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First-principles study on band structures and electrical transports of doped-SnTe

Xiao Dong^a, Hulei Yu^a, Wen Li^b, Yanzhong Pei^b, Yue Chen^{a,*}

^a Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong SAR, China

^b Key Laboratory of Advanced Civil Engineering Materials of Ministry of Education, School of Materials Science and Engineering, Tongji University, 4800 Caoan Road, Shanghai, 201804, China

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Abstract

Tin telluride is a thermoelectric material that enables the conversion of thermal energy to electricity. SnTe demonstrates a great potential for large-scale applications due to its lead-free nature and the similar crystal structure to PbTe. In this paper, the effect of dopants (i.e., Mg, Ca, Sr, Ba, Eu, Yb, Zn, Cd, Hg, and In) on the band structures and electrical transport properties of SnTe was investigated based on the first-principles density functional theory including spin–orbit coupling. The results show that Zn and Cd have a dominant effect of band convergence, leading to power factor enhancement. Indium induces obvious resonant states, while Hg-doped SnTe exhibits a different behavior with defect states locating slightly above the Fermi level.

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Keywords: Thermoelectric materials; SnTe; Band engineering; Doping

1. Introduction

The growing demand to search for alternative energy sources is becoming drastic due to the increasing awareness of greenhouse effect and global warming caused by conventional power generation. Thermoelectric materials, which enable the energy conversion from heat to electricity, have a great potential in sustainable energy industries. The conversion mechanism is based on the diffusion of mobile charge carriers in a material [1]. Metals typically have low Seebeck coefficients, while semiconductors are ideal thermoelectric materials due to their band structures and electrical transport properties. However, the efficiency is a great concern in thermoelectric applications. The development of nanostructured materials brought new concepts and inspired

approaches to improve the performance of thermoelectric materials [2,3]. Intensive studies were conducted and substantial progress was made in the past two decades [4].

Thermoelectric performance is characterized by a dimensionless figure of merit, i.e., $zT = S^2\sigma T / (\kappa_E + \kappa_L)$, where S is the Seebeck coefficient, σ is electrical conductivity, T is absolute temperature, κ_E is electronic thermal conductivity and κ_L is lattice thermal conductivity [5]. Previous studies to increase figure of merit (zT) mainly focused on minimizing the thermal conductivity. However, electronic thermal conductivity is related to the movements of electrons and holes, and it is in direct proportion to electrical conductivity σ ; hence more efforts are made to reduce the lattice thermal conductivity, which arises from phonons traveling through lattice. Many approaches, such as superlattice and nanostructure, were proved to be able to decrease lattice thermal conductivity, however, a lower limit exists [6]. Therefore, to effectively increase zT , the alternative path is to maximize the value of $S^2\sigma$, i.e., the power factor. For a given material, the Seebeck coefficient is determined by density of states (DOS) effective

* Corresponding author.

E-mail address: yuechen@hku.hk (Y. Chen).

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mass and carrier density. The electrical conductivity is determined by carrier density and carrier mobility which is related to electron scattering in imperfect crystal lattice and affected by effective mass [7]. To control these parameters, one can engineer the electrical transport properties by introducing doping elements.

The Seebeck coefficient and electrical conductivity interrelate in a contradiction way, where an increase in carrier density tends to decrease the Seebeck coefficient, yet to increase the electrical conductivity. The similar behavior exists for effective mass, where a large effective mass contributes more to the Seebeck coefficient but reduces carrier mobility, therefore reducing the electrical conductivity. Thus, it remains a challenge to settle the conflicting interrelated properties, in order to obtain the optimum value for the power factor.

Chalcogenides and skutterudites are two material categories that are most prominent in high efficiency thermoelectric applications. Skutterudites are considered as good candidates due to their “phonon-glass, electron-crystal” behavior. They are achieved by addition of filler atoms that reduce thermal conductivity, as well as provide more charge carriers [8,9]. Chalcogenide materials have been used in thermoelectric applications for a long time, where PbTe is most significantly involved. Approaches to improve the conversion efficiency of PbTe are widely studied, and one of the commonly used methods is band engineering [5,10–12]. PbTe demonstrates a significant enhancement of thermoelectric properties and is proved suitable for high-temperature applications, but the environmental impacts of its lead-containing nature result in the need of seeking an alternative material. Other chalcogenides have attracted attentions, among which SnTe has the same rock-salt structure and the similar band dispersions as PbTe [13,14].

Different routes have been considered to enhance the power factor $S^2\sigma$, with tailored electrical transport properties. The first route is to introduce resonant states [15], which refer to an impurity energy level appearing as a peak in the DOS near Fermi level. This effect can be achieved by tuning the doping elements and concentrations. Zhang et al. reported that for In-doped SnTe [16], a peak at band gap exists in the DOS, while it does not appear in Bi-doped SnTe. Resonant states result in a large DOS effective mass; thus they are beneficial to the enhancement of the Seebeck coefficients. The second route is band convergence [17]. Enhanced power factor is achieved in Cd [18] and Hg-doped SnTe [19] through the band convergence effect. Banik et al. reported that Mg enhances the thermoelectric efficiency of SnTe *via* similar modifications to the band structure [20]. He et al. demonstrated that Mn has a high solid solubility in SnTe and the doped system also exhibits band convergence behaviors [21]. In a recent study, the effects of coexisting doping atoms and Sn vacancies on the electrical transports of SnTe were investigated; it was found that the band structure of SnTe was slightly tuned by the Sn vacancies [22]. Wang et al. indicated that Eu does not enhance the thermoelectric properties of SnTe due to an unfavorable increase of carrier concentration [23].

Pei et al. demonstrated the band convergence effect on Se-doped PbTe using a two-valence band model [5]. In a two band system, band convergence represents the alignment of L band and Σ band; while the energy difference between two bands is decreased, it usually accompanies with an increase in band gap [24,25]. When two bands align, there is a local increase in DOS effective mass, resulting in an enhancement of the Seebeck coefficient at a given charge carrier concentration [17]. In addition, the total Seebeck coefficient in a two band model can be expressed as $S = (\sigma_1 S_1 + \sigma_2 S_2) / (\sigma_1 + \sigma_2)$, where S_1 , σ_1 and S_2 , σ_2 are the Seebeck coefficients and electrical conductivities of each valence bands. Electrical conductivity acts as a weight of the Seebeck coefficient in each band, therefore, the total Seebeck coefficient is usually dominated by the band that has a higher electrical conductivity. The electrical conductivity increases but the Seebeck coefficient decreases as the carrier density increases. Hence, the total Seebeck coefficient is closer to the smaller S of the two bands [5]. When the two bands converge, thus having the same Seebeck coefficient, the total S will maintain without being compromised by a high electrical conductivity [6].

In this paper, effect of dopants (i.e., Mg, Ca, Sr, Ba, Zn Cd, Hg, In, Eu and Yb) on the band structure and electrical transport of SnTe was investigated from first-principles calculations. Resonant states and band convergence were examined with spin–orbit coupling effects.

2. Computational details

First-principles calculations based on density functional theory are conducted. Band structure and DOS are calculated using VASP [26,27], where the Perdew-Burke-Ernzerh of generalized gradient approximation (GGA) method is applied [28]. The electrical conductivity and Seebeck coefficient with respect to charge carrier density are calculated based on the Boltzmann transport theory as implemented in BoltzTraP [29]. One Sn atom in a $3 \times 3 \times 3$ Rock-Salt supercell containing 54 atoms is substituted by the impurity to model the doped SnTe systems. The cut-off energy for plane wave basis is set to 350 eV. A Γ -centered Monkhorst-Pack [30] $4 \times 4 \times 4$ k-mesh is adopted to sample the Brillouin zone. For electrical transport calculations, the k-mesh is further increased to $9 \times 9 \times 9$. All the systems are fully relaxed before the calculations of electronic structures, in which spin–orbit coupling effects are included. For the systems doped with lanthanides, the f-electrons are treated implicitly and kept frozen in the atomic cores.

3. Results and discussion

Selected dopants in this study include Mg, Ca, Sr, Ba, Zn Cd, Hg, In, Eu and Yb. The effect of dopants on the band structure and electrical transport properties of SnTe was investigated.

a. SnTe:X (X = Zn, Cd)

Zinc and cadmium are taken from the group of transition metals. According to Tan et al. Cd doping enhances the Seebeck coefficient in SnTe *via* band convergence and increase of band gap [18]. From the study of Peng et al. [6], Zn-doped PbSe and Cd-doped PbSe demonstrated a higher power factor, compared to pure PbSe.

Fig. 1 shows the band structure and DOS of SnTe:X (X = Zn, Cd). By the contribution of dopant, an impurity state, which is isolated from the rest of the electronic bands, appears near the bottom of the conduction bands. As can be seen from the DOS, a sharp peak that corresponds to the impurity state arises in the doped systems at the edge of conduction bands. Also, band gap is enlarged with increased energy level of conduction band and decreased energy level of valence band at L point. In addition, the decrease of valence band maximum at L point, and the increase of Σ valence band energy result in a better band alignment.

The significant band convergence effects in the SnTe:X (X = Zn, Cd) systems may indicate a possible enhancement of the Seebeck coefficients. To further examine the doping effects on the electrical transport properties, we combined DFT band structures with the Boltzmann transport equations. The Seebeck coefficient, electrical conductivity and power factor of SnTe:X are plotted against charge carrier density at 300 K, where electrical conductivity and power factor are normalized over relaxation time τ . As relaxation time depends on various scattering mechanisms, the normalization relates doping effects on the electrical transport properties directly to the changes in band structures. As is expected, the Seebeck coefficients of SnTe:Zn and SnTe:Cd significantly increase,

compared to that of the pristine SnTe, originating from the band convergence effect. A reduction in the electrical conductivity was also observed in SnTe:X (X = Zn, Cd), which may be related to the increase of band gap. As the power factor $S^2\sigma$ is proportional to the square of the Seebeck coefficient, an overall increase in $S^2\sigma$ is realized in the doped systems.

b. SnTe:X (X = Mg, Ca, Sr, Ba)

The group of alkaline earth metals is a popular choice of dopants for IV–VI thermoelectric materials. Studies on PbTe suggested the existence of XTe (X = Mg, Ca, Sr, Ba) compounds reduces the lattice thermal conductivity [31]. The results of this group of elements could be particularly beneficial, as it may provide synergy effect that enhances power factor and reduces thermal conductivity.

Fig. 2 shows the band structures and DOS of SnTe:X (X = Mg, Ca, Sr, Ba). Clearly, this group of dopants behaves differently from Zn or Cd. The most significant changes in the band structures are found near the Γ point, particularly for Mg-doped SnTe. As the conduction and valence bands at the Γ point are relatively far from the Fermi level, their changes may not have obvious effects on the electrical transports. On the other hand, this group of doping elements has minor modifications to the band dispersions near the Fermi level, as can be seen from the band structures and DOS. The band gap, the valence band maximum at L point, and the Σ band energy are only slightly affected by these dopants. Therefore, it is anticipated that this group of dopants only have minor effects

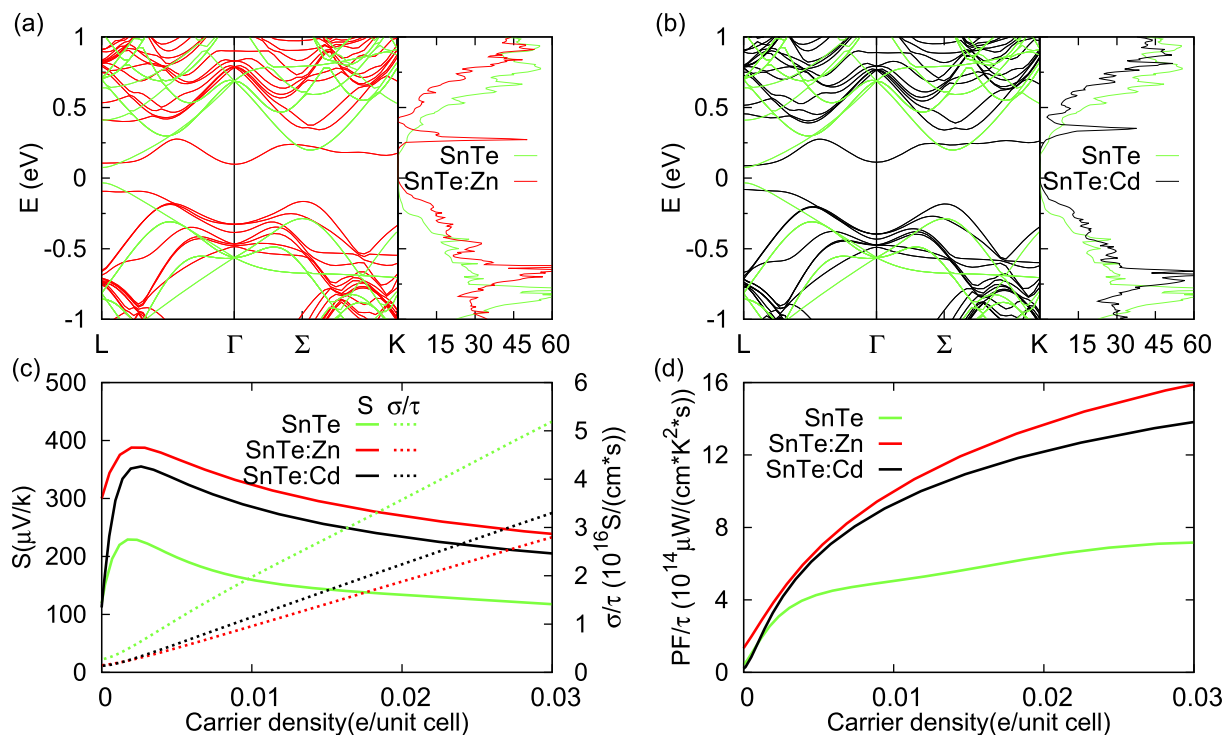


Fig. 1. Band structures and DOS of (a) SnTe:Zn and (b) SnTe:Cd. The Fermi level is located at 0 eV. (c) The Seebeck coefficients and normalized electrical conductivities by relaxation time (τ) at 300 K. (d) Normalized power factors at 300 K.

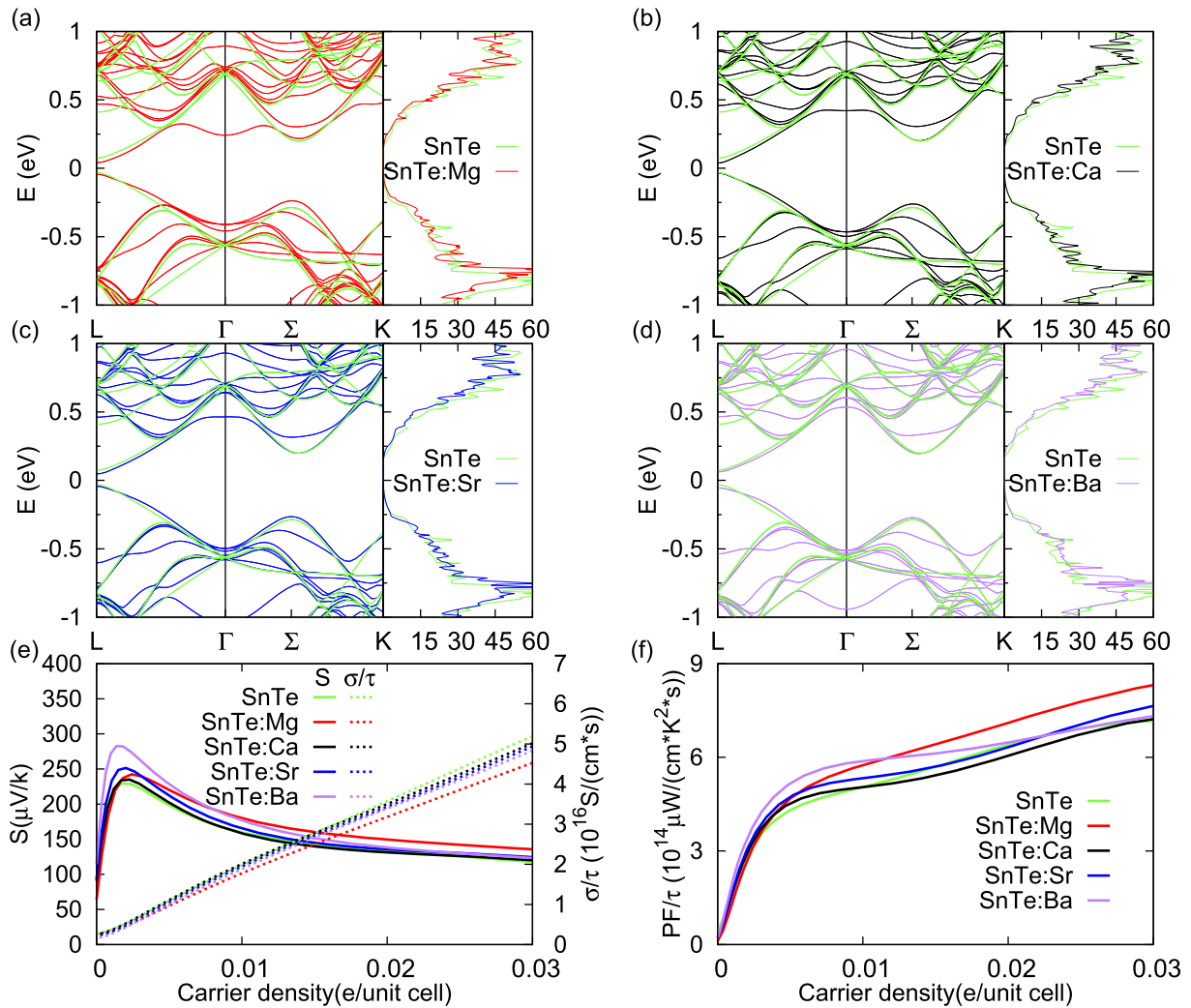


Fig. 2. Band structures and DOS of (a) SnTe:Mg, (b) SnTe:Ca, (c) SnTe:Sr, and (d) SnTe:Ba. The Fermi level is located at 0 eV. (e) The Seebeck coefficients and normalized electrical conductivities by relaxation time (τ) at 300 K. (f) Normalized power factors at 300 K.

on the electrical transport properties. This hypothesis is confirmed with further calculations based on the Boltzmann transport equations. Only minor changes in the Seebeck coefficients and electrical conductivities are observed after SnTe is doped.

c. SnTe:X (X = Eu, Yb)

Europium and ytterbium are lanthanides. They have been used as dopants in skutterudites, and showed enhancement of figure of merit [15]. Within the same group, La used as a dopant for PbTe, results in a modified band structure with a sharp peak in the DOS, which might be considered as resonant states [32].

Fig. 3 shows the band structures and DOS of SnTe:Eu and SnTe:Yb. Similar to the results of the alkaline earth dopants, the most significant changes in the band structures are found at the Γ point, where the conduction bands decrease while the valence bands increase in energy levels. Nonetheless, these bands are relatively far from the Fermi level and they do not

directly contribute to the electrical transports. The valence band maximum at L point and the Σ band energy level are only slightly affected by the dopants. In addition, no obvious change in the band gap is observed. Based on this analysis, it is anticipated that Eu and Yb do not have obvious effects on the electrical transport properties. The Seebeck coefficients and electrical conductivities of SnTe:Eu and SnTe:Yb at 300 K are calculated as functions of carrier density. It is confirmed that the electrical transport in SnTe is only slightly affected by these lanthanides.

d. SnTe:X (X = Hg, In)

The element Hg together with In, which is taken from the same group as Tl, are also included in this study. Tl-doped PbTe is a classic study that proves Tl is an effective dopant, which creates resonant states and increases the power factor [15]. Tan et al. suggested that doping In in SnTe also introduces resonant states in valence bands that enhance the Seebeck coefficient in a lower temperature region [33]. Peng

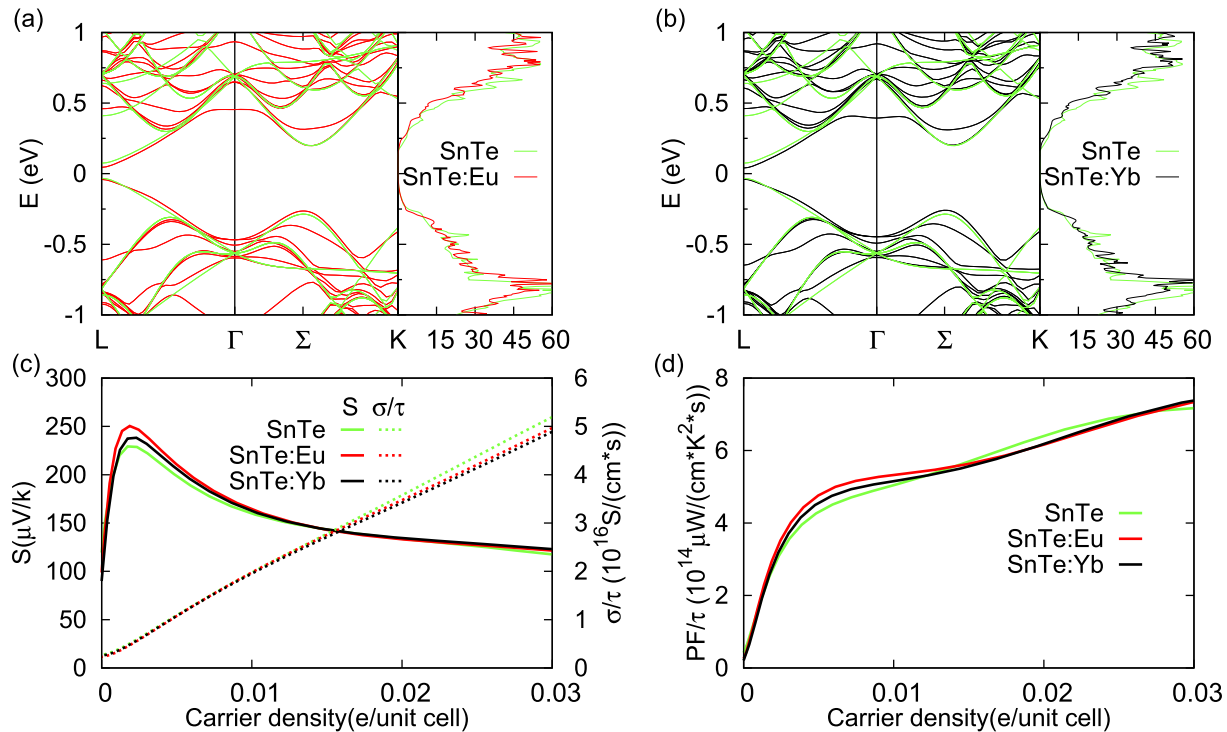


Fig. 3. Band structures and DOS of (a) SnTe:Eu and (b) SnTe:Yb. The Fermi level is located at 0 eV. (c) The Seebeck coefficients and normalized electrical conductivities by relaxation time (τ) at 300 K. (d) Normalized power factors at 300 K.

et al. pointed out that Hg and In-doped PbSe have impurity states from the valence bands penetrating through the conduction bands, thus they may be considered as metals, while more delicate investigations need to be carried out to confirm on the transport property changes [6].

Fig. 4 shows the results of SnTe:X ($X = \text{Hg}, \text{In}$). For SnTe:Hg, significant changes in the band structure are observed, compared to pristine SnTe. The Σ valence band and the conduction bands shift to higher energy levels, while a narrow impurity band lies in the band gap and overlaps with the Fermi level at K point. A relatively narrow peak slightly above the Fermi level, which corresponds to the impurity band, appears in DOS. Comparing SnTe:Hg to SnTe:Cd, which exhibits significant band convergence effects, we find that the impurity states in SnTe:Hg are closer to the top of the valence band. For SnTe:In, the effect of dopant on the band structure is similar to that of Hg except that the impurity states are even lower in energy. As a result, instead of creating a pseudo-gap in SnTe:Hg, an increase in DOS at the Fermi level is observed in SnTe:In, which is in agreement with that indium creates resonant states in SnTe [16].

To further investigate the doping effect on the electrical transport, the Seebeck coefficient, electrical conductivity and power factor were calculated. The transport properties of SnTe:Hg and SnTe:In are almost independent of charge carrier concentration. Both of the doped systems have Seebeck coefficients lower than that of pristine SnTe, while they have higher electrical conductivities. As a result, doping Hg or In into SnTe only enhances the power factor at 300 K in a low carrier concentration region. Nonetheless, the enhancement of

power factor becomes more significant at a high temperature due to the larger Seebeck coefficient (see Fig. 4 (e) and (f)).

In order to compare the band convergence effects of different dopants, we summarize the band gaps and energy differences between L and Σ bands ($\Delta E_{L-\Sigma}$) in Fig. 5. It is seen that, compared to pristine SnTe, $\Delta E_{L-\Sigma}$ is reduced in the doped systems, implying a better alignment of the L and Σ bands. In particular, Zn and Cd have the most significant band convergence effects. Also, most of the dopants have minor effects on the band gap, except Zn and Cd that cause an obvious increase in the band gap value. It is believed that a larger band gap is beneficial for the thermoelectric performance at a high temperature, as it limits the number of excited carriers to avoid rapid decline of the Seebeck coefficient [17].

4. Conclusions

The effects of ten impurity dopants from four different chemical groups on the band structure and electrical transport of SnTe were investigated using density functional theory with spin-orbit coupling. The results showed that Zn and Cd created the most significant band convergence effect and band gap enlargement, thus resulting in the enhancement of power factor. The alkali earth metals (i.e., Mg, Ca, Sr and Ba) and the lanthanides (i.e., Eu and Yb), however, only had minor effects on the band structures. For In-doped SnTe, an increase in the DOS at the Fermi level occurred, representing the typical resonant effects. Mercury created impurity states slightly higher in energy than indium, resulting in a pseudo-gap at the

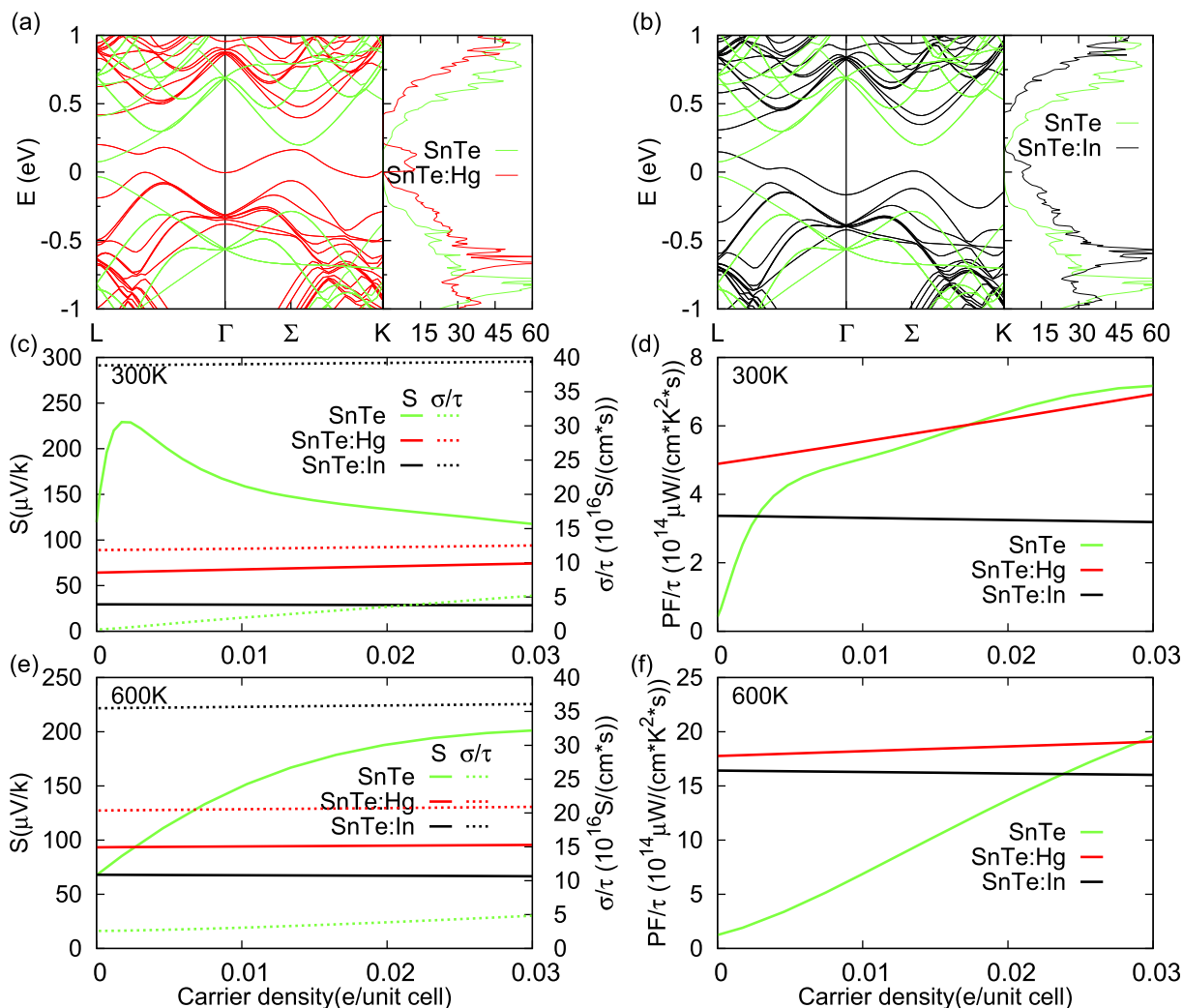


Fig. 4. Band structures and DOS of (a) SnTe:Hg and (b) SnTe:In. The Fermi level is located at 0 eV. (c) The Seebeck coefficients and normalized electrical conductivities by relaxation time (τ) at 300 K. (d) Normalized power factors at 300 K. (e) The Seebeck coefficients and normalized electrical conductivities at 600 K. (f) Normalized power factors at 600 K. Carrier density is relative to the value corresponding to unshifted Fermi level.

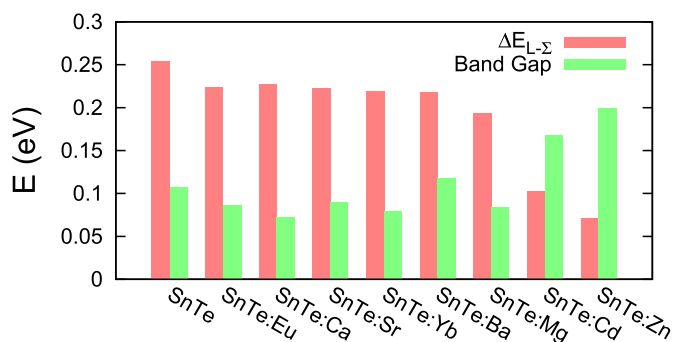


Fig. 5. Doping effect on the band gap of SnTe, and the energy differences between L and Σ bands.

Fermi level. It was believed that this work would inspire further experimental studies on SnTe, while it was worth noting that temperature and doping concentration might have significant effects on the band structure.

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Yue Chen is an assistant professor at the University of Hong Kong, Department of Mechanical Engineering. His research interests are focused on the materials physics for electrical and thermal transports, such as electronic structures and lattice dynamics. His interests stem from the studies of materials science at University of Oxford and Beihang University. He was a postdoctoral fellow at Columbia University and Institute of Metal research, Chinese Academy of Sciences before joining HKU.