It is shown that the thermal conductivity of anharmonic insulators can be derived parameter free and self-consistently from the temperature (T) dependence of the phonon—phonon scattering momentum, the phonon group velocities, and the specific heat. Using the example of SrTiO₃ the phonon mean free path is derived from the Fourier transform of the acoustic—optic mode crossing momentum. The temperature dependence of the phonon group velocities is self-consistently evaluated from the soft optic, acoustic phonon modes, which are also the input for the calculation of the specific heat. The overall quantitative agreement with experimental data suggests further applications to other anharmonic systems like, e.g., KTaO₃ PbTe, and related materials.

The thermal conductivity (TC) of solids is typically characterized by temperature dependent phonon scattering processes which at low temperatures are in the ballistic regime and follow at high temperature the normal Fourier heat conduction. The calculation of the TC is mostly based on the Callaway model [1] and modifications of it [2,3], where instead of scattering lengths relaxation times are introduced which, however, are rather difficult to evaluate explicitly for a specific system. In addition, an exact knowledge of the phonon spectrum and its temperature dependence are indispensable. Extensive studies of the TC have been devoted to ferroelectric or almost ferroelectric compounds since their lattice dynamics is governed by large anharmonicity [4–13]. A recent study of SrTiO₃ (STO) and doped STO has revealed a novel region in the TC, namely a regime of phonon Poiseuille flow where TC evolves faster than cubic in temperature [12]. A similar observation has been made before in (Ta₁₋ₓNbₓSe₄)₂I which has been attributed to extremely strong anharmonicity [14].

Here it is shown that quite generally the TC can be rather simply evaluated in ferroelectric and almost ferroelectric systems by calculating their specific heat, the temperature dependent phonon scattering processes which at low temperatures are in the ballistic regime and follow at high temperature the normal Fourier heat conduction. The calculation of the TC is mostly based on the Callaway model [1] and modifications of it [2,3], where instead of scattering lengths relaxation times are introduced which, however, are rather difficult to evaluate explicitly for a specific system. In addition, an exact knowledge of the phonon spectrum and its temperature dependence are indispensable. Extensive studies of the TC have been devoted to ferroelectric or almost ferroelectric compounds since their lattice dynamics is governed by large anharmonicity [4–13]. A recent study of SrTiO₃ (STO) and doped STO has revealed a novel region in the TC, namely a regime of phonon Poiseuille flow where TC evolves faster than cubic in temperature [12]. A similar observation has been made before in (Ta₁₋ₓNbₓSe₄)₂I which has been attributed to extremely strong anharmonicity [14].
the transverse soft optic mode frequency is derived self-consistently. Details about the 
self-consistent phonon approximation are given in Refs. [15–17], and applications to 
STO in Refs. [18–20]. The procedure outlined in these papers resembles closely the 
work of Ref. [21]. The overall features of the calculated TC are in good quantitative 
agreement with experimental data. In view of the fact that the lattice dynamics of STO 
are well understood, this compound is taken as an example. Extensions to doped STO 
are discussed.

STO is one of the best investigated perovskite oxides due to its outstanding properties 
and its wide application range. In analogy to true ferroelectric perovskites it exhibits 
long wave length transverse optic mode softening over a broad temperature interval 
[22–24], where the completion of softening is, however, inhibited by quantum fluctua-
tions which was named quantum paraelectricity [25]. Besides of the soft optic mode 
also a transverse acoustic zone boundary mode softens and freezes at 105 K, inducing a 
structural phase transition from cubic to tetragonal [26–28]. This transition is character-
ized by the oxygen octahedral rotation angle [29]. Ferroelectricity can be induced in 
STO by either isotopic replacement of 16O by 18O [30,31] or by introducing small 
amounts of Ca at the Sr lattice site thereby causing an XY pseudospin ferroelectric 
transition [32]. Also the replacement of Ba at the Sr site yields a polar transition [33]. Small 
amounts of oxygen vacancies rapidly change the system from insulating to semiconduct-
ing and metallic [34–36], where superconductivity is observed at low temperature and 
unusually small carrier density [37,38]. Similarly, superconductivity sets in with small 
amounts of Nb doping [39,40]. This superconducting state is unusual since it corre-
responds to the first two-band superconductor after its prediction.

The lattice dynamics of STO has been investigated in detail using the polarizability 
model [15–17]. This model is superior to first-principles approaches and effective 
Hamiltonian schemes, since it enables a self-consistent derivation of all relevant tem-
perature dependent properties of ferroelectric and quantum paraelectric perovskite 
oxides and IV–VI semiconductors [19]. Its basic ingredients are attractive harmonic 
interactions in the local electron-lattice coupling stabilized by long range repulsive 
fourth-order anharmonic terms [15–17]. Upon treating the latter by a cumulant expan-
sion, pseudo-harmonic temperature dependent effective interactions are obtained which 
have to be calculated self-consistently for each temperature T. In this way the soft 
modes which dominate the lattice dynamics are derived. Simultaneously, the double-
well potential of the respective compound is obtained which is characteristic for each 
compound and differs significantly between those [20].

While for a long time the focus was on the soft lattice modes only, early on an appar-
et anomaly in the related transverse acoustic mode was observed at finite momentum 
experimentally [21, 41–45], which attracted little attention. This mode-mode coupling 
induced anomalies could also be reproduced within the polarizability model and 
assigned to elastic finite size precursor dynamics. With decreasing temperature the pre-
cursors grow in size to eventually occupying the full sample size at the phase transition 
temperature [46,47]. Simultaneously, also polar nano domains emerge, which coexist 
with the soft mode and evidence that order/disorder and displacive dynamics coexist, 
however, on different time and length scales [48].
The above preliminaries are an important ingredient to calculate the TC for anharmonic almost ferroelectric compounds since from them the phonon–phonon scattering length is extracted which defines the mean free path to be used further. Basically, the TC is simply the product of specific heat $c_v$, the phonon mean free path $l_{ph}$, and the phonon group velocity. All quantities are temperature dependent, which is the main reason for the difficulties in calculating the TC. In the following the temperature dependent dispersion of the lowest transverse optic (TO) and related transverse (TA) acoustic modes in the (100) direction are used to derive these three quantities. These modes have been chosen since they are strongly temperature dependent and are coupled by higher order anharmonic interactions which cause the loss of their individual character at intermediate momentum. As such they are no longer elementary excitation like but adopt a hybrid type character which is a consequence of the strong TO softening. This softening leads to a TO–TA coupling and an avoided crossing with characteristic wave vector which defines the phonon mean free path as discussed in deeper detail below. Importantly, the strong TO mode temperature dependence induces also a temperature-dependence in the crossing region which is especially strong at low temperature where quantum fluctuations dominate the lattice dynamics of STO. The dispersion for these two modes is shown in Figure 1(a) as a function of temperature where the mode-mode coupling momentum space is highlighted by the encircled area. While detailed experimental data for the phonon mode dispersion are not available, the temperature dependence of the $q=0$ optic mode has been measured and is presented in the inset to the figure in comparison to theoretical results evidencing the convincing agreement between both. To increase the mode-mode coupling visibility, the difference between optic and acoustic modes is formed where the minimum in $\Delta(\omega) = \omega_{TO}(q) - \omega_{TA}(q)$, where the inverse of the crossing momentum of optic and acoustic modes defines the mean free path $l_{ph}$ which is identical for both modes.

The above preliminaries are an important ingredient to calculate the TC for anharmonic almost ferroelectric compounds since from them the phonon–phonon scattering length is extracted which defines the mean free path to be used further.
minimum in the mode difference moves with decreasing temperature to the long wave
length limit, whereas it saturates at an almost constant value in the high temperature
regime. In addition, the difference becomes smaller and smaller with decreasing tem-
perature. The corresponding momentum value $q$ is Fourier transformed in order to
extract the real space length scale of the scattering event as shown in the inset to Figure
1(b). This can be approximated by an exponential as displayed by the full line in the
inset which defines in the following the phonon mean free path $l_{ph}$. This definition is
related to the fact that anharmonicity induced phonon–phonon scattering takes place at
the crossing momentum value.

Furthermore, the group velocities of acoustic and optic modes are readily obtained
from Figure 1(a) by forming the derivative of both modes with respect to $q$ (Figure 2).

For both, optic and acoustic modes $\omega_{TO}$ and $\omega_{TA}$, the long wave length limit of the
velocities $v_{TO}, v_{TA}$ is taken and plotted as a function of temperature in Figure 3(a,b).
These quantities enter Equation (3) below and are the essential ingredients to evaluate
the temperature dependence of the TC [51,52]. Interestingly, their individual behavior is
grossly different also with respect to the order of magnitude of the velocities. While the
optic mode velocity increases exponentially with decreasing temperature, it increases for
the acoustic mode velocity with increasing temperature. In the high temperature region
both saturate at small values for the former and at large values for the latter.

Knowing the temperature dependent dispersion of STO, it is rather straightforward
to calculate the phonon specific heat $c_v$, which is explicitly given by:

$$c_v(q) = \frac{(\hbar \omega_{TO}(q))^2}{(kT)^2} \frac{\exp(\hbar \omega_{TO}(q))}{(\exp(\hbar \omega_{TO}(q)) - 1)^2} + \frac{(\hbar \omega_{TA}(q))^2}{(kT)^2} \frac{\exp(\hbar \omega_{TA}(q))}{(\exp(\hbar \omega_{TA}(q)) - 1)^2},$$  

where $k$ is the Boltzmann constant and $T$ temperature. Equation (1) is integrated with
respect to $q$ over the whole Brillouin zone. The dispersion as shown in Figure 1(a) is
used for each temperature. Since the phase transition from cubic to tetragonal at \( T_S = 105 \) K is driven by a zone boundary acoustic mode, which is not shown in Figure 1(a), because it corresponds to the (110) direction, the formerly calculated mode is inserted in Equation (1). The results for \( c_V \) are displayed in Figure 4 together with experimental results of Ref. [49].

Around \( T_S \) a rather tiny anomaly is observed which is more apparent in the derivative of \( c_V \) with respect to \( T \) (inset to Figure 4). This is in agreement with various measurements of \( c_V \) in STO [11, 50–53].

Now all ingredients are obtained to calculate the TC of STO. This is a simple task as only the product of the above derived quantities has to be formed for each temperature.
corresponding to the Peierls–Boltzmann transport theory:

$$\kappa_{\text{lattice}} = \frac{1}{3} \sum_{q, TO, TA} c_V(q) \nu_{q, TO, TA} l_{ph}. \quad (2)$$

Note that the contribution from the optic mode is neglected since $\nu_{\text{TO}}$ is much smaller than $\nu_{\text{TA}}$ (see Figure 3(a,b)) as has also been observed in other systems [54]. This does, however, not imply that the optic phonons are unimportant, but just the opposite, namely they represent the dominant scattering channel for the heat-carrying acoustic phonons. Omitting these [55–57] would release an enormous increase in the TC. The result for the TC is shown in Figure 5.

A comparison with experimental data [11,12] shows an overall good agreement, even though some experimentally observed fine details are not reproduced, especially for $T > 200$ K where probably further phonon branches need to be taken into account. However, in view the simplicity of this parameter free approach based on the self-consistent phonon theory the overall agreement clearly suggests that anharmonic effects in terms of phonon-phonon interactions which provide the phonon mean free path, are the basic ingredient to understand the TC of STO and related compounds. It is important to note that the mean free path changes from the order of lattice constants at high temperature to diverging at low temperature and thus provides a natural crossover from kinetic to ballistic transport regimes. The observation of a Poiseuille flow appearing above the Casimir region [12] is attributed to the enhanced quantum fluctuation effects of STO which appear just in this temperature window.

Since the key ingredient of the above theory is the phonon mean free path as deduced from the phonon-phonon scattering momentum (inset to Figure 1(b)), a similar analysis can be performed for doped STO where strong deviations in $\kappa$ as compared to the undoped system have been reported [12]. The temperature dependent exponential

Figure 5. TC as a function of temperature for STO shown on a double logarithmic scale. The experimental data of Ref. [12] of STO are represented by the black squares. The theoretically obtained results are given by the red squares.
decay of $l_{ph}$ is given by:

$$l_{ph} = l_0 + A \exp \left( - \frac{T}{T_x} \right)$$  \hspace{1cm} (2)$$

where $l_0$ is of the order of some lattice constants, $A$ is a material constant which depends on doping and decreases systematically with increasing doping, implying that the exponential gets less important, and $T_x$ is a characteristic temperature which defines the maximum in $\kappa$. This temperature scale is plotted as a function of doping in Figure 6 where obviously an almost linear increase with increasing doping takes place. Experimentally a systematic investigation has not been carried out, however, from the data in Ref. [12] it is clearly observed that indeed the maximum in $\kappa$ moves to higher temperature with increasing doping.

Simultaneously, the double-well potential of the respective compound gets shallower and narrower to be pseudo-harmonic for large doping. Details will be presented elsewhere [58].

In conclusion, a simple derivation of the TC of an anharmonic crystal has been proposed where nonlinear phonon–phonon interaction is the most important ingredient. The critical momentum at which the interaction is strongest is strongly temperature dependent and governed by higher order electron–phonon coupling. Simultaneously, it defines the phonon mean free path and thereby the temperature evolution of $\kappa$. The overall good agreement with experimental data approves this rather elementary scheme in calculating the TC and should be applicable to similar compounds with significant phonon softening, as, e.g., PbTe and KTaO$_3$ which are, however, experimentally much less investigated as compared to STO such that the important input data, as outlined above, are not available at present.

**Acknowledgements**

It is a pleasure to acknowledge valuable discussions with H. Keller.
References

[1] J. Callaway, Model for lattice thermal conductivity at low temperatures, Phys. Rev. 113 (4), 1046 (1959). DOI: 10.1103/PhysRev.113.1046.

[2] R. A. Guyer, and J. A. Krumhansl, Thermal conductivity, second sound, and phonon hydrodynamic phenomena in nonmetallic crystals, Phys. Rev. 148 (2), 778 (1966). DOI: 10.1103/PhysRev.148.778.

[3] R. A. Guyer, and J. A. Krumhansl, Solution of the linearized phonon Boltzmann equation, Phys. Rev. 148 (2), 766 (1966). DOI: 10.1103/PhysRev.148.766.

[4] M. Tachibana, T. Kolodiazhnyi, and E. Takayama-Muromachi, Thermal conductivity of perovskite ferroelectrics, Appl. Phys. Lett. 93 (9), 092902 (2008). DOI: 10.1063/1.2978072.

[5] A. J. H. Mante, and J. Volger, Phonon transport in barium titanate, Phys. Lett. 24A, 139 (1967). DOI: 10.1016/0031-8914(71)90164-9.

[6] B. Salce, J. L. Gravil, and L. A. Boatner, Disorder and thermal transport in undoped KTaO3, J. Phys. Condens. Matter 6, 4077 (1994). DOI: 10.1088/0953-8984/6/22/007.

[7] H. H. Barrett, and M. G. Holland, Thermal conductivity in perovskites, Phys. Rev. B. 2 (8), 3441 (1981). DOI: 10.1103/PhysRevB.2.3441.

[8] W. H. Huber, L. M. Hernandez, and A. M. Goldman, Electric field dependence of the thermal conductivity of quantum paraelectrics, Phys. Rev. B. 62 (13), 8588 (2000). DOI: 10.1103/PhysRevB.62.8588.

[9] D. A. Ackerman et al., Glassy behavior of crystalline solids at low temperatures, Phys. Rev. B. 23 (8), 3886 (1981). DOI: 10.1103/PhysRevB.23.3886.

[10] J. J. De Yoreo, R. O. Pohl, and G. Burns, Low-temperature thermal properties of ferroelectrics, Phys. Rev. B. 32 (9), 5780 (1985).

[11] E. F. Steigmeier, Field effect on the Cochran modes in SrTiO3 and KTaO3, Phys. Rev. 168 (2), 523 (1968). DOI: 10.1103/PhysRev.168.523.

[12] V. Martelli et al., Thermal transport and phonon hydrodynamics in strontium titanate, Phys. Rev. Lett. 120 (12), 125901 (2018).

[13] S. R. Popuri et al., Glass-like thermal conductivity in SrTiO3 thermoelectrics induced by A-site vacancies, Soc. Chem. Adv. 4, 3370 (2014).

[14] A. Smontara, J. C. Lasjaunias, and R. Maynard, Phonon Poiseuille flow in quasi-one-dimensional single crystals, Phys. Rev. Lett. 77 (27), 5397 (1996). DOI: 10.1103/PhysRevLett.77.5397.

[15] R. A. Cowley, Lattice dynamics and phase transitions of strontium titanate, Phys. Rev. 134 (4A), A981 (1964).

[16] G. Shirane, and Y. Yamada, Lattice-dynamical study of the 110°K phase transition in SrTiO3, Phys. Rev. 177 (2), 858 (1969). DOI: 10.1103/PhysRev.177.858.

[17] H. Vogt, Refined treatment of the model of linearly coupled anharmonic oscillators and its application to the temperature dependence of the zone-center soft-mode frequencies of KTaO3 and SrTiO3, Phys. Rev., B Condens. Matter 51 (13), 8046 (1995). DOI: 10.1103/physrevb.51.8046.

[18] K. A. Müller, and H. Burkard, SrTiO3: an intrinsic quantum paraelectric below 4 K, Phys. Rev. B. 19 (7), 3593 (1979). DOI: 10.1103/PhysRevB.19.3593.

[19] Y. Yamada, and G. Shirane, Neutron scattering and nature of the soft optical phonon in SrTiO 3, J. Phys. Soc. Jpn. 26 (2), 396 (1969). DOI: 10.1143/JPSJ.26.396.

[20] P. A. Fleury, J. F. Scott, and J. M. Worlock, Soft phonon modes and the 110°K phase transition in SrTiO3, Phys. Rev. Lett. 21 (1), 16 (1968). DOI: 10.1103/PhysRevLett.21.16.

[21] T. Riste et al., Critical behaviour of SrTiO3 near the 105°K phase transition, Solid State Comm. 9 (17), 1455 (1971).

[22] K. A. Müller, and W. Berlinger, Static critical exponents at structural phase transitions, Phys. Rev. Lett. 26 (1), 13 (1971). DOI: 10.1103/PhysRevLett.26.13.

[23] M. Itoh et al., Ferroelectricity induced by oxygen isotope exchange in strontium titanate perovskite, Phys. Rev. Lett. 82 (17), 3540 (1999). DOI: 10.1103/PhysRevLett.82.3540.
A. Bussmann-Holder, H. Büttner, and A. R. Bishop, Stabilization of ferroelectricity in quantum paraelectrics by isotopic substitution, *J. Phys. Condens. Matter* **12**, L115 (2000). DOI: 10.1088/0953-8984/12/6/108.

J. G. Bednorz, and K. A. Müller, Sr$_{1-x}$Ca$_x$TiO$_3$: an XY Quantum Ferroelectric with Transition to Randomness, *Phys. Rev. Lett.* **52** (25), 2289 (1984). DOI: 10.1103/PhysRevLett.52.2289.

L. Zhang *et al.*, The volume effect in barium strontium titanate, *Solid State Comm.* **104** (5), 263 (1997). DOI: 10.1016/S0038-1098(97)00289-5.

D. Bäuerle *et al.*, Soft modes in semiconducting SrTiO$_3$: II. The ferroelectric mode, *Z. Phys. B. Condens. Matter* **38**, 335 (1980). DOI: 10.1007/BF01315325.

A. Bussmann-Holder *et al.*, A polarizability model for the ferroelectric mode in semiconducting SrTiO$_3$, *Z. Phys. B. Condens. Matter* **41** (4), 353 (1981). DOI: 10.1007/BF01307326.

X. Lin *et al.*, Metallicity without quasi-particles in room-temperature strontium titanate, *NPJ Quantum Mater.* **2** (1), 1 (2017).

J. F. Schooley, W. R. Hosler, and M. L. Cohen, Superconductivity in semiconducting SrTiO$_3$, *Phys. Rev. Lett.* **12** (17), 474 (1964). DOI: 10.1103/PhysRevLett.12.474.

C. Collignon *et al.*, Superfluid density and carrier concentration across a superconducting dome: the case of strontium titanate, *Phys. Rev. B* **96** (22), 224506 (2017).

G. Binnig *et al.*, Two-band superconductivity in Nb-doped SrTiO$_3$, *Phys. Rev. Lett.* **45** (16), 1352 (1980). DOI: 10.1103/PhysRevLett.45.1352.

X. Lin *et al.*, S-wave superconductivity in optimally doped SrTi$_{1-x}$Nb$_x$O$_3$ unveiled by electron irradiation, *Phys. Rev. B.* **92** (17), 174504 (2015).

R. Migoni, H. Bilz, and D. Bäuerle, Origin of Raman scattering and ferroelectricity in oxide perovskites, *Phys. Rev. Lett.* **37** (17), 1155 (1976). DOI: 10.1103/PhysRevLett.37.1155.

H. Bilz, G. Benedek, and A. Bussmann-Holder, Theory of ferroelectricity: the polarizability model, *Phys. Rev. B Condens. Matter* **35** (10), 4840 (1987). DOI: 10.1103/physrevb.35.4840.

A. Bussmann-Holder, The polarizability model for ferroelectricity in perovskite oxides, *J. Phys. Condens. Matter* **24** (27), 273202 (2012). DOI: 10.1088/0953-8984/24/27/273202.

A. Bussmann-Holder, H. Büttner, and A. Bishop, Polar-soft-mode-driven structural phase transition in SrTiO$_3$, *Phys. Rev. Lett.* **99** (16), 167603 (2007).

A. Bussmann-Holder, Interplay of polarizability and ionicity in IV-VI compounds, *Phys. Rev. B Condens. Matter* **40** (17), 11639 (1989). DOI: 10.1103/physrevb.40.11639.

A. Bussmann-Holder, K. Roleder, and J.-H. Ko, What makes the difference in perovskite titanates?, *J. Phys. Chem. Solids.* **117**, 148 (2018). DOI: 10.1016/j.jpcs.2018.02.025.

G. Shirane, and E. Sawaguchi, On the anomalous specific heat of lead titanate, *Phys. Rev.* **81** (3), 458 (1951). DOI: 10.1103/PhysRev.81.458.2.

G. Shirane *et al.*, Soft ferroelectric modes in lead titanate, *Phys. Rev. B.* **2**, 155 (1970). DOI: 10.1103/PhysRevB.2.155.

J. Harada, J. D. Axe, and G. Shirane, Neutron-scattering study of soft modes in cubic BaTiO$_3$, *Phys. Rev. B* **4** (1), 155 (1971). DOI: 10.1103/PhysRevB.4.155.

E. Courtens *et al.*, New excitations in quantum paraelectrics, *Phys. B Condens. Matter* **219-220**, 577 (1996). doi:10.1016/0921-4526(95)00817-9.

A. Bussmann-Holder, Electron-phonon-interaction-driven anharmonic mode-mode coupling in ferroelectrics: the origin of acoustic-mode anomalies, *Phys. Rev. B.* **56** (17), 10762 (1997). DOI: 10.1103/PhysRevB.56.10762.

J. L. Servoin *et al.*, ed. Devrees, J., Recent developments in condensed matter physics. In *Low-Dimensional Systems, Phase Changes and Experimental Techniques* (Plenum Press, New York, 1982), Vol. 4, p. 157.

A. Bussmann -Holder, K. Roleder, and J.-H. Ko, Instabilities in the ferro- and antiferroelectric lead perovskites driven by transition metal ion mass: from PbTiO$_3$ via PbZrO$_3$ to PbHfO$_3$, *J. Phys. Condens. Matter* **26** (27), 275402 (2014). DOI: 10.1088/0953-8984/26/27/275402.
[47] J.-H. Ko et al., Mode softening, precursor phenomena, and intermediate phases in PbZrO₃, Phys. Rev. B. 87 (18), 184110 (2013).

[48] M. Stachiotti et al., Crossover from a displacive to an order-disorder transition in the nonlinear-polarizability model, Phys. Rev. B Condens. Matter 47 (5), 2473 (1993). DOI: 10.1103/physrevb.47.2473.

[49] J. Petzelt et al., Dielectric, infrared, and Raman response of undoped SrTiO₃ ceramics: evidence of polar grain boundaries, Phys. Rev. B. 64 (18), 184111 (2001).

[50] J. L. Servoin, Y. Luspin, and F. Gervais, Infrared dispersion in SrTiO₃ at high temperature, Phys. Rev. B. 22 (11), 5501 (1980). DOI: 10.1103/PhysRevB.22.5501.

[51] G. Lang et al., Anharmonic line shift and linewidth of the Raman mode in covalent semiconductors, Phys. Rev. B. 59 (9), 6182 (1999). DOI: 10.1103/PhysRevB.59.6182.

[52] A. Bussmann-Holder et al., Relation between structural instabilities in EuTiO₃ and SrTiO₃, Phys. Rev. B. 83 (21), 212102 (2011).

[53] A. Debernardi, S. Baroni, and E. Molinari, Anharmonic phonon lifetimes in semiconductors from density-functional perturbation theory, Phys. Rev. Lett. 75 (9), 1819 (1995). DOI: 10.1103/PhysRevLett.75.1819.

[54] D. A. Broido et al., Intrinsic lattice thermal conductivity of semiconductors from first principles, Appl. Phys. Lett. 91 (23), 231922 (2007). DOI: 10.1063/1.2822891.

[55] M. Omini, and A. Sparavigna, Beyond the isotropic-model approximation in the theory of thermal conductivity, Phys. Rev. B. 53 (14), 9064 (1996).

[56] M. Omini, and A. Sparavigna, Heat transport in dielectric solids with diamond structure, Nuovo Cimento D. 19, 1537 (1997).

[57] D. A. Broido, A. Ward, and N. Mingo, Lattice thermal conductivity of silicon from empirical interatomic potentials, Phys. Rev. B. 72 (1), 014308 (2005).

[58] A. Bussmann-Holder, to be published.