High throughput thermal conductivity of high temperature solid phases: 
The case of oxide and fluoride perovskites
Supplemental Material

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In this supplemental material, we provide more data to analyze the discrepancy in thermal conductivity between fluorides and oxides, a few details about the method we have used to calculate the finite-temperature force constants, the phonon spectra that we have calculated and a benchmark of our machine-learning scheme.

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Table I: List of elements considered in the high-throughput study of perovskites $ABX_3$. Elements in green and in yellow were considered for the $A$ and $B$ sites, and elements in yellow for the $X$ site.

Figure 1: Left panel: Thermal conductivities and specific heats of all mechanically stable fluorides (blue dots) and oxides (red dots). Right panel: Thermal conductivities and lattice parameters of all mechanically stable fluorides (blue dots) and oxides (red dots).

I. LIST OF COMPOUNDS

Table I displays the list of elements considered for the construction of the list of cubic perovskites that we have calculated. Density functional theory calculations were performed using the GGA functional with DFT+U corrections as described in Ref. [1].

II. THERMAL CONDUCTIVITY OF FLUORIDES VS OXIDES

We show on Fig. 1 the relationship between the thermal conductivities and the specific heats of all mechanically stable oxides and fluorides. We see an overall tendency of increasing thermal conductivity with a higher specific heat. This plays a role in the observed higher thermal conductivity of oxides. As shown in Fig. 1, it can also be related to the larger lattice parameters in fluorides, since at 1000 K the specific heat is negatively correlated to the lattice parameter (see correlograms in the main text).

In Fig. 2, we show the relationship between the thermal conductivities and the mean phonon group velocities of all mechanically stable oxides and fluorides. Here, we also see a trend driving larger thermal conductivities with high mean velocities. It is linked to the smaller inter-atomic force constants in fluorides which show lower ionic charge (see main text).

Finally, we display in Fig. 2 the values of the thermal conductivities and root mean square Grüneisen parameters
Figure 2: Left panel: Thermal conductivities and mean phonon group velocities of all mechanically stable fluorides (blue dots) and oxides (red dots). Right panel: Thermal conductivities and root mean square Grüneisen parameters of all mechanically stable fluorides (blue dots) and oxides (red dots).

of all mechanically stable oxides and fluorides. In contrast to the figures shown above, it is difficult to distinguish a global trend, although there is a negative correlation between the root mean square Grüneisen parameter and the thermal conductivity within each family of compounds (see the main text).

III. DETAILS ABOUT THE METHOD

We give a few details about the method we used to compute the finite-temperature phonon spectra. In the harmonic approximation, the probability of finding the system in a configuration in which each ion \(i\) is displaced in direction \(\alpha\) by \(u_{i\alpha}\) is \(\rho_h \left( \{u_{i\alpha}\} \right) \propto \exp \left( -\frac{1}{2} u^T \Sigma^{-1} u \right)\), with \(\Sigma (i\alpha, j\beta)\) the quantum covariance for atoms \(i, j\) and directions \(\alpha, \beta\). Due to computational limitations, we have used a 3x3x3 supercell, such that the \(\Gamma\) point of this supercell does not include the zone corners of the cubic Brillouin zone. This can be a problem when we want to renormalize soft modes appearing at those corners, since they are not sampled. For this reason, we sum over a 19x19x19 q-point grid when we compute the thermal displacement matrix as:

\[
\Sigma (i\alpha, j\beta) = \frac{\hbar}{2\sqrt{M_i M_j}} \sum_m \omega_m^{-1} (1 + 2n_B (\omega_m)) \epsilon_{m\alpha} \epsilon^*_{m\beta} (1)
\]

where \(M\) is the atomic mass, \(\omega_m\) the phonon frequency of mode \(m\) (comprising both wavevector and branch degrees of freedom), \(\epsilon_m\) the corresponding wavefunction and \(n_B\) the Bose-Einstein distribution. We also estimate the thermal expansion by calculating the mean stress tensor from density functional theory

\[
<P^{DFT}> = \frac{1}{N} \sum_{n<N} P^{DFT} \left( \{u^n_{i\alpha}\} \right) (2)
\]

and updating the lattice parameter such that it becomes negligible.

Finally, the computation of the thermal displacement matrix from equation 1 can be a problem if there are modes with imaginary frequencies. When it is the case, we renormalize these particular frequencies to 0.5 THz. After a few cycles, if the compound is stable in the cubic perovskite structure, the converged phonon spectrum will no longer display imaginary frequencies and the consistency of the approach is thus guaranteed. On the other hand, for unstable compounds the computed spectrum will still present imaginary frequencies and instability is the only conclusion.
We show below all phonon spectra calculated via the following approaches: finite displacements (entitled “0K”), our model combining principal component analysis and regression of the force constants from 0K to 1000 K (entitled “Model 1000 K”), and our finite-temperature method at 300 K and 1000 K when the compound is found mechanically stable (entitled “300 K” and “1000 K”, respectively).

Figure 3: Phonon spectra of AgBaF$_3$

Figure 4: Phonon spectra of AgBeF$_3$
Figure 5: Phonon spectra of AgCaF$_3$

Figure 6: Phonon spectra of AgCdF$_3$

Figure 7: Phonon spectra of AgIO$_3$
Figure 8: Phonon spectra of AgMgF$_3$
Figure 9: Phonon spectra of AgNbO₃

Figure 10: Phonon spectra of AgSrF₃
Figure 11: Phonon spectra of AgTaO$_3$

Figure 12: Phonon spectra of AgVO$_3$
Figure 13: Phonon spectra of AgZnF₃

Figure 14: Phonon spectra of AlBaF₃
Figure 15: Phonon spectra of AlBeF$_3$

Figure 16: Phonon spectra of AlCaF$_3$

Figure 17: Phonon spectra of AlCdF$_3$
Figure 18: Phonon spectra of AlFeF$_3$

Figure 19: Phonon spectra of AlGeF$_3$
Figure 20: Phonon spectra of AlHgF$_3$

Figure 21: Phonon spectra of AlMgF$_3$
Figure 22: Phonon spectra of AlOsF₃

Figure 23: Phonon spectra of AlPbF₃

Figure 24: Phonon spectra of AlRuF₃
Figure 25: Phonon spectra of AlSiF$_3$

Figure 26: Phonon spectra of AlSnF$_3$

Figure 27: Phonon spectra of AlSrF$_3$
Figure 28: Phonon spectra of AlTaO$_3$

Figure 29: Phonon spectra of AlZnF$_3$
Figure 30: Phonon spectra of AsAlO$_3$

Figure 31: Phonon spectra of AsBO$_3$

Figure 32: Phonon spectra of AsCoO$_3$
Figure 33: Phonon spectra of AsGaO$_3$

Figure 34: Phonon spectra of AuBaF$_3$

Figure 35: Phonon spectra of AuBeF$_3$
Figure 36: Phonon spectra of AuCF\textsubscript{3}

Figure 37: Phonon spectra of AuCaF\textsubscript{3}

Figure 38: Phonon spectra of AuCdF\textsubscript{3}
Figure 39: Phonon spectra of AuMgF$_3$
Figure 40: Phonon spectra of AuNbO$_3$

Figure 41: Phonon spectra of AuSrF$_3$
Figure 42: Phonon spectra of AuTaO$_3$

Figure 43: Phonon spectra of AuVO$_3$
Figure 44: Phonon spectra of AuZnF$_3$

Figure 45: Phonon spectra of BBeF$_3$
Figure 46: Phonon spectra of BCF$_3$

Figure 47: Phonon spectra of BCaF$_3$

Figure 48: Phonon spectra of BCdF$_3$
Figure 49: Phonon spectra of BFeF₃

Figure 50: Phonon spectra of BHgF₃

Figure 51: Phonon spectra of BIO₃
Figure 52: Phonon spectra of BMgF$_3$

Figure 53: Phonon spectra of BNbO$_3$

Figure 54: Phonon spectra of BSrF$_3$
Figure 55: Phonon spectra of BTaO$_3$

Figure 56: Phonon spectra of BZnF$_3$

Figure 57: Phonon spectra of BaAgF$_3$
Figure 58: Phonon spectra of BaAlF$_3$

Figure 59: Phonon spectra of BaCsF$_3$
Figure 60: Phonon spectra of BaCuF$_3$

Figure 61: Phonon spectra of BaGaF$_3$
Figure 62: Phonon spectra of BaHfO$_3$

Figure 63: Phonon spectra of BaInF$_3$
Figure 64: Phonon spectra of BaKF$_3$

Figure 65: Phonon spectra of BaLiF$_3$
Figure 66: Phonon spectra of BaNaF$_3$

Figure 67: Phonon spectra of BaRbF$_3$

Figure 68: Phonon spectra of BaSeO$_3$
Figure 69: Phonon spectra of BaSiO$_3$

Figure 70: Phonon spectra of BaTeO$_3$
Figure 71: Phonon spectra of BaTiO$_3$

Figure 72: Phonon spectra of BaTlF$_3$
Figure 73: Phonon spectra of BaZrO$_3$
Figure 74: Phonon spectra of BeAlF$_3$

Figure 75: Phonon spectra of BeBiF$_3$
Figure 76: Phonon spectra of BeInF$_3$

Figure 77: Phonon spectra of BeLiF$_3$

Figure 78: Phonon spectra of BeNaF$_3$
Figure 79: Phonon spectra of BeSbF$_3$

Figure 80: Phonon spectra of BeScF$_3$
Figure 81: Phonon spectra of BeSiO$_3$

Figure 82: Phonon spectra of BeYF$_3$
Figure 83: Phonon spectra of BiAlO$_3$

Figure 84: Phonon spectra of BiCoO$_3$

Figure 85: Phonon spectra of BiGaO$_3$
Figure 86: Phonon spectra of BiInO$_3$

Figure 87: Phonon spectra of BiNO$_3$

Figure 88: Phonon spectra of BiScO$_3$
Figure 89: Phonon spectra of BiYO$_3$

Figure 90: Phonon spectra of BrHfF$_3$

Figure 91: Phonon spectra of BrZrF$_3$
Figure 92: Phonon spectra of CLiF$_3$

Figure 93: Phonon spectra of CNaF$_3$

Figure 94: Phonon spectra of CaAgF$_3$
Figure 95: Phonon spectra of CaBF$_3$

Figure 96: Phonon spectra of CaCsF$_3$

Figure 97: Phonon spectra of CaGeO$_3$
Figure 98: Phonon spectra of CaHfO$_3$

Figure 99: Phonon spectra of CaK$_3$F

Figure 100: Phonon spectra of CaLiF$_3$
Figure 101: Phonon spectra of CaNaF$_3$

Figure 102: Phonon spectra of CaRbF$_3$
Figure 103: Phonon spectra of CaSeO₃
Figure 104: Phonon spectra of CaSiO$_3$ 

Figure 105: Phonon spectra of CaSnO$_3$
Figure 106: Phonon spectra of CaTeO$_3$

Figure 107: Phonon spectra of CaTiO$_3$

Figure 108: Phonon spectra of CaZrO$_3$
Figure 109: Phonon spectra of CdAlF$_3$

Figure 110: Phonon spectra of CdBiF$_3$
Figure 111: Phonon spectra of CdGeO$_3$

Figure 112: Phonon spectra of CdLiF$_3$

Figure 113: Phonon spectra of CdNaF$_3$
Figure 114: Phonon spectra of CdSbF$_3$
Figure 115: Phonon spectra of CdScF$_3$

Figure 116: Phonon spectra of CdSiO$_3$
Figure 117: Phonon spectra of CdYF$_3$

Figure 118: Phonon spectra of ClHfF$_3$
Figure 119: Phonon spectra of CsBaF$_3$
Figure 120: Phonon spectra of CsCaF$_3$
Figure 121: Phonon spectra of CsCdF$_3$
Figure 122: Phonon spectra of CsHgF$_3$
Figure 123: Phonon spectra of CsSrF$_3$

Figure 124: Phonon spectra of CsVO$_3$
Figure 125: Phonon spectra of CsZnF$_3$

Figure 126: Phonon spectra of CuBaF$_3$
Figure 127: Phonon spectra of CuBeF$_3$

Figure 128: Phonon spectra of CuCF$_3$
Figure 129: Phonon spectra of CuCaF$_3$

Figure 130: Phonon spectra of CuCdF$_3$

Figure 131: Phonon spectra of CuIO$_3$
Figure 132: Phonon spectra of CuMgF$_3$

Figure 133: Phonon spectra of CuNbO$_3$

Figure 134: Phonon spectra of CuSrF$_3$
Figure 135: Phonon spectra of CuTaO$_3$

Figure 136: Phonon spectra of CuZnF$_3$

Figure 137: Phonon spectra of GaBaF$_3$
Figure 138: Phonon spectra of GaBeF$_3$

Figure 139: Phonon spectra of GaCF$_3$

Figure 140: Phonon spectra of GaCaF$_3$
Figure 141: Phonon spectra of GaCdF₃

Figure 142: Phonon spectra of GaGeF₃

Figure 143: Phonon spectra of GaHgF₃
Figure 144: Phonon spectra of GaIO$_3$

Figure 145: Phonon spectra of GaMgF$_3$
Figure 146: Phonon spectra of GaNbO$_3$

Figure 147: Phonon spectra of GaOsF$_3$

Figure 148: Phonon spectra of GaPbF$_3$
Figure 149: Phonon spectra of GaRuF$_3$

Figure 150: Phonon spectra of GaSiF$_3$
Figure 151: Phonon spectra of GaSnF$_3$

Figure 152: Phonon spectra of GaSrF$_3$
Figure 153: Phonon spectra of GaTaO$_3$
Figure 154: Phonon spectra of GaZnF$_3$

Figure 155: Phonon spectra of GeHfO$_3$
Figure 156: Phonon spectra of GeKF₃

Figure 157: Phonon spectra of GeLiF₃

Figure 158: Phonon spectra of GeNaF₃
Figure 159: Phonon spectra of GeRbF$_3$

Figure 160: Phonon spectra of GeSO$_3$

Figure 161: Phonon spectra of GeSeO$_3$
Figure 162: Phonon spectra of GeSiO$_3$

Figure 163: Phonon spectra of GeSnO$_3$

Figure 164: Phonon spectra of GeTiO$_3$
Figure 165: Phonon spectra of GeZrO$_3$

Figure 166: Phonon spectra of HfBeO$_3$

Figure 167: Phonon spectra of HfCaO$_3$
Figure 168: Phonon spectra of HfMgO$_3$

Figure 169: Phonon spectra of HgAlF$_3$

Figure 170: Phonon spectra of HgAsF$_3$
Figure 171: Phonon spectra of HgBiF$_3$
Figure 172: Phonon spectra of HgInF$_3$

Figure 173: Phonon spectra of HgLiF$_3$
Figure 174: Phonon spectra of HgSbF$_3$

Figure 175: Phonon spectra of HgScF$_3$
Figure 176: Phonon spectra of HgYF$_3$

Figure 177: Phonon spectra of IHfF$_3$
Figure 178: Phonon spectra of InBaF$_3$

Figure 179: Phonon spectra of InBeF$_3$

Figure 180: Phonon spectra of InCaF$_3$
Figure 181: Phonon spectra of InCdF₃

Figure 182: Phonon spectra of InGeF₃
Figure 183: Phonon spectra of InHgF₃

Figure 184: Phonon spectra of InMgF₃
Figure 185: Phonon spectra of InOsF$_3$

Figure 186: Phonon spectra of InPbF$_3$
Figure 187: Phonon spectra of InSiF$_3$

Figure 188: Phonon spectra of InSnF$_3$

Figure 189: Phonon spectra of InSrF$_3$
Figure 190: Phonon spectra of InZnF$_3$

Figure 191: Phonon spectra of KBaF$_3$
Figure 192: Phonon spectra of KBeF$_3$

Figure 193: Phonon spectra of KBrO$_3$

Figure 194: Phonon spectra of KCF$_3$
Figure 195: Phonon spectra of KCaF$_3$
Figure 196: Phonon spectra of KCdF$_3$

Figure 197: Phonon spectra of KClO$_3$
Figure 198: Phonon spectra of KFeF₃

Figure 199: Phonon spectra of KGeF₃
Figure 200: Phonon spectra of KHgF$_3$
Figure 201: Phonon spectra of KMgF$_3$
Figure 202: Phonon spectra of KNbO$_3$
Figure 203: Phonon spectra of KPbF$_3$

Figure 204: Phonon spectra of KSiF$_3$
Figure 205: Phonon spectra of KSnF₃

Figure 206: Phonon spectra of KSrF₃
Figure 207: Phonon spectra of KZnF$_3$

Figure 208: Phonon spectra of LiBaF$_3$
Figure 209: Phonon spectra of LiBeF$_3$

Figure 210: Phonon spectra of LiBrO$_3$

Figure 211: Phonon spectra of LiCF$_3$
Figure 212: Phonon spectra of LiCaF$_3$

Figure 213: Phonon spectra of LiCdF$_3$

Figure 214: Phonon spectra of LiGeF$_3$
Figure 215: Phonon spectra of LiHgF$_3$

Figure 216: Phonon spectra of LiIO$_3$

Figure 217: Phonon spectra of LiMgF$_3$
Figure 218: Phonon spectra of LiNbO$_3$

Figure 219: Phonon spectra of LiPbF$_3$

Figure 220: Phonon spectra of LiRuF$_3$
Figure 221: Phonon spectra of LiSiF$_3$

Figure 222: Phonon spectra of LiSnF$_3$

Figure 223: Phonon spectra of LiSrF$_3$
Figure 224: Phonon spectra of LiZnF$_3$

Figure 225: Phonon spectra of MgBiF$_3$

Figure 226: Phonon spectra of MgGeO$_3$
Figure 227: Phonon spectra of MgHfO$_3$

Figure 228: Phonon spectra of MgKF$_3$

Figure 229: Phonon spectra of MgLiF$_3$
Figure 230: Phonon spectra of MgNaF$_3$

Figure 231: Phonon spectra of MgYF$_3$

Figure 232: Phonon spectra of NaBaF$_3$
Figure 233: Phonon spectra of NaBeF$_3$

Figure 234: Phonon spectra of NaBrO$_3$
Figure 235: Phonon spectra of NaCF$_3$

Figure 236: Phonon spectra of NaCaF$_3$

Figure 237: Phonon spectra of NaCdF$_3$
Figure 238: Phonon spectra of NaClO$_3$

Figure 239: Phonon spectra of NaGeF$_3$

Figure 240: Phonon spectra of NaHgF$_3$
Figure 241: Phonon spectra of NaIO$_3$

Figure 242: Phonon spectra of NaMgF$_3$
Figure 243: Phonon spectra of NaNbO$_3$

Figure 244: Phonon spectra of NaPbF$_3$
Figure 245: Phonon spectra of NaSiF$_3$

Figure 246: Phonon spectra of NaSnF$_3$

Figure 247: Phonon spectra of NaSrF$_3$
Figure 248: Phonon spectra of NaTaO$_3$

Figure 249: Phonon spectra of NaVO$_3$
Figure 250: Phonon spectra of NaZnF$_3$

Figure 251: Phonon spectra of PBO$_3$

Figure 252: Phonon spectra of PCoO$_3$
Figure 253: Phonon spectra of PbAgF$_3$

Figure 254: Phonon spectra of PbHfO$_3$
Figure 255: Phonon spectra of PbKF₃

Figure 256: Phonon spectra of PbLiF₃

Figure 257: Phonon spectra of PbNaF₃
Figure 258: Phonon spectra of PbRbF$_3$

Figure 259: Phonon spectra of PbSO$_3$

Figure 260: Phonon spectra of PbSeO$_3$
Figure 261: Phonon spectra of PbSiO$_3$

Figure 262: Phonon spectra of PbSnO$_3$
Figure 263: Phonon spectra of PbTiO$_3$

Figure 264: Phonon spectra of PbZrO$_3$
Figure 265: Phonon spectra of PdAsF$_3$

Figure 266: Phonon spectra of PdBiF$_3$

Figure 267: Phonon spectra of PdPF$_3$
Figure 268: Phonon spectra of PdSbF$_3$

Figure 269: Phonon spectra of PdScF$_3$
Figure 270: Phonon spectra of PdYF$_3$

Figure 271: Phonon spectra of RbBaF$_3$
Figure 272: Phonon spectra of RbBeF₃

Figure 273: Phonon spectra of RbBrO₃

Figure 274: Phonon spectra of RbCF₃
Figure 275: Phonon spectra of RbCaF$_3$
Figure 276: Phonon spectra of RbCdF$_3$
Figure 277: Phonon spectra of RbFeF₃

Figure 278: Phonon spectra of RbGeF₃
Figure 279: Phonon spectra of RbHgF$_3$
Figure 280: Phonon spectra of RbMgF$_3$

Figure 281: Phonon spectra of RbNbO$_3$
Figure 282: Phonon spectra of RbPbF$_3$

Figure 283: Phonon spectra of RbSiF$_3$
Figure 284: Phonon spectra of RbSnF$_3$
Figure 285: Phonon spectra of RbSrF$_3$
Figure 286: Phonon spectra of RbTaO₃

Figure 287: Phonon spectra of RbVO₃
Figure 288: Phonon spectra of RbZnF$_3$

Figure 289: Phonon spectra of SbAlO$_3$
Figure 290: Phonon spectra of SbBO$_3$

Figure 291: Phonon spectra of SbCoO$_3$

Figure 292: Phonon spectra of SbGaO$_3$
Figure 293: Phonon spectra of SbInO$_3$

Figure 294: Phonon spectra of SbScO$_3$

Figure 295: Phonon spectra of ScAlO$_3$
Figure 296: Phonon spectra of ScBO$_3$

Figure 297: Phonon spectra of ScCoO$_3$

Figure 298: Phonon spectra of ScGaO$_3$
Figure 299: Phonon spectra of ScInO$_3$

Figure 300: Phonon spectra of ScNO$_3$

Figure 301: Phonon spectra of ScRhO$_3$
Figure 302: Phonon spectra of ScYO₃

Figure 303: Phonon spectra of SiGeO₃

Figure 304: Phonon spectra of SiHfO₃
Figure 305: Phonon spectra of SiKF$_3$

Figure 306: Phonon spectra of SiLiF$_3$

Figure 307: Phonon spectra of SiNaF$_3$
Figure 308: Phonon spectra of SiRbF$_3$

Figure 309: Phonon spectra of SiSO$_3$

Figure 310: Phonon spectra of SiSnO$_3$
Figure 311: Phonon spectra of SiTiO$_3$

Figure 312: Phonon spectra of SiZrO$_3$

Figure 313: Phonon spectra of SnHfO$_3$
Figure 314: Phonon spectra of SnKF₃

Figure 315: Phonon spectra of SnLiF₃

Figure 316: Phonon spectra of SnNaF₃
Figure 317: Phonon spectra of SnRbF$_3$

Figure 318: Phonon spectra of SnSO$_3$

Figure 319: Phonon spectra of SnSeO$_3$
Figure 320: Phonon spectra of SnSiO$_3$

Figure 321: Phonon spectra of SnTiO$_3$
Figure 322: Phonon spectra of SnZrO$_3$

Figure 323: Phonon spectra of SrAgF$_3$

Figure 324: Phonon spectra of SrBF$_3$
Figure 325: Phonon spectra of SrCsF$_3$

Figure 326: Phonon spectra of SrHfO$_3$
Figure 327: Phonon spectra of SrKF$_3$ 

Figure 328: Phonon spectra of SrLiF$_3$ 

Figure 329: Phonon spectra of SrNaF$_3$
Figure 330: Phonon spectra of SrRbF$_3$

Figure 331: Phonon spectra of SrSeO$_3$
Figure 332: Phonon spectra of SrSiO$_3$

Figure 333: Phonon spectra of SrSnO$_3$
Figure 334: Phonon spectra of SrTeO$_3$

Figure 335: Phonon spectra of SrTiO$_3$
Figure 336: Phonon spectra of SrZrO$_3$

Figure 337: Phonon spectra of TeBeO$_3$

Figure 338: Phonon spectra of TlBaF$_3$
Figure 339: Phonon spectra of TlBeF$_3$

Figure 340: Phonon spectra of TlCF$_3$
Figure 341: Phonon spectra of TlCaF$_3$
Figure 342: Phonon spectra of TlCdF₃

Figure 343: Phonon spectra of TlGeF₃
Figure 344: Phonon spectra of TlHgF$_3$

Figure 345: Phonon spectra of TlIO$_3$
Figure 346: Phonon spectra of TlMgF$_3$
Figure 347: Phonon spectra of TlNbO$_3$
Figure 348: Phonon spectra of TlOsF$_3$
Figure 349: Phonon spectra of TlPbF$_3$

Figure 350: Phonon spectra of TlSiF$_3$
Figure 351: Phonon spectra of TlSnF$_3$

Figure 352: Phonon spectra of TlSrF$_3$
Figure 353: Phonon spectra of TlTaO$_3$
Figure 354: Phonon spectra of TlZnF$_3$
Figure 355: Phonon spectra of XeBiF₃

Figure 356: Phonon spectra of XePF₃
Figure 357: Phonon spectra of XeScF$_3$

Figure 358: Phonon spectra of YAlO$_3$
Figure 359: Phonon spectra of YBO$_3$

Figure 360: Phonon spectra of YCoO$_3$

Figure 361: Phonon spectra of YGaO$_3$
Figure 362: Phonon spectra of YInO$_3$

Figure 363: Phonon spectra of YIrO$_3$

Figure 364: Phonon spectra of YNO$_3$
Figure 365: Phonon spectra of YRhO$_3$

Figure 366: Phonon spectra of YScO$_3$
Figure 367: Phonon spectra of ZnAlF$_3$
Figure 368: Phonon spectra of ZnBiF$_3$
Figure 369: Phonon spectra of ZnInF$_3$

Figure 370: Phonon spectra of ZnLiF$_3$
Figure 371: Phonon spectra of ZnNaF$_3$

Figure 372: Phonon spectra of ZnSbF$_3$
Figure 373: Phonon spectra of ZnScF$_3$
Figure 374: Phonon spectra of ZnYF$_3$

Figure 375: Phonon spectra of ZrBeO$_3$
Figure 376: Phonon spectra of ZrMgO$_3$
V. MACHINE LEARNING PERFORMANCE

We display on Fig. 377 some statistics about the performance of the model described in Section III of the main text. The left panel shows the variation of the final precision and recall depending on the number of principal components taken into account. For the 10 components considered in our study, both trends show convergence. On the middle panel, we gauge the performance of the model as a function of the size of the training set by skipping the iterative inclusion of newly found compounds in the training set. Considering the marginal cost of training the model, the iterative procedure shows a clear advantage. Those two benchmarks were performed in the framework described in Fig. 3 of the main text, that is to say starting from compounds that are stable at 0 K and progressively including new ones as they are detected to be stabilized by temperature. The right panel shows the mean relative error between the calculated and the predicted force constants, \( \frac{\| \Phi_{SCFCS}^{1000 K} - \Phi_{model}^{1000 K} \|}{\| \Phi_{SCFCS}^{1000 K} \|} \). In this last panel, the values are calculated within 2-fold, 3-fold, 5-fold, 10-fold and n-fold cross-validation, for 2, 4, 6, 8 and 10 principal components. We observe that while the mean error is importantly reduced by including more principal components, a relatively small training set is already sufficient to obtain convergence. This is in contrast to the results for the iterative procedure, that are seen to improve with the size of training set. We explain this by the fact that the original training set of the iterative procedure is biased since it contains only compounds that are stable at 0 K – which is the only option in practice since they are the only ones that are known. Indeed, the mean relative error for 10 principal components and using this original training set is 0.21, higher than within the cross-validation. At the end of the procedure this bias is suppressed, showing again the interest of adding more compounds iteratively.

![Figure 377: Left panel: Precision and recall of the model as a function of the number of principal components. Middle panel: Number of true and false positives as a function of the size of the training set, for 9 principal components. Right panel: Mean relative error between the calculated and the predicted force constants, as a function of the size of the training set and of the number of principal components, using 2-fold, 3-fold, 5-fold, 10-fold and n-fold cross-validation.](image)

Finally, to verify the model’s predictive power, we performed a 10-fold cross-validation. We have arranged the 92 mechanically stable compounds at random and successively tested the ability of the model to predict the stability of each series of 9 compounds when it was trained with the data of all the other materials. We obtained a mean recall of 72%, similar to the final performance of the iterative procedure. The 90 phonon spectra predicted during the cross-validation process are shown below, along with the 0 K and 1000 K spectra calculated \textit{ab initio} and that obtained with the final model (already presented above).
Figure 378: Cross validation of model phonon spectra of AgMgF₃
Figure 379: Cross validation of model phonon spectra of AgNbO$_3$
Figure 380: Cross validation of model phonon spectra of AgTaO₃
Figure 381: Cross validation of model phonon spectra of AlFeF$_3$
Figure 382: Cross validation of model phonon spectra of AlMgF$_3$
Figure 383: Cross validation of model phonon spectra of AlZnF$_3$
Figure 384: Cross validation of model phonon spectra of AuMgF$_3$
Figure 385: Cross validation of model phonon spectra of AuNbO$_3$
Figure 386: Cross validation of model phonon spectra of AuZnF$_3$
Figure 387: Cross validation of model phonon spectra of BaCuF₃
Figure 388: Cross validation of model phonon spectra of BaHfO$_3$
Figure 389: Cross validation of model phonon spectra of BaLiF$_3$
Figure 390: Cross validation of model phonon spectra of BaSiO$_3$
Figure 391: Cross validation of model phonon spectra of BaTiO$_3$
Figure 392: Cross validation of model phonon spectra of BaZrO$_3$
Figure 393: Cross validation of model phonon spectra of BeAlF$_3$. 
Figure 394: Cross validation of model phonon spectra of BeScF$_3$
Figure 395: Cross validation of model phonon spectra of BeYF\textsubscript{3}
Figure 396: Cross validation of model phonon spectra of CaSeO$_3$
Figure 397: Cross validation of model phonon spectra of CaSiO$_3$
Figure 398: Cross validation of model phonon spectra of CdBiF$_3$
Figure 399: Cross validation of model phonon spectra of CdSbF$_3$
Figure 400: Cross validation of model phonon spectra of CdScF₃
Figure 401: Cross validation of model phonon spectra of CdYF$_3$
Figure 402: Cross validation of model phonon spectra of CsBaF$_3$
Figure 403: Cross validation of model phonon spectra of CsCaF$_3$
Figure 404: Cross validation of model phonon spectra of CsCdF₃
Figure 405: Cross validation of model phonon spectra of CsHgF$_3$
Figure 406: Cross validation of model phonon spectra of CsSrF$_3$
Figure 407: Cross validation of model phonon spectra of CsZnF$_3$
Figure 408: Cross validation of model phonon spectra of CuCF$_3$
Figure 409: Cross validation of model phonon spectra of GaMgF$_3$
Figure 410: Cross validation of model phonon spectra of GaRuF₃
Figure 411: Cross validation of model phonon spectra of GaZnF₃
Figure 412: Cross validation of model phonon spectra of \(\text{HgBiF}_3\)
Figure 413: Cross validation of model phonon spectra of HgInF$_3$. 
Figure 414: Cross validation of model phonon spectra of HgScF₃
Figure 415: Cross validation of model phonon spectra of HgYF₃
Figure 416: Cross validation of model phonon spectra of InCdF$_3$
Figure 417: Cross validation of model phonon spectra of InMgF$_3$
Figure 418: Cross validation of model phonon spectra of InOsF$_3$
Figure 419: Cross validation of model phonon spectra of InZnF$_3$
Figure 420: Cross validation of model phonon spectra of KCaF$_3$
Figure 421: Cross validation of model phonon spectra of KCdF$_3$
Figure 422: Cross validation of model phonon spectra of KFeF$_3$
Figure 423: Cross validation of model phonon spectra of KHgF$_3$
Figure 424: Cross validation of model phonon spectra of KMgF$_3$
Figure 425: Cross validation of model phonon spectra of KNbO₃
Figure 426: Cross validation of model phonon spectra of KPbF$_3$
Figure 427: Cross validation of model phonon spectra of KSnF$_3$
Figure 428: Cross validation of model phonon spectra of KZnF₃
Figure 429: Cross validation of model phonon spectra of NaBeF$_3$
Figure 430: Cross validation of model phonon spectra of NaNbO₃
Figure 431: Cross validation of model phonon spectra of NaTaO₃
Figure 432: Cross validation of model phonon spectra of PbHfO$_3$
Figure 433: Cross validation of model phonon spectra of PbSiO$_3$
Figure 434: Cross validation of model phonon spectra of PbTiO₃
Figure 435: Cross validation of model phonon spectra of PdScF$_3$
Figure 436: Cross validation of model phonon spectra of PdYF$_3$
Figure 437: Cross validation of model phonon spectra of RbCaF$_3$
Figure 438: Cross validation of model phonon spectra of RbCdF$_3$
Figure 439: Cross validation of model phonon spectra of RbFeF$_3$
Figure 440: Cross validation of model phonon spectra of RbHgF$_3$
Figure 441: Cross validation of model phonon spectra of RbMgF$_3$
Figure 442: Cross validation of model phonon spectra of RbPbF$_3$
Figure 443: Cross validation of model phonon spectra of RbSnF₃
Figure 444: Cross validation of model phonon spectra of RbSrF$_3$
Figure 445: Cross validation of model phonon spectra of RbTaO₃
Figure 446: Cross validation of model phonon spectra of RbZnF$_3$
Figure 447: Cross validation of model phonon spectra of SnSiO$_3$
Figure 448: Cross validation of model phonon spectra of SrHfO$_3$
Figure 449: Cross validation of model phonon spectra of SrSiO$_3$
Figure 450: Cross validation of model phonon spectra of SrTiO$_3$
Figure 451: Cross validation of model phonon spectra of TICaF$_3$
Figure 452: Cross validation of model phonon spectra of TlCdF$_3$
Figure 453: Cross validation of model phonon spectra of TlHgF$_3$
Figure 454: Cross validation of model phonon spectra of TlMgF$_3$
Figure 455: Cross validation of model phonon spectra of TlNbO$_3$
Figure 456: Cross validation of model phonon spectra of TlOsF$_3$
Figure 457: Cross validation of model phonon spectra of TlPbF$_3$
Figure 458: Cross validation of model phonon spectra of TlSnF₃
Figure 459: Cross validation of model phonon spectra of TlTaO$_3$
Figure 460: Cross validation of model phonon spectra of TlZnF$_3$
Figure 461: Cross validation of model phonon spectra of XeBiF$_3$
Figure 462: Cross validation of model phonon spectra of XeScF$_3$
Figure 463: Cross validation of model phonon spectra of ZnAlF$_3$
Figure 464: Cross validation of model phonon spectra of ZnBiF$_3$
Figure 465: Cross validation of model phonon spectra of ZnInF$_3$
Figure 466: Cross validation of model phonon spectra of ZnScF$_3$
Figure 467: Cross validation of model phonon spectra of ZnYF$_3$