

Supplementary Information for
“Database and deep-learning scalability of anharmonic phonon properties by
automated brute-force first-principles calculations”

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I. FORMULATIONS FOR LATTICE THERMAL CONDUCTIVITY

Lattice thermal conductivity was calculated by solving Peierls-Boltzmann transport equation¹ for the particle-like contribution and the Wigner transport formula² for the wave-like contribution, both implemented in the ALAMODE package^{3,4}. Considering the second-order perturbation within the relaxation approximation, the phonon linewidth due to the three-phonon scattering for phonon mode q is derived as

$$\Gamma_q = \frac{\pi}{16N} \sum_{q_1, q_2} |V_3(-q, q_1, q_2)|^2 [(n_1 + n_2 + 1)\delta(\omega_q - \omega_1 - \omega_2) - 2(n_1 - n_2)\delta(\omega_q - \omega_1 + \omega_2)], \quad (S1)$$

where the subscripts ($i = 1, 2$) denote phonon modes contributing to the scattering of the target mode q , n_i is the Bose-Einstein distribution function, ω_i is the phonon frequency, N is the number of q points, and $\pm q = (\pm \mathbf{q}, s)$ with $\mathbf{q}$ and s being the wavevector and branch index, respectively. The three-phonon coupling matrix element V_3 is given by

$$V_3(q, q_1, q_2) = \left(\frac{\hbar}{\omega\omega_1\omega_2}\right)^{\frac{1}{2}} \times \sum_{\mathbf{R}_i l_i p_i} \Psi_{0l_0, \mathbf{R}_1 l_1, \mathbf{R}_2 l_2}^{p_0 p_1 p_2} \times \frac{\mathbf{e}_{l_0}^{p_0}(q) \mathbf{e}_{l_1}^{p_1}(q_1) \mathbf{e}_{l_2}^{p_2}(q_2)}{\sqrt{M_{l_0} M_{l_1} M_{l_2}}} \times \exp[i(\mathbf{q} \cdot \mathbf{R}_0 + \mathbf{q}_1 \cdot \mathbf{R}_1 + \mathbf{q}_2 \cdot \mathbf{R}_2)], \quad (S2)$$

where $\hbar$ is the reduced Planck constant, $\mathbf{R}_i$ is the position of the primitive cell, l_i is the atom index, p_i is the direction of the displacement of atom l_i , M is the atomic mass, Ψ is the cubic force constants, and $\mathbf{e}(q)$ is the eigenvector of the mode q . The phonon lifetime due to three phonon scattering τ_{pp} is given by $\tau_{pp}(q) = 1/(2\Gamma_q)$. The total phonon lifetime of mode q is obtained with Matthiessen's rule: $\tau_q^{-1} = \tau_{q,pp}^{-1} + \tau_{q,iso}^{-1}$, where $\tau_{q,iso}^{-1}$ is the scattering rate due to isotopes⁵. Finally, the Peierls term is calculated as $\kappa_p^{\alpha\beta, scp}(T) = (NV)^{-1} \sum_q c_q(T) v_q^\alpha(T) v_q^\beta(T) \tau_q(T)$. Here, V is the volume of the primitive unit cell, c is the mode specific heat, v is the group velocity, and α and β are the Cartesian directions.

In the automated workflow, the coherence contribution (κ_c), corresponding to the nondiagonal terms of the heat flux operator, was also considered. Its contribution can be obtained as

$$\kappa_c^{\alpha\beta} = \frac{\hbar^2}{k_B T^2 V N} \sum_q \sum_{s_1 \neq s_2} \frac{\omega_1 + \omega_2}{4} V_{12}^\alpha(\mathbf{q}) V_{21}^\beta(\mathbf{q}) \frac{\omega_1 n_1(n_1 + 1) + \omega_2 n_2(n_2 + 1)}{(\omega_1 - \omega_2)^2 + (\Gamma_1 + \Gamma_2)^2} (\Gamma_1 + \Gamma_2), \quad (S3)$$

where k_B is the Boltzmann constant. The subscripts (1 and 2) denote the phonon modes $(\mathbf{q}, s_1)$ and $(\mathbf{q}, s_2)$, respectively. The generalized group velocity operator $V(\mathbf{q})$ is given as

$$V_{12}(\mathbf{q}) = \frac{1}{\omega_1 + \omega_2} \left\langle \mathbf{e}(q_1) \left| \frac{\partial D(\mathbf{q})}{\partial \mathbf{q}} \right| \mathbf{e}(q_2) \right\rangle, \quad (S4)$$

where $D(\mathbf{q})$ is the dynamical matrix.

II. ELEMENTAL OCCURRENCE FREQUENCY

The elemental occurrence frequency in the materials for which anharmonic properties were calculated in *Phonix*, a database for anharmonic phonon interactions, is illustrated in the periodic table shown in Fig. S1. The number shown for each element represents the number of materials that include that element. For example, the most frequently occurring element, oxygen, is found in 2,534 out of the 6,641 materials in the current version of Phonix.

This figure shows that chalcogens (group 16) and alkali metals (group 1) are the two most frequently occurring groups of elements. It also indicates that elements from groups 1–2 and 11–17 are commonly present in the Phonix materials, whereas transition metals occur less frequently—likely due to the absence of magnetic materials in the current version of Phonix.

Overall, Phonix contains a broad range of elements, which is important for improving data quality and enabling its application to diverse fields—not only for thermal properties, but also for various other material properties, including mechanical, electronic, electrical, optical, and magnetic characteristics.

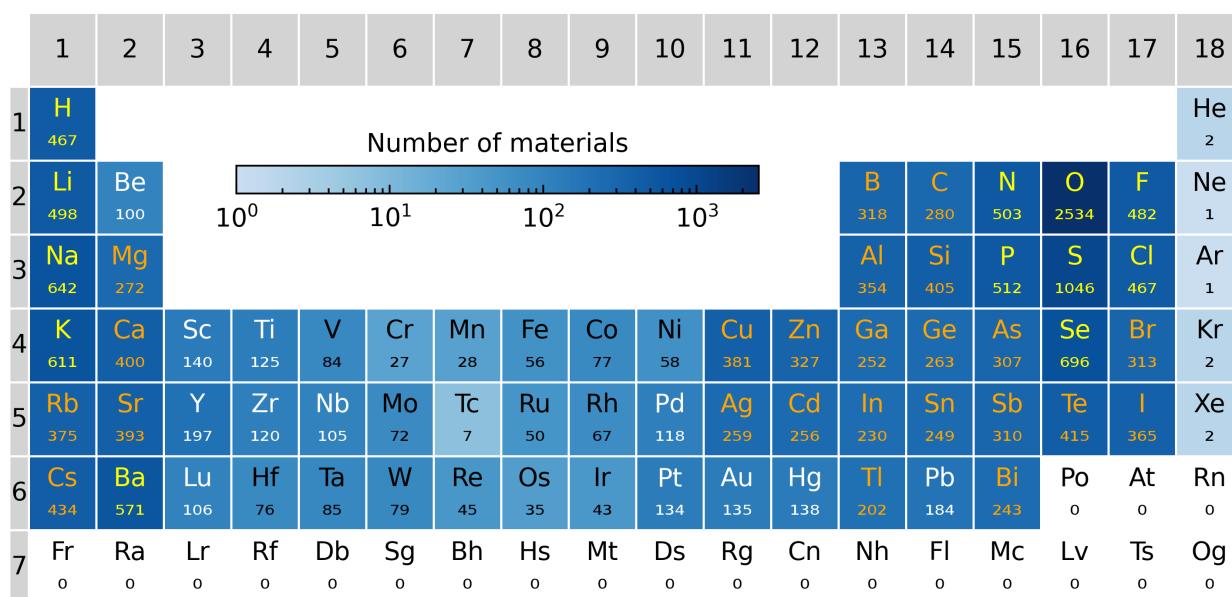


Fig. S1. Elemental occurrence frequency in the database for anharmonic phonon interactions (Phonix). The number in each cell indicates how frequently each element appears in the materials included in the Phonix database, with the magnitude visualized using a logarithmic blue color scale. Element symbols are colored according to their occurrence: yellow for elements appearing in more than 500 materials, orange for more than 200, white for more than 100, and black for all others.

III. LIST OF MATERIALS WITH HIGH AND LOW THERMAL CONDUCTIVITIES

The target materials consist of non-metallic, non-magnetic materials from the Materials Project⁶⁻⁸, as well as those from Phonondb⁹, totaling 21,452 materials. To construct Phonix, we developed an automated calculation software package, auto-kappa, for anharmonic phonon properties. So far, we have calculated the anharmonic phonon properties of approximately 6,500 materials, while harmonic phonon properties have been computed for an even larger set of materials.

Among the calculated high- κ materials, the following materials, including their polymorphs, are novel or have been rarely discussed as high- κ materials: triclinic $\text{Hg}(\text{BiS}_2)_2$ ($\kappa_{p,\{xx,yy,zz\}} = 292, 2.5, \text{ and } 943 \text{ Wm}^{-1}\text{K}^{-1}$), cubic HC (306 $\text{Wm}^{-1}\text{K}^{-1}$), cubic BiB (235 $\text{Wm}^{-1}\text{K}^{-1}$), and trigonal CsHoS_2 ($\kappa_{p,\{zz,xx(yy)\}} = 22 \text{ and } 657 \text{ Wm}^{-1}\text{K}^{-1}$). Only 105 materials (1.6%) has a κ_{lat} exceeding 100 $\text{Wm}^{-1}\text{K}^{-1}$, as shown in Table S1. On the other hand, discovering novel materials with low thermal conductivity appears to be much easier. In the Phonix database, approximately 1,800 materials (28%) have κ_{lat} below 1.0 $\text{Wm}^{-1}\text{K}^{-1}$. Even when limited to binary compounds, 201 materials (3.1%) have a $\kappa_{\text{lat}} \leq 1.0 \text{ Wm}^{-1}\text{K}^{-1}$. Considering that the thermal conductivities of typical thermoelectric materials Bi_2T_3 and PbTe are 1.2¹⁰ and 2.2¹¹⁻¹³ $\text{Wm}^{-1}\text{K}^{-1}$, the constructed database provides an exciting opportunity to search for materials with low- κ for applications such as thermal insulators and thermoelectric materials.

Phonon properties of the fifty-five high- κ materials ($\kappa_{\text{lat}} \geq 200 \text{ Wm}^{-1}\text{K}^{-1}$) and fourteen low- κ materials ($\kappa_{\text{lat}} \leq 0.1 \text{ Wm}^{-1}\text{K}^{-1}$) are shown in Fig. S2 and Fig. S3, respectively.

Table S1. Number of materials exhibiting high and low thermal conductivity in Phonix. The lattice thermal conductivity is evaluated as $\kappa_{\text{lat}} = (\kappa_{xx} + \kappa_{yy} + \kappa_{zz})/3$ for all materials, including anisotropic ones, for simplicity. For this analysis, duplicated material data and data with fitting errors larger than 10% for both harmonic and cubic force constants were omitted.

High thermal conductivity		Low thermal conductivity	
Range of κ_{lat} ($\text{Wm}^{-1}\text{K}^{-1}$)	Number of materials	Range of κ_{lat} ($\text{Wm}^{-1}\text{K}^{-1}$)	Number of materials
>1,000	11 (0.17%)	<0.1	15 (0.23%)
>500	25 (0.38%)	<0.2	200 (3.0%)
>200	67 (1.02%)	<0.5	966 (15%)
>100	105 (1.6%)	<1.0	1,815 (28%) (201 for binary)

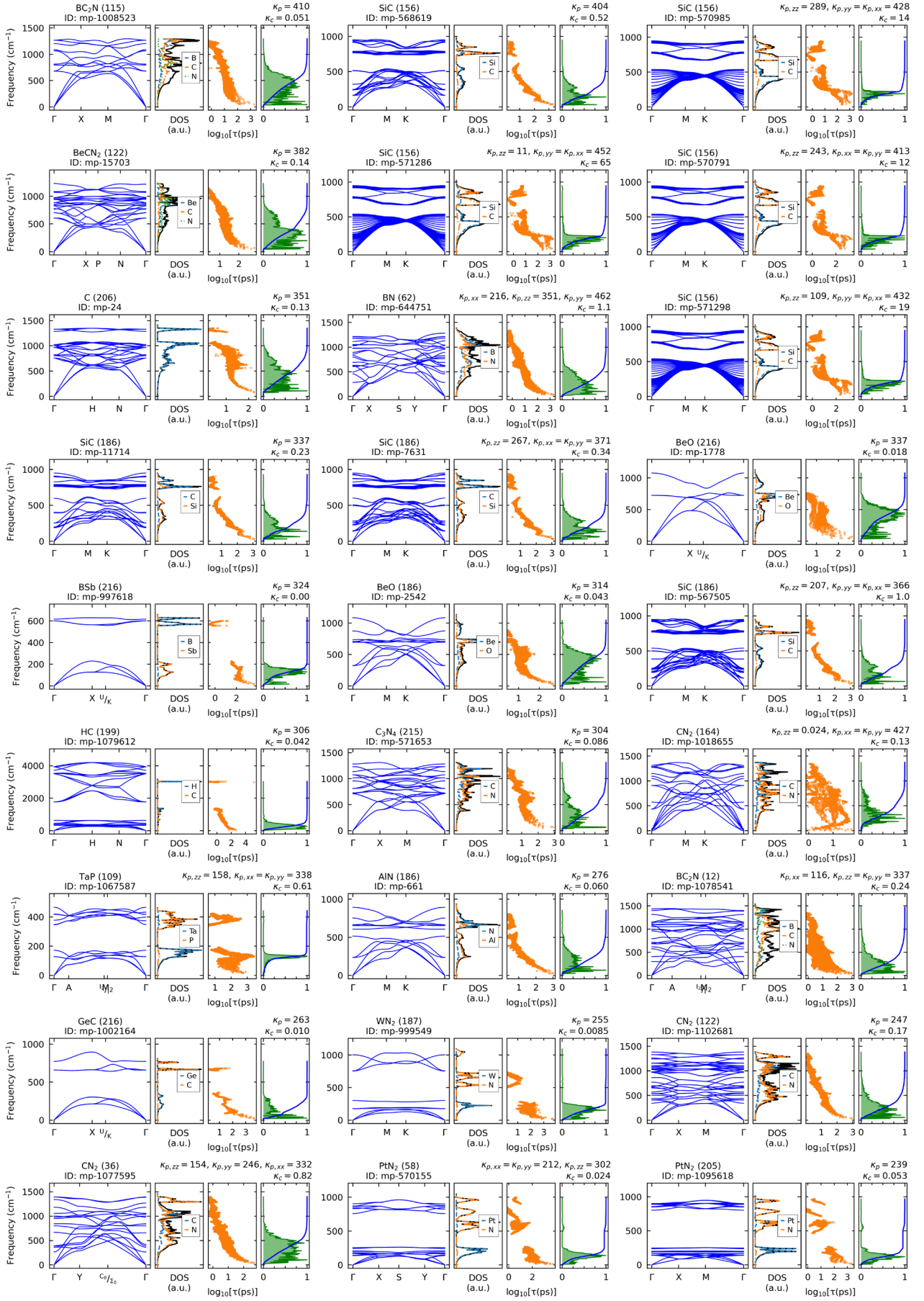


Fig. S2 (2/3). List of phonon properties for materials with high thermal conductivity.

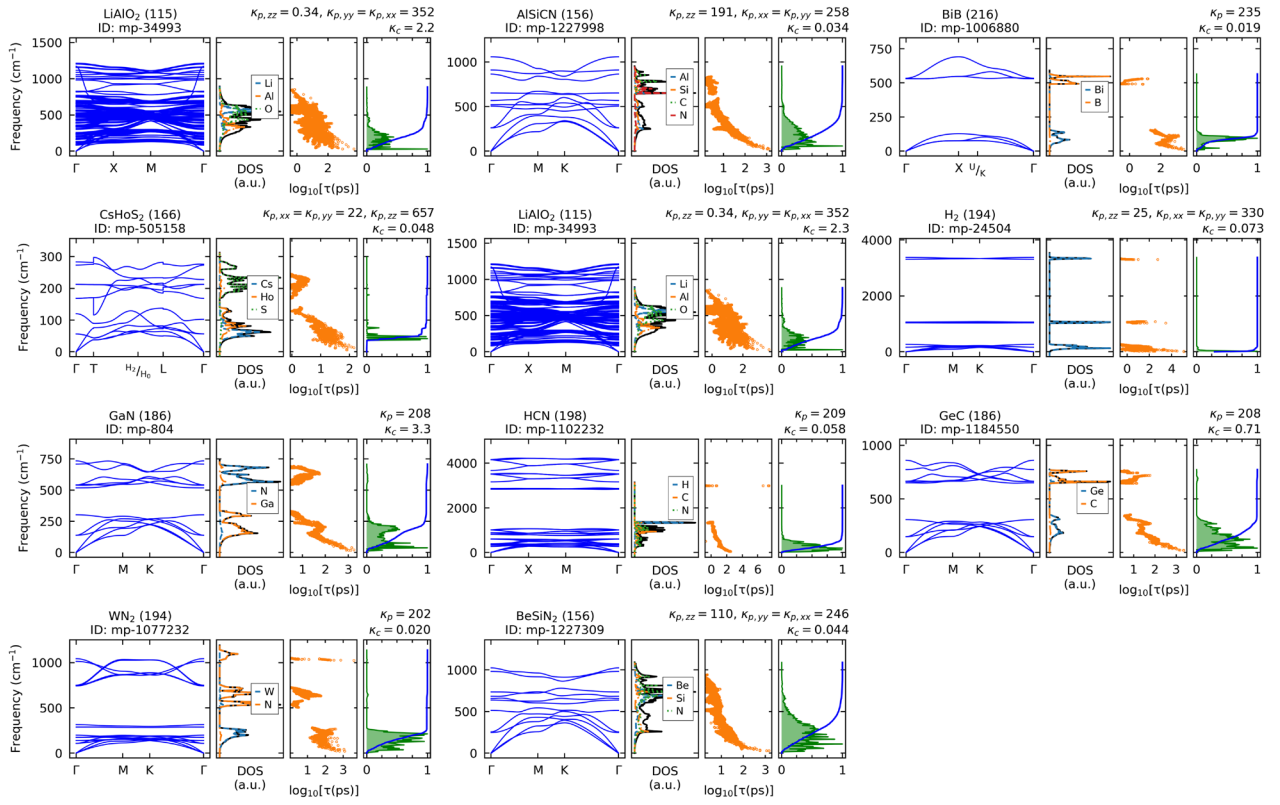


Fig. S2 (3/3). List of phonon properties for materials with high thermal conductivity ($> 200 \text{ Wm}^{-1}\text{K}^{-1}$), ordered by magnitude. Each panel includes phonon dispersion, density of states (DOS), phonon lifetime (in logarithmic scale), and spectral (green) and cumulative (blue) thermal conductivity for Peierls component (κ_p), which are normalized by their respective maximum and total values. The chemical formula, space group number (in parentheses), and Materials Project ID are shown in the top-left corner, while the magnitudes of the Peierls (κ_p) and coherent (κ_c) components are displayed in the top-right corner of each panel.

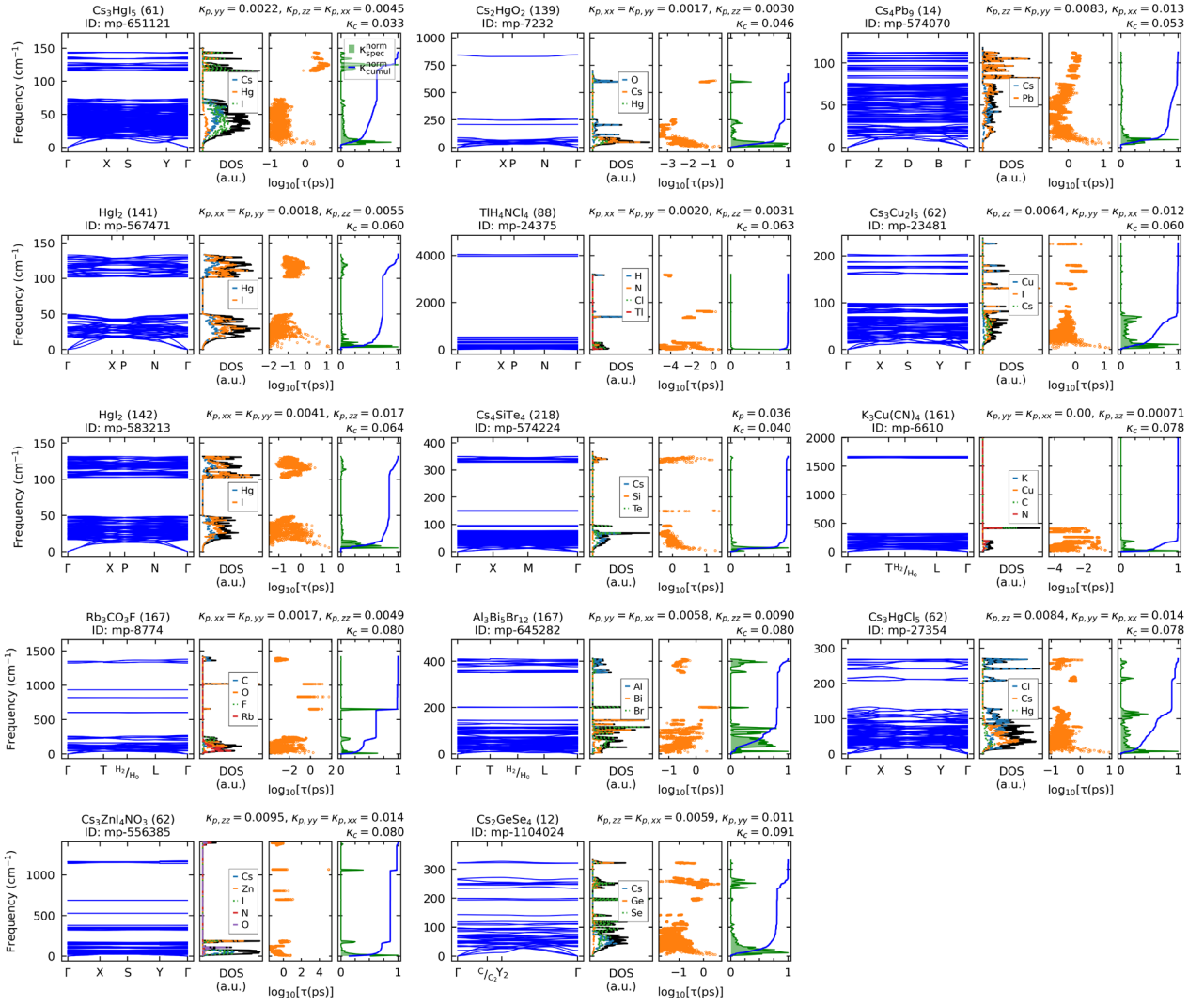


Fig. S3. List of phonon properties for materials with low thermal conductivity ($< 0.1 \text{ W m}^{-1} \text{ K}^{-1}$), arranged in ascending order. See the caption of Fig. S2 for a detailed description of the figure.

IV. COMPARISON BETWEEN PARTICLE AND COHERENT CONTRIBUTIONS TO HEAT TRANSPORT

Lattice thermal conductivity is governed by both particle-like phonon gas transport and wave-like tunneling mechanisms^{2,14}. In the early stages of first-principles phonon analysis, calculating the coherent component arising from wave-like tunneling was challenging. However, since Simoncelli *et al.* proposed a unified theory (also known as the Wigner heat transport formula) to evaluate both the Peierls component (κ_p) from particle-like phonons and the coherent component (κ_c)², this approach has been widely adopted for analysis¹⁵.

Among the materials calculated in Phonix, we identified that materials with a large coherent component (κ_c) are polymorphs of SiC and related structures with the space group $P3m1$ (156). While the relative contribution of κ_c to total heat transport remains small due to the relatively large κ_p , the absolute magnitude of κ_c exceeds $50 \text{ Wm}^{-1}\text{K}^{-1}$. This significant coherent contribution arises from densely packed phonon branches, which result from the large number of atoms in the primitive cell. Their thermal conductivities (κ_p and κ_c) and phonon dispersions are shown in Fig. S4.

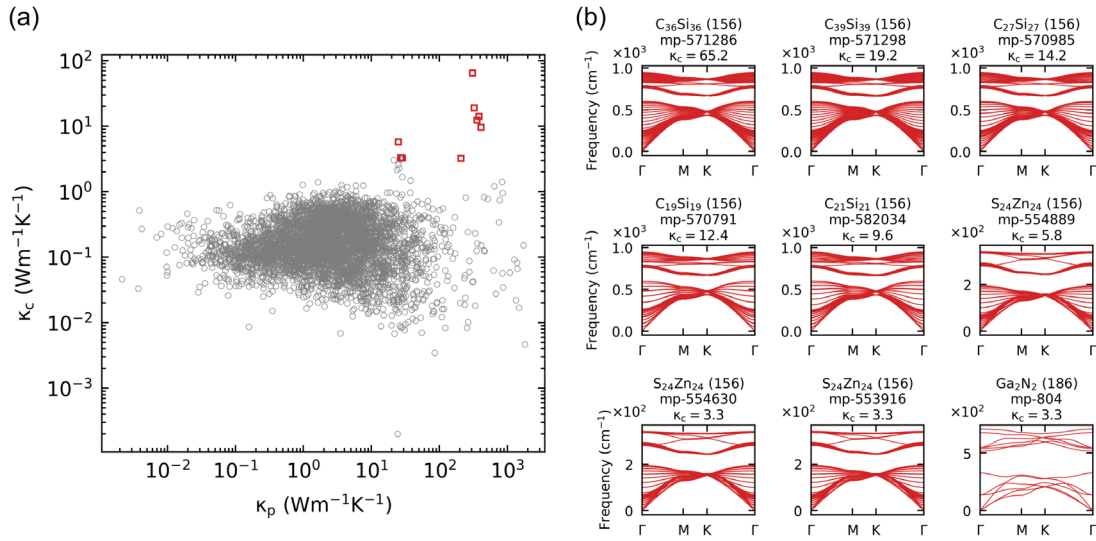
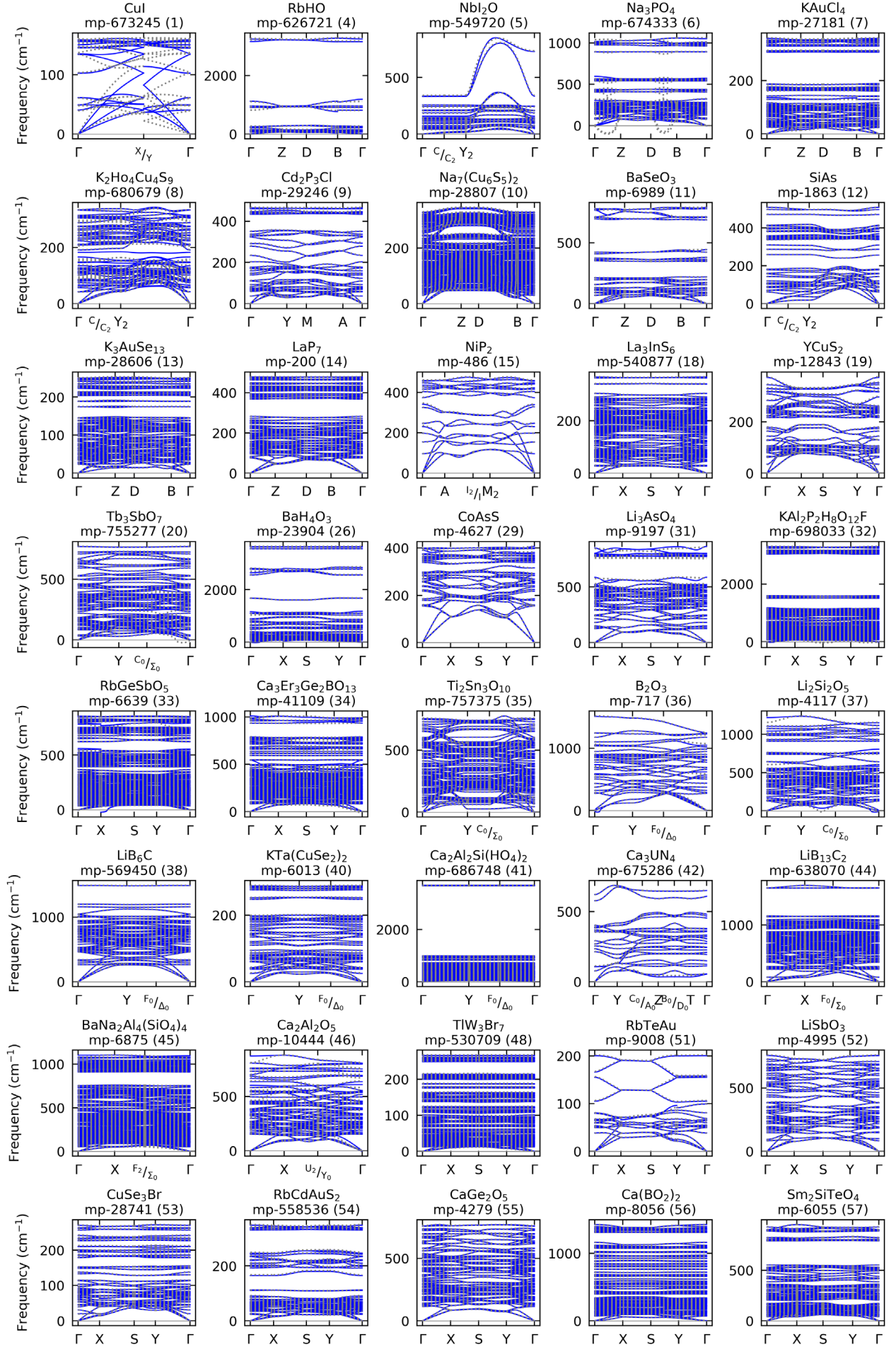
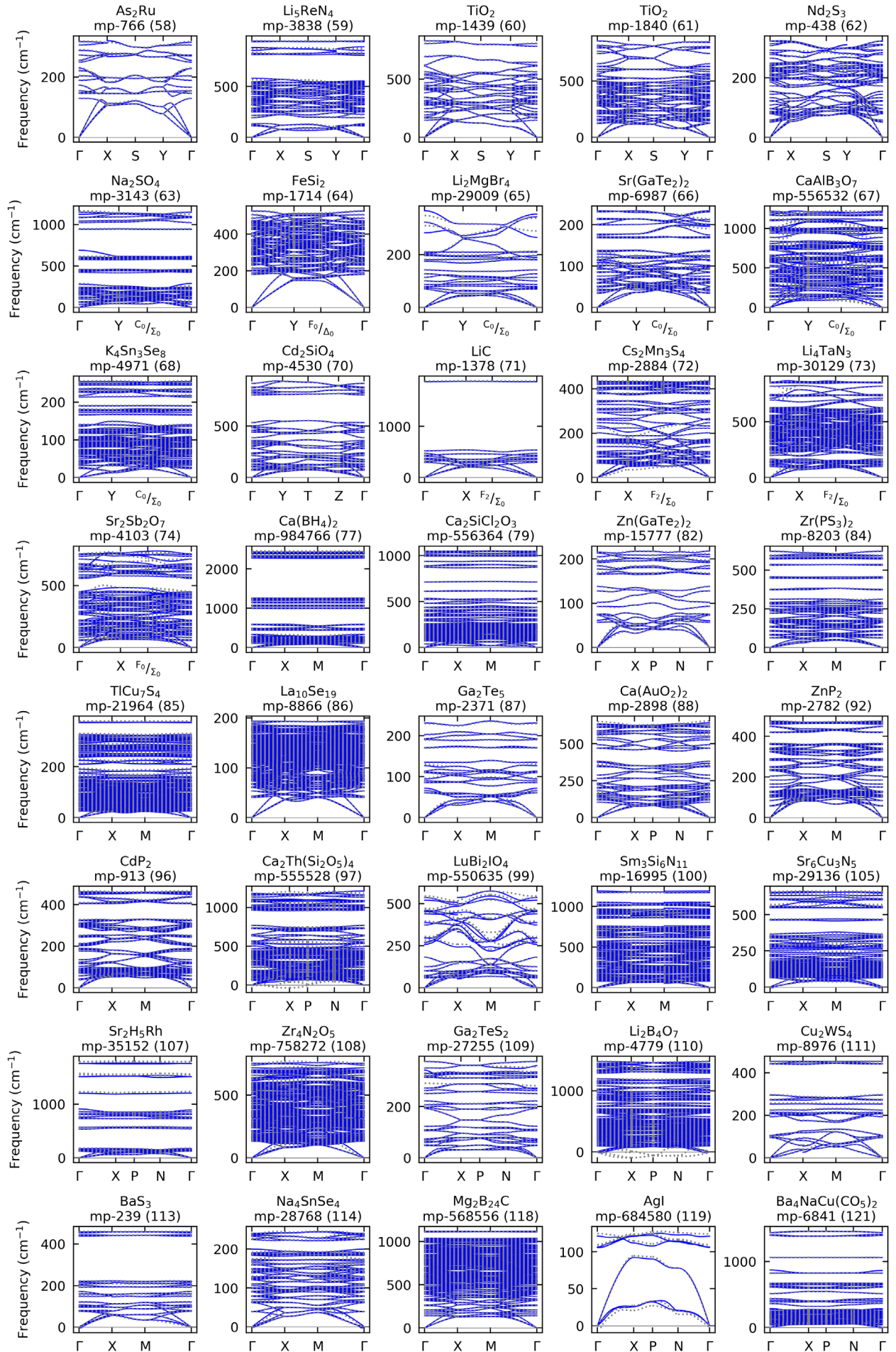


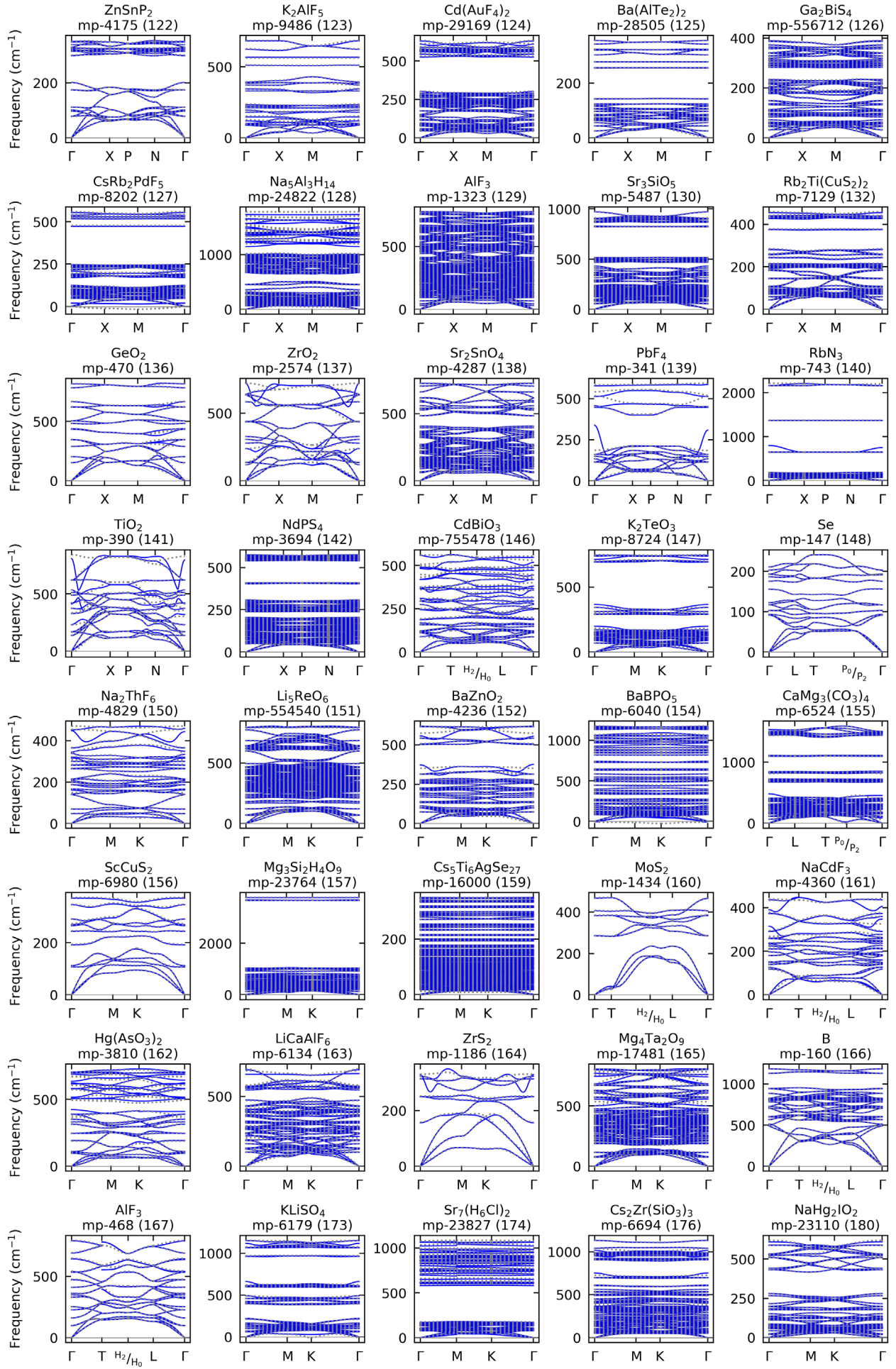
Fig. S4. Materials exhibiting large coherent thermal conductivity. (a) Distribution of Peierls (κ_p) and coherent (κ_c) thermal conductivity. Red markers indicate the top nine materials with the highest κ_c . (b) Phonon dispersion for these nine materials.

V. COMPARISON WITH PHONONDB

Phonon dispersions obtained in this study using automated calculations were compared with those in Phonondb⁹. Comparisons were possible for 155 out of 230 space groups. The Phonondb results were calculated using Phonopy¹⁶ with displacement–force datasets stored in the database. The parameters used in this study for first-principles calculations, including the pseudopotentials, were largely the same as those in Phonondb, although the structures were re-relaxed in this study. The two sets of results are in excellent agreement, as shown in Fig. S5. The remaining discrepancies are likely attributable to differences in the relaxed structures, particularly the lattice constants. Overall, this comparison demonstrates the reliability of both datasets.







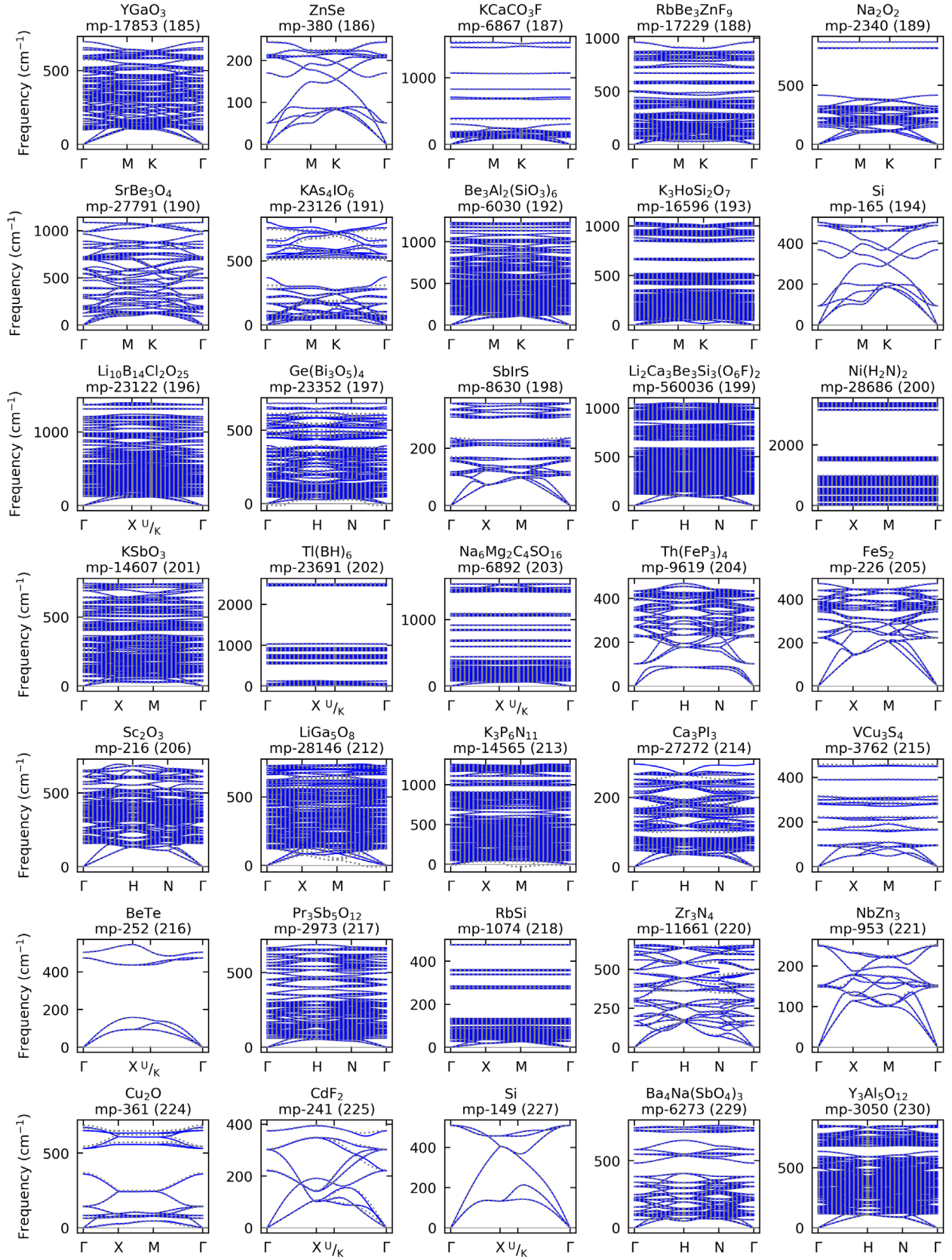


Fig. S5. Comparison of phonon dispersions obtained in this study (blue solid line) with those reported in Phonondb (grey dotted line) for all available space groups. The chemical formula, material ID in Materials Project, and space group number (in parentheses) are shown in the top of each panel.

VI. COMPARISON WITH EXPERIMENTAL RESULTS

The calculated room-temperature lattice thermal conductivities ($\kappa_{\text{lat}}^{\text{RT}}$) were compared with experimental results for 101 single-crystal compounds, comprising 162 data points, as shown in Fig. S6. In this figure, the deviation of the calculated data (κ_{DFT}) from the experimental data (κ_{exp}) is evaluated in different formats, as described below.

Mean absolute error (MAE) in log scale:

$$\text{MAE (log scale)} = \frac{1}{N} \sum (\log_{10} \kappa_{\text{exp}} - \log_{10} \kappa_{\text{DFT}})$$

coefficient of determination (R^2):

$$R^2 = 1 - \frac{\sum (\kappa_{\text{exp}} - \kappa_{\text{DFT}})^2}{\sum (\kappa_{\text{exp}} - \overline{\kappa_{\text{exp}}})^2}$$

symmetry mean absolute percentage error (SMAPE):

$$\text{SMAPE} = \frac{100}{N} \sum \frac{|\kappa_{\text{DFT}} - \kappa_{\text{exp}}|}{(|\kappa_{\text{exp}}| + |\kappa_{\text{DFT}}|)/2}$$

mean symmetry relative error (MSRE):

$$\text{MSRE} = \frac{2}{N} \sum \frac{|\kappa_{\text{DFT}} - \kappa_{\text{exp}}|}{\kappa_{\text{DFT}} + \kappa_{\text{exp}}}$$

where N is the number of data points.

While certain materials—for example, those with significant long-range interactions such as PbX ($X = \text{S, Se, Te}$)—exhibit relatively large discrepancies between calculated and experimental values, the calculated data overall show good agreement with the experimental results. For materials with large discrepancies, including PbX and ZnGeP_2 , the computational conditions employed in the automated calculations may not be sufficiently accurate; therefore, careful treatment with higher-level computational settings is required for more reliable predictions, as discussed in Supplementary Sec. VIII-A. Experimental data used in Fig. S6 are listed in Table S2.

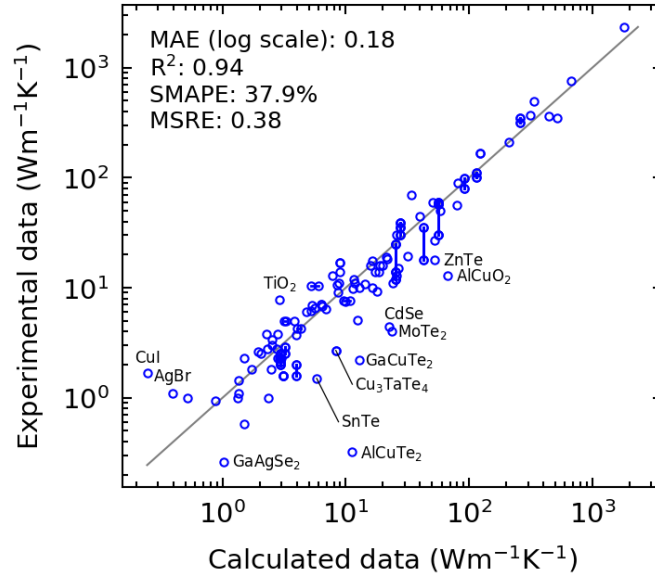


Fig. S6 Room-temperature lattice thermal conductivity of single-crystal compounds compared with experimental and computational data. The dataset includes 101 materials and 162 data points. Chemical formulas of materials exhibiting significant discrepancies are indicated in the figure.

Table S2 List of experimental data in Fig. S6.

Material ID	Formula	Space-group	κ_{lat} ($\text{W m}^{-1} \text{K}^{-1}$)	Reference	DOI or book title
mp-66	C	227	2340	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-149	Si	227	166	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-216	Sc2O3	206	17	Li (2005) ¹⁸	DOI:10.1111/j.1551-2916.2005.00162.x
mp-241	CdF2	225	4.3	Popov (2010) ¹⁹	DOI: 10.1134/S1063783410030091
mp-361	Cu2O	224	5	Lide (2004) ²⁰	RC handbook of chemistry and physics
mp-406	CdTe	216	7.5	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-463	KF	225	6.43	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-602	MoTe2	194	4.02	Miller (2017) ²¹	DOI: 10.1021/acs.chemmater.6b04179
mp-643	ThO2	225	14	Mann (2010) ²²	DOI: 10.1021/cg901308f
mp-661	AlN	186	319	Slack (1987) ²³	DOI: 10.1016/0022-3697(87)90153-3
mp-661	AlN	186	350	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-672	CdS	186	16	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-682	NaF	225	18.4	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-804	GaN	186	210	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-856	SnO2	136	98/55	Turkes (1980) ²⁴	DOI: 10.1088/0022-3719/13/26/015.
mp-981	SrF2	225	9.035	Popov (2010) ¹⁹	DOI: 10.1134/S1063783410030091
mp-1029	BaF2	225	6.8	Popov (2010) ¹⁹	DOI: 10.1134/S1063783410030091
mp-1138	LiF	225	17.6	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-1143	Al2O3	167	35	Lide (2004) ²⁰	CRC handbook of chemistry and physics
mp-1143	Al2O3	167	30	Slack (1962) ²⁵	DOI: 10.1103/PhysRev.126.427

mp-1143	Al ₂ O ₃	167	39	Langenbert (2016) ²⁶	DOI: 10.1063/1.4966220
mp-1190	ZnSe	216	19	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-1239	IrSb ₃	204	16	Slack (1994) ²⁷	DOI: 10.1063/1.357750
mp-1265	MgO	225	60	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-1265	MgO	225	57	Langenberg (2016) ²⁶	DOI: 10.1063/1.4966220
mp-1265	MgO	225	30	Slifka (1998) ²⁸	DOI: 10.6028/jres.103.021
mp-1317	CoSb ₃	204	10	Toberer (2011) ²⁹	DOI: 10.1039/C1JM11754H
mp-1342	BaO	225	2.3	Surplice (1963) ³⁰	DOI: 10.1088/0508-3443/14/10/333
mp-1479	BP	216	350	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-1550	AlP	216	90	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-1639	BN	216	760	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-1883	SnTe	225	1.5	Toberer (2011) ²⁹	DOI: 10.1039/C1JM11754H
mp-1960	Li ₂ O	225	11	Takahashi (1980) ³¹	DOI: 10.1016/0022-3115(80)90036-7
mp-1986	ZnO	216	50	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-2133	ZnO	186	60	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-2172	AlAs	216	80	Steigmeier (1966) ³²	DOI: 10.1103/PhysRev.141.767
mp-2172	AlAs	216	98	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-2176	ZnTe	216	18	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-2201	PbSe	225	2	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-2201	PbSe	225	1.6	El-Sharkawy (1983) ¹³	DOI: 10.1007/BF00502357
mp-2469	CdS	216	16	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-2472	SrO	225	12	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-2490	GaP	216	110	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-2490	GaP	216	100	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-2534	GaAs	216	45	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-2542	BeO	186	370	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-2605	CaO	225	30	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-2624	AlSb	216	56	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-2652	Y ₂ O ₃	206	14	Fornasiero et al., (2000) ³³	DOI: 10.1016/S0272-8842(99)00101-7
mp-2657	TiO ₂	136	7.8	Langenbert (2016) ²⁶	DOI: 10.1063/1.4966220
mp-2691	CdSe	216	4.4	Toberer (2011) ²⁹	DOI: 10.1039/C1JM11754H
mp-2741	CaF ₂	225	9.91	Popov (2010) ¹⁹	DOI: 10.1134/S1063783410030091
mp-3050	Y ₃ Al ₅ O ₁₂	230	10.4	Langenberg (2016) ²⁶	DOI: 10.1063/1.4966220
mp-3196	NdGaO ₃	62	6	Langenberg (2016) ²⁶	DOI: 10.1063/1.4966220
mp-3359	Ba ₂ SnO ₄	139	6.13	Miller (2017) ²¹	DOI: 10.1021/acs.chemmater.6b04179
mp-3536	MgAl ₂ O ₄	227	19.4	Langenberg (1962) ²⁶	DOI: 10.1063/1.4966220
mp-3595	ZnSiAs ₂	122	14	Beasley (1994) ³⁴	DOI: 10.1364/AO.33.001000
mp-3668	CdGeP ₂	122	11	Beasley (1994) ³⁴	DOI: 10.1364/AO.33.001000
mp-3748	AlCuO ₂	166	13	Yanagiya (2010) ³⁵	DOI: 10.3390/ma3010318
mp-3792	YAlO ₃	62	10.7	Langenberg (2016) ²⁶	DOI: 10.1063/1.4966220
mp-3839	GaCuTe ₂	122	2.2	Toberer (2011) ²⁹	DOI: 10.1039/C1JM11754H

mp-4524	ZnGeP2	122	35.5	Beasley (1994) ³⁴	DOI: 10.1364/AO.33.001000
mp-4524	ZnGeP2	122	18	Masumoto (1966) ³⁶	DOI: 10.1016/0022-3697(66)90124-7
mp-4840	GaCuSe2	122	12.9	Beasley (1994) ³⁴	DOI: 10.1364/AO.33.001000
mp-5238	GaCuS2	122	5.09	Beasley (1994) ³⁴	DOI: 10.1364/AO.33.001000
mp-5342	AgGaS2	122	1.45	Beasley (1994) ³⁴	DOI: 10.1364/AO.33.001000
mp-5518	GaAgSe2	122	0.26	Garbato (1979) ³⁷	DOI: 10.1016/0009-2614(79)80529-1
mp-5837	LaGaO3	62	5	Langenberg (2016) ²⁶	DOI: 10.1063/1.4966220
mp-5967	TiCoSb	216	14	Sekimoto (2005) ³⁸	DOI: 10.2320/matertrans.46.1481
mp-5967	TiCoSb	216	25	Xia (2000) ³⁹	DOI: 10.1063/1.1305829
mp-5967	TiCoSb	216	12	Kawaharada (2004) ⁴⁰	DOI: 10.1016/j.jallcom.2004.04.096
mp-7631	SiC	186	490	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-8017	AlCuTe2	122	0.32	Rincón (1995) ⁴¹	DOI: 10.1002/pssa.2211470212
mp-8062	SiC	216	360	Harris (1995) ⁴²	Properties of Silicon Carbide
mp-9295	Cu3TaTe4	215	2.69	Miller (2017) ²¹	DOI: 10.1021/acs.chemmater.6b04179
mp-10695	ZnS	216	27	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-10760	MgSe	225	7.69	Pawlak ⁴³	DOI: 10.1007/s10765-009-0590-6
mp-11718	RbF	225	2.27	Hakansson (1989) ⁴⁴	DOI: 10.1088/0953-8984/1/25/009
mp-19717	PbTe	225	2.1	Pei (2011) ⁴⁵	DOI: 10.1039/C0EE00456A
mp-19717	PbTe	225	2.5	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-19717	PbTe	225	2.0	El-Sharkawy (1983) ¹³	DOI: 10.1007/BF00502357
mp-20194	CeO2	225	10.8	Jha (2019) ⁴⁶	DOI: 10.1201/b17045
mp-20352	Ba3In2O6	139	3.76	Miller (2017) ²¹	DOI: 10.1021/acs.chemmater.6b04179
mp-20485	InSe	194	6.9	El-Sharkawy (1983) ¹³	DOI: 10.1016/0022-3697(70)90284-2
mp-21276	PbS	225	2.9	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-21276	PbS	225	2.5	El-Sharkawy (1983) ¹³	DOI: 10.1007/BF00502357
mp-22220	LaLuO3	62	2.5	Langenberg (2016) ²⁶	DOI: 10.1063/1.4966220
mp-22862	NaCl	225	7.1	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-22867	RbBr	225	3.8	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-22895	CuI	225	1.68	Lide (2004) ²⁰	CRC handbook of chemistry and physics
mp-22898	KI	225	2.6	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
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mp-23209	SrCl2	225	2.3	Moore (1985) ⁴⁷	DOI: 10.1007/978-1-4684-4916-7_12
mp-23231	AgBr	225	1.1	Mamran (2007) ⁴⁸	DOI: 10.1088/0022-3727/40/3/027
mp-23251	KBr	225	3.4	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-23259	LiBr	225	1.83	Hakansson (1989) ⁴⁴	DOI: 10.1088/0953-8984/1/25/009.
mp-23268	NaI	225	1.8	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-23295	RbCl	225	2.8	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2
mp-23703	LiH	225	15	Morelli (2005) ¹⁷	DOI: 10.1007/0-387-25100-6_2

mp-31117	NdScO ₃	62	4	Langenbert et al. ²⁶	DOI: 10.1063/1.4966220
mp-31118	SmScO ₃	62	3.5	Langenbert et al. ²⁶	DOI: 10.1063/1.4966220
mp-31119	TbScO ₃	62	3	Langenberg et al. ²⁶	DOI: 10.1063/1.4966220
mp-31120	DyScO ₃	62	2.9	Langenberg et al. ²⁶	DOI: 10.1063/1.4966220
mp-34202	Bi ₂ Te ₃	166	1.6	Toberer (2011) ²⁹	DOI: 10.1039/C1JM11754H
mp-540688	SrIn ₂ O ₄	62	6.53	Miller (2017) ²¹	DOI: 10.1021/acs.chemmater.6b04179
mp-559756	PrScO ₃	62	3.7	Langenberg (2016) ²⁶	DOI: 10.1063/1.4966220
mp-567636	VFeSb	216	13	Young (2000) ⁴⁹	DOI: 10.1063/1.371863
mp-568560	TlBr	63	0.58	Zhu (2021) ⁵⁰	DOI: 10.1039/D1EE00442E
mp-571222	CsBr	225	0.94	Gerlich (2000) ⁵¹	DOI: 10.1088/0022-3719/15/25/013
mp-573697	CsCl	225	1	Gerlich (2000) ⁵¹	DOI: 10.1088/0022-3719/15/25/013
mp-614603	CsI	225	1.1	Gerlich (2000) ⁵¹	DOI: 10.1088/0022-3719/15/25/013
mp-755574	LuAlO ₃	62	11	Langenberg (2016) ²⁶	DOI: 10.1063/1.4966220
mp-924130	TiNiSn	216	9.3	Hohl (1999) ⁵²	DOI: 10.1088/0953-8984/11/7/004
mp-1017439	SrSiO ₃	221	10.1	Xiao (2013) ⁵³	DOI: 10.1103/PhysRevB.96.161201

VII. PRECAUTIONS FOR AUTOMATED CALCULATIONS

In high-throughput calculations, there is always a trade-off between computational accuracy and speed. Based on our knowledge and experience with first-principles phonon calculations, we have aimed to ensure the highest possible computational accuracy in the automated calculations conducted in this study. However, we found that some materials still exhibit implausible data, as shown in Fig. S7.

Implausible data led to excessively high κ_p , exceeding a few thousand $\text{Wm}^{-1}\text{K}^{-1}$. In most cases, this overestimation arises from excessively long phonon lifetimes in isolated flat branches or low-frequency acoustic modes, as well as from excessively high group velocities. To eliminate the excessively long lifetimes, the increase in $\mathbf{q}$ -mesh density and consideration of four-phonon interaction⁵⁴ are necessary. The computational cost of four-phonon interactions is excessively high, but machine-learning prediction⁵⁵ may be an effective strategy for accurately predicting high κ_p values. In contrast, excessively large group velocities are likely due to insufficient structural optimization. For example, implausible changes in phonon branches can be observed around the T point of $\text{Sr}_2\text{CuBrO}_2$ in Fig. S7. While these implausible data can be automatically handled in future versions of the software, they were manually excluded from the discussion in this study.

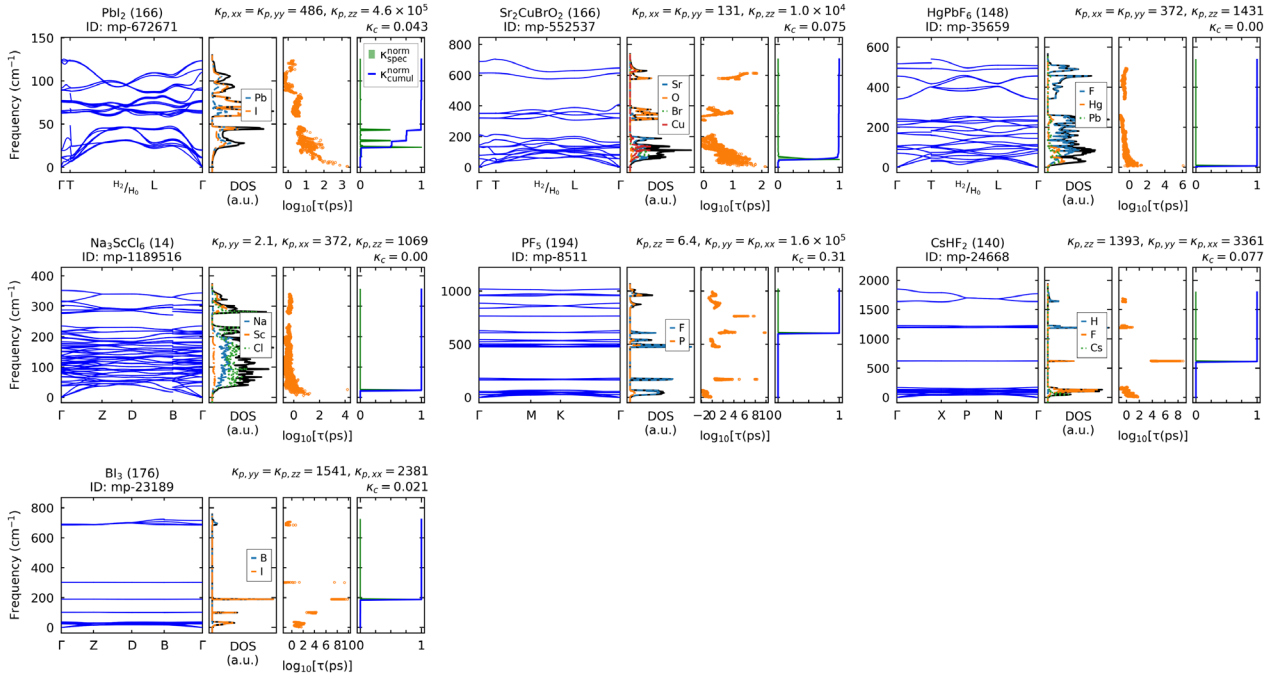


Fig. S7. Results of the automated calculations, including implausible data.

VIII. COMPUTATIONAL ACCURACY

A. Effect of Supercell Size on Phonon Properties

In the first loop of the automated calculations conducted in this study, the maximum number of atoms in a supercell was set to 150, and the supercell size for harmonic force constants (FCs) was subsequently increased if imaginary frequencies appeared. Each supercell was generated from the conventional cell so as to maximize the number of atoms within this limit. Because all possible harmonic FCs in the generated supercell were included in the phonon analysis, the maximum atomic distance of the harmonic FCs depended on the supercell size. In contrast, the cutoff distance for cubic FCs was set to the larger of 4.3 Å or the third-shortest atomic distance. The criterion for determining the cubic-FC cutoff was optimized based on insights gained during the automated calculations, ensuring that the dominant cubic FCs were captured for most materials. In this Supplementary section, we present calculations of phonon properties for selected materials using different supercell sizes. We demonstrate that the above criteria—namely, the choice of supercell size (which determines the harmonic-FC cutoff) and the cubic-FC cutoff length—were reasonable for most materials. Nevertheless, we note that these parameters may require careful verification when analyzing specific materials

We analyzed the size dependence of phonon properties in a set of randomly selected materials. Most of these materials showed no significant size dependence at the supercell size used in this study (≈ 150 atoms), as illustrated in Fig. S8(a). Specifically, the phonon dispersion, phonon lifetime, and temperature-dependent Peierls lattice thermal conductivity exhibited no appreciable size dependence. To further investigate size effects, we next focused on rocksalt PbX (X = S, Se, Te), which are well known to exhibit long-range interactions^{56–59}. Figure S8(b) shows that the phonon dispersion does not converge with increasing supercell size in these compounds. While the phonon dispersion of PbTe exhibits a relatively moderate size dependence compared with PbS and PbSe, its thermal conductivity fluctuates considerably with changes in supercell size. Conversely, even for relatively small supercells ($2 \times 2 \times 2$ and $3 \times 3 \times 3$ supercells containing 64 and 216 atoms, respectively), the anharmonic phonon properties (phonon lifetime and thermal conductivity) of PbS and PbSe show no appreciable size dependence. These results demonstrate that the criteria adopted for cubic FCs ensure convergence in most materials, including those with significant long-range interactions, owing to the much shorter interaction range of cubic FCs compared with harmonic FCs⁵⁹. In contrast, for harmonic FCs, convergence was not achieved even in large systems (e.g., a $5 \times 5 \times 5$ supercell with 1,000 atoms). Therefore, the use of the density functional perturbation theory (DFPT) approach may be necessary to further improve computational accuracy.

Finally, examples of materials whose phonon properties did not converge within our criteria are shown in Fig. S8(c). In certain materials, slight changes in the phonon dispersion—typically in modes with large Grüneisen parameters—affect the resulting lattice thermal conductivity, as in the case of CsAu. In PrRh, the phonon dispersion exhibits an anomalous change with increasing supercell size, leading to the emergence of imaginary frequencies. For ZnGeP₂, the thermal conductivity fluctuates by an order of magnitude, despite meeting the criteria adopted in this study.

In summary, the computational criteria for the automated calculations were determined by balancing computational cost and accuracy. While most materials showed good convergence under different computational conditions, including supercell size, the dataset for certain materials contains substantial errors. Therefore, when using data for specific

materials, it is necessary to examine the detailed results and, if required, to recalculate with more stringent conditions. It may also be of interest to use the Phonix database to optimize the computational conditions for each material.

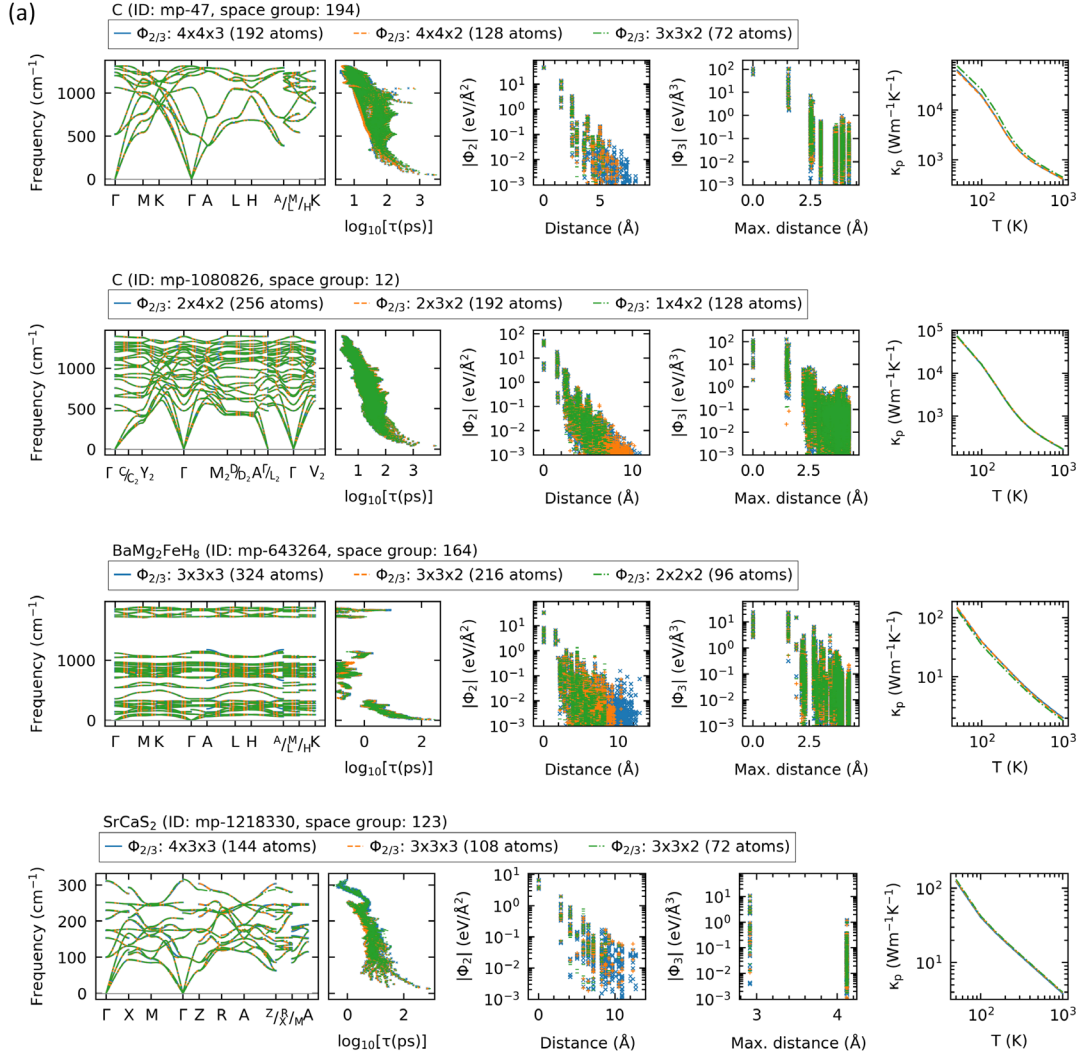


Fig. S8. Effect of supercell size on phonon properties. Each panel shows phonon dispersion, phonon lifetime on a logarithmic scale ($|\log_{10} \tau \text{ (ps)}|$), harmonic (Φ_2) and cubic (Φ_3) force constants, and Peierls lattice thermal conductivity (κ_p). At the top of each panel, the chemical formula, material ID, and space group number are shown. In the legend, each color denotes the supercell size (relative to the primitive cell) used for force constant calculations, as well as the number of atoms in the supercell. In several cases, different supercell sizes were used to compute Φ_2 and Φ_3 constants. (a) Examples of materials showing convergence of phonon properties with respect to the supercell size.

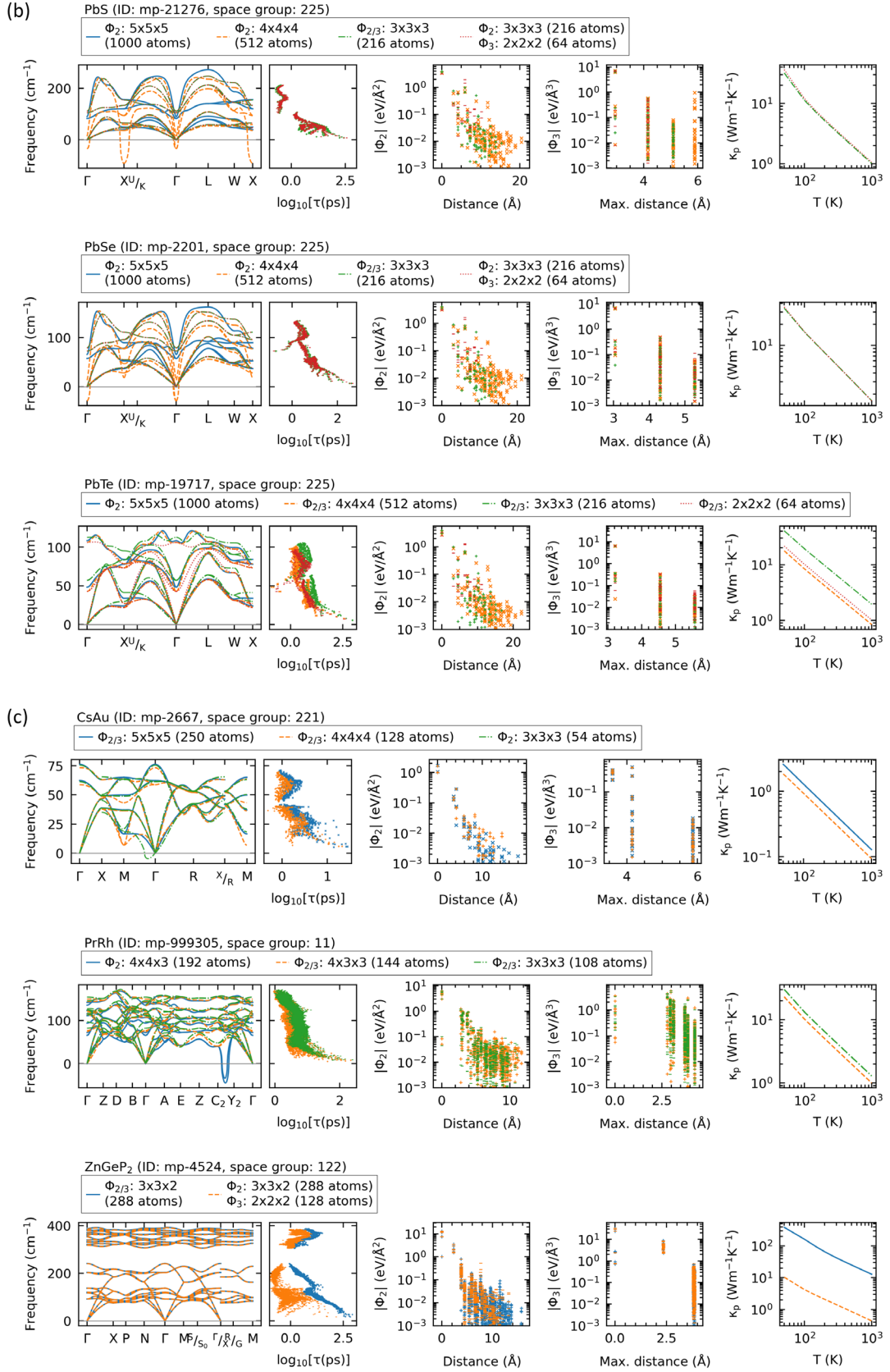


Fig. S8. (contd.) (b) Phonon properties of PbX (X = S, Se, Te) calculated for different supercell sizes. These compounds are known to exhibit significant long-term interactions. (c) Examples of materials with a significant size effect in phonon properties.

B. Comparison between the Finite-Displacement Method and LASSO Regression

In the automated calculations performed in this study, the least absolute shrinkage and selection operator (LASSO) regression was applied when the number of suggested displacement patterns for the finite-displacement (FD) method exceeded 100; otherwise, the FD method was used. To obtain cubic force constants, one or two atoms were displaced in the FD method, whereas all atoms in the supercell were randomly displaced in the LASSO approach. The displacement magnitudes were set to 0.03 Å in both cases.

We compared the force constants and the resulting temperature-dependent thermal conductivity obtained from these approaches, as illustrated in Fig. S9. To reduce the computational cost, particularly for the FD method, the comparison was conducted for relatively simple materials. The force constants obtained with both approaches were in excellent agreement. Although certain materials may exhibit small discrepancies between the two approaches—for example, NaF (mp-682) in Fig. S9—the results are generally comparable. This comparison suggests that, although both methods were employed in this study, LASSO regression may be a suitable choice for future high-throughput calculations, as it reduces computational time and improves methodological consistency across materials.

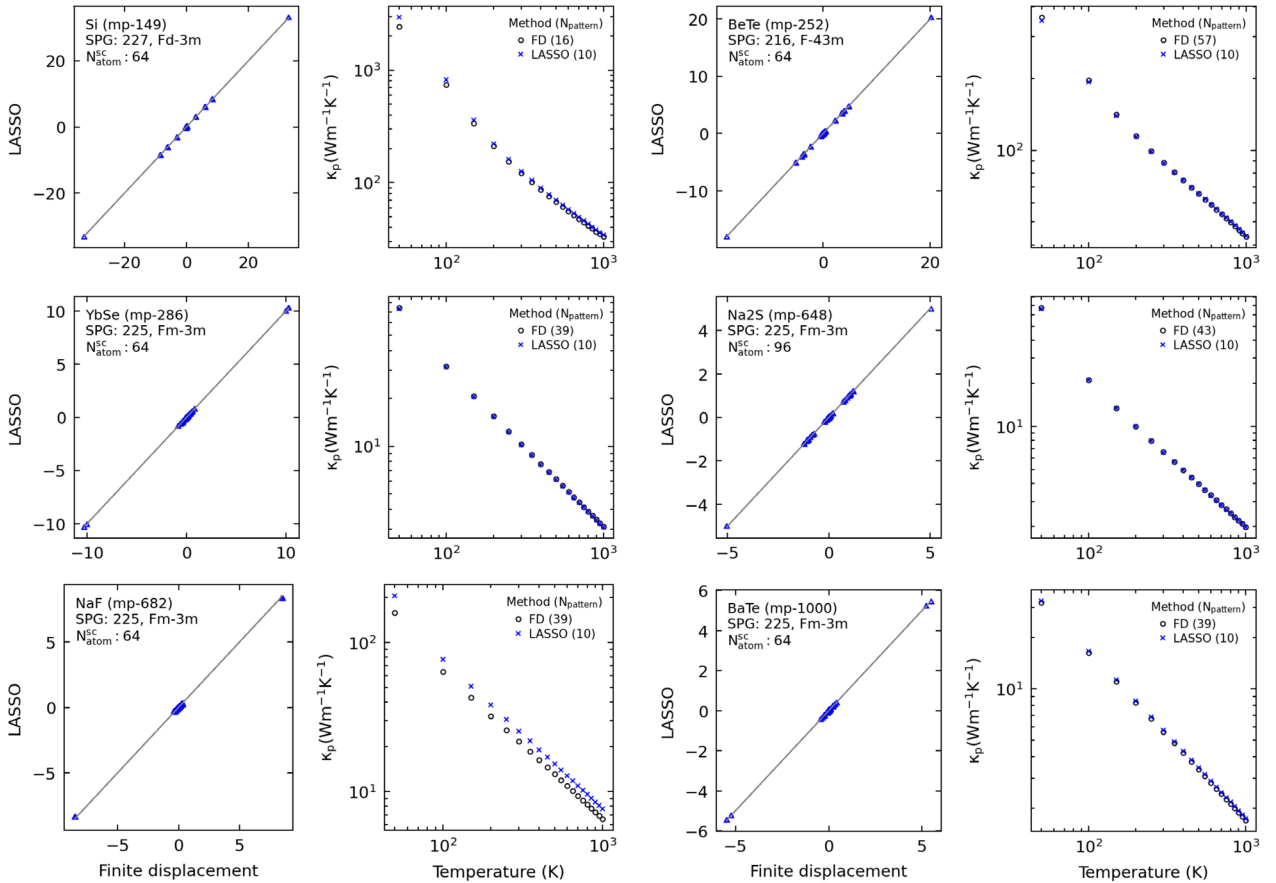


Fig. S9. Comparison of anharmonic phonon properties—force constants (left) and Peierls lattice thermal conductivity (right)—obtained using the finite displacement (FD) method and LASSO regression. In each left panel, the chemical formula, material ID (in parentheses), space group (SPG) number and name, and the number of atoms in the supercell are shown. In each right panel, the numbers of displacement patterns used for each method are indicated in parentheses.

IX. MACHINE LEARNING-BASED PREDICTION OF PHONON PROPERTIES

Using the Phonix database, we predicted the Peierls lattice thermal conductivity (κ_p) and its cumulative value with respect to the mean free path (κ_{cumul}), as mentioned in the main text. In addition to these properties, we also conducted the prediction for the coherent component (κ_c), maximum phonon frequency (ω_{max}), and spectral κ_p as a function of frequency ($\kappa_{\text{spec}}(\omega)$). For training of these properties, we used $\log_{10}(\kappa_c + \varepsilon)$ (where $\varepsilon = 0.001 \text{ Wm}^{-1}\text{K}^{-1}$), $\log_{10} \omega_{\text{max}}$, and $\kappa_{\text{spec}}(\omega)$ normalized by its maximum value, respectively. For $\kappa_{\text{spec}}^{\text{norm}}(\omega)$, the data were prepared from 0 to ω_{max} with 51 points. In the study on phonon density of states (DOS) prediction⁶⁰, which we referred to for the prediction method using the Euclidean neural networks (e3nn)⁶¹, DOS data were discretized into 51 points from 0 to $1,000 \text{ cm}^{-1}$. In contrast, in our prediction, the frequency was normalized by its maximum value because the maximum frequency does not reach $1,000 \text{ cm}^{-1}$ in most materials. Spectral thermal conductivity as a function of the absolute frequency can be obtained by combining the predicted values of ω_{max} and $\kappa_{\text{spec}}^{\text{norm}}(\omega/\omega_{\text{max}})$. For the machine learning technique, CGCNN⁶² was applied to the prediction of κ_c and ω_{max} and e3nn⁶¹ was applied to κ_{spec} .

We observed deep learning scaling laws for these three phonon properties, similar to those for κ_p and $\kappa_{\text{cumul}}^{\text{norm}}(\Lambda)$, as discussed in the main text. In every case, the prediction accuracy increased as the training dataset size increased. The scaling factor was 0.075 to 0.28, which are compatible magnitude as those observed for large language model (0.095)⁶³ and deep learning for materials in a previous study (0.21)⁶⁴. Notably, since the prediction accuracy for ω_{max} was remarkably high (with an MAE of 0.035 in log-scaled ω_{max} (cm^{-1})), integrating the predictions of ω_{max} and $\kappa_{\text{spec}}^{\text{norm}}(\omega/\omega_{\text{max}})$ may provide more valuable information than directly predicting $\kappa_{\text{spec}}^{\text{norm}}(\omega)$, which approaches zero at high frequencies.

While the prediction accuracy for $\kappa_{\text{spec}}(\omega)$ (with an MAE of 0.070) was slightly lower than that for $\kappa_{\text{cumul}}(\Lambda)$ (with an MAE of 0.063), Phonix enables accurate prediction of the spectral anharmonic property, as shown in Fig. S10. The figure illustrates that spectral thermal conductivity was excellently predicted for half of the materials (green and blue), whereas predicting spectra with multiple peaks remains challenging, as indicated by the orange and red lines in Fig. S10.

Consequently, these data clearly show that Phonix opens up multiple possibilities for predicting not only phonon properties but also their interactions with other quasiparticles or related properties. At the same time, further increasing the dataset size or developing advanced machine learning techniques for phonon properties remains essential.

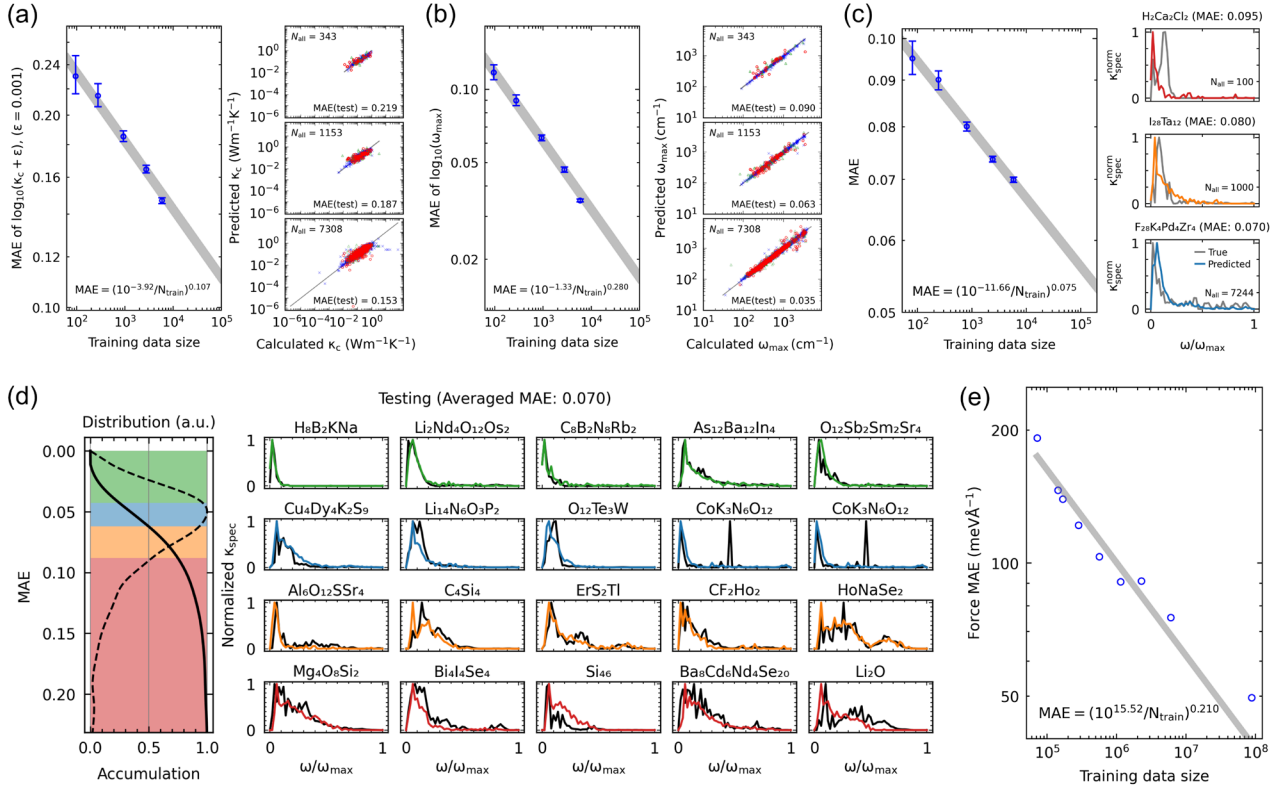


Fig. S10. Deep learning scaling law for phonon properties with respect to the training data size. (a) Coherent thermal conductivity (κ_c), (b) maximum frequency (ω_{max}), and (c) normalized spectral Peierls thermal conductivity ($\kappa_{\text{spec}}^{\text{norm}}$) were predicted. The MAEs were evaluated with $\log_{10}(\kappa_c + \epsilon)$, where $\epsilon = 0.001$ $\text{Wm}^{-1}\text{K}^{-1}$, $\log_{10}[\omega_{\text{max}} (\text{cm}^{-1})]$, and $\kappa_{\text{spec}}^{\text{norm}}$, respectively. (d) $\kappa_{\text{spec}}^{\text{norm}}$ prediction for the test data using all available data ($N_{\text{all}} \approx 7,000$). See the caption of Fig. 3 in the main text for details. (e) Prediction accuracy for atomic forces as a function of training data size, reproduced from Ref.⁶⁴ to compare scalability.

X. LIST OF SCREENED MATERIALS WITH HIGH AND LOW THERMAL CONDUCTIVITY

Using the prediction models built with Phonix, we screened materials with high and low κ_p from the GNoME database, as discussed in the main text. Through this screening, we identified three materials with $\kappa_{\text{lat}}^{3\text{ph}} > 200 \text{ Wm}^{-1}\text{K}^{-1}$ and nine materials with $\kappa_{\text{lat}}^{3\text{ph}} < 0.2 \text{ Wm}^{-1}\text{K}^{-1}$. Their phonon properties are presented in Fig. S11. For the three high- κ materials, we considered four-phonon scattering in addition to three-phonon scattering using the ALAMODE package. Although four-phonon scattering significantly reduces the thermal conductivity—for example, from 277 to 78 $\text{Wm}^{-1}\text{K}^{-1}$ in NpPH—the three compounds still exhibit relatively high values ($>50 \text{ Wm}^{-1}\text{K}^{-1}$) compared with the entire set of materials in Phonix (see Fig. 2(b)).

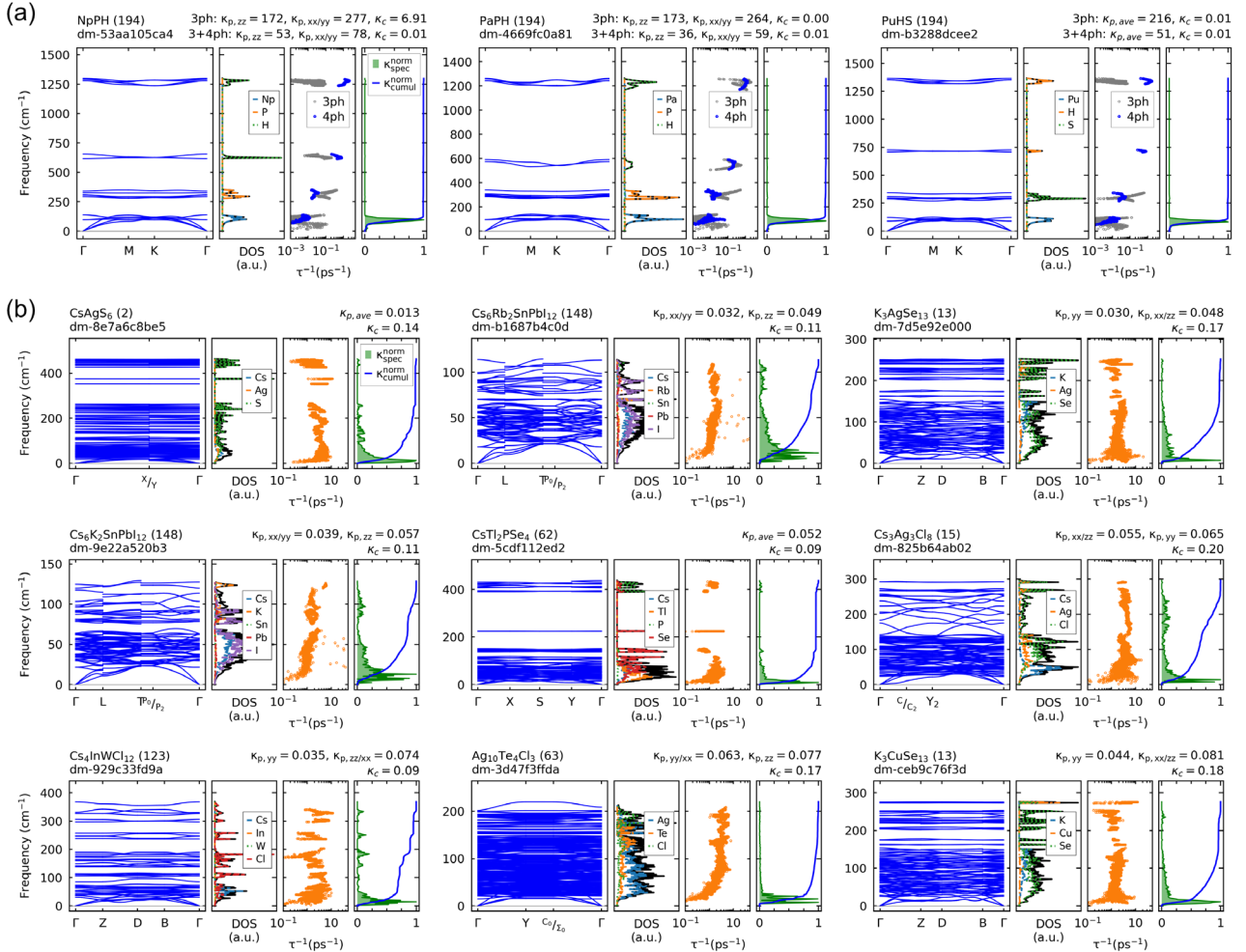


Fig. S11. Novel materials exhibiting extreme thermal conductivity. (a) A list of materials with $\kappa_{\text{lat}} > 200 \text{ Wm}^{-1}\text{K}^{-1}$ and (b) materials with $\kappa_{\text{lat}} < 0.2 \text{ Wm}^{-1}\text{K}^{-1}$. The materials were identified through screening of the GNoME database⁶⁴.

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