1. Introduction

Searching for high-performance thermoelectric materials is challenging and urgent, as these materials can make essential contributions to the energy crisis and global warming by directly converting heat to electricity. The dimensionless thermoelectric figure of merit $ZT$, which determines the performance of thermoelectric materials [1, 2], can be written as

$$ZT = S^2\sigma T/(\kappa_\text{e} + \kappa_\text{L})$$

(1)

where $S$, $\sigma$, $T$, $\kappa_\text{e}$ and $\kappa_\text{L}$ are the Seebeck coefficient, electrical conductivity, absolute working temperature, and the electronic and lattice thermal conductivities, respectively. To attain a high $ZT$, a high power factor ($S^2\sigma$) and a low thermal conductivity ($\kappa = \kappa_\text{e} + \kappa_\text{L}$) is required. Unfortunately, the Seebeck coefficient and electrical conductivity are generally coupled to each other, and they are oppositely proportional to the carrier density. Therefore, an appropriate carrier density is neither too big nor too small, and can lead to the maximum power factor.

The narrow band-gap materials are potential for efficient thermoelectric applications [3]. Topological insulators, characterized by a full insulating bulk gap and gapless edge states [4, 5], share similar material properties with thermoelectric materials, such as heavy elements and narrow gaps. For example, bismuth-tellurium systems are both famous topological insulators [6] and good thermoelectric materials [7]. It has been demonstrated that the $ZT$ of topological insulators is strongly
size dependent, and can be improved to be greater than 1 by tuning the size parameter \[8\].

Recently, \(\text{BaSn}_2\) has been predicted to be a strong topological insulator \[9, 10\], which is composed of alternating buckled honeycomb Sn layers and flat triangular Ba layers. A topological band inversion occurs at high symmetry A point; this is different from known strong topological insulators which invert at the high symmetry \(\Gamma\) point. It is interesting and urgent to investigate thermoelectric properties of \(\text{BaSn}_2\). Another important cause is that \(\text{BaSn}_2\) contains buckled honeycomb Sn layers known as stanene, which has been realized via molecular beam epitaxy on a \(\text{Bi}_2\text{Te}_3\) substrate \[11\]. Stanene with buckled honeycomb structure like silicene \[12\] and germanene \[13\] has been also predicted to be a topological insulator, supporting a large-gap two-dimensional (2D) quantum spin Hall state \[14\].

The thermoelectric properties of Stanene have also been investigated \[8, 15\], and the corresponding room-temperature lattice thermal conductivity is \(11.6 \text{ W m}^{-1} \text{K}^{-1}\) \[15\]. It is also interesting to know whether Ba layers can produce reduced effects on lattice thermal conductivity.

Here, we investigate the thermoelectric properties of \(\text{BaSn}_2\), including both the electron and phonon parts. Calculated results show that the electronic transport coefficients along \(a\) and \(c\) axes exhibit strong anisotropy. At room temperature, the lattice thermal conductivity is \(1.77 \text{ W m}^{-1} \text{K}^{-1}\) along the \(a\) axis and \(1.54 \text{ W m}^{-1} \text{K}^{-1}\) along the \(c\) axis, which is lower than the \((11.6 \text{ W m}^{-1} \text{K}^{-1})\) of Stanene. This is also comparable or lower than those of good thermoelectric materials, such as lead chalcogenides and bismuth-tellurium systems. The additional result is that the structural stability of \(\text{BaSn}_2\) is proved by phonon dispersion and mechanical stability criterion within elastic constants. According to calculated \(ZT\) values, it is found that n-type doping may provide better thermoelectric performance.

The rest of the paper is organized as follows. In the next section, we shall describe computational details for first-principle and transport coefficient calculations. In section 3, we shall present the electronic structures and thermoelectric properties of \(\text{BaSn}_2\). Finally, we shall give our discussions and conclusion in the section 4.

2. Computational detail

A full-potential linearized augmented-plane-waves method within the density functional theory (DFT) \[16\] is employed to study electronic structures of \(\text{BaSn}_2\), as implemented in the package WIEN2k \[17\]. An improved Tran and Blaha’s mBJ exchange potential plus local-density approximation (LDA) correlation potential for the exchange-correlation potential \[18\] is employed to produce more accurate band gaps. The free atomic position parameters are optimized using GGA of Perdew, Burke and Ernzerhof (GGA–PBE) \[19\] with a force standard of 2 mRy a.u.\(^{-1}\). The full relativistic effects are calculated using the Dirac equations for core states, and the scalar relativistic approximation is used for valence states \[20–22\]. The SOC was included self-consistently by solving the radial Dirac equation for the core electrons and evaluated by the second-variation method \[23\]. The convergence results are determined using 6000 k-points in the first Brillouin zone for the self-consistent calculation, making a harmonic expansion up to \(l_{\max} = 10\) in each of the atomic spheres, and setting \(R_{\text{cut}} \times k_{\max} = 8\) for the plane-wave cut-off. The self-consistent calculations are considered to be converged when the integration of the absolute charge-density difference between the input and output electron density is less than 0.0001\(e\) per formula unit, where \(e\) is the electron charge. Based on the results of electronic structure, transport coefficients for the electron part are calculated through solving Boltzmann transport equations within the constant scattering time approximation (CSTA), as implemented in the BoltzTrap \[24\], which shows reliable results in many classic thermoelectric materials \[25–27\]. To obtain accurate transport coefficients, we set the parameter LPFAC for 10, and use 32000 k-points \((35 \times 35 \times 25\) k-point mesh\) in the first Brillouin zone for the energy band calculation. The lattice thermal conductivities are performed by using Phono3py+VASP codes \[28–31\]. For the third-order force constants, \(2 \times 2 \times 2\) supercells are built, and reciprocal spaces of the supercells are sampled by \(4 \times 4 \times 3\) meshes. To compute lattice thermal conductivities, the reciprocal spaces of the primitive cells are sampled using the \(20 \times 20 \times 19\) meshes.

3. Main calculated results and analysis

\(\text{BaSn}_2\) crystallizes in \(\text{EuGe}_2\)-type hexagonal structures with space group being \(P\bar{3}m1\) (No.164), which is composed of alternating buckled honeycomb Sn and flat triangular Ba layers (see figure 1.). According to stacking of Sn, the Sn layer is actually a famous stanene \[11\], a monolayer with buckled honeycomb structure like silicene and germanene \[12, 13\]. In our calculations, the experimental values \((a = 4.652 \text{ Å}, c = 5.546 \text{ Å})\) \[2\] are used for \(a, b\), and \(c\), and the free atomic position of Sn is optimized within GGA–PBE. The optimized position of Sn \((1/3, 2/3, 0.107)\) is in good agreement with the experimental value of Sn \((1/3, 2/3, 0.103)\). An improved mBJ exchange potential is employed to investigate electronic structures of \(\text{BaSn}_2\), which is superior to GGA and LDA for gap

\[2\] The experimental crystal structure is attained from the Inorganic Crystal Structure Database (ICSD).
calculations. \(\text{BaSn}_2\) is predicted to be a topological insulator \([9, 10]\), so SOC is included for the electron part. The energy band structures of \(\text{BaSn}_2\) using both mBJ and mBJ + SOC are plotted in figure 2. It is found that SOC has observable effects on energy bands around the high symmetry A point. The mBJ results show that the valence band extrema (VBE) and conduction band extrema (CBE) along the H-A line almost coincide, while a gap of 156 meV is produced with mBJ + SOC. Notably, \(\text{BaSn}_2\) contains many CBE with their energies being very close, which is beneficial for high Seebeck coefficients \([1]\).

The transport coefficients for the electron part, including the Seebeck coefficient and electrical conductivity, are carried out using the CSTA Boltzmann theory. The Seebeck coefficients as a function of doping level (N) along a and c axes are plotted in figure 3. At room temperature (300 K), transport coefficients as a function of doping level (N) along a and c axes: Seebeck coefficient \(S\), electrical conductivity with respect to scattering time \(\sigma \tau\), power factor with respect to scattering time \(S^2/\sigma \tau\) and electronic thermal conductivity with respect to scattering time \(\kappa /\kappa \tau\) calculated with mBJ and mBJ + SOC.
The Seebeck coefficient is independent of scattering time, while electrical conductivity is dependent on the scattering time. Within the framework of the rigid band approach, the doping level can be achieved by simply shifting the Fermi level, which is reasonable in the low doping level in many thermoelectric materials [32–34]. The doping level is defined as electrons (minus value) or holes (positive value) per unit cell. The n-type doping (negative doping levels) can be simulated by shifting the Fermi level into conduction bands, producing the negative Seebeck coefficient. When the Fermi level moves into valence bands, the p-type doping (positive doping levels) with the positive Seebeck coefficient can be achieved.

Due to the crystal symmetry of BaSn$_2$, the physical properties along $a$ and $b$ axes (the in-plane direction) are equivalent, which are different from those along the $c$ axis (the cross-plane direction), so we only show transport coefficients along $a$ and $c$ axes. At 300 K, the doping level dependence of the Seebeck coefficient $S$, electrical conductivity with respect to scattering time $\sigma/\tau$, power factor with respect to scattering time $S^2\sigma/\tau$ and electrical thermal conductivity with respect to scattering time $\kappa_0/\tau$ along the $a$ and $c$ axes using mBJ and mBJ+SOC are plotted in figure 3. It is found that SOC has an enhanced effect on the Seebeck coefficient, which can be explained by the fact that some VBE or CBE are more close to each other at the presence of SOC. However, SOC has a reduced influence on the electrical conductivity and electrical thermal conductivity. Calculated results show that SOC has a mildly improved effect on the power factor, except for n-type one along the $a$ axis in low doping. The n-type doping has a larger Seebeck coefficient than the p-type, which is because the numbers of CBE with adjacent energies are more than those of VBE, and then the n-type power factor is much larger than the p-type.

\begin{table}[h]
\centering
\begin{tabular}{cccccccc}
\hline
$C_{11}$ & $C_{12}$ & $C_{13}$ & $C_{14}$ & $C_{33}$ & $C_{44}$ & $B$ \\
\hline
71.89 & 31.81 & 23.39 & 12.46 & 43.10 & 27.91 & 36.63 \\
19.39 & 42.28 & 32.55 & 1.89 & 1.39 & 1.64 & \\
\hline
\end{tabular}
\caption{The calculated elastic constants $C_{ij}$, bulk modulus $B$, shear modulus $G$ and Young’s modulus $E_x$, $E_y$ (their unit: GPa); $B/G$ and anisotropy factor $A_1$, $A_2$.}
\end{table}

The anisotropy of the Seebeck coefficient along the $a$ and $c$ axes is tiny, while electrical conductivity shows strong anisotropy. The electrical conductivity along the $a$ axis is almost three times as large as the electrical conductivity along the $c$ axis, which implies that the in-plane direction is a much more conductive direction. The power factor and electrical thermal conductivity show the same anisotropy with electrical conductivity. It is observed that electrical thermal conductivity has similar trends with electrical conductivity, which is due to the Wiedemann–Franz law: $\kappa_0 = L\sigma T$, where $L$ is the Lorenz number.

The phonon band structure and density of states (DOS) of BaSn$_2$ using GGA–PBE are shown in figure 4. The unit cell of BaSn$_2$ contains one Ba and two Sn atoms, resulting in 3 acoustic and 6 optical phonon branches. The maximum optical frequency of 5.13 THz is comparable with the corresponding values of good thermoelectric materials, such as Bi$_2$Te$_3$ [35] (4.5 THz) and SnSe [36] (5.6 THz). The maximal acoustic vibration frequency in BaSn$_2$ is only 2.36 THz, which is beneficial to low thermal conductivities. It is found that the phonon dispersions are separated into two regions with a gap around 0.47 THz. According to projected DOS in Ba and Sn atoms, it can be noted that the lower (upper) part of phonon dispersions is mainly due to the vibrations of the heavy Ba (light Sn) atoms. Calculated results show that no imaginary frequency modes are produced, suggesting no structural instability at low temperatures for BaSn$_2$.

Based on the following mechanical stability criterion for a rhombohedral structure [38]:

\begin{equation}
C_{11} - |C_{12}| > 0 \tag{2}
\end{equation}

\begin{equation}
(C_{11} + C_{12})C_{33} - 2C_{13}^2 > 0 \tag{3}
\end{equation}

The phonon band structure and DOS of BaSn$_2$ using GGA–PBE.

Table 1. The calculated elastic constants $C_{ij}$, bulk modulus $B$, shear modulus $G$ and Young’s modulus $E_x$, $E_y$ (their unit: GPa); $B/G$ and anisotropy factor $A_1$, $A_2$. 

![Figure 4. Phonon band structure and DOS of BaSn$_2$ using GGA–PBE.](image-url)

![Figure 5. The lattice thermal conductivities of BaSn$_2$ along $a$ and $c$ axes using GGA–PBE.](image-url)

Table 2. Lattice thermal conductivities (Unit: W m$^{-1}$K$^{-1}$) of BaSn$_2$, lead chalcogenides [40] and bismuth-tellurium systems [41, 42] at 300 K.

| Material | PbS | PbSe | PbTe | Bi$_2$Te$_3$ | Sb$_2$Te$_3$ | Bi$_2$Se$_3$ |
|----------|-----|------|------|-------------|-------------|-------------|
| $\kappa_a$ | 1.69 | 2.9  | 2.0  | 2.5         | 1.6         | 2.4         |
| $\kappa_c$ | 2.4  | 1.34 | 1.6  | 2.5         | 1.6         | 2.4         |

The phonon band structure and DOS of BaSn$_2$ using GGA–PBE.
The $C_{ij}$ are five independent elastic constants, and the calculated values are listed in table 1. It is easy to conclude that these criteria are satisfied for $\text{BaSn}_2$, implying mechanical stability of $\text{BaSn}_2$. Based on calculated elastic constants $C_{ij}$, the bulk modulus $B$, shear modulus $G$, and Young's modulus $E_x$ and $E_z$ can be attained (table 1). The lattice thermal conductivity can be qualitatively correlated with Young's modulus $E$ and shear modulus $G$ [37], low $E$ and $G$ can produce low group velocities, giving rise to low lattice thermal conductivities. The predicted $E$ and $G$ implies that $\text{BaSn}_2$ should have low lattice thermal conductivity. $B/G$ can measure ductility and brittleness, and the critical value separating ductile and brittle materials is $\sim 1.75$ [38]. The calculated ratio is 1.89, indicating the ductile nature of $\text{BaSn}_2$. The anisotropy ratios can also be calculated by the following expressions:

$$A_1 = 2C_{44}/(C_{11} - C_{12})$$

$$A_2 = 4C_{44}/(C_{11} + C_{33} - 2C_{13})$$

The numeric values of $A_1$ and $A_2$ are 1.39 and 1.64, which are close to unity, suggesting relatively small anisotropy. The related data are also summarized in table 1. Moreover, it is very interesting that the elastic parameters of $\text{BaSn}_2$ are very close to those of the good thermoelectric material $\text{Bi}_2\text{Te}_3$ [25], which may mean they share similar lattice thermal conductivities.

Based on harmonic and anharmonic interatomic force constants, the lattice thermal conductivities of $\text{BaSn}_2$ can be obtained along the $a$ and $c$ axes as a function of temperature (figure 5). It is assumed that the lattice thermal conductivity is independent of the doping level, and typically goes as $1/T$, which can be found in many thermoelectric materials [27, 39]. It is found that the lattice thermal conductivity exhibits little anisotropy, where the lattice thermal conductivity along the $c$ axis is lower than that along the $a$ axis, which conforms to predicted Young's modulus $E_c < E_a$. The room-temperature lattice thermal conductivity is 1.77 $\text{W m}^{-1}\text{K}^{-1}$ along the $a$ axis and 1.54 $\text{W m}^{-1}\text{K}^{-1}$ along the $c$ axis, which is much lower than that of (11.6 $\text{W m}^{-1}\text{K}^{-1}$) of Stanene [15] due to Ba layers. The average lattice thermal conductivity $1.69 $\text{W m}^{-1}\text{K}^{-1}$ along three axes can match with ones of lead chalcogenides and bismuth-tellurium systems as classic thermoelectric materials [40–42], we summarize related lattice thermal conductivities in table 2. The lattice thermal conductivity of $\text{BaSn}_2$ is even lower than ones of conventional good thermoelectric materials except for $\text{Bi}_2\text{Se}_3$ and $\text{Bi}_2\text{Te}_3$. Such a
low lattice thermal conductivity implies that \( \text{BaSn}_2 \) may be a potential thermoelectric material.

Finally, we consider the possible efficiency of thermoelectric conversion based on calculated transport coefficients of electron and phonon parts. The power factor and electronic thermal conductivity with respect to scattering time \( \tau \) and \( \sigma \tau_S^2 \) and \( \kappa_e \tau \) along the \( a \) and \( c \) axes as a function of doping levels with temperatures at 300, 600 and 900 K (figure 6). To attain the figure of merit \( ZT \), an unknown parameter is scattering time \( \tau \). Calculating scattering time \( \tau \) from the first-principle calculations is difficult because of the complexity of various carrier scattering mechanisms. If some experimental transport coefficients are available, the scattering time can be attained by comparing experimental transport coefficients with calculated coefficients, such as electrical conductivity. Unfortunately, the related experimental transport coefficients of \( \text{BaSn}_2 \) are unavailable, and we use an empirical scattering time \( \tau = 10^{-14} \) s to estimate possible \( ZT \) values (a similar order of magnitude for scattering time of topological insulator \( \text{Bi Te}_2 \) is used in theoretical calculations [32]). The thermal conductivity \( \kappa = \kappa_e + \kappa_L \) and \( ZT \) along \( a \) and \( c \) axes as a function of doping level with temperatures at 300, 600 and 900 K are shown in figure 7. In n-type doping, the figure of merit along the \( a \) axis is always larger than the figure of merit along the \( c \) axis. In p-type doping, the \( a \) axis figure of merit is larger than the \( c \) axis figure of merit at low temperatures. The \( c \) axis figure of merit becomes larger with increasing temperature. It is found that n-type doping exhibits more superior thermoelectric performance than p-type doping due to more higher n-type power factor. The peak \( ZT \) along \( a \) and \( c \) axes and corresponding doping concentrations at three different temperatures for both n- and p-type are shown in table 3. It is found that the doping concentration of peak \( ZT \) increases with increasing temperature. In n-type doping, at 900 K, the \( a \) axis \( ZT \) is as high as 0.46, and 0.40 for the \( c \) axis \( ZT \). These results make us believe that \( \text{BaSn}_2 \) may be a potential thermoelectric material. Finally, the effect on \( ZT \) caused by different scattering times \( \tau \) are considered, and the related \( ZT \) along \( a \) and \( c \) axes as a function of doping level with the temperatures 300, 600 and 900 K are plotted in figure 8. With increasing scattering time \( \tau \), the \( ZT \) moves toward its upper limit, which can be expressed as \( ZT = S^2 \sigma T / \kappa_e \), neglecting lattice thermal conductivity. This can be explained by the relation \( ZT = ZT_e \times \kappa_e / (\kappa_e + \kappa_L) \). The \( \kappa_e \) equals \( \kappa_e / \tau \times \tau_e \), where \( \tau_e, \tau \) are true and empirical scattering time, respectively. The \( \kappa_e \) increases with increasing scattering time \( \tau \). When \( \kappa_e \) becomes larger, the \( ZT \) is closer to \( ZT_e \) due to \( \kappa_e / (\kappa_e + \kappa_L) \) being more close to one.
4. Discussions and conclusion

As is well known, energy band gap produces important effects on transport coefficients for the electron part. Narrow gaps with high carrier mobility favours high electrical conductivity [43], but gapless behavior leads to a vanishing Seebeck coefficient [44]. Seebeck coefficient and electrical conductivity are oppositely proportional to the carrier density. The electronic thermal conductivity is proportional to electrical conductivity using the Wiedemann–Franz law. So, an appropriate energy band gap is needed to attain high $ZT_\tau$, like $\text{Bi}_2\text{Te}_3$ (0.15 eV) [45], but the mBJ+SOC gap of $\text{BaSn}_2$ is only 0.065 eV. At 300 K, the best n-type Seebeck coefficient (about 150 $\mu$V K$^{-1}$) is much weaker than the p-type (about 300 $\mu$V K$^{-1}$) and n-type (about 250 $\mu$V K$^{-1}$) of $\text{Bi}_2\text{Te}_3$ [45], due to too small energy band gap. However, the narrow energy band gap induces high electronic conductivity for $\text{BaSn}_2$, which also indicates high electronic thermal conductivity. Due to high electrical conductivity, the average best n-type power factor (about $25 \times 10^{-14} \mu$W cm$^{-1}$ K$^{-2}$ s$^{-1}$) of $\text{BaSn}_2$ is larger than best p-type (about $15 \times 10^{-14} \mu$W cm$^{-1}$ K$^{-2}$ s$^{-1}$) of $\text{Bi}_2\text{Te}_3$ at room temperature [45]. In spite of higher power factors, the average best n-type $ZT_\tau$ (about 0.42, see figure 9) is lower than the best p-type (about 0.70) of $\text{Bi}_2\text{Te}_3$ at 300 K [46]; this is because of higher electronic thermal conductivity.

For gap calculations, mBJ is usually superior to GGA or LDA, but it may still underestimate the energy band gap of $\text{BaSn}_2$. So, $\text{BaSn}_2$ may have better thermoelectric performance. The energy band gap can also be tuned by strain. For example LaPtBi [46], when a stretched uniaxial strain is applied, it changes from a semimetal into a real topological insulator, achieving comparable thermoelectric performance with $\text{Bi}_2\text{Te}_3$ by an 8% stretched uniaxial strain. It is possible for $\text{BaSn}_2$ to achieve enhanced thermoelectric performance by strain. In [8], Xu et al pointed out that $ZT_\tau$ is no longer an intrinsic material property in topological insulators, but is strongly size dependent. The tuning size parameter can dramatically increase $ZT_\tau$, being significantly greater than 1. Here, we have ignored the gapless edge states contribution to conducting channels, which helps to great improve thermoelectric performance by tuning size parameter. Experimentally, it is possible to achieve further enhanced thermoelectric performance of $\text{BaSn}_2$ by tuning size parameter.

In summary, the thermoelectric properties of $\text{BaSn}_2$, including both electron and phonon parts, are investigated and based mainly on the reliable first-principle calculations. It was found that SOC has little influence on electronic transport coefficients. Calculated results show obvious anisotropy of power factor and electronic thermal conductivity between the in-plane and cross-plane directions, while a slight anisotropy of lattice thermal conductivity is observed. The low lattice thermal conductivity is predicted, and the average is 1.69 W m$^{-1}$ K$^{-1}$ at room temperature, which highlights the possibility for $\text{BaSn}_2$ as a potential thermoelectric material. From 600 K to 900 K, the n-type figure of merit $ZT_\tau$ is up to about 0.45 with empirical $\tau = 10^{-14}$ s by optimizing doping levels, and it is possible to achieve improved thermoelectric performance by strain and tuning size parameter experimentally. The present work may be useful to encourage further theoretical and experimental efforts to achieve high thermoelectric performance of $\text{BaSn}_2$.

Acknowledgments

This work is supported by the Fundamental Research Funds for the Central Universities (2015QNA44). We are grateful to the Advanced Analysis and Computation Center of CUMT for the award of CPU hours to accomplish this work.

References

[1] Pei Y, Shi X, LaLonde A, Wang H, Chen L and Snyder G J 2011 Nature 473 66
[2] Bell L E 2008 Science 321 1457
[3] Snyder G J and Toberer E S 2008 Nat. Mater. 7 105
[4] Hasan M Z and Kane C L 2010 Rev. Mod. Phys. 82 3045
[5] Qi X L and Zhang S C 2011 Rev. Mod. Phys. 83 1057
[6] Zhang H J, Liu C X, Qi X L, Dai X, Fang Z and Zhang S C 2009 Nat. Phys. 5 438
[7] Ko D K, Kang Y J and Murray C B 2011 Nano Lett. 11 2841
[8] Xu Y, Gan Z and Zhang S C 2014 Phys. Rev. Lett. 112 226801
[9] Young S M, Shao J P and Kolmogorov A N 2016 arXiv:1607.05234
[10] Shao J P, Beaufils C and Kolmogorov A N 2016 Sci. Rep. 6 28369
[11] Zhu F F et al 2015 Nat. Mater. 14 1020
[12] Hauge H I T et al 2015 Nano Lett. 15 5855
[13] Dávila M E et al 2014 New J. Phys. 16 095002
[14] Xu Y et al 2013 Phys. Rev. Lett. 111 136804
[15] Peng B et al 2016 Sci. Rep. 6 20225
[16] Hohenberg P and Kohn W 1964 Phys. Rev. 136 B864
[17] Kohn W and Sham L J 1965 Phys. Rev. 140 A1133
[18] Blaha P, Schwarz K, Madsen G K H, Kvasnicka D and Luitz J 2001 WIEN2k, An Augmented Plane Wave – Local Orbitals Program for Calculating Crystal Properties (Karlsruhe, Schwarz Technische Universität Wien, Austria)
[19] Tran F and Blaha P 2009 Phys. Rev. Lett. 102 226401
[20] Perdew J P, Burke K and Ernzerhof M 1996 Phys. Rev. Lett. 77 3865
[21] MacDonald A H, Pickett W E and Koelling D D 1980 J. Phys. C: Solid State Phys. 13 2675
[22] Singh D J and Nordstrom L 2006 Plane Waves, Pseudopotentials and the LAPW Method 2nd edn (New York: Springer)
[23] Kunes J, Novak P, Schmid R, Blaha P and Schwarz K 2001 Phys. Rev. B 64 153102
[24] Koepping D D and Harmon B N 1977 J. Phys. C: Solid State Phys. 10 3107
[25] Madsen G K H and Singh D J 2006 Comput. Phys. Commun. 175 67
[26] Huang B L and Kaviani M 2008 Phys. Rev. B 77 125209
[27] Xu L Q, Zheng Y P and Zheng J C 2010 Phys. Rev. B 82 195102
[28] Polliott K J, Singh D J, Auluck S, Saravanan M, Misra D K, Dhar A and Budhani R C 2012 Phys. Rev. B 86 155204
[29] Kresse G 1995 J. Non-Cryst. Solids 193 222
[30] Kresse G and Furthmüller J 1996 Comput. Mater. Sci. 6 15
[31] Kresse G and Joubert D 1999 Phys. Rev. B 59 1758
[32] Togo A, Chaput L and Tanaka I 2015 Phys. Rev. B 91 094306
[33] Scheidemann T J, Ambrosch-Draxl C, Thonhauser T, Togo A, Chaput L and Tanaka I 2015 Phys. Rev. B 91 155210
[34] Madsen G K H 2006 J. Am. Chem. Soc. 128 12140
[34] Gao X, Uehara K, Klug D, Patchkovskii S, Tse J and Tritt T 2005 Phys. Rev. B 72 125202
[35] Qiu B and Ruan X 2009 Phys. Rev. B 80 165203
[36] Carrete J, Mingo N and Curtarolo S 2014 Appl. Phys. Lett. 105 101907
[37] Kim W 2015 J. Mater. Chem. C 3 10336
[38] Shang S L, Sheng G, Wang Y, Chen L Q and Liu Z K 2009 Phys. Rev. B 80 052102
[39] Parker D and Singh D J 2010 Phys. Rev. B 82 035204
[40] Morelli D T and Slack G A 2006 High Thermal Conductivity Materials ed S L Shindé and J S Goela (New York: Springer)
[41] Toberer E S, Zevalkink A and Snyder G J 2011 J. Mater. Chem. 21 15843
[42] Springer Materials: The Landolt–Börnstein Database www.springermaterials.com/docs/index.html
[43] Mächler L, Casper F, Yan B, Chadow S and Felser C 2013 Phys. Status Solidi RRL 7 91
[44] Bilc D I and Ghosez P 2011 Phys. Rev. B 83 205204
[45] Shi H, Parker D, Du M H and Singh D J 2015 Phys. Rev. Appl. 3 014004
[46] Ding G Q, Gao G Y, Yu L, Ni Y and Yao K L 2016 J. Appl. Phys. 119 025105