Thermoelectric materials are capable to directly convert heat into electricity and vice versa, which have received intensive attention for energy harvesting and cooling applications.\cite{1–3} The dimensionless thermoelectric figure of merit (ZT) is defined as $\text{ZT} = S^2\sigma / (\kappa_{\text{lat}} + \kappa_{\text{ele}})/T$, where $S$, $\sigma$, $\kappa_{\text{lat}}$, $\kappa_{\text{ele}}$, and $T$ are Seebeck coefficient, electrical conductivity, lattice thermal conductivity, electronic thermal conductivity, and absolute temperature, respectively. For half of the century, ZT around the unit is regarded as the benchmark value in the thermoelectric community. Thanks to these recently developed strategies,\cite{4–8} nowadays ZTs close or above 2 have been experimentally realized in the group IV–VI chalcogenides, e.g., Pb(Se, Te) polycrystals\cite{9–16} and SnSe crystals,\cite{17,18} as well as some ionic copper chalcogenides.\cite{19,20} These newly discovered thermoelectric materials fulfill these selection rules recently proposed by Xiao and Zhao.\cite{21}

The numerator $S^2\sigma$ in the ZT equation, known as the power factor (PF), corresponds to the microscopic transport process of charge carriers and dominates the output power of thermoelectric devices in real applications in addition to the leg length.\cite{22,23} The conventional viewpoint is that both carrier concentration and electronic band structure codetermine the potential of experimentally measured power factor.\cite{24} Convergence of electronic bands, as one of the most important strategies, could achieve the maximization of power factor with the help of carrier concentration optimization.\cite{24–27} One promising approach is the manipulation of crystal structure toward higher symmetry, thereby possessing a higher band degeneracy and reducing the defect formation energy, in the targeted material. This, in turn, favorably or adversely affects the effective transport process of charge carriers in semiconductors. However, the significance of point defect chemistry has long been neglected or underestimated in the thermoelectric area.\cite{31–33} Recently, the persistent p-type conduction in Zintl phase Mg$_2$Sb$_2$ reflect the critical role of intrinsic point defects in thermoelectric properties.\cite{34,35}

Currently, PbTe is the most efficient thermoelectric for intermediate-temperature power generation.\cite{16,37} Considering the toxic problem of Pb element, GeTe, one of the analogs of PbTe, attracts renewed research attention for the replacement of PbTe.\cite{38–40} Due to the similarly beneficial band structure...
and strong phonon anharmonicity with PbTe arising from the same chemical bonding mechanism, comparable high peak ZTs =2 have continuously been reported in the system of GeTe. One important difference between these two compounds is that GeTe undergoes the structural phase transition from the low-temperature rhombohedral to the high-temperature cubic phase at a critical temperature around 700 K. The rhombohedral structure refers to a unit cell with parameters \( a = b = c \) and \( \alpha = \beta = \gamma \approx 90^\circ \), belonging to the hexagonal crystal family. It can be regarded as a slightly distorted rock-salt lattice along the [111] direction with an interaxial angle less than 90\(^\circ\). As the rhombohedral angle increases to 60\(^\circ\), GeTe approaches the cubic rock-salt lattice with interaxial angle close to 90\(^\circ\). Although the rhombohedral structure is a slightly distorted cubic packing, GeTe shows the intrinsically strong p-type conduction owing to the high-concentration Ge vacancies, as a result of the large population of the occupied antibonding state. Therefore, optimizing the carrier concentration by aliovalent dopants, e.g., Bi or Sb doping on the Ge site, can significantly enhance the thermoelectric performance. Very recently, Li et al. proposed a new perspective of tuning the crystal symmetry by Pb alloying and Bi doping to enable the convergence of the low-symmetry valence bands, which contributed to a record ZT =2 at 600 K for the rhombohedral phase. Similarly, some transition metals, e.g., Mn, Ti, and Cd, are also thought to be effective in reducing the valence band offset of rhombohedral phase, leading to the increased Seebeck coefficient. However, most of the previous work neglected the role of Ge vacancies in the properties optimization. The concentration of Ge vacancies plays an important role in carrier transport properties, affecting the doping effectiveness, doping limit, carrier mobility, etc. Tuning the structure and/or composition may alter the native formation energy of Ge vacancies and result in the different Ge-vacancies concentration. For instance, it is found that Cr doping significantly reduced the formation energy from 1.02 to \(-0.08 \) eV at the valence band maximum (VBM). As is known, suppressing the Ge vacancies is essential to ensure high charge carrier mobility that will be beneficial to achieve a high power factor. 

Herein, we provided a deep understanding of the relationship among the crystal symmetry, defect chemistry, and properties optimization in the rhombohedral GeTe. First principles calculations revealed the substantially reduced formation energy of Ge vacancies as the crystal symmetry approached cubic. Two key factors, namely, carrier concentration and rhombohedral distortion degree, were found to determine the potential power factor of rhombohedral GeTe-based materials, in which the dynamic change of Ge-vacancies concentration was first considered. We discovered that Sc doping was the most effective dopant to increase the power factor, the room-temperature value around 23.3 \( \mu \text{W cm}^{-1} \text{K}^{-2} \) higher than other dopants. The underlying mechanism for the achieved high power factor was due to the efficient optimization of carrier concentration without significantly affecting the rhombohedral distortion degree. Further Bi doping contributed to the reduced thermal properties and an ultrahigh average ZT =1.2 that surpassed the majority of the Pb-free GeTe system. 

Pristine GeTe possesses a high hole concentration close to \(10^{21} \) cm\(^{-3}\) owing to the intrinsic Ge vacancies. In order to understand the defect chemistry in rhombohedral GeTe (R-GeTe), the formation energies of these typical defects, including Te vacancy \( \text{V}_{\text{Te}} \), Ge vacancy \( \text{V}_{\text{Ge}} \), antisite defects \( \text{T}_{\text{Ge}} \), and \( \text{Ge}_{\text{Te}} \), are calculated based on density functional theory (DFT) calculations, as shown in Figure 1a. Two rhombohedral structures are considered in theoretical calculations. One is the original or perfect structure with the rhombohedral angle \( \alpha = \beta = \gamma \approx 57.802^\circ \) while the others are the less distorted or higher-symmetry structure with the increased rhombohedral angle degrees of 58, 58.5, 59, and 59.5, respectively. It is obvious that the Ge vacancy exhibits the lowest formation energy as the most possible native defect, even in the Ge-rich growth environment. More importantly, as the rhombohedral structure approaches cubic, the formation energy of Ge vacancy is substantially decreased, which becomes negative at the entire range of Fermi energy. It should be noted that there is almost no difference between rhombohedral angle degrees 59 and 59.5. This indicates that Ge vacancy spontaneously forms in the higher-symmetry rhombohedral structure, as revealed by the schematic diagram in Figure 1c. Since Ge vacancies significantly reduce the charge carrier mobility \( \mu_{\text{d}} \) and thereby deteriorate the power factor, this newly discovered crystal symmetry-defect chemistry relationship could be helpful to explain the unusual transport behavior and to rationally design higher-performance GeTe.

As a consequence of native Ge vacancies, most of previous studies utilized the aliovalent dopant on the Ge site to reduce the hole concentration, such as Bi, Sb, Sn, In, and transition metals (Ti, Cr, Cd, and Cu). Among them, some dopants also obviously contributed to modifying the structure symmetry from rhombohedral to cubic, represented by means of the increased interaxial angle \( \alpha \). Figure 2a summarizes the measurement data of temperature-dependent power factor in rhombohedral GeTe-based materials. Apparently, Sc doping is currently most effective to enhance the power factor at the rhombohedral-temperature range. The room-temperature power factor is about 23.3 \( \mu \text{W cm}^{-1} \text{K}^{-2} \) higher than twice the value of undoped GeTe. To elucidate the underlying mechanism of high power factor occurring in Sc doping, the contour plot of the room-temperature power factor as a function of interaxial angle \( \alpha \) and Hall carrier concentration \( n_{\text{H}} \) is displayed in Figure 2b. The X-ray diffraction (XRD) refinement results and the obtained lattice parameters of Sc doping are shown in Figure S1 and Table S1 in the Supporting Information, respectively. Generally, the optimum carrier concentration range is around 2 \( \times \) \(10^{20} \) cm\(^{-3}\), consistent with the previous estimation. The most important observation here is that the increased interaxial angle \( \alpha \) leads to the reduced power factor, which is contradicted to the conventional understanding of the symmetry engineering in GeTe. It has to be noted, however, that the previous studies do not take into account the simultaneously increased Ge-vacancies concentration during the structural change. As a result of the compromise between the optimized carrier concentration and the reduced charge carrier mobility from the increased Ge-vacancies concentration, the observed high power factor is confined in a relatively small range, indicated by the red color in Figure 2b. To further analyze the different doping behavior in detail, the interaxial angle...
Figure 1. The relationship between Ge-vacancies formation energy and rhombohedral distortion degree. a,b) Calculated low-energy intrinsic defects formation energies GeTe using the primitive cell of rhombohedral structure (rhombohedral degrees of \( a = b = \gamma = 57.802, 58, 58.5, 59, \) and \( 59.5 \)) as a function of Fermi energy at the Ge-rich and Te-rich environment, respectively. The Fermi energy equal to 0 is referenced to the valence band maximum (VBM). c) Schematic diagram of the spontaneous formation of Ge vacancies on increasing the interaxial angle.

Figure 2. Analysis and understanding of high power factor of Sc-doped GeTe by comparison with previous literature results of rhombohedral GeTe-based materials, including Ti doping,\(^{67}\) In doping,\(^{74}\) Bi doping,\(^{84}\) Ag doping,\(^{74}\) Cr doping,\(^{59}\) Mn alloying,\(^{65}\) Cd alloying,\(^{70}\) and Pb alloying.\(^{59}\) a) Temperature dependent power factor. b) Contour plot representation of the room-temperature power factor as a function of interaxial angle \( \alpha \) and Hall carrier concentration \( n_H \). c,d) Interaxial angle \( \alpha \) and Hall carrier concentration \( n_H \) as a function of alloying or doping concentration, respectively.
\( \alpha \) and Hall carrier concentration \( n_H \) as a function of alloying or doping concentration is shown in Figure 2c,d, respectively. To clearly display the different slope value, the calculated interaxial angle \( \alpha \) of each dopant in Figure 2c is after the normalization process by removing the difference of these starting points in each dopant curve. The original curve is presented in Figure S2 in the Supporting Information. It is surprising that all the reported dopants lead to increased interaxial angle, which needs to be further investigated for this structural change. Among them, Ti doping,\(^{67,68}\) Bi doping,\(^{61,64}\) and Sb doping\(^{71}\) substantially increase the interaxial angle while Pb alloying\(^{29}\) and Cd alloying\(^{69,70}\) slightly alter the interaxial angle. Sc doping lies in between these two ends. Here, it should be noted that Pb or Cd alloying could not optimize the carrier concentration efficiently,\(^{29,69,70}\) leading to the lower power factor. One representative feature of Sc doping is the effective optimization of carrier concentration in comparison to the other dopants. For example, Sc doping with 2 at\% (atomic percentage) significantly reduced the hole concentration from \( 8.6 \times 10^{20} \) cm\(^{-3} \) for pristine GeTe to \( 3.2 \times 10^{20} \) cm\(^{-3} \), as shown in Table S1 in the Supporting Information. The reason of Sc as a good n-type dopant in GeTe is due to the following triple roles: First, the electron configuration of Sc element usually possesses the valence state of 3+, as the electron donor effect when substituting on the Ge site. Second, Sc doping slightly increases the interaxial angle. Third, Sc doping itself does not significantly reduce the formation energy of Ge vacancy. Both of them means that Sc doping would not obviously alter the concentration of Ge vacancies, ensuring the high doping effectiveness.

Previous discussions are based on the fact that Sc doping does not significantly affect the electronic band structure. To thoroughly elucidate the effect of Sc doping, their corresponding electronic band structure and density of states (DOS) are calculated by DFT calculations. Figure 3a,b compares the band structure and DOS between supercell R-Ge\(_{27}\)Te\(_{27}\) and supercell R-Ge\(_{26}\)Sc\(_1\)Te\(_{27}\), respectively. After Sc doping, the

**Figure 3.** The calculated electronic band structure and DOS of R-GeTe and Sc-doped R-GeTe. a,b) Comparison of band structure and DOS between supercell R-Ge\(_{27}\)Te\(_{27}\) and supercell R-Ge\(_{26}\)Sc\(_1\)Te\(_{27}\), respectively. c,d) The unfolded band structure of R-Ge\(_{27}\)Te\(_{27}\) and R-Ge\(_{26}\)Sc\(_1\)Te\(_{27}\), respectively. The plot size in the band structure reflects the unfolded spectral weight.
curvatures of valence band maximum at $F$ point show no clear change while the band offset between the secondary (and third) valence band edge and VBM is enlarged by 0.08 eV. However, considering the high hole concentration of GeTe, i.e., the Fermi level into the valence band, as well as the thermal broadening of the Fermi distribution, the slight change of relative position of these three valence bands would not impact the transport properties. The unfolded band structures in the primitive cell of pristine and Sc-doped rhombohedral GeTe are displayed in Figure 3c,d, respectively, to recover the electronic states satisfying the translation symmetry of the primitive cell. The same conclusion that Sc doping would not significantly alter the band structure can be more conveniently obtained. This observation is distinct from some transition-metal dopants, like Mn$^{65,66}$ and Cd$^{69-71}$ in rhombohedral GeTe that lead to the obvious converged valence bands and largely enhance the overall DOS. From the orbital projection of the Sc states, we find the main orbital contribution of Sc near the bandgap comes from its 3d orbitals, but they are located within a 1 eV window above the conduction band minimum (Figure S3, Supporting Information), therefore small influence for the p-type transport. In addition, the effect of Sc doping on the defect formation energy of Ge vacancy at both Ge-rich and Te-rich condition is also theoretically investigated. It was found that Sc doping also reduces the defect formation energy of Ge vacancy, but not significantly (Figure S4, Supporting Information). It should be noted that there is almost no difference between rhombohedral angle degrees 59 and 59.5.

Figure 4 shows the electrical transport properties of Sc-doped samples and also compares them with other representative

![Figure 4](image)

Figure 4. Electrical transport properties in rhombohedral GeTe-based materials. a,c,e) Temperature dependent electrical resistivity $\rho$, Seebeck coefficient $S$, and power factor PF of Ge$_{1-x}$Sc$_x$Te ($x = 0, 0.02, 0.04, 0.06,$ and 0.08), respectively. b,d,f) Room-temperature hall carrier mobility $\mu_H$, Seebeck coefficient $S$, and power factor PF as a function of hall carrier concentration $n_H$ in rhombohedral GeTe-based materials, including Sc doping, Sb doping, and Ge$_{1+x}$Te from Li et al.$^{73}$ Cu doping from Bu et al.$^{73}$ as well as Cu doping from Xie et al.$^{54}$ The solid lines in (b) and (f) are included to guide the eye whereas the solid and dashed lines in (d) represent the modified two-band model$^{73}$ and the single parabolic band (SPB) model calculations, respectively.
dopants in GeTe. Sc doping increases the electrical resistivity $\rho$ with almost the same temperature dependence (Figure 4a). As above-mentioned, this is due to the significantly decreased carrier concentration after Sc doping. Nevertheless, the charge carrier mobility still shows the increased tendency (Figure 4b), which may be related to the microstructural modulation, e.g., Ge precipitates,[50,53] Ge-vacancies thin layer,[54] and nanoscale domains,[50,52,72] to reduce the grain boundary scattering for charge carriers. Compared to other dopants, the unusual high values of the charge carrier mobility of Sc-doped samples are caused by the weak scattering from fewer Ge vacancies. This can be qualitatively understood by the abovementioned slight variation of the interaxial angle. The critical role of Sc doping on charge carrier transport is similar to Cu doping from Bu et al.[51] and Xie et al.[54] Although their data look somewhat different. Indeed, the superior properties obtained by Sc doping and Cu doping represent the inherently high potential of rhombohedral GeTe.

Figure 5. Thermoelectric properties of rhombohedral GeTe with Sc and Bi codoping. a–c) Temperature dependent power factor $PF$, total thermal conductivity $\kappa_{\text{tot}}$, and ZT of $\text{Ge}_{0.94-x}\text{Bi}_x\text{Sc}_{0.06}\text{Te}$ ($x = 0, 0.04, 0.06$, and $0.08$), respectively. d) Comparison of average ZT at the entire measured temperature range in advanced GeTe-based materials, containing Pb-free and Pb-alloying two main categories.[29,43,44,48,51,65,66,77]

The enhanced total effective mass originating from the converged valence bands,[59,65–67,76] Since Sc doping efficiently optimizes the carrier concentration and concurrently enhances the charge carrier mobility, power factor $PF$ largely increases at the rhombohedral-temperature range (Figure 4e). For instance, room-temperature $PF$ increases from 10.4 $\mu$W cm$^{-1}$ K$^{-2}$ for GeTe to 23.3 $\mu$W cm$^{-1}$ K$^{-2}$ for $\text{Ge}_{0.94}\text{Sc}_{0.06}\text{Te}$. It should be noted that the worsened properties of $\text{Ge}_{0.92}\text{Sc}_{0.08}\text{Te}$ was caused by the appearance of impurity phase $\text{Sc}_2\text{Te}_3$ due to the limited solid solubility of Sc in the lattice (Figure S5, Supporting Information). At the same carrier concentration range, both Sc doping and Cu doping exhibit a higher power factor than the other dopants (Figure 4f), originated from the abovementioned dual roles. These high-temperature properties are out of our current discussion due to the rhombohedral to cubic phase transition that may lead to the appearance of increased carrier concentration and/or bipolar effect.

Although Sc doping largely enhances the power factor, the total thermal conductivity $\kappa_{\text{tot}}$ still maintains at the relatively high level (Figure 5a; Figure S6, Supporting Information), mainly due to the high electronic thermal conductivity $\kappa_{\text{ele}}$ (Figure S6, Supporting Information). Lorenz number ($L$) is estimated based on a SPB model approximation with acoustic phonon scattering and the detailed information can be found in Figure S7 in the Supporting Information. In addition, the calculated lattice thermal conductivity $\kappa_{\text{lat}}$ shows the negligible reduction as the small difference between atomic mass and radius of Sc and Ge leads to the weak scattering from mass fluctuation and the related strain fluctuation (Figure S6, Supporting Information). The reduction of $\kappa_{\text{tot}}$ predominantly arises from the decreased $\kappa_{\text{ele}}$ due to the increased $\rho$. In this scenario, Bi
doping, known as a good dopant to enable the large reduction of carrier concentration and obvious suppression of thermal conductivity,[61,64,66] was further utilized to enhance ZT. After Bi doping, the total thermal conductivity shows further suppression (Figure 5a). Moreover, the lattice thermal conductivity was further reduced to a certain extent after Bi doping as a result of the strong point defect scattering (Figure S8, Supporting Information). However, Bi doping simultaneously induces a gradual decrease of power factor (Figure 5b). For instance, the room-temperature power factor decreases down to 16.8 μW cm⁻¹ K⁻² for Ge₀.₉₈Sc₀.₀₆Bi₀.₀₆Te, around two-thirds of Ge₀.₉₄Sc₀.₀₆Te sample. The lower power factor after Bi doping is because n₁₁ is a little out of optimized range together with the increased inter-axial angle. The corresponding electrical resistivity and Seebeck coefficient can be found in Figure S8 in the Supporting Information. Thanks to the substantially suppressed total thermal conductivity, Bi doping further enhances ZT at the entire measured temperature range (Figure 5c). The highest average ZT calculated by the integral method from 300 to 723 K is significantly boosted to 1.2, which surpasses the majority of Pb-free GeTe system and even can be comparable to some composition with heavily Pb alloying (Figure 5d).[29,43,44,48,51,53,65,66,77] Pb alloying induces the phonon softening in addition to generating point-defect scattering, contributing to the higher ZT in comparison to Pb-free counterpart.[29,78] It is widely acknowledged that high average ZT at a wide temperature is beneficial for achieving a high thermoelectric conversion efficiency in real conditions.[20] Therefore, using the codoping of Sc and Bi contributes to further pushing the GeTe system for intermediate-temperature range power generation.

In conclusion, we provided new insights into the influence of rhombohedral distortion degree on the charge carrier transport in rhombohedral GeTe, in which DFT calculations revealed that the rhombohedral lattice closer to cubic counterpart led to the significantly decreased formation energy of Ge vacancies. Experimentally, a record-high power factor, e.g., the room-temperature value around 23.3 μW cm⁻¹ K⁻², at the rhombohedral range was realized by Sc doping. The corresponding mechanism is the dual role of Sc doping that efficiently reduces the carrier concentration without obviously affecting the rhombohedral distortion degree. Further Bi doping contributed to the reduced thermal properties and an ultrahigh average ZT =1.2 that surpassed the majority of the Pb-free GeTe system. Our studies not only provide the design principle for high-performance rhombohedral GeTe, but also unravel the hidden role of the relationship between crystal symmetry and defect chemistry in thermoelectrics that may be also applicable to other systems.

Supporting Information
Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest
The authors declare no conflict of interest.

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defect formation energy, Ge vacancies, germanium telluride, scandium doping, thermoelectric materials

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