

# Thermoelectric Properties of Metallic Antiperovskites $AXD_3$ (A=Ge, Sn, Pb, Al, Zn, Ga; X=N, C; D=Ca, Fe, Co)

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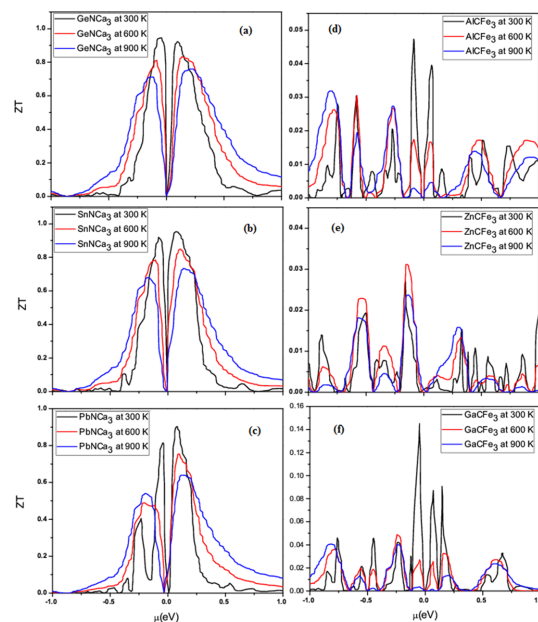
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In this paper we communicate the thermoelectric properties of carbon and nitrogen based metallic antiperovskites  $ANCa_3$  (A=Ge, Sn, Pb),  $BCFe_3$  (B=Al, Zn, Ga) and  $SnCD_3$  (D=Co and Fe) using the ab-initio calculations to explore efficient metallic thermoelectric materials. The consistency of the calculated results of  $SnCCo_3$  and  $SnCFe_3$  with the experimental results confirms the reliability of our theoretical calculations for the other investigated metallic antiperovskites. The results indicate that the thermopower of these materials can be enhanced by changing the chemical potential. The dimensionless figure of merit for the three nitrides approaches 0.96 at room temperature, which proves the usefulness of these materials in thermoelectric generators. Furthermore, the thermal conductivity is minimum at room temperature for chemical potential values between  $-0.25 \mu\text{eV}$  and  $0.25 \mu\text{eV}$ , and provides the maximum values of dimensionless figure of merit in this range. The striking feature of these studies is identifying a metallic compound,  $SnNCa_3$ , with the highest value of Seebeck coefficient at room temperature out of all metals. The results anticipate that these materials could be efficient in thermoelectric generators; however, this needs experimental verification.

**Keywords:** thermoelectric properties, metallic antiperovskites, electrical conductivity, ab-initio calculations, spin orbit coupling



## 1. INTRODUCTION

Energy is the resource used to exploit all other resources, with increasing demand in recent years because of population growth and industrial development. Over the past decade, there has been a keen interest in exploring efficient thermoelectric (TE) materials for power generation.<sup>[1]</sup> A sufficiently big quantity of heat is converted into useful energy in TE devices, which makes them a good source of green energy.<sup>[2]</sup> A key material parameter, related to efficiency is the dimensionless figure of merit,  $ZT = \sigma S^2 T / k$ , where  $\sigma$  is

the electrical conductivity,  $S$  is the Seebeck coefficient, and  $k = k_e + k_l$  is the thermal conductivity, composed of electronic and lattice parts.<sup>[3]</sup> Materials with  $ZT$  above unity are considered excellent candidates for TE applications.<sup>[4,5]</sup> TE generators have no moving parts so there is complete absence of friction in TE devices which makes them more environment-friendly.<sup>[6]</sup>

Antiperovskites have the general formula  $AXB_3$ , where A is a main group (III-V) element, X is carbon or nitrogen, and B is a transition (s-d) metal.<sup>[7,8]</sup> These materials usually crystallize in space group  $Pm\bar{3}m$  (221) where the A atom is located at (0, 0, 0), the X atom at (1/2, 1/2, 1/2) and B atom at (0, 1/2, 1/2).<sup>[9]</sup> Different research groups have investigated thermoelectric properties of various crystal structures like

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Skutterudites,<sup>[10]</sup> Clathrates,<sup>[11]</sup> Half-Heusler Alloys,<sup>[12]</sup> Chalcogenides,<sup>[13]</sup> Complex Oxide,<sup>[14,15]</sup> and Perovskites.<sup>[16,17]</sup> A variety of physical properties of antiperovskite structural compounds have been studied after the discovery of the first antiperovskite superconductor  $\text{MgCNi}_3$  in 2001.<sup>[18-30]</sup> However, there are very few reports available<sup>[31-35]</sup> on TE properties of antiperovskites. Very recently, Lin *et al.*<sup>[36]</sup> investigated TE properties of Cobalt based antiperovskites. The authors claim that the metallic antiperovskite  $\text{SnCCo}_3$  has the largest Seebeck coefficient of about  $50 \mu\text{V/K}$  at room temperature in the antiperovskite family.

High values of figure of merit are achieved in materials having large Seebeck coefficient. Literature clearly shows that there is a vast room for exploring TE properties of metallic antiperovskites. In this paper we study the density of states of  $\text{SnCCo}_3$ , the  $\text{ANCa}_3$  ( $\text{A}=\text{Ge}, \text{Sn}$  and  $\text{Pb}$ ) and the  $\text{BCFe}_3$  ( $\text{B}=\text{Al}, \text{Zn}, \text{Ga}$  and  $\text{Sn}$ ) antiperovskite materials. The effects of spin-orbit coupling (SOC) on the density of states are also explored. Using these results, we calculate the TE properties of these materials and discuss the effects of SOC on the TE properties. The calculated Seebeck coefficient of  $\text{SnCX}_3$  ( $\text{X}=\text{Co}$  and  $\text{Fe}$ ) match well with the experimental data.<sup>[36]</sup> There is no other experimental evidence available on the TE properties of these materials to the best of our knowledge. We predict high values of ZT for these materials. The TE properties of  $\text{ANCa}_3$  ( $\text{A}=\text{Ge}, \text{Sn}$  and  $\text{Pb}$ ) is enhanced due to SOC effects with highest absolute Seebeck coefficient of  $730 \mu\text{V/K}$  for  $\text{SnNCa}_3$  at room temperature whereas the TE properties diminish in  $\text{SnCCo}_3$  and  $\text{BCFe}_3$  ( $\text{B}=\text{Al}, \text{Zn}, \text{Sn}$  and  $\text{Ga}$ ) with the SOC. Until now, the metallic material  $\text{CePd}_3$  has had the highest experimentally reported Seebeck coefficient of  $125 \mu\text{V/K}$  among metals,<sup>[37,38]</sup> at 140 K. Therefore, we predict and report a new class of metals which show high Seebeck coefficient. Our results show that figure of merit of these materials can be enhanced at room temperature by changing chemical potential.

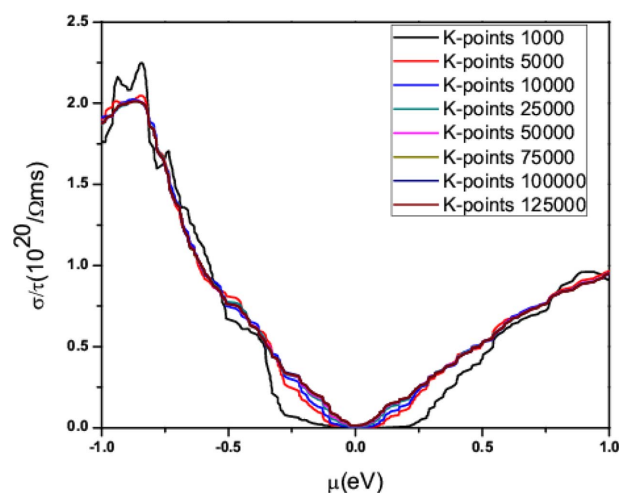
## 2. COMPUTATIONAL DETAILS

To calculate the electronic properties, we used the full potential linearized augmented plane waves (FP-LAPW) method, based on density functional theory<sup>[39,40]</sup> as implemented in WIEN2k.<sup>[41]</sup> The experimental values of lattice constants of these materials are taken from ref<sup>[36,42,43]</sup> and used as input

variables to calculate theoretical lattice constants. The calculated relaxed lattice parameters are then used to calculate the electronic properties of these compounds. The exchange-correlation effects for the electronic properties are treated by a generalized gradient approximation (GGA).<sup>[44]</sup> Our results show that all these materials are metallic in nature. Band structures of these materials show that there are dense electronic states at Fermi level, which play critical role in transport properties.

The separation energy between the core and valence states is kept  $-6.0 \text{ Ry}$ . The wave functions inside the atomic spheres in the full potential scheme for these materials are expanded in terms of spherical harmonics up to  $l_{\text{max}} = 10$ . The convergence parameter  $R_{\text{MT}}K_{\text{max}}$ , is set to 7. The plane wave cut off value for the charge density and potential is selected to be  $G_{\text{Max}} = 12 (\text{Ry})^{1/2}$ . 1000 k-points are used for electronic properties calculations within WBZ. The RMT's used for these materials are presented in Table 1.

The calculated electronic structures are further used to calculate thermoelectric properties like Seebeck coefficients, electronic thermal conductivities and electrical conductivities using the BoltzTraP code.<sup>[45]</sup> Kim *et al.*<sup>[46]</sup> have already shown that metallic phases need large number of k-points to ensure the convergence of the transport properties. Here, due to this important point, we first verify the convergence of our reported transport properties by plotting electrical conductivity



**Fig. 1.** Electrical conductivity for  $\text{PbNCa}_3$  at different k-points without SOC.

**Table 1.** RMT values for each element of  $\text{AlCFe}_3$ ,  $\text{GaCFe}_3$ ,  $\text{GeNCa}_3$ ,  $\text{PbNCa}_3$ ,  $\text{SnCCo}_3$ ,  $\text{SnCFe}_3$ ,  $\text{SnNCa}_3$  and  $\text{ZnCFe}_3$ .

| Compounds | $\text{AlCFe}_3$    | $\text{GaCFe}_3$     | $\text{GeNCa}_3$    | $\text{PbNCa}_3$    | $\text{SnCCo}_3$    | $\text{SnCFe}_3$     | $\text{SnNCa}_3$    | $\text{ZnCFe}_3$    |
|-----------|---------------------|----------------------|---------------------|---------------------|---------------------|----------------------|---------------------|---------------------|
| Elements  | Al C<br>Fe          | Ga C<br>Fe           | Ge N<br>Ca          | Pb N<br>Ca          | Sn C<br>Co          | Sn C<br>Fe           | Sn N<br>Ca          | Zn C<br>Fe          |
| RMT's     | 2.21<br>1.48<br>1.9 | 2.32<br>1.47<br>1.89 | 2.5<br>2.07<br>2.18 | 2.5<br>2.16<br>2.27 | 2.4<br>1.49<br>1.91 | 2.46<br>1.52<br>1.96 | 2.5<br>2.15<br>2.26 | 2.42<br>1.5<br>1.92 |

versus chemical potential for various number of k-points. Figure 1 presents electrical conductivity for different k-points for PbNca<sub>3</sub> without considering spin-orbit coupling effects. Our results show that 100000 k-points are suitable for providing an acceptable accuracy for transport properties calculations, since the curve obtained by 125000 k-points follows the trend of 100000 k-points. Therefore, for the transport properties of all the compounds we used 100000 k-points within WBZ. The transport coefficients based on the rigid band approach to conductivity are explained by using equation (1) as given below:

$$\sigma_{\alpha\beta}(\varepsilon) = \frac{1}{N} \sum_{i,k} \sigma_{\alpha\beta}(i,k) \frac{\delta(\varepsilon - \varepsilon_{i,k})}{\delta(\varepsilon)} \quad (1)$$

$$\sigma_{\alpha\beta}(i, \vec{k}) = e^2 \tau_{i,k} v_{\alpha}(i, \vec{k}) v_{\beta}(i, \vec{k}) \quad (2)$$

where  $N$  is the number of k-points. Equation 2 explains k-dependent transport tensors, where  $\tau$  is the relaxation time, and  $v_{\alpha}(i, \vec{k})$  is a component of group velocities. Transport coefficients, which are a function of temperature ( $T$ ) and chemical potential ( $\mu$ ), i.e. electrical conductivity and Seebeck coefficient tensors, can be found by integrating the transport distribution:<sup>[45,47]</sup>

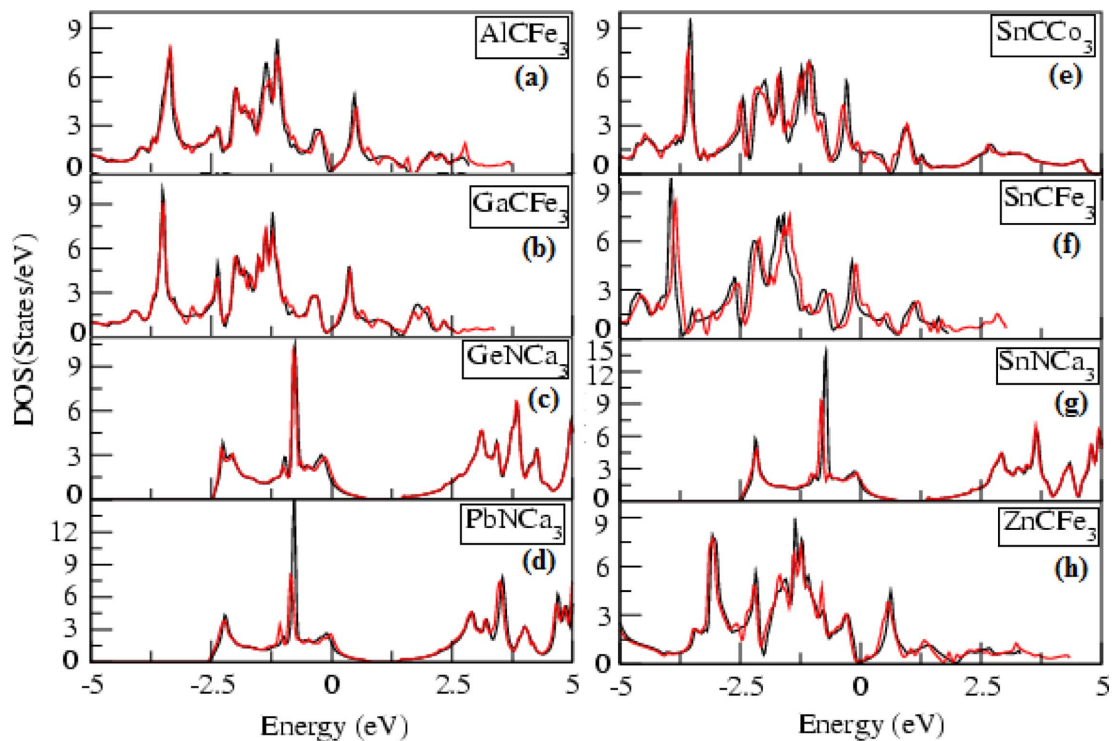
$$\sigma_{\alpha\beta}(T, \mu) = \frac{1}{\Omega} \int \sigma_{\alpha\beta}(\varepsilon) \left[ -\frac{\partial f_0(T, \varepsilon, \mu)}{\partial \varepsilon} \right] d\varepsilon \quad (3)$$

$$S_{\alpha\beta}(T, \mu) = \frac{1}{eT\Omega\sigma_{\alpha\beta}(T, \mu)} \int \sigma_{\alpha\beta}(\varepsilon) (\varepsilon - \mu) \left[ -\frac{\partial f_0(T, \varepsilon, \mu)}{\partial \varepsilon} \right] d\varepsilon \quad (4)$$

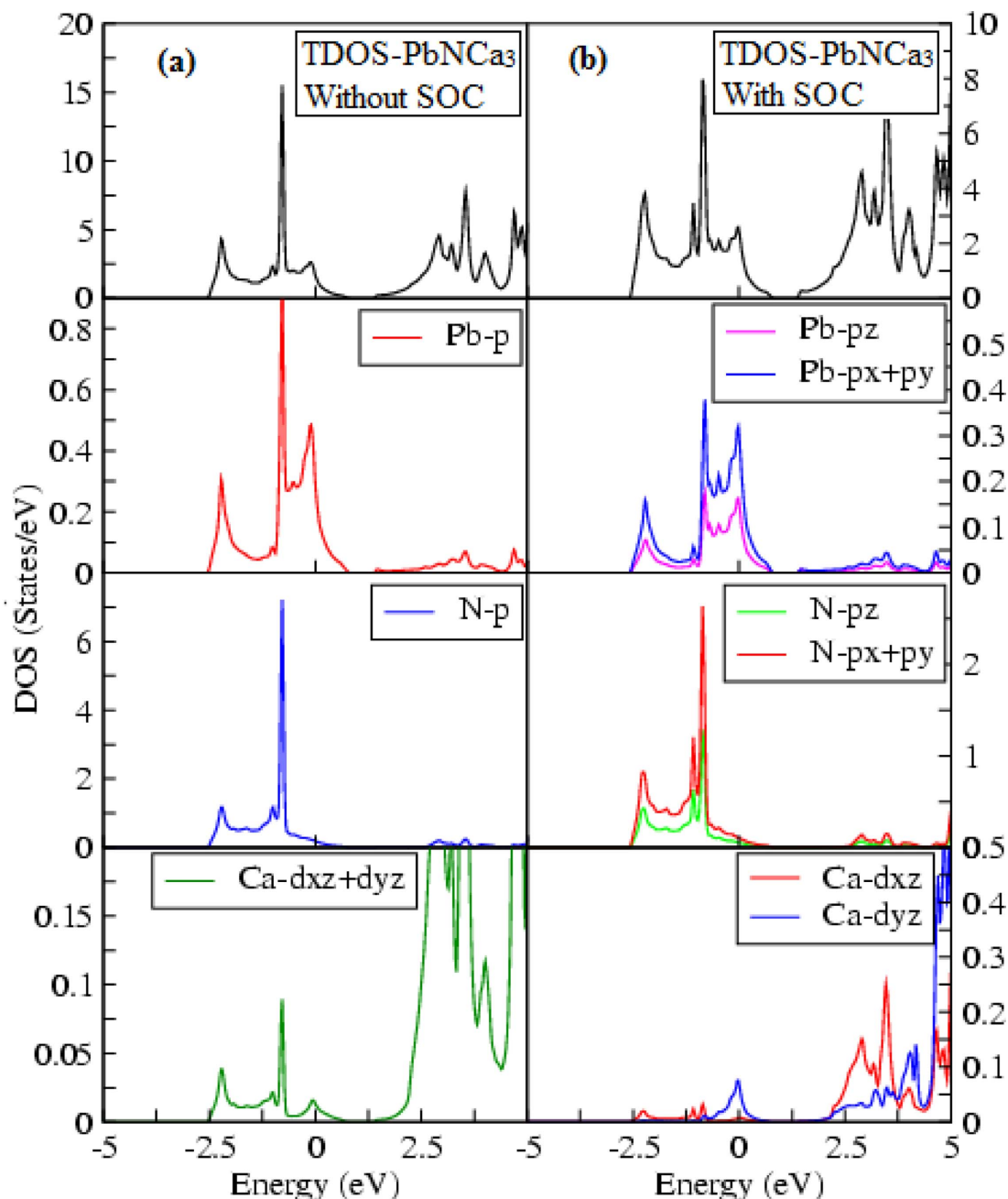
where  $\alpha$  and  $\beta$  are the tensor indices,  $e$  is the electron charge,  $\Omega$  is the volume of the unit cell,  $\mu$  is the carrier concentration and  $f_0$  is the Fermi-Dirac distribution function. The relaxation time,  $\tau$ , is kept constant in this study. The Seebeck coefficient is calculated by the band structure calculation as it does not depend on relaxation time (under the assumption that relaxation time is constant) but electrical conductivity needs to be calculated with respect to the relaxation time.

### 3. RESULTS AND DISCUSSION

The total density of states of these materials in spin-up states, with the effect of spin orbit coupling (SOC) and without SOC are presented in Fig. 2.1. For the deep understanding of the effects of SOC on the different states of these materials, the partial density of states (PDOS) for PbNca<sub>3</sub> and AlCFe<sub>3</sub> are presented in Figs. 2.2 and 2.3, respectively. The PDOS of GeNca<sub>3</sub> and SnNca<sub>3</sub> are similar to the PDOS of PbNca<sub>3</sub> while the PDOS of ZnCFe<sub>3</sub>, SnCCo<sub>3</sub>, SnCFe<sub>3</sub> and GaCFe<sub>3</sub> are similar to AlCFe<sub>3</sub> and are not presented to avoid repetition. It is evident from Fig. 2.2 that the SOC effect splits the Pb-p state into Pb-p<sub>z</sub> and Pb-p<sub>x+y</sub> states in PbNca<sub>3</sub>. After splitting, the combined effect



**Fig. 2.1.** Total density of states, in spin up state, for (a) AlCFe<sub>3</sub> (b) GaCFe<sub>3</sub> (c) GeNca<sub>3</sub> (d) PbNca<sub>3</sub> (e) SnCCo<sub>3</sub> (f) SnCFe<sub>3</sub> (g) SnNca<sub>3</sub> and (h) ZnCFe<sub>3</sub>. Black lines represent density of states without SOC while red lines represents density of states with SOC.

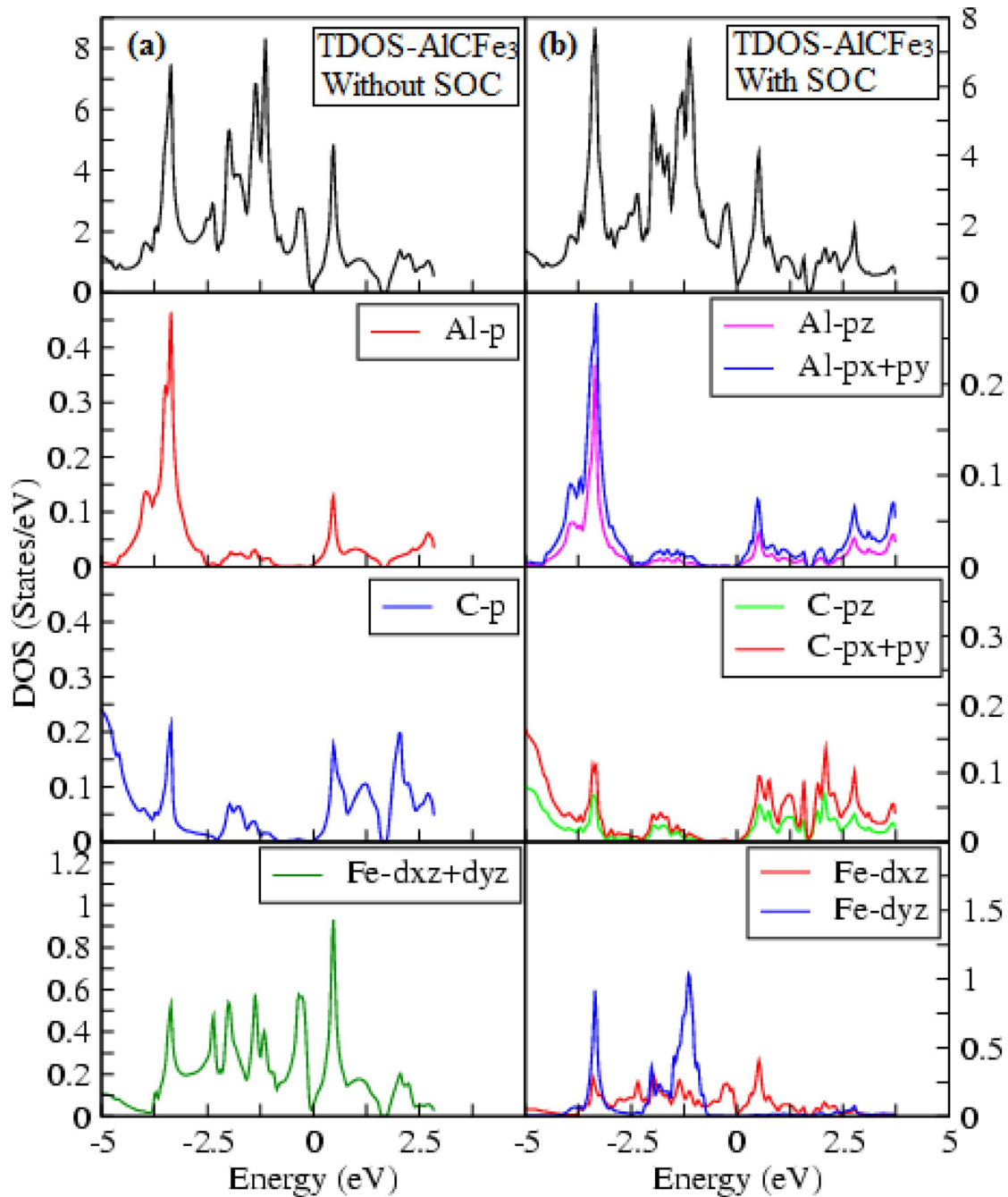


**Fig. 2.2.** Total and partial density of states, in spin up state, for PbNCa<sub>3</sub> (a) without SOC effects and (b) with SOC.

of Pb- $p_z$  and Pb- $p_x+p_y$  states increases the density of Pb-p states at the Fermi level. A very small increase in the width of Pb-p states is also observed due to SOC effects. Similarly, SOC effect splits N-p states into N- $p_z$  and N- $p_x+p_y$  states whereas a small increase in the width of N-p states is also observed. In case of calcium, Ca- $d_{xz}+d_{yz}$  states are split into Ca- $d_{xz}$  and Ca- $d_{yz}$  states at the Fermi level due to SOC effect. The Ca- $d_{yz}$  states shift towards the Fermi level which increases the density of states at the Fermi level. Therefore, the effect of SOC increases the density of states at the Fermi

level in PbNCa<sub>3</sub>, which logically enhances the thermoelectric properties of the material.

Figure 2.3 shows the PDOS for AlCFe<sub>3</sub>. Though the Al-p state and C-p states split due to SOC effect, the splitting does not increase the density of states at the Fermi level. Secondly, the contribution of these states at the Fermi level is very small for these elements. Fe-d states are dominant as compared to Al and C states where Fe- $d_{xz}+d_{yz}$  states split into Fe- $d_{xz}$  and Fe- $d_{yz}$  states due to SOC effect. In contrast to Ca- $d_{yz}$  states in PbNCa<sub>3</sub>, Fe- $d_{yz}$  states in AlCFe<sub>3</sub> shift away

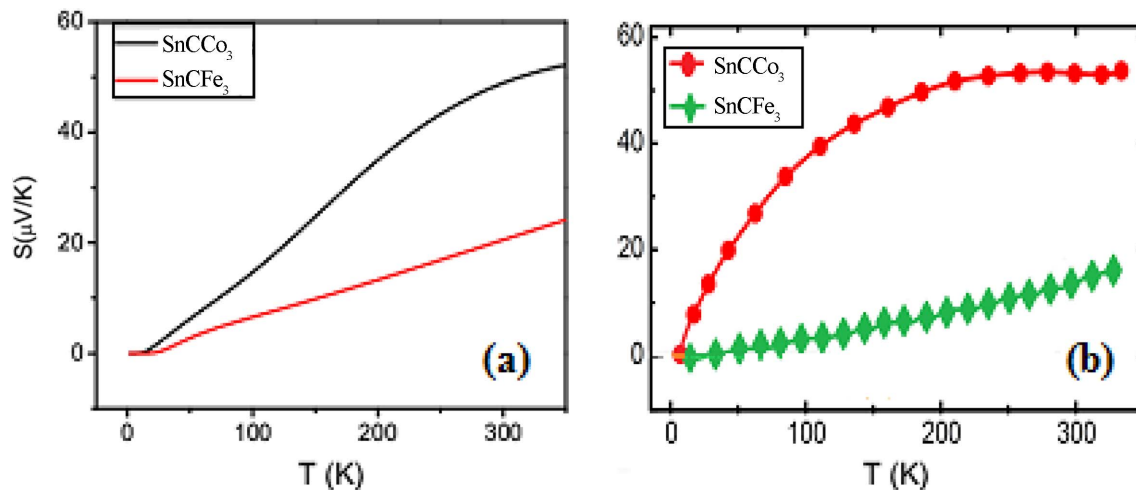


**Fig. 2.3.** Total and partial density of states, in spin up state, for AlCFe<sub>3</sub> (a) without SOC effects and (b) with SOC.

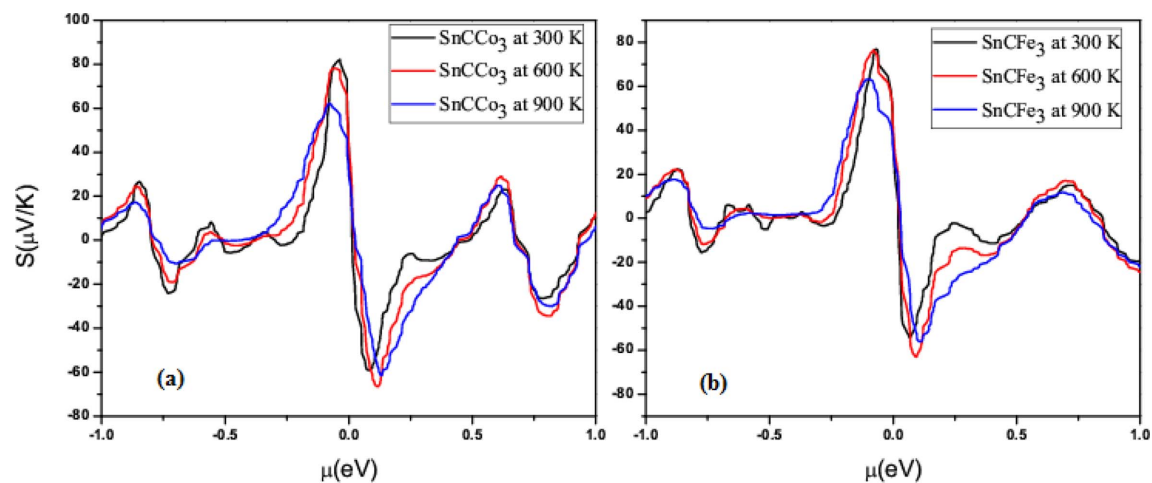
from the Fermi level, hence decreasing the density of states at the Fermi level which eventually diminishes the TE properties of this material.

The Seebeck coefficient is an important tool, which provides a sensitive test of the electronic structures of the materials in close proximity to the Fermi energy. Large values of Seebeck coefficient are desired for efficient TE devices. In Fig. 3.1 the calculated Seebeck coefficient of SnCCo<sub>3</sub> and SnCFe<sub>3</sub> against temperature are compared with

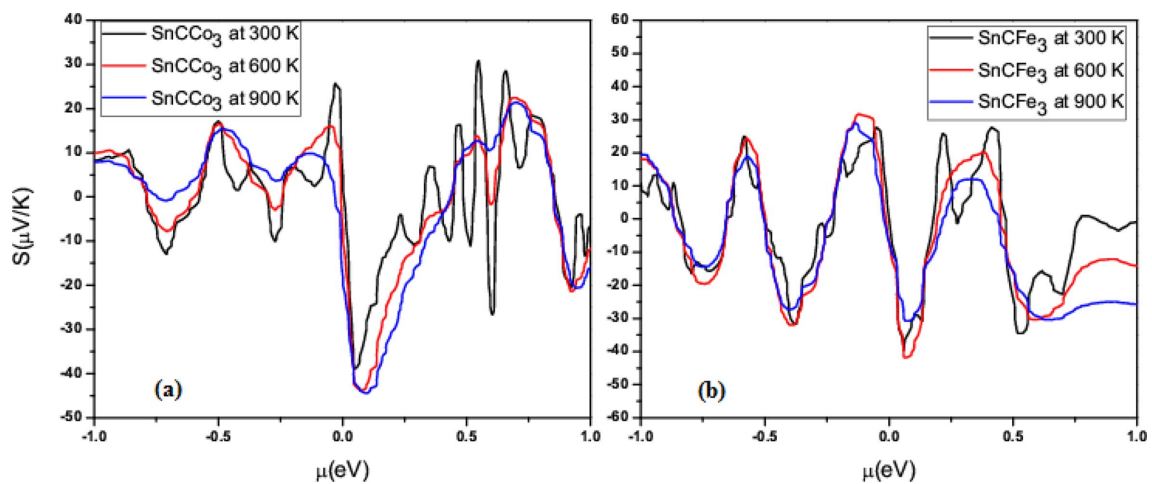
the experimental results<sup>[36]</sup> presented, where Fig. 3.1(a) shows calculated and Fig. 3.1(b) shows experimental results. At room temperature, the Seebeck coefficients for SnCCo<sub>3</sub> and SnCFe<sub>3</sub> are 50  $\mu$ V/K and 20  $\mu$ V/K, respectively. In comparison with the available experimental results,<sup>[36]</sup> we found that our results follow the experimental curves almost in the entire temperature range. The positive values of the Seebeck coefficient show that these materials favor *p*-type doping. A small difference between calculated and experi-



**Fig. 3.1.** Calculated (a) and experimental<sup>36</sup> (b) Seebeck coefficients for  $\text{SnCCo}_3$  and  $\text{SnCFE}_3$  as a function of temperature without SOC.



**Fig. 3.2.** Seebeck coefficients for (a)  $\text{SnCCo}_3$  and (b)  $\text{SnCFE}_3$  at 300, 600 and 900 K as a function of chemical potential without SOC.

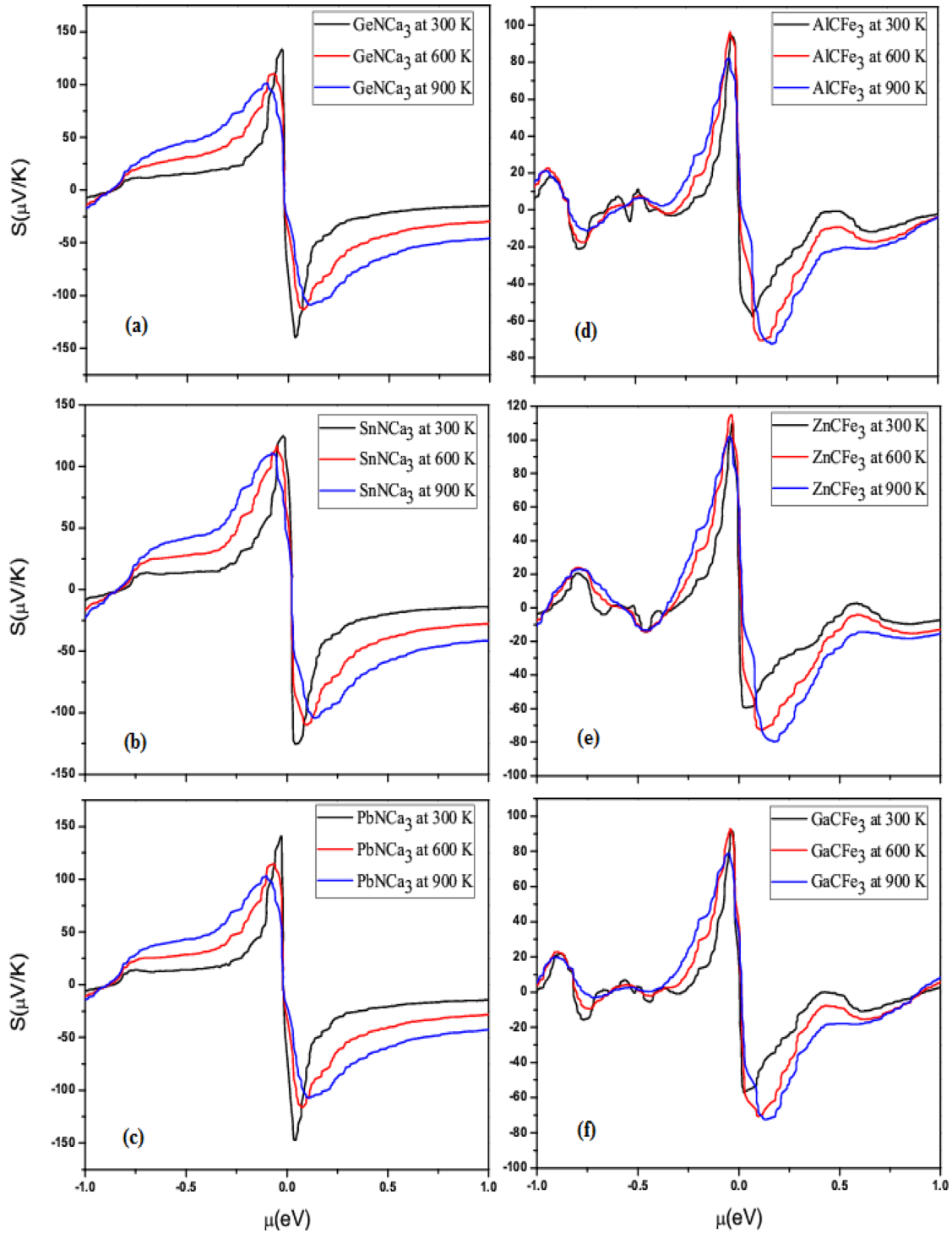


**Fig. 3.3.** Seebeck coefficients for (a)  $\text{SnCCo}_3$  and (b)  $\text{SnCFE}_3$  at 300, 600 and 900 K as a function of chemical potential with SOC.

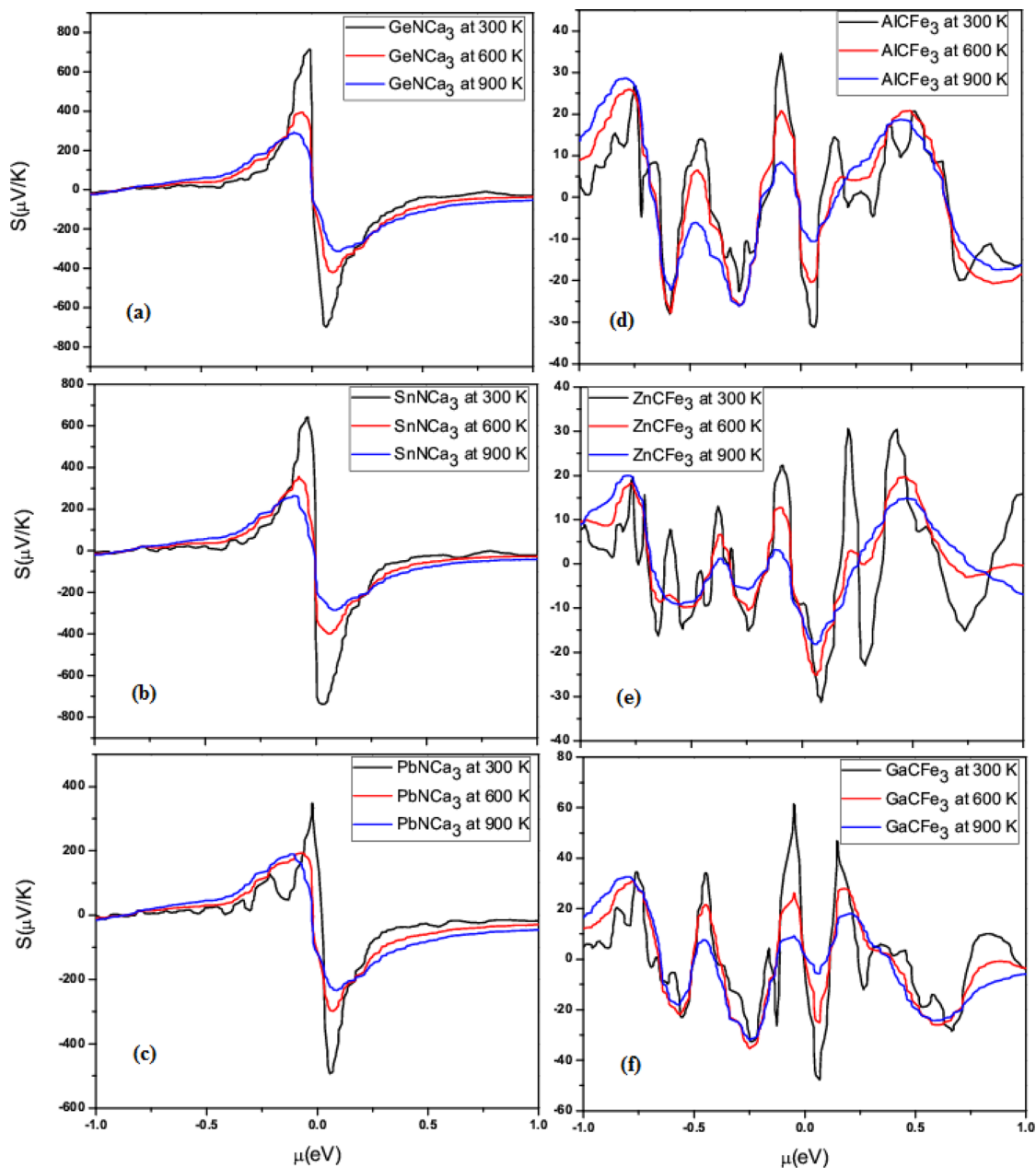
mental results can be attributed to the fact that DFT produces results after the materials are optimized at the ground state, while the experimental results are not obtained from the ground state. Secondly, only pseudo-eigenvalues are available in the DFT approximation.<sup>[48]</sup> Therefore, it is important to

note that besides its advantages, DFT has its limitations.<sup>[49,50]</sup>

We also calculated the Seebeck coefficient of these materials against chemical potential at 300, 600 and 900 K temperature for better understanding of its behavior, as presented in Figs. 3.2(a) and (b). It is clear from the figure



**Fig. 4.1.** Seebeck coefficients for (a) GeNCa<sub>3</sub> (b) SnNCa<sub>3</sub> (c) PbNCa<sub>3</sub> (d) AlCFe<sub>3</sub> (e) ZnCFe<sub>3</sub> and (f) GaCFe<sub>3</sub> at 300, 600 and 900 K as a function of chemical potential without SOC.

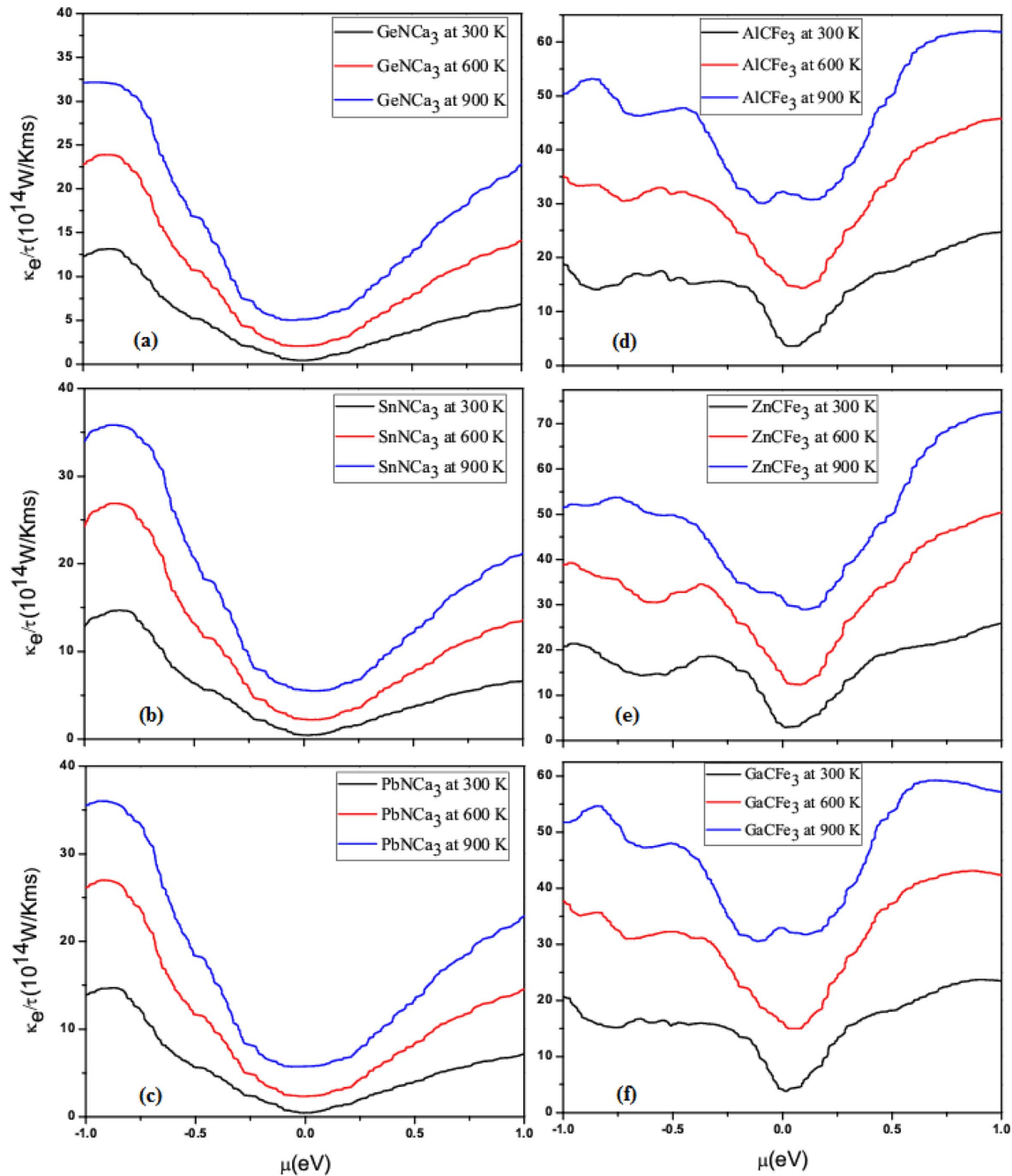


**Fig. 4.2.** Seebeck coefficients for (a)  $\text{GeNCa}_3$ ; (b)  $\text{SnNCa}_3$ ; (c)  $\text{PbNCa}_3$ ; (d)  $\text{AlCFe}_3$ ; (e)  $\text{ZnCFe}_3$  and (f)  $\text{GaCFe}_3$  at 300, 600 and 900 K as a function of chemical potential with SOC.

that the values of Seebeck coefficient can be tuned by chemical potential. At room temperature we achieve the maximum values of  $82 \mu\text{V/K}$  and  $78 \mu\text{V/K}$  for  $\text{SnCCo}_3$  and  $\text{SnCFe}_3$ , respectively, at  $-0.1 \mu\text{eV}$  chemical potential without considering the effects of SOC. Further, it is clear from the figure that high values of Seebeck are achieved between  $-0.25 \mu\text{eV/K}$  and  $0.25 \mu\text{eV/K}$  while beyond these points the Seebeck coefficient decreases. Thus, it is obvious that we shall get the best TE response of these materials in this region. Figure 3.3 shows that SOC diminishes the Seebeck

coefficient of these materials.

Figures 4.1 and 4.2 present Seebeck coefficients without considering the effects of SOC and with the effects of SOC respectively, for  $\text{ANCa}_3$  ( $A=\text{Ge, Sn, Pb}$ ) and  $\text{BCFe}_3$  ( $B=\text{Al, Zn, Ga}$ ), against chemical potential at 300, 600 and 900 K. All materials show high values for the Seebeck coefficient. We see approximately similar behavior of the Seebeck coefficient in both  $p$ -type and  $n$ -type regions. The Seebeck coefficients of  $\text{ANCa}_3$  ( $A=\text{Ge, Sn, Pb}$ ) are enhanced while they are diminished for  $\text{BCFe}_3$  ( $B=\text{Al, Zn, Ga}$ ) due to the

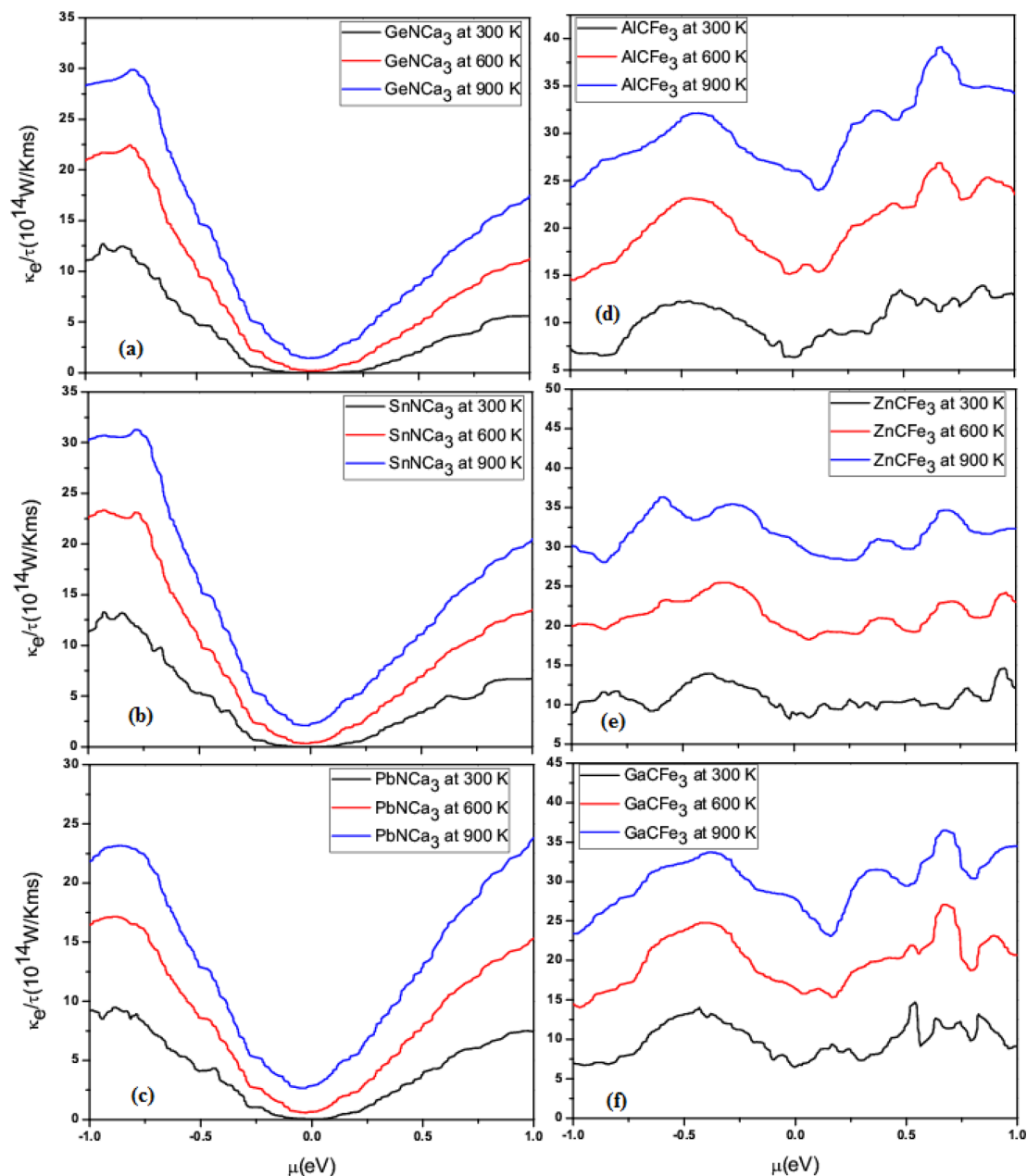


**Fig. 5.1.** Thermal conductivity for (a)  $\text{GeNCa}_3$  (b)  $\text{SnNCa}_3$  (c)  $\text{PbNCa}_3$  (d)  $\text{AlCFe}_3$  (e)  $\text{ZnCFe}_3$  and (f)  $\text{GaCFe}_3$  at 300, 600 and 900 K as a function of chemical potential without SOC.

SOC. At  $0.1 \mu(\text{eV})$  chemical potential, considering the effects of SOC,  $\text{SnNCa}_3$  shows the highest value of  $-730 \mu\text{V/K}$  at room temperature among all nitride and carbide antiperovskites investigated in this work. Therefore, we can predict that this material will show better TE response than the other materials discussed in this paper.

Heat is transferred in a material through electrons and lattice vibrations. In semiconductors, lattice vibrations are

mostly responsible for the conduction of heat while in metals free electrons are good sources of thermal conductivity.<sup>[4]</sup> In metals, the lattice part of the thermal conductivity is less than 2% of the total thermal conductivity and can be safely neglected.<sup>[51,52]</sup> For materials used in TE generators, thermal conductivity is desired to be small so that the temperature gradient could be maintained across the material. Figure 5.1 and 5.2 present electronic thermal conductivity, without

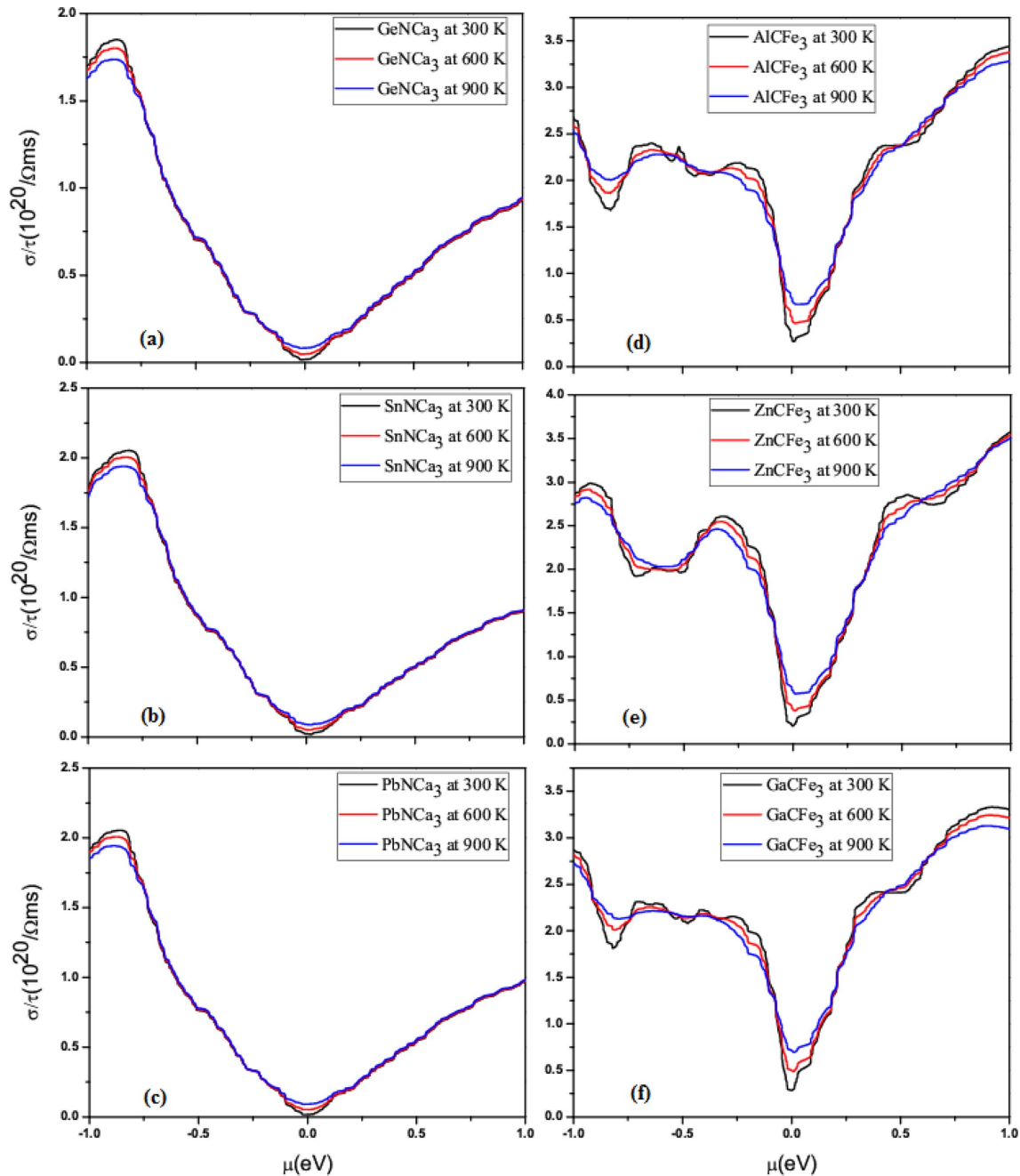


**Fig. 5.2.** Thermal conductivity for (a) GeNCa<sub>3</sub> (b) SnNCa<sub>3</sub> (c) PbNCa<sub>3</sub> (d) AlCFE<sub>3</sub> (e) ZnCFE<sub>3</sub> and (f) GaCFE<sub>3</sub> at 300, 600 and 900 K as a function of chemical potential with SOC.

considering the effects of SOC and with the effects of SOC respectively, for ANCa<sub>3</sub> (A=Ge, Sn, Pb) and BCFE<sub>3</sub> (B=Al, Zn, Ga), against chemical potential at 300, 600 and 900 K. The same behavior is observed for all materials as thermal conductivity is minimum at zero chemical potential and increases as chemical potential is increased. As we need small values of thermal conductivity to achieve higher figure of merit, it is clear from the figure that the materials will give good TE response in the region between  $-0.25$  and  $0.25$   $\mu$ (eV) chemical potential, as in this region thermal conductivities

are minimum. In particular, for nitrides with SOC effects, the graph remains zero between  $-0.2$  and  $0.2$   $\mu$ (eV) chemical potential at room temperature. Further, we see that the thermal conductivity increases with temperature for all materials because by increasing temperature free electrons gain energy and result in more transfer of heat. The figure shows that nitride antiperovskites have lower values of thermal conductivity as compared to carbide antiperovskites.

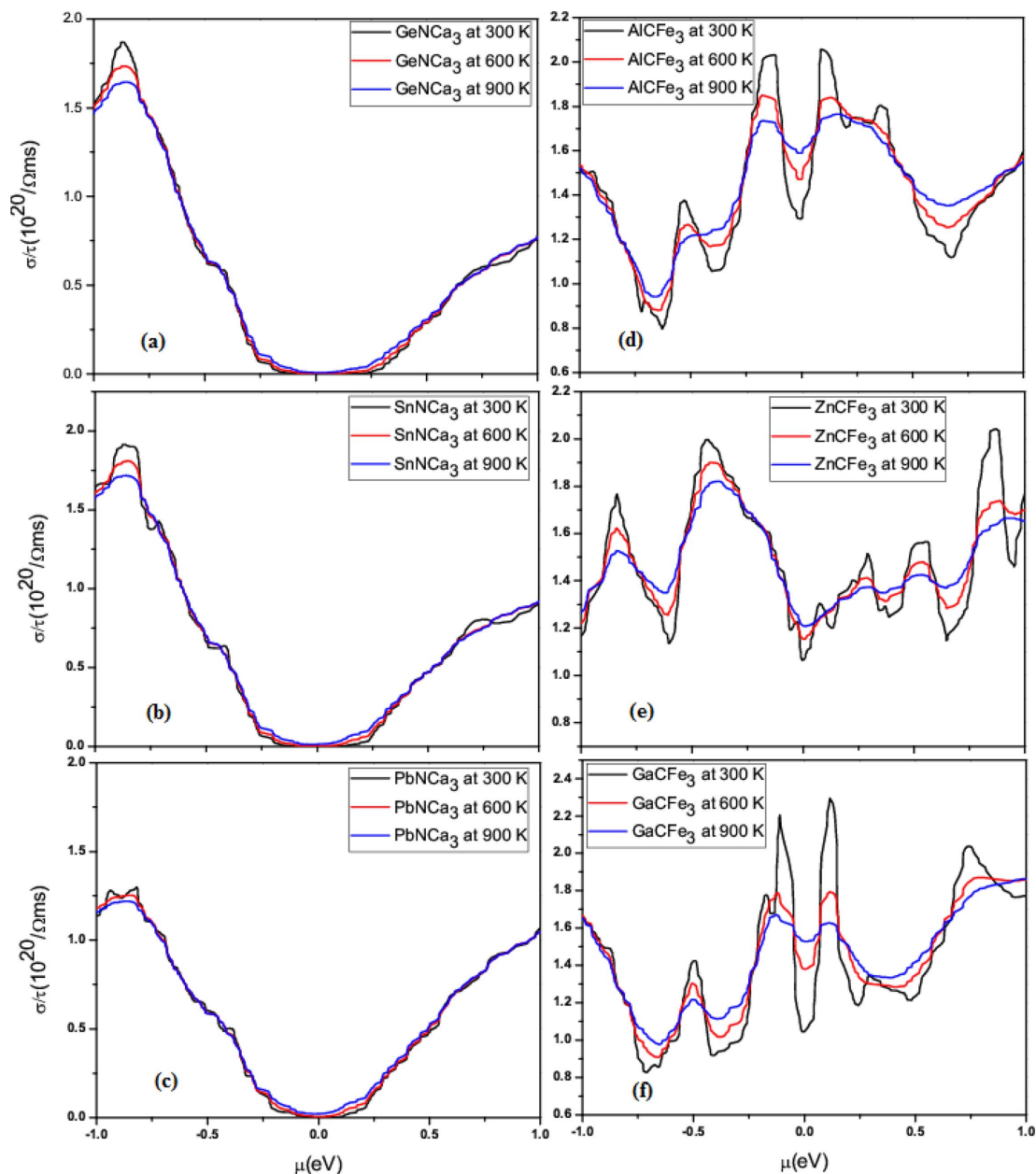
Electrical conductivity is the flow of charge carriers in a material. Electrons move from the hot regions of a material



**Fig. 6.1.** Electrical conductivity for (a) GeNCa<sub>3</sub> (b) SnNCa<sub>3</sub> (c) PbNCa<sub>3</sub> (d) AlCFe<sub>3</sub> (e) ZnCFe<sub>3</sub> and (f) GaCFe<sub>3</sub> at 300, 600 and 900 K as a function of chemical potential without SOC.

to the cold regions. In TE devices current is produced as a result of this phenomena. Therefore, for good TE performance we need materials having high values of electrical conductivity. Figure 6.1 and 6.2 present electrical conductivity, without considering the effects of SOC and with the effects of SOC respectively, of ANCa<sub>3</sub> (A=Ge, Sn, Pb) and BCFe<sub>3</sub> (B=Al, Zn, Ga) against chemical potential at 300, 600 and 900 K. It is clear from the figures that electrical conductivity is minimum for all materials near zero chemical potential and

increases as chemical potential is increased. This means that we can achieve desired values of electrical conductivity for these materials by changing chemical potential. Further, we see that carbide antiperovskites have higher values of electrical conductivity than nitride antiperovskites. In carbides, *n*-type materials show good response, with peak value of  $3.5 \times 10^{20} / \Omega\text{ms}$  at  $1 \mu\text{eV}$ , while in nitrides, this is true for *p*-type materials, with peak value of  $2.1 \times 10^{20} / \Omega\text{ms}$  at  $0.9 \mu\text{eV}$  chemical potential. Further, we see that SOC



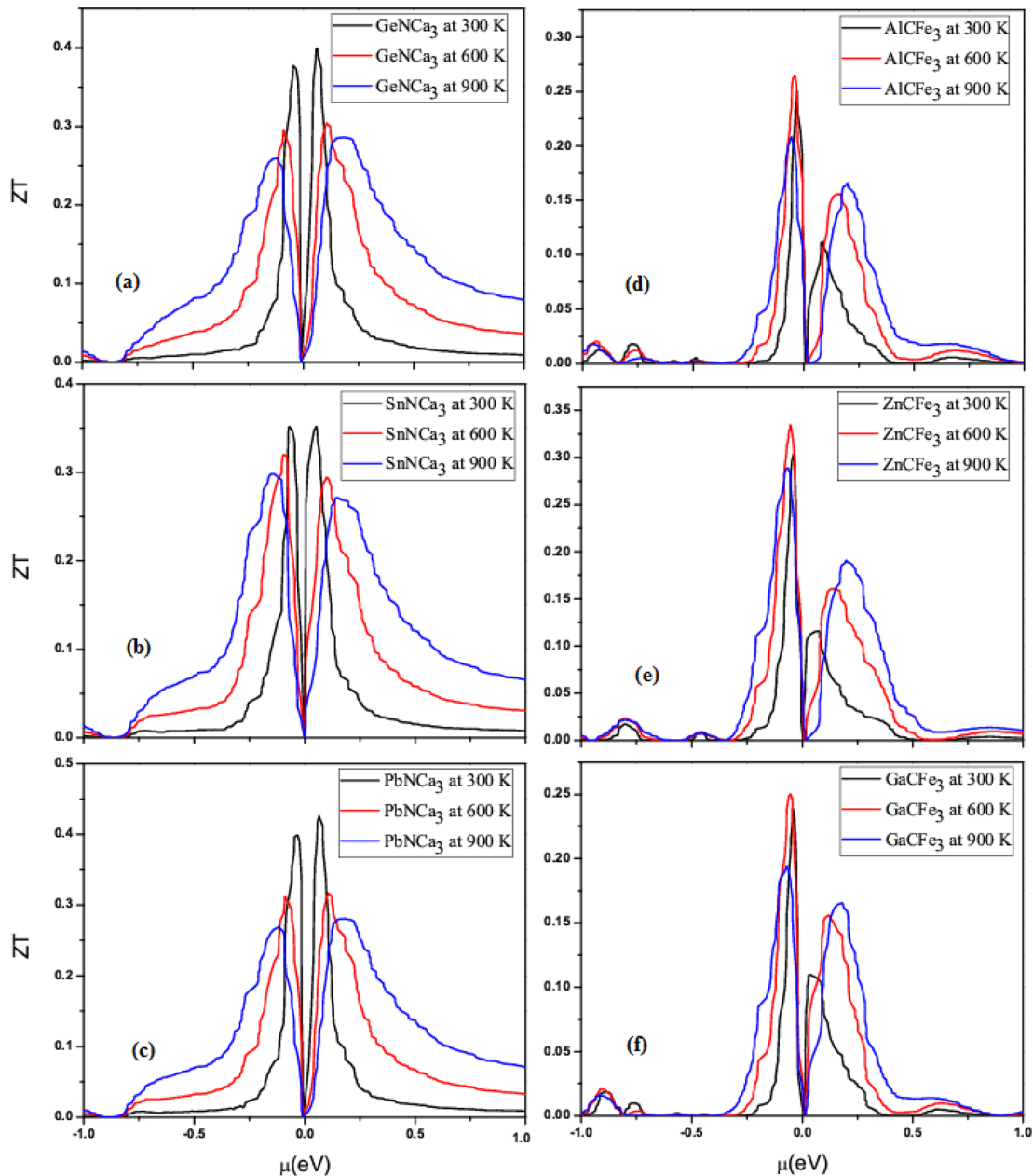
**Fig. 6.2.** Electrical conductivity for (a) GeNCa<sub>3</sub> (b) SnNCa<sub>3</sub> (c) PbNCa<sub>3</sub> (d) AlCFe<sub>3</sub> (e) ZnCFe<sub>3</sub> and (f) GaCFe<sub>3</sub> at 300, 600 and 900 K as a function of chemical potential with SOC.

slightly decreases electrical conductivity for all materials.

The efficiency of a TE generator can be measured by its figure of merit  $ZT$ , which is large for high Seebeck coefficient, high electrical conductivity and low thermal conductivity.

Figures 7.1 and 7.2 present dimensionless figure of merit, without considering the effects of SOC and with the effects of SOC respectively, for ANCa<sub>3</sub> (A=Ge, Sn, Pb) and BCF<sub>3</sub> (B=Al, Zn, Ga) against chemical potential at 300, 600 and 900 K.  $ZT$  is calculated from the Seebeck coefficient ( $S$ ), the electrical conductivity ( $\sigma/\tau$ ) and the electronic part of thermal

conductivity ( $k_e/\tau$ ), presented above. It is clear from the figures that the figure of merit increases due to SOC in nitride antiperovskites while it decreases in carbide antiperovskites. SnNCa<sub>3</sub> has the highest value of figure of merit among all materials and at room temperature - it reaches to 0.96 at 0.1  $\mu$ (eV) chemical potential, considering the effects of SOC. The result is apparent (understandable?) because this material has the highest Seebeck coefficient. As the Seebeck coefficient and electronic thermal conductivity show good response between  $-0.25$  and  $0.25$   $\mu$ (eV) chemical



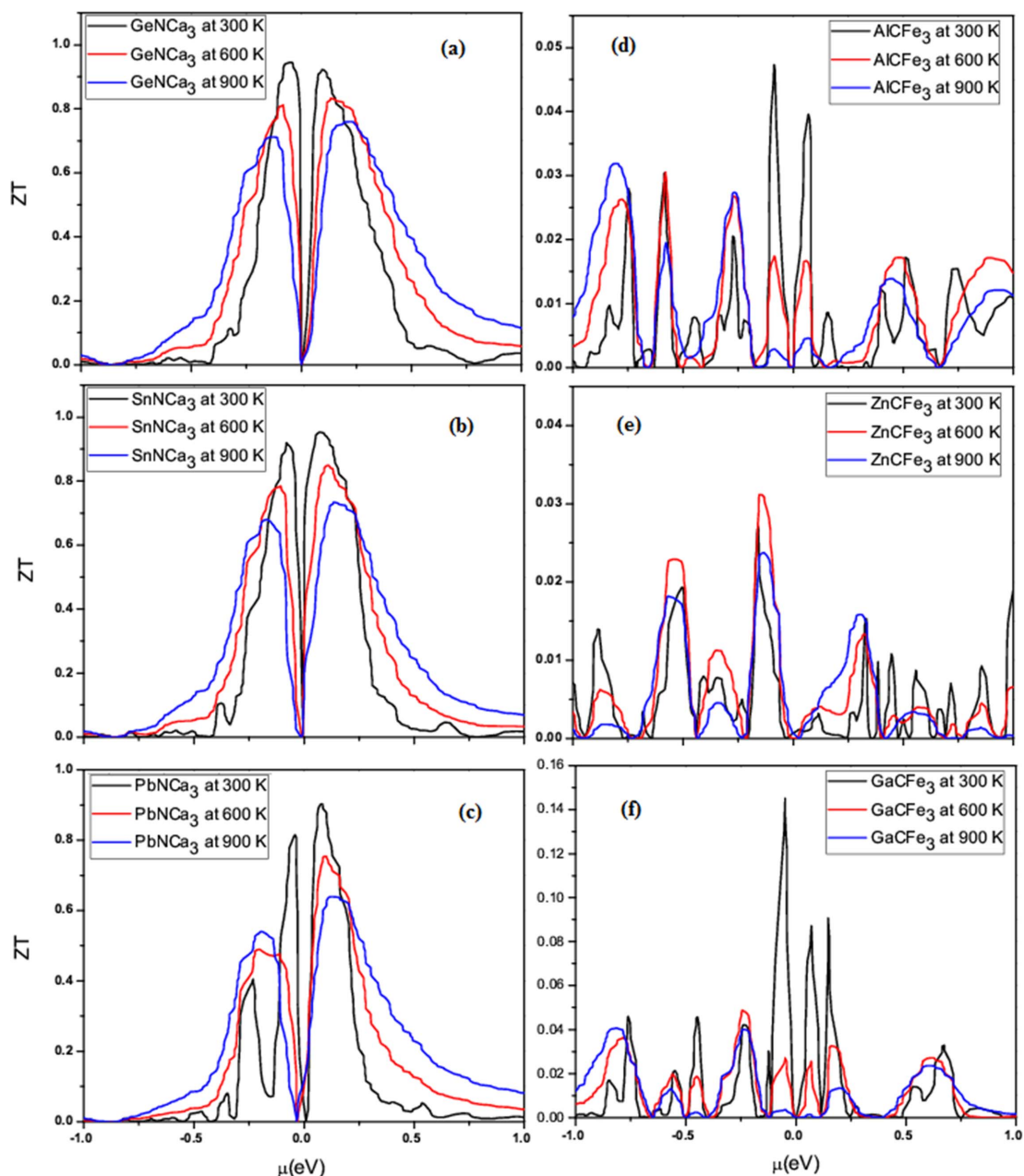
**Fig. 7.1.** Dimensionless figure of merit for (a)  $\text{GeNCa}_3$  (b)  $\text{SnNCa}_3$  (c)  $\text{PbNCa}_3$  (d)  $\text{AlCFe}_3$  (e)  $\text{ZnCFe}_3$  and (f)  $\text{GaCFe}_3$  at 300, 600 and 900 K as a function of chemical potential without SOC.

potential, we get the peak values of figure of merit in this region. Small values of figure of merit, beyond this region, may be attributed to the large values of electrical conductivity. Furthermore, it is clear from the figure that nitride antiperovskites show good response in *p*-type while carbide antiperovskites show good response in *n*-type materials.

#### 4. CONCLUSIONS

In conclusion, the thermoelectric properties of carbon and

nitrogen based metallic antiperovskites  $\text{ANCa}_3$  ( $A=\text{Ge, Sn, Pb}$ ),  $\text{BCFe}_3$  ( $B=\text{Al, Zn, Ga}$ ) and  $\text{SnCD}_3$  ( $D=\text{Co and Fe}$ ) are calculated using first principle calculations. The effects of spin orbit coupling are also presented. The high values of Seebeck coefficients between  $-0.25$  and  $0.25 \mu\text{eV}$  chemical potential and low thermal conductivities, i.e. almost zero in this region, confirm the maximum values of figure of merit in this region. Nitride antiperovskites give figures of merit of about 0.96 from which we conclude that these materials maybe useful in thermoelectric power generation.



**Fig. 7.2.** Dimensionless figure of merit for (a) GeNCa<sub>3</sub> (b) SnNCa<sub>3</sub> (c) PbNCa<sub>3</sub> (d) AlCFe<sub>3</sub> (e) ZnCFe<sub>3</sub> and (f) GaCFe<sub>3</sub> at 300, 600 and 900 K as a function of chemical potential with SOC.

Electrical conductivity gives maximum values beyond  $-0.5$  and  $0.5$   $\mu$ (eV) chemical potential in  $p$ -type and  $n$ -type regions, respectively. For this reason, we see small values of figure of merit beyond these points. The overall pattern of figure of merit clearly shows that these materials can be used in industrial applications for power generation. The most remarkable conclusion of this studies is identifying a metallic compound SnNCa<sub>3</sub>, considering SOC effects, with the highest value of Seebeck coefficient ( $-730$   $\mu$ V/K), at room temperature, out of all metals.

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