃ | 607.88 | 4.94 | 21.08 | 3.74 | 3.74 | 3.74 | 90.00 | 90.00 | 90.00 | <i>Pm-3m</i> |

| Name | F_b (MV/m) | E_g (eV) | ω_{\max} (THz) | a (Å) | b (Å) | c (Å) | α (°) | β (°) | γ (°) | Space group |
|----------------------|--------------|------------|-----------------------|---------|---------|---------|--------------|-------------|--------------|---------------|
| LaAlONF | 191.28 | 2.05 | 20.85 | 3.78 | 3.70 | 3.91 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| LaBO ₂ S | 1197.94 | 3.94 | 38.75 | 4.29 | 3.90 | 4.78 | 89.21 | 79.49 | 81.19 | <i>P1</i> |
| LaBO ₃ | 2784.29 | 5.89 | 38.39 | 3.89 | 3.89 | 3.89 | 81.08 | 81.08 | 81.08 | <i>R3m</i> |
| LaBONF | 1583.79 | 4.10 | 42.73 | 3.84 | 3.59 | 4.41 | 80.97 | 81.20 | 83.32 | <i>P1</i> |
| LaGaO ₂ S | 173.83 | 2.56 | 15.13 | 3.83 | 3.83 | 5.49 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| LaGaONF | 272.55 | 2.68 | 21.83 | 3.93 | 3.92 | 4.02 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| LaGeO ₂ N | 107.47 | 0.92 | 23.91 | 3.84 | 3.84 | 3.79 | 90.00 | 90.00 | 90.00 | <i>P4/mmm</i> |
| LaHfO ₂ N | 293.66 | 3.14 | 19.84 | 3.95 | 4.20 | 4.17 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| LaInO ₂ S | 217.83 | 2.97 | 16.21 | 3.99 | 3.99 | 5.77 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| LaIrO ₂ S | 41.61 | 0.16 | 17.83 | 4.00 | 4.87 | 4.00 | 95.37 | 89.85 | 95.78 | <i>P1</i> |
| LaSiO ₂ N | 313.55 | 2.80 | 23.44 | 3.69 | 3.69 | 3.66 | 90.00 | 90.00 | 90.00 | <i>P4/mmm</i> |
| LaTaON ₂ | 141.00 | 1.51 | 20.56 | 4.06 | 4.02 | 4.02 | 90.00 | 89.92 | 89.92 | <i>Cm</i> |
| LaYO ₂ S | 329.63 | 4.22 | 16.15 | 4.02 | 4.02 | 5.96 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| LaZnO ₂ F | 315.67 | 3.98 | 16.57 | 3.93 | 3.93 | 4.26 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| MgSiO ₃ | 658.97 | 4.13 | 26.46 | 3.29 | 3.29 | 4.34 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| MgTeO ₂ S | 229.94 | 2.55 | 19.86 | 3.81 | 3.81 | 5.57 | 85.63 | 94.60 | 91.03 | <i>P1</i> |
| NaTeO ₂ F | 191.51 | 3.21 | 13.31 | 3.95 | 3.95 | 4.82 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| NbAlON ₂ | 264.53 | 2.02 | 28.30 | 5.38 | 3.74 | 3.74 | 90.21 | 72.61 | 72.61 | <i>Cm</i> |
| PbAlO ₂ F | 459.31 | 4.50 | 19.25 | 3.68 | 3.68 | 4.39 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| PbBO ₂ F | 1657.54 | 4.29 | 41.74 | 4.10 | 3.68 | 4.10 | 83.41 | 82.21 | 83.42 | <i>Cm</i> |
| PbGaO ₂ F | 359.01 | 3.84 | 18.93 | 3.79 | 3.79 | 4.43 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| PbHfONF | 188.69 | 2.43 | 17.35 | 4.00 | 4.14 | 4.30 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| PbInO ₂ F | 342.39 | 3.59 | 19.57 | 4.09 | 4.50 | 4.09 | 89.97 | 90.00 | 90.02 | <i>Cm</i> |
| PbLaO ₂ F | 185.56 | 2.88 | 14.39 | 4.28 | 4.91 | 4.28 | 90.68 | 90.07 | 91.14 | <i>P1</i> |
| PbNbO ₂ N | 193.59 | 1.99 | 21.68 | 3.95 | 4.25 | 3.95 | 89.36 | 89.39 | 89.37 | <i>Cm</i> |
| PbScO ₂ F | 284.73 | 3.82 | 15.92 | 4.02 | 4.02 | 4.24 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| PbSiO ₃ | 391.30 | 3.02 | 25.68 | 3.45 | 4.67 | 3.45 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| PbSnO ₂ S | 57.18 | 0.43 | 16.89 | 3.93 | 3.93 | 5.59 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| PbSnO ₃ | 276.05 | 2.91 | 20.33 | 4.06 | 4.06 | 4.06 | 89.67 | 89.67 | 89.67 | <i>R3m</i> |
| PbTaO ₂ N | 181.89 | 2.09 | 19.45 | 4.00 | 4.09 | 4.00 | 89.86 | 88.88 | 89.87 | <i>Cm</i> |
| PbVO ₂ N | 82.29 | 0.52 | 28.41 | 3.68 | 4.49 | 3.68 | 89.91 | 90.00 | 89.93 | <i>Cm</i> |
| PbZrONF | 183.50 | 2.38 | 17.17 | 4.03 | 4.15 | 4.44 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| RbHfO ₂ F | 307.36 | 4.39 | 14.73 | 4.07 | 4.07 | 4.22 | 90.00 | 90.00 | 90.00 | <i>P4/mmm</i> |

| Name | F_b (MV/m) | E_g (eV) | ω_{\max} (THz) | a (Å) | b (Å) | c (Å) | α (°) | β (°) | γ (°) | Space group |
|----------------------------------|--------------|------------|-----------------------|---------|---------|---------|--------------|-------------|--------------|-------------|
| RbNbO ₂ S | 166.09 | 1.87 | 19.77 | 4.21 | 4.76 | 4.20 | 89.99 | 89.47 | 89.99 | <i>Amm2</i> |
| RbNbO ₃ | 266.59 | 3.46 | 16.61 | 4.02 | 4.02 | 4.02 | 89.93 | 89.93 | 89.93 | <i>R3m</i> |
| RbSiO ₂ F | 312.38 | 2.75 | 23.80 | 3.41 | 3.41 | 5.25 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| RbTaONF | 179.33 | 1.80 | 22.22 | 3.97 | 4.18 | 4.18 | 89.98 | 90.00 | 90.00 | <i>Pmm2</i> |
| RbTiO ₂ F | 216.54 | 2.78 | 17.24 | 3.91 | 4.12 | 3.91 | 90.00 | 89.83 | 90.00 | <i>Amm2</i> |
| RbWO ₂ N | 267.85 | 1.90 | 30.33 | 3.85 | 4.75 | 3.85 | 89.98 | 90.00 | 89.99 | <i>P4mm</i> |
| Sb ₂ ON ₂ | 105.73 | 0.98 | 22.06 | 4.62 | 3.85 | 3.85 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| SbAlO ₃ | 443.78 | 3.99 | 21.23 | 3.79 | 3.79 | 3.79 | 89.08 | 89.08 | 89.08 | <i>R3m</i> |
| SbBO ₃ | 1293.17 | 4.38 | 36.26 | 3.92 | 3.92 | 3.92 | 80.68 | 80.69 | 80.69 | <i>R3m</i> |
| SbBONF | 786.00 | 3.25 | 37.35 | 3.28 | 4.22 | 4.49 | 89.32 | 83.72 | 87.79 | <i>P1</i> |
| SbGaO ₃ | 529.09 | 4.50 | 21.20 | 3.93 | 3.93 | 3.93 | 88.88 | 88.88 | 88.88 | <i>R3m</i> |
| SbGeO ₂ N | 398.12 | 3.23 | 24.30 | 4.52 | 3.31 | 4.52 | 89.99 | 79.75 | 89.99 | <i>Amm2</i> |
| SbInO ₃ | 512.13 | 4.39 | 21.25 | 4.25 | 4.25 | 4.25 | 88.17 | 88.22 | 88.22 | <i>R3m</i> |
| SbNbON ₂ | 185.62 | 1.74 | 23.81 | 4.69 | 3.82 | 3.82 | 90.00 | 89.85 | 89.85 | <i>Cm</i> |
| SbScO ₂ S | 202.59 | 2.55 | 17.70 | 3.92 | 5.48 | 3.92 | 87.30 | 89.67 | 87.39 | <i>Cm</i> |
| SbSiO ₂ N | 542.71 | 3.79 | 25.56 | 4.45 | 3.14 | 4.45 | 89.99 | 80.09 | 89.99 | <i>Amm2</i> |
| SbTaON ₂ | 216.82 | 2.09 | 22.98 | 4.58 | 3.85 | 3.85 | 90.00 | 90.07 | 90.07 | <i>Cm</i> |
| SbTiO ₂ N | 257.59 | 2.24 | 25.01 | 4.57 | 3.61 | 3.84 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| SbYO ₃ | 540.88 | 4.69 | 20.62 | 4.38 | 4.38 | 4.38 | 89.21 | 89.21 | 89.21 | <i>R3m</i> |
| ScBO ₂ S | 1183.81 | 4.15 | 36.58 | 3.57 | 4.92 | 3.57 | 84.26 | 85.84 | 84.26 | <i>Cm</i> |
| ScGaO ₂ S | 316.43 | 3.38 | 19.57 | 3.57 | 3.57 | 5.41 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| ScInO ₂ S | 232.98 | 2.83 | 18.11 | 3.69 | 3.69 | 5.81 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| ScSbON ₂ | 122.45 | 1.10 | 23.76 | 5.38 | 3.85 | 3.85 | 90.47 | 79.45 | 79.45 | <i>Cm</i> |
| ScSiO ₂ N | 764.90 | 4.40 | 27.17 | 3.25 | 3.25 | 4.52 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| ScTaON ₂ | 208.15 | 2.09 | 22.11 | 4.47 | 3.82 | 3.82 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| Si ₂ O ₃ | 307.19 | 2.81 | 22.94 | 3.58 | 3.58 | 3.58 | 89.56 | 89.56 | 89.56 | <i>R3m</i> |
| SiBO ₂ F | 1150.67 | 3.80 | 39.34 | 3.97 | 4.04 | 3.98 | 89.06 | 76.42 | 89.06 | <i>Cm</i> |
| SiGeO ₃ | 28.65 | 0.01 | 21.52 | 3.82 | 3.84 | 3.84 | 87.63 | 87.67 | 87.67 | <i>Cm</i> |
| SiHfO ₂ S | 134.43 | 1.52 | 19.30 | 3.40 | 5.45 | 3.40 | 107.89 | 90.04 | 107.89 | <i>Cm</i> |
| SiInO ₂ F | 284.82 | 2.64 | 23.01 | 4.14 | 4.33 | 4.14 | 87.74 | 88.88 | 87.85 | <i>Cm</i> |
| SiNbO ₂ N | 209.89 | 1.84 | 25.35 | 3.89 | 3.78 | 3.89 | 83.96 | 81.53 | 96.03 | <i>Cm</i> |
| Sn ₂ O ₂ S | 29.20 | 0.02 | 16.84 | 3.92 | 3.92 | 5.46 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| SnAlO ₂ F | 369.81 | 3.86 | 19.27 | 3.64 | 3.64 | 4.51 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |

| Name | F_b (MV/m) | E_g (eV) | ω_{\max} (THz) | a (Å) | b (Å) | c (Å) | α (°) | β (°) | γ (°) | Space group |
|----------------------|--------------|------------|-----------------------|---------|---------|---------|--------------|-------------|--------------|---------------|
| SnBO ₂ F | 1041.70 | 3.63 | 39.09 | 3.90 | 4.09 | 3.90 | 87.23 | 84.63 | 87.25 | <i>Cm</i> |
| SnGaO ₂ F | 268.64 | 3.07 | 18.86 | 3.73 | 3.73 | 4.55 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| SnHfO ₂ S | 147.01 | 1.96 | 16.58 | 3.97 | 5.29 | 3.97 | 90.76 | 89.97 | 90.74 | <i>Cm</i> |
| SnHfONF | 151.03 | 1.81 | 18.44 | 3.90 | 4.05 | 4.45 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| SnInO ₂ F | 221.18 | 2.52 | 19.40 | 3.98 | 4.64 | 3.98 | 89.92 | 90.00 | 90.01 | <i>Cm</i> |
| SnLaO ₂ F | 288.89 | 3.58 | 17.16 | 4.35 | 4.68 | 4.35 | 96.24 | 91.71 | 96.51 | <i>P1</i> |
| SnScO ₂ F | 233.31 | 3.06 | 16.76 | 3.94 | 3.94 | 4.38 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| SnTaO ₂ N | 136.76 | 1.51 | 19.81 | 4.02 | 3.99 | 4.04 | 89.99 | 88.46 | 90.00 | <i>P1</i> |
| SnTiO ₃ | 155.90 | 1.48 | 23.31 | 3.79 | 3.79 | 4.27 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| SnZrONF | 145.40 | 1.76 | 18.23 | 3.92 | 4.06 | 4.57 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| SrBiO ₂ F | 176.48 | 3.02 | 13.04 | 4.20 | 4.98 | 4.20 | 91.21 | 90.00 | 92.64 | <i>P1</i> |
| SrBO ₂ F | 5977.17 | 6.86 | 44.40 | 4.10 | 3.62 | 4.10 | 81.79 | 81.73 | 81.80 | <i>Cm</i> |
| SrGaO ₂ F | 381.00 | 3.70 | 20.53 | 3.85 | 3.85 | 3.91 | 90.00 | 90.00 | 90.00 | <i>P4/mmm</i> |
| SrGeO ₃ | 185.86 | 2.12 | 19.61 | 3.78 | 3.78 | 3.78 | 90.00 | 90.00 | 90.00 | <i>Pm-3m</i> |
| SrNbO ₂ N | 225.19 | 2.16 | 23.04 | 3.92 | 4.26 | 3.92 | 89.96 | 90.00 | 89.96 | <i>Cm</i> |
| SrSiO ₃ | 574.72 | 5.14 | 19.55 | 3.62 | 3.62 | 3.62 | 90.00 | 90.00 | 90.00 | <i>Pm-3m</i> |
| SrSiONF | 669.58 | 3.86 | 28.65 | 4.85 | 3.91 | 3.07 | 90.00 | 89.99 | 89.79 | <i>Pm</i> |
| SrSnO ₃ | 357.32 | 3.39 | 21.40 | 4.03 | 4.03 | 4.03 | 90.00 | 90.00 | 90.00 | <i>Pm-3m</i> |
| SrTaO ₂ N | 197.87 | 2.07 | 21.25 | 3.95 | 4.15 | 3.95 | 89.95 | 90.00 | 89.95 | <i>Cm</i> |
| TaAlON ₂ | 348.99 | 2.50 | 28.49 | 5.41 | 3.76 | 3.76 | 90.18 | 71.97 | 71.97 | <i>Cm</i> |
| TaBeO ₂ N | 287.20 | 2.58 | 23.74 | 3.12 | 4.45 | 3.13 | 89.84 | 90.00 | 89.99 | <i>Pm</i> |
| TeBeO ₃ | 908.12 | 4.76 | 27.67 | 3.94 | 3.94 | 3.94 | 83.30 | 83.32 | 83.32 | <i>R3m</i> |
| TeBO ₂ N | 644.07 | 2.97 | 36.29 | 3.75 | 4.18 | 3.75 | 80.90 | 80.52 | 80.97 | <i>Cm</i> |
| TeGeON ₂ | 72.92 | 0.54 | 22.25 | 4.57 | 3.65 | 3.65 | 90.00 | 89.58 | 89.58 | <i>Cm</i> |
| TeSiON ₂ | 80.72 | 0.55 | 26.26 | 4.36 | 3.55 | 3.55 | 90.00 | 89.95 | 89.95 | <i>P1</i> |
| TeWON ₂ | 34.73 | 0.05 | 24.79 | 4.72 | 3.76 | 3.76 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| TiBO ₂ N | 404.10 | 2.85 | 27.83 | 4.35 | 2.77 | 4.40 | 89.99 | 65.35 | 89.99 | <i>Pm</i> |
| TiLiO ₂ N | 30.33 | 0.02 | 20.12 | 2.85 | 2.85 | 5.41 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| TiSnON ₂ | 247.18 | 1.98 | 27.24 | 5.51 | 3.87 | 3.87 | 90.38 | 74.95 | 74.95 | <i>Cm</i> |
| YAlO ₂ S | 519.58 | 4.80 | 19.63 | 3.62 | 3.62 | 5.37 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| YAlONF | 499.49 | 4.18 | 21.95 | 3.65 | 3.93 | 3.70 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| YBONF | 1910.51 | 4.42 | 43.33 | 3.53 | 3.35 | 4.53 | 81.85 | 81.18 | 86.43 | <i>P1</i> |
| YGaO ₃ | 574.62 | 4.72 | 21.29 | 4.66 | 3.59 | 3.59 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |

| Name | F_b (MV/m) | E_g (eV) | ω_{\max} (THz) | a (Å) | b (Å) | c (Å) | α (°) | β (°) | γ (°) | Space group |
|---------------------------------|--------------|------------|-----------------------|---------|---------|---------|--------------|-------------|--------------|---------------|
| YGaONF | 370.15 | 3.42 | 21.78 | 3.41 | 5.08 | 3.46 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| YGeO ₂ N | 324.34 | 2.88 | 23.38 | 3.47 | 3.47 | 4.85 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| YInONF | 213.66 | 2.18 | 21.74 | 4.10 | 4.86 | 4.07 | 86.58 | 90.83 | 90.04 | <i>P1</i> |
| YScO ₂ S | 392.22 | 4.36 | 17.81 | 3.77 | 5.72 | 3.77 | 90.03 | 90.00 | 90.08 | <i>P4mm</i> |
| YSiO ₂ N | 343.35 | 2.79 | 25.18 | 3.55 | 3.55 | 3.65 | 90.00 | 90.00 | 90.00 | <i>P4/mmm</i> |
| YSnO ₂ N | 234.94 | 2.56 | 20.18 | 3.61 | 3.61 | 5.19 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| YTaN ₂ O | 167.40 | 1.75 | 21.30 | 4.14 | 3.95 | 3.95 | 90.00 | 89.36 | 89.36 | <i>Cm</i> |
| YTiO ₂ N | 476.41 | 3.55 | 25.07 | 3.59 | 3.59 | 4.71 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| YTlO ₂ S | 114.02 | 1.54 | 15.52 | 3.90 | 3.90 | 6.02 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| ZnAlO ₂ F | 256.87 | 2.77 | 20.13 | 3.77 | 3.77 | 3.71 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| Zr ₂ ON ₂ | 299.60 | 2.62 | 24.17 | 5.78 | 3.97 | 3.97 | 90.36 | 76.07 | 76.07 | <i>Cm</i> |
| ZrBeO ₃ | 537.77 | 4.16 | 23.17 | 4.20 | 3.30 | 3.30 | 90.00 | 90.00 | 90.00 | <i>P4mm</i> |
| ZrHfON ₂ | 334.30 | 2.82 | 24.49 | 5.75 | 3.94 | 3.94 | 90.34 | 75.57 | 75.57 | <i>Cm</i> |
| ZrSiON ₂ | 408.56 | 2.84 | 28.10 | 3.29 | 4.52 | 3.38 | 90.00 | 90.00 | 90.00 | <i>Pmm2</i> |
| ZrSnON ₂ | 225.43 | 2.02 | 24.68 | 5.66 | 3.97 | 3.97 | 90.52 | 76.93 | 76.93 | <i>Cm</i> |
| ZrTiON ₂ | 221.46 | 1.90 | 25.72 | 5.46 | 3.84 | 3.84 | 90.31 | 76.18 | 76.18 | <i>Cm</i> |