Inertial effective mass as an effective descriptor for thermoelectrics via data-driven evaluation†

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Effective mass has been touted as an important descriptor in thermoelectric transport. Based on theoretical intuition, some reports demonstrate that low effective mass is preferable in thermoelectrics, while others propose that a large density of states effective mass for high Seebeck is the pathway to better thermoelectric materials. Leveraging on the available data from Materials Project, we present a data-driven conclusion that corroborates the central role of effective mass in high-throughput thermoelectric materials screening. The efficacy of the Fermi surface complexity factor in enhancing power factor is analyzed in relation to the effective mass for a large number of compounds. Here, we show that starting with a low inertial effective mass material, any changes in Fermi surface complexity factor will have a pronounced effect on its thermoelectric power factor and verify this strategy in recently discovered thermoelectric materials. This can be accomplished by employing band engineering using doping, or symmetry distortion, and starting with a base material that intrinsically possesses a low inertial effective mass.

Introduction

In order to make thermoelectric materials commercially viable for green energy harvesting and cooling applications, decades of efforts have been focused on improving the dimensionless figure of merit $zT = S^2 \sigma T / (\kappa_L + \kappa_e)$, where $S$, $\sigma$, $T$, $\kappa_L$, and $\kappa_e$ are the Seebeck coefficient, electrical conductivity, absolute temperature, and lattice and electronic contributions to the total thermal conductivity, respectively. A lot of these efforts are based on a heuristic approach, guided by chemical and physical understanding and intuition. However, little progress has been made in terms of pushing the $zT$ high enough for thermoelectrics to be workable for wide ranging applications, especially at ambient temperatures. Traditional experimental-based thermoelectric materials discovery is an arduous task due to a vast unexplored chemical space, exploring which is time and resource intensive. This is down to the fact that there are many interdependent parameters making up the $zT$, making it difficult to establish predictive guidelines with few independent descriptors, especially true in regards to the optimization of the electronic properties.1 The intricate interdependencies can be best illustrated by Mott’s formula for Seebeck coefficient and Drude model in the degenerate limit of carrier concentration (i.e. $n > 1 \times 10^{20}$ cm$^{-3}$):

$$S = \frac{8\pi^2 k_B^2 T}{3e\hbar^2} m^* \left(\frac{\pi}{3n}\right)^{2/3}$$

(1)

$$\sigma = ne\mu = \frac{ne^2 \tau}{m_e^*}$$

(2)

As both eqn (1) and (2) make up the numerator of $zT$, the Seebeck and electrical conductivity have an inverse relationship through the effective mass ($m^*$) and carrier concentration ($n$). While high effective mass and low carrier concentration translate to higher Seebeck, they reduce the electrical conductivity, and vice versa. Therefore, the carrier concentration needs to be optimized to maximize the power factor. On the other hand, the $m^*$ in Seebeck and the $m^*$ in electrical conductivity are not the same. The effective mass that contributes to Seebeck can be expressed as $m^*_s$, or Seebeck effective mass, while the effective mass that affects the electrical conductivity is $m^*_e$ (also defined as inertial effective mass, $m^*_i$). These two effective masses are related through:

$$m^*_s = \left(N_e^* K^* m_e^* \right)^{1/3}$$

(3)

Image 232x591 to 243x601
This relation was discussed extensively in recent work by Gibbs, et. al. \(^2\) \(N_v K^*\) in eqn (3) represents the Fermi surface complexity factor, which encompasses the effective contribution of both the effective valley degeneracy \(N_v\) as well as effective carrier pocket anisotropy \(K^*\). Consequently, it is arguable that ideal thermoelectric materials ought to possess high \(N_v K^*\) value, which translates to higher Seebeck for a particular value of electrical conductivity. The term \(N_v\) (effective valley degeneracy) is expressed in order to quantify the effective contribution from all carrier pockets at a given chemical potential \(i.e\.\) Fermi level at non-zero temperature and temperature, and hence represents the importance of band convergence in achieving high power factor.

The term \(K^*\) represents the effective anisotropy \(K^*\) is obtained from the averaged contribution of \(m^*_{\text{xx}}, m^*_{\text{yy}}\) and \(m^*_{\text{zz}}\,\) as shown in eqn (11) in ESI\(^{\dagger}\) of the Fermi surface of a carrier pocket. A highly symmetric/isotropic electronic band structure yields \(K^*\) close to unity. For instance, \(K^* = 1\) represents spherical Fermi pockets. On the contrary, low-dimensional electronic band structure generally results in high \(K^*\) value.\(^{\text{1-3}}\) Indeed, many high-performance thermoelectric compounds have been reported to possess \(K^* > 1.6-11\)

Together, \(N_v K^*\) represents an important electronic descriptor for thermoelectrics. In fact, for many scattering mechanisms such as acoustic deformation potential, optical deformation potential, strongly screened ionized impurities as well as intervalley scattering, band effective mass is also intrinsically linked to the scattering times: a higher band effective mass \(\text{(larger density of states)}\) at the band extrema typically translates to higher scattering \(\text{(and thus lower mobility)}\) of the mobile charge carriers as many states are available to scatter into.\(^{\text{12}}\) However, a lower inertial effective mass does not provide a higher Seebeck coefficient. Hence, an additional band at a different symmetry point in the crystal \(\text{(higher } N_v)\) within the Fermi-dirac distribution energy windows of transport can significantly enhance the Seebeck coefficient while maintaining low scattering \(\text{(thus high mobility)}\), therefore significantly enhancing the power factor.

The state-of-the-art data-driven efforts to discover compounds with high \(N_v K^*\) values was built on earlier efforts in high-throughput thermoelectric compounds screening using DFT and BoltzTraP\(^{\text{2,3,14}}\). Other efforts focused on band-structure as descriptor.\(^{\text{15}}\) While \(N_v K^*\) and band-structure are relatively robust electronic descriptors for thermoelectrics, their interdependence with the scattering times renders them less comprehensive. Thus, a simple and independent descriptor is vital to further constrain the chemical search space for screening purposes.

In this work, we report our data-driven approach that reveals the crucial role of the inertial effective mass \(m^*\). More importantly, we point out that the efficacy of tuning \(N_v K^*\) largely hinges on \(m^*\). Ultimately, we observe a strong correlation between power factor and \(m^*\), which provides a new paradigm that \(m^*\) in itself is a robust independent descriptor for electronic transport in thermoelectrics and semiconductors in general. We find that this is consistent with several reports on selected materials using deformation potential theory as well as electron-phonon averaging computations.\(^{\text{16-37}}\) As the database used for our analysis was obtained from Materials Project,\(^{\text{14,38}}\) it is important to take note of some assumptions made in the earlier works, which includes constant relaxation time \((10^{-14} \text{ s})\) that does not account for energy-dependent carrier scattering \((i.e.\ r = 0)\) and a rigid band, therefore, a carrier concentration-independent \(m^*\). Note that rigid band approximation is employed to simplify high throughput calculations. Caution must be taken while choosing the type of dopants as some types, particularly those that create resonant states near band edges, have been shown to alter the band structure appreciably.\(^{\text{19}}\)

In addition, we constrain our discussions to bulk polycrystalline thermoelectric properties since we perform averaging on thermoelectric properties in all directions \(\text{(see ESI\dagger)}\).\(^{\text{20}}\) It is noteworthy that in practical situations, some degree of texturing may be observed in bulk polycrystalline samples. For a more accurate averaging, this requires additional weight factors to be considered depending on the preferred orientation of a particular sample.

**Results and discussions**

As an extension to Gibbs et. al.\(^{\text{2}}\) where a list of \(\sim 2300\) cubic semiconductor compounds was considered, the importance of \(N_v K^*\) as an electronic descriptor is corroborated further in Fig. 1(a), which shows the correlation between \(N_v K^*\) and power factor for 1617 p-type and n-type compounds from all crystal structures, moving beyond the cubic crystal structure assumption. Thermoelectric transport properties as well as other fundamental physical properties was obtained from earlier works by Ricci et. al. as well as Matminer.\(^{\text{12,22}}\) The plot is represented at 300 K to emphasize near room-temperature applications. In addition, only data with energy above the convex hull of \(<0.03 \text{ eV per atom}\) \(\text{(in order to remove unstable compounds, }\sim 0.03 \text{ eV corresponds roughly to room temperature thermal energy)}\) and band gap ranging from 0.1 eV to 1.0 eV was presented due to the well-known discrepancies between DFT values and actual experimental values. The maximum power factor was estimated using linearized Boltzmann transport equations within the constant relaxation time approximation \((r \sim 10^{-14} \text{ s})\).

Some of the traditionally high performing thermoelectric compounds are also labelled, with most of them lying in the high \(N_v K^*\) region. Clear correlation can be observed between \(N_v K^*\) and maximum power factor, which lends credibility to Fermi surface complexity factor as an effective electronic transport descriptor. In addition, p-type compounds have systematically slightly higher power factor as compared to n-type counterparts, which can be associated with the generally higher valley degeneracy for p-type materials.\(^{\text{14}}\)

Fig. 1(b) shows the interdependencies of Seebeck coefficient and electrical conductivity through carrier concentration. The plot is divided into two regions: to the left and right of the peak power factor, respectively. At low carrier concentration, the power factor increases with increasing carrier concentration all the way until peak power factor is reached. Subsequently, the power factor decreases as carrier concentration increases, as
represented by the formula which was derived from Mott formula for highly degenerate semiconductors. It is important to take precaution that Mott formula is only accurate in the degenerate regime; for more accurate representation of thermoelectric transport, full Boltzmann transport equations should be used.

In order to search for high $N^*V$ compounds, it is important to understand the physical origin of both $N^*V$ and $K^*$ as well as possible correlation between these two parameters. In general, highly-symmetric crystal structures such as cubic tend to have high value of $N^*V$ due to the high level of carrier pocket multiplicity in each energy band. Fig. 2 illustrates the multiplicity of each energy band in face-centered-cubic structure, showing a high multiplicity band. (i.e. $\Delta$ band with $N_V = 6$, $L$ band with $N_V = 4$, and $\Sigma$ band with $N_V = 12$).

The effective anisotropy in the shape of carrier pockets in Fig. 2 can be represented by $K^*$. It is important to draw a distinction between crystal structure anisotropy and electronic band structure anisotropy. A highly anisotropic band structure does not necessarily require low-symmetry crystal structure. In fact, recent reports associate the types of chemical bonding to the anisotropy in the Fermi surface (i.e. a mixture of metallic and covalent bonding tends to result in increased anisotropy in the Fermi surface). Therefore, it is entirely plausible to have both high $N^*V$ (via high-symmetry crystal structure as well as band convergence) and high $K^*$ (via metavalent bonding).

Going further, we elucidate the importance of $m^*_c$ on the electronic transport properties in thermoelectrics, especially in relation to $N^*V K^*$. Fig. 3 illustrates $m^*_c$ as an effective avenue for power factor enhancement, together with band engineering tuning of $N^*V K^*$. In Fig. 3(a), the effective Seebeck coefficients for all compounds is plotted as a function of their effective $m^*_c$ at fixed temperature and carrier concentration ($T = 300$ K; $n = 1 \times 10^{20}$ cm$^{-3}$). The effective Seebeck coefficient and average conductivity for polycrystalline compounds can be calculated by...

Fig. 1 (a) Maximum power factor at optimal doping vs. Fermi surface complexity factor at 300 K for 1617 p-type and n-type compounds. $(S^2 \sigma)_{max}$ is expressed in ($\mu$W cm$^{-1}$ K$^{-2}$). (b) Plot of Seebeck, electrical conductivity, and power factor as a function of carrier concentration illustrating optimization of carrier concentration to yield peak power factor. The plot is divided into two regions by the dotted line: to the left and right of peak power factor, respectively. The dependency of power factor on carrier concentration is given in each side of the plot. In the left hand side equation, the exponent, $a$ represents the dependence of power factor on carrier concentration with value lies from 0 to 1.

Fig. 2 Illustration showing Fermi pockets for $\Delta$, $L$ and $\Sigma$ bands and their respective multiplicity, $N_V$ in FCC crystal structure.
assessing diagonal Seebeck and conductivity tensors (ESI†), which takes into account the contribution from crystal structure anisotropy.20 The solid lines represent Seebeck as a function of $m_\text{c}^*$ for $N'_c K^* = 1$ and $N'_c K^* = 10$. It is clear from this figure, contrary to Mott’s formula for Seebeck coefficient, that the relation between $S$ and $m_\text{c}^*$ is not linear. This is due to the fact that at $1 \times 10^{20}$ cm$^{-3}$ doping, some compounds are not in the highly degenerate region, especially for compounds that possess high Seebeck effective mass, $m_\text{c}^*$ (i.e. higher doping is required to shift the chemical potential energy into the band). Thus, an accurate description of the relationship between $S$ and $m_\text{c}^*$ is better represented by using Boltzmann transport equations, as applied in our case. An important ramification of the non-linear relationship between Seebeck and $m_\text{c}^*$ is that the power factor of compounds with low $m_\text{c}^*$ has more room to be enhanced via $N'_c K^*$, as illustrated by the size of the green arrows in Fig. 3(a). For instance, by increasing the $N'_c K^*$ value from 1 to 10, a more dramatic enhancement in Seebeck (1.98 times enhancement) can be achieved at low effective mass ($m_\text{c}^* = 1$) as compared to the enhancement (1.40 times enhancement) at high effective mass ($m_\text{c}^* = 5$) region. (This applies to a wide range of different carrier concentrations, as shown in Fig. S1 and S2†). In summary, low $m_\text{c}^*$ serves as an avenue for sensitive enhancement of power factor through band engineering. It is therefore, not a coincidence that reports on high-performing thermoelectricities and the enhancements achieved through doping or band engineering lie in the low $m_\text{c}^*$ region, as shown in Fig. 3(b).

From a band structure point of view, it is useful to examine the rate of change in $N'_c K^*$ as $n$ increases for different values of $m_\text{c}^*$. Fig. 4(a) shows the slope of $N'_c K^*/n$ as a function of $m_\text{c}^*$ at 300 K. The slope is calculated within carrier concentration range of $1 \times 10^{19}$ cm$^{-3}$ to $1 \times 10^{20}$ cm$^{-3}$. Details of the estimation of $N'_c K^*/n$ slope can be found in ESL†. Intuitively, the slope of $N'_c K^*/n$ represents the change in the effective number of bands participating in the electronic transport (and therefore the change in Seebeck effective mass) as a function of the change in carrier concentration (i.e. as chemical potential moves into conduction/valence band). $N'_c K^*/n$ is quantitatively equivalent to DOS (density of states) shape factor26 and energy differential of DOS.27 Note, these theoretical models assume a rigid-band approximation and experimentally the actual effective masses could be altered owing to dopant and defect-induced electronic states. Nevertheless, the slope of $N'_c K^*/n$ serves as a proxy to probe the “steepness” of the density of states, which has been demonstrated to be crucial in power factor enhancement, most often due to an enhancement in the Seebeck coefficient.22,28,29 Interestingly, $N'_c K^*$ was also found to be higher at low $m_\text{c}^*$ (Fig. S4† plotted at $1 \times 10^{20}$ cm$^{-3}$), which represents the “ease” with which the chemical potential shifts as carrier concentration changes, as illustrated in Fig. 4(b). At lower $m_\text{c}^*$, when extra carriers are injected into the system via doping, the change in the chemical potential is higher than that for a material with high $m_\text{c}^*$, explained by the Moss-Burstein effect.31 This then provides an opportunity to utilize more carrier pockets for the low $m_\text{c}^*$ material, therefore resulting in higher $N'_c K^*$ as higher doping is achieved. Therefore, in addition to providing the dramatic enhancement to power factor via $N'_c K^*$, low $m_\text{c}^*$ compounds also tend to provide a higher slope of $N'_c K^*/n$, which provides an extra dimension to enhance power factor via doping manipulation.

It is worth noting that some exceptions are also observed, as shown in the red box of Fig. 4(a). These compounds have high $N'_c K^*/n$ slope as well as high power factor (represented by the size of the symbols) despite having a wide range of inertial effective masses. The high power factor in these compounds is an anomaly as far as the trends are concerned, and we speculate that the highly complex crystal structures (mostly quaternary compounds) along with high $N'_c K^*$ values (ESI Table T1†) implies a large number of bands with similar energies lie near the band edge.
The overall role of $m^*_c$ in power factor is summarized in Fig. 5. Fig. 5(a) shows the correlation between $N^*_vK^*$ and $m^*_c$. Low $m^*_c$ tends to lead to high $N^*_vK^*$, which eventually leads to higher power factor, which is shown in Fig. 5(b) for optimally doped compounds as a function of $m^*_c$ for both p-type and n-type compounds at 300 K. At high $m^*_c$, the distribution of the power factor values is very narrow as compared to the distribution at low $m^*_c$. This reinforces the earlier evaluation that low $m^*_c$ is an effective avenue for enhancing power factor. The presence of many high performing compounds at low $m^*_c$
further corroborates this hypothesis. In addition, in the low $m^*_e$ region, besides some traditionally high performing compounds, some relatively rarely studied compounds are shown to have potentially high power factor.

A list of the top few promising compounds for both p-type and n-type with lowest $m^*_e$ and potentially high power factor (and $zT$) at 300 K are presented in Table 1 together with their corresponding mpid (materials project ID). To ensure sensitive power factor enhancement, only compounds $m^*_e$ below 0.25 are taken into account. The criteria $\frac{m^*_e}{m_e} < 0.25$ is chosen because an order of enhancement in $N^*_eK^*$ will result in at least a commensurate (or order or higher) enhancement in power factor. Only Sulfides, Selenides, and Tellurides based compounds are displayed in the table considering their relatively good potential for synthesis, as laid out in works by Chen, et.al. It is noteworthy that while some of these compounds may have low $m^*_e$ and favorable power factor, it is equally important to screen for low lattice thermal conductivity compounds, which is not quantitatively expressed in this study. However, conventional wisdom dictates that generally compounds with light elements tend to possess high lattice thermal conductivity due to larger acoustic phonon group velocities. Also, only compounds with average molecular weight $>100$ g mol$^{-1}$ are considered because most good thermoelectric compounds have average molecular weight above this level (high average molecular weight also partially correlates to reasonable band gap). Lastly, to further filter out less-promising compounds, only peak power factor with values larger than 10 $\mu$W cm$^{-1}$ K$^{-2}$ (corresponding to $zT$ of 0.1 at 300 K with thermal conductivity of 3 W mK$^{-1}$) are considered. The optimum power factor estimated here is just for qualitative purposes and does not reflect the true potential of a particular compound, which will depend on bandgap and optimized working temperature. The full dataset for both p-type and n-type compounds with average molecular weight higher than 100 g mol$^{-1}$ is provided in ESI Table T2,† which shows many traditionally high-performing compounds, lending credibility to our selection process.

Also, some of these compounds that possess low $m^*_e$ as well as reasonable power factor are from the ABX$_2$ system, some of those were shown to possess extremely low lattice thermal conductivity due to high degree of anharmonicity caused by the presence of lone pairs in this material class. Besides thermal conductivity, the dopability of certain compounds maybe limited in reality. To date, although it is possible to predict dopability accurately in relation to intrinsic and extrinsic defect chemistry, it still requires in depth domain knowledge. To a certain extent, dopability is inversely correlated to band gap (i.e. low band gap results in higher dopability, and vice versa), hence, it is reasonable in our selection process to limit the maximum band gap to 1.0 eV. Given these considerations, we conclude that the inertial effective mass is indeed a good descriptor towards further tunability of the power factor by band/strain engineering and/or crystal structure distortion. The caveat is that the data from Materials project lacks the information about scattering times, which will also depend upon the inertial effective mass, hence affecting the mobility. For acoustic phonon scattering, the deformation potential can provide a measure of the charge carrier scattering times. However the relationship between electron-phonon relaxation times and the inertial effective mass as well as deformation potential is still not well understood, although recent work on a large number of half-heusler compounds shows that crystal symmetry safeguards orbital interactions resulting in large mobilities. In addition to the acoustic phonon scattering that can be determined via the deformation potential, most thermoelectric compounds are of multivalent bonding nature, which has strong polar characteristics and consequently may

Table 1 List of 7 p-type and 5 n-type compounds with lowest $m^*_e$ ($m_e$) and high power factor (>10 $\mu$W cm$^{-1}$ K$^{-2}$). Interestingly, many of the top p-type compounds have experimentally synthesized and have been shown to have high thermoelectric performance. Additional filters such as band gap ranging from 0.1 eV to 1.0 eV was used and energy above the convex hull of <0.03 eV per atom have been applied to remove unstable compounds. Average molecular weight of >100 g mol$^{-1}$ is also applied. The power factor is estimated at 300 K for polycrystalline compounds, assuming relaxation time of $10^{-14}$ s. The material quality factor ($\beta_{SE}$) as well as thermal conductivity ($\kappa_{total}$) data were obtained from TE Design Lab database. Data from TE Design Lab. Alkali metal compounds are excluded.

<table>
<thead>
<tr>
<th>Compound</th>
<th>mpid</th>
<th>$m^*_e$ ($m_e$)</th>
<th>$(S\epsilon)^{max}$ ((\mu)W cm$^{-1}$ K$^{-2}$)</th>
<th>$\beta_{SE}$</th>
<th>$\kappa_{total}$ (Wm$^{-1}$ K$^{-1}$)</th>
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</thead>
<tbody>
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<td>p-type</td>
<td></td>
<td></td>
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<td>TiNiO$_3$</td>
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<td>0.08</td>
<td>29.5</td>
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<td>SnSe</td>
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<td>21.3</td>
<td>23.9</td>
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<td>2.51</td>
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result in non-negligible polar optical phonon scattering, especially at temperatures higher than the Debye temperature. Hence, future screening metrics will include both scattering times by electron-phonon interaction considerations, as well as $N_e^*K^*$ and $m_e^*$ as the comprehensive descriptors.

Conclusions

In conclusion, our data-driven study shows that the inertial effective mass is a crucial parameter that has profound impact on thermoelectrics performance and is a vital an electronic transport descriptor towards achieving high power factor, along with the previously studied $N_e^*K^*$ as well as puddling mold-like band structure.33 Starting from low $m_e^*$ compounds, aided by chemical intuition, experiments can be performed to dope compounds either to achieve band convergence or to provide low symmetry to high symmetry distortion, both of which will enhance the power factor.48 Furthermore, recent experimental studies that leverage upon magnetic interaction to tune effective masses as well as enhancing power factor adds an exciting possibility to engineer low $m_e^*$ compounds.44–46 Lastly, it has been demonstrated that it is also possible to tune the inertial effective mass by altering the atomic basis states using solid solutions.45

Conflicts of interest

The authors declare no competing financial interest.

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