Two functionals approach in DFT for the prediction of thermoelectric properties of Fe$_2$ScX (X = P, As, Sb) full-Heusler compounds

Shivprasad S Shastri and Sudhir K Pandey

School of Engineering, Indian Institute of Technology Mandi, Kamand—175005, India

E-mail: shastri1992@gmail.com and sudhir@iitmandi.ac.in

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Abstract

In the quest for new thermoelectric materials with high power factors, full-Heusler compounds having flat band are found to be promising candidates. In this direction, Fe$_2$ScX (X = P, As, Sb) compounds are investigated using mBJ for the band gap and SCAN to describe the electronic bands and phonon properties for thermoelectric applications. The band gaps obtained from mBJ are 0.81 eV, 0.69 eV and 0.60 eV for Fe$_2$ScX compounds. The phonon dispersion, phonon density of states (DOS) and partial DOS are calculated. The phonon contributions to specific heat are obtained as a function of temperature under harmonic approximation. The electronic band structure calculated from mBJ and SCAN functionals are qualitatively compared. The effective mass values are calculated at the band extrema from SCAN functional. The thermoelectric parameters are calculated for both hole and electron dopings under semiclassical theory. We use a simple, but reasonable method to estimate the phonon relaxation time ($\tau_{\text{ph}}$). Using the specific heat, estimated $\tau_{\text{ph}}$ and slopes (phase velocity) of acoustic branches in the linear region, lattice thermal conductivity ($\kappa_{\text{ph}}$) at 300 K is calculated for three compounds. The obtained values of $\kappa_{\text{ph}}$ with constant $\tau_{\text{ph}}$ are 18.2, 13.6 and 10.3 Wm$^{-1}$K$^{-1}$, respectively. Finally, the temperature dependent figure of merit $ZT$ values are calculated for optimal carrier concentrations in the doping range considered, to evaluate the materials for thermoelectric application. The $ZT$ values for n-type Fe$_2$ScX, in 900–1200 K, are 0.34–0.43, 0.40–0.48 and 0.45–0.52, respectively. While, the p-type Fe$_2$ScX have $ZT$ values of 0.25–0.34, 0.20–0.28 and 0.18–0.26, respectively in the same temperature range. The $ZT$ values suggest that, Fe$_2$ScX compounds can be promising materials in high temperature power generation application on successful synthesis and further $\kappa_{\text{ph}}$ reduction by methods like nanostructuring.

Keywords: thermoelectric materials, lattice thermal conductivity, density functional theory, figure of merit, phonons, power factor

(Some figures may appear in colour only in the online journal)
Research in the area of developing thermoelectric materials is important since they can be a very good alternative energy sources in many small scale applications. TEGs are green energy sources compared to the conventional fossil fuel based energy sources. The thermoelectric materials with dimensionless figure of merit $ZT \geq 1.0$ are considered as suitable for thermoelectric applications. But, the bottleneck in implementing the most of the existing thermoelectric materials into technological applications is due to their poor value of $ZT$. Therefore, there has been continuous efforts in thermoelectric area of research to enhance the efficiency as well as in searching for new thermoelectric materials.

Efficiency of a thermoelectric can be increased by maximizing its electrical power and by reducing the heat transport by electrons and phonons. The electrical power depends on the electrical conductivity $\sigma$, and Seebeck coefficient $S$ of the material [3]. The transport of heat in a material is decided by the electronic and phonon contributions to thermal conductivity. Thus, in order to have a thermoelectric with high $ZT$, given by the relation,

$$ZT = \frac{S^2\sigma T}{\kappa}$$  \hspace{1cm} (1)

the power factor $S^2\sigma$ must be higher and thermal conductivity $\kappa$ should be lower. The thermal conductivity $\kappa$ in a material is a sum of electronic and lattice part of thermal conductivities denoted by $\kappa_e$ and $\kappa_{ph}$ respectively. Many methods like alloying, nanostructuring are employed to reduce the $\kappa_{ph}$ by increasing phonon scattering without or least affecting its electronic structure [4]. Another method towards improving efficiency is to improve the power factor of the material. The power factor of a material is mainly decided by its electronic structure and such materials are being searched which could have electronic structure that yields high power factor [5].

The studies of electronic structure and thermoelectric properties carried out on many Heusler alloys suggested that, they possess a flat conduction band along $\Gamma - X$ direction and hence larger effective mass of carriers and higher Seebeck coefficient values [6, 7, 8, 9]. These works suggested that full-Heusler alloys with a semiconducting ground states could be used for thermoelectric applications. Sharma et al [10] reported three new full-Heusler alloys having flat conduction band viz. Fe$_2$ScP, Fe$_2$ScAs and Fe$_2$ScSb with their electronic structure and thermoelectric properties using density functional theory (DFT) calculations. In a DFT calculation, generally band gaps are underestimated and Fe$_2$ScSb compound in the work of [10] was predicted to be a semimetal. The transport coefficients to be calculated in first-principles calculations are highly dependent on the band gap and band structure of the compound. The electronic structure changes depending on the exchange-correlation (XC) functional used in the DFT calculations. Therefore, in the computational discovery of thermoelectric materials, selection and benchmarking of XC functional becomes an important step.

In our previous work [11], electronic structure of two iron based Heusler alloys Fe$_2$VAI and Fe$_2$TiSn were studied using five XC functionals. The effective mass values estimated showed the dependence of band features on XC functionals and usefulness of mBJ in predicting accurate band gaps. Buchelnikov et al studied Fe$_2$VAI and other ternary Heusler alloys using SCAN and PBE functionals [12]. The differences in ground state electronic structure as given by two functionals were observed in their work. In semiconductors and insulators, transport of heat is mainly through the phonons and thus study of phonon properties is important to understand the thermal conductivity. The phonon calculations are useful in extracting information about stability of the crystal, lattice contribution to specific heat and other thermal properties, and thermal expansion of crystals. A computational study of phonon dispersion of a material along with its electronic structure would completely describe thermoelectric material which makes phonon calculations, desirable in a study of thermoelectric properties. Recently, in the work of Sk et al [13], the $S$ value of Fe$_2$VAI was measured in the range 300–620 K. This experimental $S$ values were explained using DFT and Boltzmann transport calculations using different XC functionals. The best matching between the experimental and theoretical values was found, for using the band gap obtained from mBJ and band structure from SCAN or PBEsol. Therefore, motivated by the results of the work of Sk et al [13], we take up the combination of mBJ and SCAN functionals to investigate the electronic structure and thermoelectric properties of the Fe$_2$ScX (X = P, As, Sb) compounds.

To investigate the electronic structure and dependent properties mBJ and SCAN functionals are used. Using the mBJ, band gaps of 0.81, 0.69 and 0.60 eV are obtained for Fe$_2$ScX (X = P, As, Sb) compounds, respectively. Using SCAN, phonon dispersion, total density of states (DOS) and partial DOS are also calculated. The specific heat contribution from the lattice part of compounds are calculated. The Debye temperatures estimated from the highest phonon frequency for three compounds are $\sim$637 K, $\sim$556 K and $\sim$498 K, respectively. Seebeck coefficient, electrical conductivity per relaxation time, power factor per relaxation time and electronic thermal conductivity per relaxation time are calculated with temperature for different values of electron and hole dopings. The effective mass values are calculated at the band extrema. The electronic band structures obtained from mBJ and SCAN are qualitatively compared. We make use of simple method in this work to estimate phonon relaxation time $\tau_{ph}$. Using calculated specific heat, $\tau_{ph}$ and slopes of acoustic branches in the linear region close to $\Gamma$, $\kappa_{ph}$ values at 300 K are calculated. Then to further evaluate the materials for thermoelectric applications, we calculate temperature dependent $ZT$ for three compounds for the highest power factor giving electron and hole doping concentrations.

2. Computational details

In our work, full-potential linearized augmented plane wave (FP-LAPW) method based first-principles DFT program WIEN2k [14] is used for the calculation of ground state energy, electronic structure and total forces on atoms. mBJ exchange potential with LDA correlation [15] and SCAN [16] XC functionals are chosen for the calculations. Here, The
lattice parameters are taken from [10] and used for electronic properties calculation. Since, phonon frequency is sensitive to the lattice parameter, it is optimized for force calculations with SCAN functional. For force constants and phonon properties calculations phonopy [17] code is used. Phonon properties are calculated under finite displacement method (FDM) and supercell approach in phonopy. To capture the long-range force constant between atoms a supercell of size $2 \times 2 \times 2$ with 128 atoms is constructed. To create the forces artificially in the system each of inequivalent atoms in the formula unit of Fe$_2$ScX is displaced by 0.02 Bohr in x-direction. To obtain the forces on the atoms in the created supercell, force convergence criteria of 0.1 mRy/Bohr is set in the force calculator (WIEN2k). A k-mesh of size $5 \times 5 \times 5$ is used for the force calculations in supercell. The calculations of band structure dependent transport coefficients are done using BoltzTraP program [18]. The ground state total energy calculations are done on dense k-mesh of $50 \times 50 \times 50$ size in order to facilitate transport calculations. The convergence criteria to meet the self-consistency in iterations for total energy is $10^{-3}$ Ry/ cell and for charge/cell is $10^{-2}$ electronic charges, respectively are used.

3. Results and discussion

Heusler compounds are known to be found in tetragonally distorted D0$_2$, L1$_0$ (disordered) structures and also in cubic D0$_3$, B2 and A2 disordered structures apart from the the perfectly ordered cubic L2$_1$ structure [19, 20]. Thus, in order to confirm the actual ground state of Fe$_2$ScX ($X = P, As, Sb$) compounds, we carried out structural optimization calculations to find out the lowest energy structure. The total energy calculations are performed using Korringa–Kohn–Rostoker (KKR) method implemented in AkaiKKR program [21]. The disordered systems were treated using coherent potential approximation. We used Vosko–Wilk–Nusair XC functional for these calculations [22].

The difference in ground state energy of the optimized structures with respect to cubic L2$_1$ structure are tabulated in table 1 along with the optimized lattice parameters. The calculations showed that other possible structures have higher energy compared to ordered cubic L2$_1$ structure. Therefore, confirming the ground state of Fe$_2$ScX compounds to be ordered cubic L2$_1$ structure which is used in the present work.

We built the crystal structure of Fe$_2$ScX ($X = P, As, Sb$) full-Heusler compounds in the cubic L2$_1$ phase with space group $Fm\overline{3}m$ [10]. In [10] the ground state formation energy of the static lattices have been calculated. The obtained negative values of formation energies supported the feasibility of synthesis of Fe$_2$ScX ($X = P, As, Sb$) in laboratories. Further, to study the structural stability of the compounds we have carried out phonon calculations. The phonon frequencies are sensitive to lattice parameter and XC functional [23] used in the computation (which was also observed in our previous work [24]). Therefore, the lattice parameters taken from [10] were optimized to get the ground state lattice parameters for SCAN functional. The equilibrium lattice parameters after fitting the B-M EOS [25] for the energy-volume curves are 5.704, 5.828, and 6.085 Å for Fe$_2$ScP, Fe$_2$ScAs and Fe$_2$ScSb, respectively. Using these lattice parameters from SCAN phonon dispersion, density of states (DOS) and electronic dispersions are studied.

3.1. Phonon properties

The phonon dispersions for Fe$_2$ScX ($X = P, As, Sb$) compounds are presented in figures 1(a)–(c). The calculated phonon spectrum does not show any negative frequency (or energy) which suggests that crystal is stable for any small atomic displacements about the mean position. Dynamical stability of the compounds found out with phonon calculations and formation energy values from [10] further supports the possibility of preparation of samples in laboratories.

In the figure, one can observe that maximum phonon energy is decreasing from Fe$_2$ScP to Fe$_2$ScSb. The highest energy phonons are of $\sim 55$, $\sim 48$ and $\sim 43$ meV for Fe$_2$ScP, Fe$_2$ScAs and Fe$_2$ScSb, respectively. The observed decreasing trend in phonon frequency can be mainly due to the following reasons. The radius of atoms $X$ ($P, As, Sb$) in the unit cell of Fe$_2$ScX is increasing from P to Sb making the distance between atoms to increase and hence, the lattice constant to increase from Fe$_2$ScP to Fe$_2$ScSb. Also, the X atoms in the unit cell are heavier in mass on going from P to Sb. Since, the mass of atoms and distance between them are increased the frequency of vibrations of atoms is expected to reduce from first to last compound in the Fe$_2$ScX family. The phonon properties and electronic structure for Fe$_2$ScAs are discussed in our earlier work [26] but, to study the family of Fe$_2$ScX with $X = P, As, Sb$ atoms for thermoelectric applications, we included Fe$_2$ScAs here, for the purpose of completeness in the discussion.

The phonon dispersion for Fe$_2$ScP in figure 1(a) shows three acoustic branches, out of which one branch is degenerate with optical branch at k-points nearer to X-point in the F-X direction. Three optical branches starting at 45 meV are well separated from the rest of the branches along the k-path directions shown in the plot except near L-point, around 43 meV, where the separation is very much reduced ($\sim 0.14$ meV). This separation is also noted in the dispersions of Fe$_2$ScAs and Fe$_2$ScSb. In Fe$_2$ScAs above 40 meV and in Fe$_2$ScSb above 35 meV optical branches with clear separation are situated. In case of Fe$_2$ScSb, optical and acoustic branches are touching only near L-point at $\sim 22$ meV unlike in other two compounds. From phonon dispersion we can also observe that the maximum energy for acoustic phonons in a given compound is reducing from Fe$_2$ScP to Fe$_2$ScSb.

Figures 2(a)–(c) and (d)–(f) show the calculated phonon total density of states (TDOS) and partial DOS for Fe$_2$ScX ($X = P, As, Sb$), respectively. From the atom specific phonon DOS of Fe$_2$ScP (figure 2(d)), we can see that higher energy optical phonon branches ($\sim 45–55$ meV) are contributed mainly from Sc atom. The considerable number of states for phonons due to the vibrations of lighter mass P atom are in the energy range $\sim 30–40$ meV. The lower energy acoustic phonons in the range $\sim 10–22$ meV are mainly due to the Sc and Fe atoms in the unit cell. The contributions to
different branches in the phonon dispersion from the atoms in the unit cell of Fe$_2$ScAs can be understood from phonon PDOS in figure 2(e). The higher energy states of optical phonons in ∼40–50 meV are mainly contributed from lighter Sc atom in the formula unit. The major number of vibrational states lying in the intermediate energy region ∼25–30 meV can be attributed to Fe and As atoms. For Fe$_2$ScSb, TDOS and PDOS of phonon states are shown in figures 2(c) and (f), respectively. The heavier Sb atom is contributing considerably to the phonon states in ∼10–22 meV region. Like in the case of Fe$_2$ScAs, there is a small region in the neighborhood of 35 meV with no phonon states. The higher energy states of optical phonon states (∼36–43 meV) are primarily due to the Sc atoms (figure 2(f)). Fe atom contribution is mainly to phonons of energy ∼22–34 meV. The vibrational contribution of atoms X (X = P, As, Sb) in the unit cell of Fe$_2$ScX is shifting...
towards the phonons of lower energy on crossing to Fe$_2$ScSb from Fe$_2$ScP. The increase in the atomic mass of X elements as well as increase in lattice constant mainly being the reason for this observed shift. But, in all the three cases the peaks in the higher energy range in DOS plots corresponding to three optical branches are substantially due to vibrations of the Sc atom.

The lattice contributions to the constant volume specific heat $c_v$ of Fe$_2$ScX compounds calculated under harmonic approximation are shown in figure 3. At higher temperatures (above 800 K) $c_v$ curves are approaching the classical Dulong and Petit limit of $\sim 100$ J mol$^{-1}$ K$^{-1}$ for Fe$_2$ScX compounds. Similar trend in $c_v$ is also observed for Fe$_2$VAl and Fe$_2$TiSn compounds in our previous work [24]. The $c_v$ is reaching Dulong and Petit value at $\sim 800$ K and $\sim 700$ K for two compounds, respectively. Therefore, it appears that this is generic feature for this class of compounds. It would have been interesting to verify these observations experimentally also. But, we could not come across any high temperature experimental data to the best of our knowledge to compare with. This behavior in $c_v$ appears to vary from material to material as can be seen in the work of Togo et al [17] (and reference [35] there in) where the experimental and calculated specific heat of Al is compared. It is observed that for Al, Dulong and Petit limit is reached at $\sim 300$ K.

At any temperature, one can see that $c_v$ values for Fe$_2$ScSb $>$ Fe$_2$ScAs $>$ Fe$_2$ScP compound. The $\kappa_{ph}$ is directly proportional to $c_v$ and hence calculation of $c_v$ is essential for an estimation of $\kappa_{ph}$ of a thermoelectric material. From the nature of the curves, one can estimate that at higher temperatures the differences in $\kappa_{ph}$ of Fe$_2$ScX compounds should be mainly due to group velocity and phonon relaxation time rather than due to $c_v$ which are closer to each other in this case. Considering the definition of Debye frequency as a measure of the maximum phonon frequency and Debye temperature, $\Theta_D$, to be the temperature above which all phonon modes begin to be excited [27], the calculated values of $\Theta_D$ for Fe$_2$ScX are $\sim 637$ K, $\sim 556$ K and $\sim 498$ K, respectively. The maximum phonon energy is decreasing from Fe$_2$ScP to Fe$_2$ScSb as mentioned earlier which is the reason for observed trend of $\Theta_D$.

### 3.2. Electronic structure

The band gaps of semiconductors and insulators in Kohn–Sham DFT calculations are generally underestimated. But, in a theoretical study or in prediction of new compounds with a band gap for thermoelectric applications, accurate calculation of band gap is essential since the number of carriers thermally excited varies exponentially with band gap. Also, in a DFT calculation, the curvature of bands at the band extrema and band features of electronic dispersion depend on the approximation used for the exchange-correlation part [11]. The transport coefficients calculated, depend on the effective mass and group velocity, which are derived from the band structure. Therefore, proper selection of XC functional for any DFT study of thermoelectric material is crucial. The question of which functional to choose was addressed in the work of Sk et al [13] as mentioned in the introduction which proposed that the combination of mBJ and SCAN (or PBEsol) functional would better explain the Seebeck coefficient. Thus, to calculate electronic band structure and dependent transport properties, two functionals viz. SCAN and mBJ are used.

The electronic bandstructure of Fe$_2$ScX ($X = P$, As, Sb) compounds are shown in figures 4(a)–(c), respectively. In the plots, the zero energy corresponds to the Fermi level, $E_F$, and is set to the middle of the gap. For each compound the indirect band gaps obtained from both functionals are listed in table 2. The indirect band gaps of Fe$_2$ScP and Fe$_2$ScAs obtained in the work of Sharma et al [10] are also included for comparison. Fe$_2$ScSb was predicted as semimetallic while former two compounds as semiconducting from PBEsol calculations in [10]. As can be seen in table 2, the band gap values predicted by SCAN and PBEsol are closer to each other but, much lesser than that from mBJ. The band gaps of Fe$_2$ScP, Fe$_2$ScAs and Fe$_2$ScSb are 0.81, 0.69 and 0.60 eV, respectively as obtained from mBJ calculations. The mBJ is constructed to give accurate band gaps and the literatures show the good agreement between the experimental and mBJ calculated band gaps [11, 28]. Thus, band gaps predicted in this work could be useful numbers to experimentalists for comparison in case samples are prepared.

The band gap is reducing from Fe$_2$ScP to Fe$_2$ScSb by a value of approximately 0.1 eV in case of mBJ. Therefore, at a given temperature the number of electrons excited into the conduction band are relatively lower in Fe$_2$ScP compared to other two compounds with the relatively least number being in Fe$_2$ScSb. A band gap of mBJ ground state band structure has been introduced into the band structure of SCAN in such a way that conduction band minimum (CBM) at $\Gamma$-point and valence band maximum (VBM) at $\Gamma$-point from both functionals coincide. This representation of band structure from two functionals depicts (figure 4) the differences in the features of dispersion curves at different points along the k-path. The bands numbered 1 to 5 in figure 4 are denoted with symbols B1 to B5 in the description. The X atom in the compound does not found to significantly affect the electronic states in the $\sim −4$ to $−0.3$ eV energy range of valence band region. Similarly, bands B1 and B2 in CB region are also slightly altered. This is discernible in the plots since the features of...
bands qualitatively does not show much difference in energy range mentioned.

In the plots the valence band maximum (VBM) is at Γ-point and CBM is at X-point giving indirect band gaps. In all three compounds, the VBM is triply degenerate at Γ-point. Fe$_2$ScX compounds possess a band B2 which is almost flat along the Γ-X direction and is dispersive in the direction Γ-L-W. The bands B1 and B2 are degenerate at Γ-point and continue to show degeneracy till L-point. The bands B1 and B2 start at the same energy at W but along the W-Γ and Γ-X directions, the bands of SCAN are elevated in energy relative to the mBJ bands. The three valence bands of SCAN starting from Γ and along the directions L-W and X-W-K are higher in energy relative to mBJ bands. In other words, in the VB region nearer to $E_F$, SCAN bands are narrower compared to mBJ bands (B3-B5) which implies density of states should be higher near $E_F$ in electronic structure calculated from SCAN. The CBM at Γ-point is doubly degenerate, but the bands B1 and B2 obtained from mBJ are relatively more narrower compared to the bands of SCAN. This implies the density of states in the CB region near $E_F$ is more in mBJ approximated electronic ground state.

The relatively small number of electrons excited into the conduction band decide the transport behavior in a semiconductor [27]. Since, the excited carriers are found almost in the neighborhood of the CB minima or VB maxima, for the three compounds the band extrema are approximated with a parabola to calculate the effective mass. Under the parabolic approximation, effective mass is inversely proportional to the curvature of the parabolic band. Thus, the effective mass values of carriers in a band indicates the curvature of the band. The Seebeck coefficient $S$ is directly proportional to the effective mass of charge carriers in the material according to the equation [4],

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

In the above relation, $h$ is Planck’s constant, $k_B$ is Boltzmann constant, $e$ is electronic charge and $n$ is carrier concentration, respectively.

The direct band gap from mBJ in these materials are 0.85, 0.72 and 0.62 eV, respectively (figure 4). These values of energy gap are much close to the indirect band gaps of mBJ listed in table 2 and hence there is finite probability that electron transition takes place between these points too. In order to quantify the curvature of bands from SCAN, the parabola were fitted at band extrema according to the free electron energy equation $E = \frac{h^2k^2}{2m_e}$, where $m_e$ is rest mass of electron and $m^*$ effective mass in terms of mass of electron. The bands numbered 1 to 5 (labeled B1 to B5 in table 3) in figure 4 which significantly participate in the transport are fitted with parabola in the vicinity of CB minima at Γ and X-points and VB maximum at Γ-point for SCAN functional. The obtained values of effective mass along different directions for Fe$_2$ScX for SCAN bands are listed in table 3. The notation, for instance, Γ–ΓL denotes the effective mass calculated at Γ-point along Γ to L direction.

The effective mass values in table 3 clearly highlight the large $m^*$ for band B2 in all three compounds. Along X – Γ direction $m^*$ are 39.91, 36.67 and 37.69 for three compounds, respectively. For the same band along Γ-X direction carriers have $m^*$ greater than along X – W direction. In Fe$_2$ScP, effective mass $m^*$ of the bands B1-B4 is 0.26 and B5 is 0.22.
respectively along $\Gamma - L$ directions. Along the $\Gamma - X$ direction $m^*$ of bands B1, B5, B3 and B4 are 0.13, 0.14, 0.43 and 0.42, respectively. As can be seen from the table, the band B2 has very large value of effective mass ($m^*$) along $\Gamma - X$ and $X - \Gamma$ directions and can be called heavy band in Fe$_2$ScX. From figure 4 one can observe that at CBM and VBM at the $\Gamma$-point, the curvature of mBJ bands are lesser compared to that of SCAN bands. This implies that effective mass if estimated from mBJ should be higher for these compounds. In the work of Kim et al [28] for III-V semiconductors effective mass values were estimated using mBJ and found that mBJ effective masses are overestimated with respect to experimental data by $\sim$30$\%$–50$\%$. Thus, one may predict that effective mass calculated for SCAN should be nearer to experimental value since these band features also explained the $S$ of Fe$_2$VAI in [13]. For a given compound, along the $\Gamma - L$ direction the bands B1 to B5 have nearly same curvature. While, along $\Gamma - L$ direction, B3 and B4 bands are of similar curvature which is justified by the $m^*$ values in the table.

### 3.3. Thermoelectric properties

The thermoelectric parameters Seebeck coefficient $S$, electrical conductivity per relaxation time $\sigma/\tau$ and power factor per relaxation time $S^2 \sigma/\tau$ (PF), are calculated for Fe$_2$ScX compounds under semiclassical transport theory. In order to calculate thermoelectric properties, the band structure from SCAN functional and band gap obtained from the mBJ have been used. In figures 5(a)–(c), for three compounds the variation in $S$ with the shifts in chemical potential ($\mu$) are presented at 300 K. The dashed line normal to $\mu$ axis indicates chemical potential for the intrinsic compounds at 0 K. The positive and negative values of $\mu$ in plots correspond to electron and hole doping, respectively. At the temperature of 300 K, $S$ versus $\mu$ curve cuts the $\mu = 0$ line, for Fe$_2$ScP, at $\sim$1134 $\mu$V K$^{-1}$ and for Fe$_2$ScAs and Fe$_2$ScSb at $\sim$1068 and $\sim$963 $\mu$V K$^{-1}$, respectively. This indicates intrinsic Fe$_2$ScX at 300 K will show negative $S$ values which is attributed mainly due to presence of flat conduction band in these compounds. The values of extrema in the $S$ curves are reducing from Fe$_2$ScP to Fe$_2$ScSb which implies in Fe$_2$ScP maximum $S$ can be obtained either by electron or hole doping.

The maximum value of $S$ (at 300 K) for the three compounds are $\sim$1421, $\sim$1230 and $\sim$1080 $\mu$V K$^{-1}$ in the order, for shift in $\mu$ of $\sim$34, $\sim$23 and $\sim$24 meV, respectively. At a given temperature, $S$ is inversely proportional to carrier concentration ($n$) and directly proportional to $m^*$. The band gap of Fe$_2$ScP is 0.81 eV and is the highest in the family of Fe$_2$ScX (table 2) making $n$ to be smaller compared to other compounds at a given temperature. This explains the reason for the observed higher $S$ in figure 5(a) for Fe$_2$ScP compared to other two compounds. We compare the $S$ versus $\mu$ curves with the work of Sharma et al [10] wherein PBEsol functional was used. We observe that the extrema of $S$ values calculated as a function of $\mu$ at 300 K are very much lower compared to that of our work. The maximum value of $S$ in [10] for undoped compounds (at $\mu = 0$) was $\sim$770, $\sim$386, $\sim$192 $\mu$V K$^{-1}$ for Fe$_2$ScP, Fe$_2$ScAs and Fe$_2$ScSb, respectively. This can be mainly due to the lower band gap predicted by PBEsol (table 2) for Fe$_2$ScX compounds.

In order to find out the proper carrier concentration that would yield $S$ and $\sigma/\tau$ values which maximize the PF, we have computationally considered doping in Fe$_2$ScX compounds with electrons and holes in the range $\sim$1 $\times$ 10$^{19}$ – $\sim$ 5 $\times$ 10$^{21}$ cm$^{-3}$. Doping in BoltzTraP was considered by the shift in the position of the chemical potential from the middle of the band gap. At 0 K, chemical potential at the middle of the gap represents the undoped case. For the electron doping, chemical potential positions above the middle of the gap are considered and the doping concentration corresponds to that particular shift in chemical potential. Higher the shift in the position of the chemical potential towards conduction band, higher is the doping. Similarly, hole dopings are considered for chemical potential positions towards valence band region.

For the three compounds $S$, $\sigma/\tau$ and PF values are calculated for various dopings in the temperature range 250–1200 K. Seebeck coefficient values for electron doped compounds are shown in figures 5 (d)–(f). For Fe$_2$ScX, values of $S$ are decreasing continuously with the increase in the temperature for a given electron doping from $\sim$1 $\times$ 10$^{19}$ cm$^{-3}$ to $\sim$1 $\times$ 10$^{20}$ cm$^{-3}$. For $\sim$5 $\times$ 10$^{20}$ cm$^{-3}$ of doping, the range of $S$ (max. $S$-min.$S$) for temperature range under study is reduced. For $\sim$1 $\times$ 10$^{21}$ cm$^{-3}$ of doping the $S$ is not varying substantially with temperature. But, slow increasing nature of $S$ is observed for $\sim$5 $\times$ 10$^{21}$ cm$^{-3}$. This is the general trend of $S$ observed in case of electron doping. Also, with increase in the electron doping $S$ curves are shifting towards lower values since $S$ varies inversely with carrier concentration as given by equation (2). The maximum values of $S$ are $\sim$743, $\sim$645, $\sim$637 $\mu$V K$^{-1}$ for $\sim$1 $\times$ 10$^{19}$ cm$^{-3}$ electron doping for Fe$_2$ScX compounds, respectively at 250 K. At any temperature lower doping of $\sim$1 $\times$ 10$^{19}$ cm$^{-3}$ has higher $S$ value. In [10], nature of the $S$ curves for $\sim$1 $\times$ 10$^{19}$ – $\sim$1 $\times$ 10$^{21}$ cm$^{-3}$

### Table 3. Effective mass ($m^*$) of charge carriers calculated for Fe$_2$ScX (X = P, As, Sb) compound at $\Gamma$ and X points respectively, in various bands from SCAN.

| Fe$_2$ScP | Fe$_2$ScAs | Fe$_2$ScSb |
|-----------|------------|------------|
| $\Gamma-\Gamma$ | $\Gamma-X$ | $\Gamma-X$ | $\Gamma-X$ |
| B1 | 0.26 | 0.10 | 0.16 | 0.09 |
| B2 | 0.26 | 0.10 | 0.16 | 0.22 | 0.45 |
| B3 | 0.26 | 0.14 | 0.16 | 0.16 |
| B4 | 0.26 | 0.14 | 0.16 |
| B5 | 0.22 | 0.14 | 0.16 | 0.16 | 0.09 |
Figure 5. Seebeck Coefficient ($S$) versus chemical potential ($\mu$) plots (figures (a)–(c)) and $S$ as a function of temperature ($T$) for electron doping (figures (d)–(f)) and hole doping (figures (g)–(i)). Each of three vertical panel in the figure shows the plots for Fe$_2$ScP, Fe$_2$ScAs and Fe$_2$ScSb, respectively.

of doping are different which can be due the lower band gaps considered compared to the present work. The maximum $S$ values at $\sim 1 \times 10^{19}$ cm$^{-3}$ doping are $\sim 500$, $\sim 400$ and $\sim 25 \mu$ V K$^{-1}$ for Fe$_2$ScX, respectively.

The nature of $S$ curves for different hole dopings are shown in figures 5(g)–(i) for three compounds. The maximum $S$ is obtained for doping of $\sim 1 \times 10^{19}$ cm$^{-3}$ in the temperature range considered and the increment in $S$ with the increase in the temperature is less compared to higher dopings. For $\sim 5 \times 10^{19}$ to $5 \times 10^{21}$ cm$^{-3}$ range, $S$ is increasing with the lower doping values. In [10], $S$ curves for hole doping do not show linear increase behavior as in this work, instead there are peaks in the $S$ curves. The reason for the observed differences may be due to the large band gap considered in this work. Comparing the $S$, for hole and electron doped case, one can observe that from figure 5, for a given doping electron doping gives larger $S$ for Fe$_2$ScX.

The figure 6 shows the $\sigma$/τ and PF plots for different carrier concentrations as a function of temperature. The electron and hole doping values considered for both $\sigma$/τ and PF are shown only in the respective PF plots, represented in same colors (or symbols). The highlighting feature of $\sigma$/τ plots (figures 6(a)–(f)) is that, for any doping values $\sigma$/τ curves are nearly linearly increasing from 250 to 1200 K for all compounds. For doping of $\sim 1 \times 10^{19}$ to $\sim 1 \times 10^{20}$ cm$^{-3}$, $\sigma$/τ curves are close to each other for both electron and hole doping. For higher dopings $\sigma$/τ curves are shifting towards higher values. The highest $\sigma$/τ is obtained for doping concentration of $\sim 5 \times 10^{21}$ cm$^{-3}$ of both electron and hole type. From $\sim 5 \times 10^{20}$ to $\sim 5 \times 10^{21}$ cm$^{-3}$, the obtained value of $\sigma$/τ, for a given doping concentration is higher for hole type doping compared to electron type. This can be understood as because of the lesser effective mass of holes in valence bands (B3–B5) (table 3) compared to that of electrons with high effective mass in band B2. Since, the charge carrier with higher effective mass has lower mobility and electrical conductivity in semiconductors is related to mobility as, $\sigma = ne\mu$, where $\mu$ is mobility of charge carriers, higher electrical conductivity of holes is expected in these compounds.

The $S^2\sigma$/τ (PF) plots for Fe$_2$ScX are presented in figures 6(g)–(l) for electron and hole doping in $10^{14}$ $\mu$ W K$^{-2}$ cm$^{-1}$ s$^{-1}$ (1 PF unit, PFU). For electron doped cases, the PF curves are shifted to higher values with the increased doping concentration except for doping of $\sim 5 \times 10^{21}$ cm$^{-3}$. For a given doping, the PF is increasing with temperature from 250 to 1200 K. For temperatures of practical applications, for instance, in automobiles where temperature of heat source, to install TEG is considered as 800 K [29], PF values...
at these temperatures are, \( \sim 121 \), \( \sim 125 \) and \( \sim 131 \) PFU, for
doping of \( \sim 1 \times 10^{22} \) cm\(^{-3} \) for Fe\(_2\)ScP, Fe\(_2\)ScAs, and Fe\(_2\)ScSb,
respectively. Thus, for Fe\(_2\)ScX compounds, to get a high PF from
electron doping, \( \sim 1 \times 10^{21} \) cm\(^{-3} \) can be considered as
optimal doping concentration in the doping range considered.

For hole doped case also an increasing trend in PF with
temperature is observed in figures 6(j)–(l). For doping range \( \sim 1 \times 10^{19} \)–\(1 \times 10^{20} \) cm\(^{-3} \), the PF values are
close to each other. At any temperature, for the hole doping
of \( \sim 5 \times 10^{21} \) cm\(^{-3} \) highest PF is obtained for these com-
ounds. At 800 K, the values of PF for \( \sim 5 \times 10^{21} \) cm\(^{-3} \) doped
ings are, \( \sim 118 \), \( \sim 83 \) and \( \sim 63 \) PFU for Fe\(_2\)ScP, Fe\(_2\)ScAs, and
Fe\(_2\)ScSb, respectively. From figures 6(j)–(l) we can observe that PF values for a given doping is decreasing from Fe\(_2\)ScP
to Fe\(_2\)ScSb. The power factor curves in the work of [10] shows
gradual increasing behavior for the carrier concentration of
\( \sim 1 \times 10^{17} \) to \( \sim 1 \times 10^{19} \) cm\(^{-3} \). But, for doping of \( \sim 1 \times 10^{20} \)
to \( \sim 1 \times 10^{21} \) cm\(^{-3} \), there are peaks in the PF curves. The
maximum PF is obtained for a doping of \( \sim 5 \times 10^{21} \) cm\(^{-3} \) in
all three compounds. The maximum values of PF obtained
for p-type doping is \( \sim 90–24 \) PFU and for n-type doping
is \( \sim 85–54 \) PFU from Fe\(_2\)ScP to Fe\(_2\)ScSb compound in [10].
The values of maximum PFs obtained by using PBEsol func-
tional in the work of [10] are lesser compared to the present
work. The band gaps obtained by PBEsol are lesser compared
to mBJ as can be seen in table 2, may be the reason for the
observed differences in PF values calculated in two works.

From the nature of the PF curves (figures 6(g)–(l)), which
are showing increasing behavior with temperature, we can
propose these materials for high temperature thermoelectric
applications.

Electronic thermal conductivity per relaxation time \( (\kappa_e/\tau) \)
of Fe\(_2\)ScX compounds for electron and hole dopings consid-
ered in this study are shown in figures 7(a)–(c) and (d)–(f),
respectively. For three compounds, \( \kappa_e/\tau \) curves are showing
increasing trend with temperature. For optimal doping cases

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure6.png}
\caption{Electrical conductivity per relaxation time \( (\sigma/\tau) \) and power factor per relaxation time \( (S^2\sigma/\tau) \) as a function of temperature (T) for electron doping (figures (a)–(c) and (g)–(i)) and hole doping (figures (d)–(f) and (j)–(l)) for Fe\(_2\)ScP, Fe\(_2\)ScAs and Fe\(_2\)ScSb, respectively.}
\end{figure}
Figure 7. Electronic thermal conductivity per relaxation time ($\kappa_e/\tau$) as a function of temperature (T) for electron doping (figures (a)–(c)) and hole doping (figures (d)–(f)) for Fe$_2$ScP, Fe$_2$ScAs and Fe$_2$ScSb, respectively.

Table 4. Phase velocity ($c$) of three acoustic branches (S1–S3) in $\Gamma$-W and $\Gamma$-L directions and average of phase velocities, $c_{\text{avg}}$, for Fe$_2$ScX (X = P, As, Sb), Fe$_2$VAl and Fe$_2$TiSn compounds in THz·Bohr

|        | Fe$_2$ScP | Fe$_2$ScAs | Fe$_2$ScSb | Fe$_2$VAl | Fe$_2$TiSn |
|--------|-----------|------------|------------|-----------|------------|
| $\Gamma$-W | $\Gamma$-L | $\Gamma$-W | $\Gamma$-L | $\Gamma$-W | $\Gamma$-L |
| S1 69.9 | 102.4 | 71.0 | 86.5 | 73.4 | 78.5 | 96.7 | 101.4 | 80.1 | 93.1 |
| S2 95.5 | 102.4 | 84.4 | 86.5 | 78.1 | 78.5 | 101.4 | 101.4 | 90.4 | 93.1 |
| S3 161.9 | 141.0 | 138.7 | 128.3 | 120.6 | 117.1 | 151.1 | 147.8 | 146.2 | 139.9 |
| $c_{\text{avg}}$ | 112.2 | 99.2 | 91.0 | 116.6 | 107.1 |

giving the highest PFs viz. $\sim 1 \times 10^{21}$ cm$^{-3}$ of electron doping, $\kappa_e/\tau$ is increasing from first to last compound while, for hole doping of $\sim 5 \times 10^{21}$ cm$^{-3}$ reverse trend is observed. At 800 K, $\kappa_e/\tau$ values for electron doping of $\sim 1 \times 10^{21}$ cm$^{-3}$ which yields the highest PF are 0.13, 0.14 and $0.15 \times 10^{16}$ W m$^{-1}$ K$^{-1}$ s$^{-1}$ for Fe$_2$ScX compounds, respectively.

Calculation of $\kappa$ of thermoelectric material is important to fully evaluate it for thermoelectric application. But, calculation of $\kappa_{\text{avg}}$ is a difficult and computationally demanding task [30]. Therefore, any simple method predicting fairly good value of $\kappa_{\text{avg}}$ is of much help. Here for a quantitative estimation of $\kappa_{\text{ph}}$ in Fe$_2$ScX compounds we resort to a simple method which turns out to provide reasonably good estimation of $\kappa_{\text{ph}}$. The relation for $\kappa_{\text{ph}}$ is given by [27],

$$\kappa_{\text{ph}} = \frac{1}{3} c_{\text{ph}} c^2 \tau_{\text{ph}}, \quad (3)$$

where $c_{\text{ph}}$ is constant volume specific heat per unit volume, $c$ is phonon phase velocity in linear dispersion and $\tau_{\text{ph}}$ is phonon relaxation time.

Now, to calculate $\kappa_{\text{ph}}$ from equation (3), the values of $c_{\text{ph}}$, $c$ and $\tau_{\text{ph}}$ are needed. The specific heat, $c_{\text{ph}}$ is obtained as function of temperature from the phonon calculations. To calculate $c$, three acoustic branches are approximated with linear dispersion, by fitting with straight line in the neighborhood of $\Gamma$ ($k = 0$) of the calculated phonon dispersions. Then $c$ is calculated as

$$c = \omega/k ,$$

the slope of the linear dispersion. To find out $c$, acoustic branches in the $\Gamma$-W and $\Gamma$-L directions are considered. Values of $c$ of three acoustic branches in two directions are averaged, which we denote by $c_{\text{avg}}$ and used to estimate $\kappa_{\text{ph}}$ instead of $c$ in equation (3). Table 4 shows the values of $c$ calculated for three acoustic branches in two directions and $c_{\text{avg}}$ values for Fe$_2$ScX, Fe$_2$VAl and Fe$_2$TiSn compounds. The branch notations followed are shown in the inset of figure 1(b).

The table 4 shows that the $c$ of phonons of three acoustic branches in $\Gamma$-L directions are reducing from Fe$_2$ScP to Fe$_2$ScSb. In $\Gamma$-W direction, similar trend in $c$ is noted for branch S2 and S3 (which are degenerate), except for S1 in which opposite trend is observed. In $\Gamma$-L direction, branches S1 and S2 are degenerate and have value of $c$, 102.4, 86.5 and 78.5 THz · Bohr for Fe$_2$ScX, respectively. The $c_{\text{avg}}$ for Fe$_2$ScX are 112.2, 99.2, and 91.0 THz · Bohr, respectively. The observed trend is due to reduction in phonon frequencies on going from first to last compound. In both directions considered, $c$ of phonons in Fe$_2$VAl is greater than that in Fe$_2$TiSn for all branches.

The calculated $c_{\text{avg}}$ are 116.6 and 107.1 THz · Bohr for Fe$_2$VAl and Fe$_2$TiSn, respectively. The phonon $c_{\text{avg}}$ of Fe$_2$ScX compounds are lesser compared to Fe$_2$VAl and Fe$_2$TiSn except, for Fe$_2$ScP with $c_{\text{avg}}$ of 112.2 THz · Bohr.

Once, the quantities $c_{\text{ph}}$ and $c$ are known, $\tau_{\text{ph}}$ needs to be found out which is the computationally more difficult part. At
this step, to estimate the value of $\tau_{ph}$, we considered Fe$_2$VAl and later the $\tau_{ph}$ is benchmarked using Fe$_2$TiSn compound. For this estimation, $c_v$ values are taken from our previous work [24] and $c_{\text{avg}}$ and $c_{v}$ are used which are calculated are tabulated in table 4. Using the experimental $\kappa$ of Fe$_2$VAl [31] at 300 K of $\sim 25$ Wm$^{-1}$K$^{-1}$, the $\tau_{ph}$ estimated, is $\sim 5 \times 10^{-13}$s. The calculated value of $\tau_{ph}$ for Fe$_2$TiSn using the estimated $\tau_{ph}$ at the same temperature is $\sim 14.8$ Wm$^{-1}$K$^{-1}$. This value is close to the experimental $\kappa$ value of Leu et al. [32] ($\sim 7$ Wm$^{-1}$K$^{-1}$) at 300 K. This suggests that the $\tau_{ph}$ estimated by this method can predict reasonably accurate values of $\kappa_{ph}$ for other three compounds using such a simple approach. It is important to note here that, Fe$_2$VAl, Fe$_2$TiSn and Fe$_2$ScX compounds have same crystal structure and belong to the same class of compounds with similar phonon dispersions which led us to select the former two compounds in the estimation. With the calculated $\tau_{ph}$ of $5 \times 10^{-13}$s and using $c_{\text{avg}}$ and $c_{v}$ values, the estimated $\kappa_{ph}$ at 300 K for three compounds are 18.2, 13.6 and 10.3 Wm$^{-1}$K$^{-1}$, respectively. The $\kappa_{ph}$ is reducing from Fe$_2$ScP to Fe$_2$ScSb, which may be mainly due to the larger sized and heavier mass elements in the latter compounds.

The assessment of TE applicability of Fe$_2$ScX Heusler compounds is done by calculating temperature dependent $ZT$ in 300–1200 K range. For the calculation of $ZT$ from equation (1), the estimated $\kappa_{ph}$ at 300 K of the pure compounds are used for all temperatures, which is generally expected to reduce at higher temperatures. Constant electron relaxation time $\tau$ of $1 \times 10^{-14}$s is used [27] in the estimation of $S^2\sigma$ and $\kappa_e$. The temperature dependent $ZT$ values of Fe$_2$ScX compounds are calculated for the highest PF yielding optimal electron (n-type) doping of $\sim 1 \times 10^{21}$ cm$^{-3}$ and hole (p-type) doping of $\sim 5 \times 10^{21}$ cm$^{-3}$, out of the doping range considered in this study. The obtained $ZT$ for doped Fe$_2$ScX compounds are presented in figure 8. The $ZT$ values suggest that Fe$_2$ScX compounds could be promising materials for TE applications with $ZT$ showing the increasing nature with temperature.

From the figure we can see that for electron doping shown, Fe$_2$ScSb has the highest $ZT$ while, for hole doping Fe$_2$ScP shows the highest $ZT$ among the family. The highest $ZT$ is obtained from Fe$_2$ScSb, which in 300–500 K is 0.11–0.25, in the mid-temperature range of 500–900 K is 0.25–0.45 and in high temperature range 900–1200 K is 0.45–0.52. The $ZT$ values obtained from the hole doping of $\sim 5 \times 10^{21}$ cm$^{-3}$ for these compounds are lower compared to electron doping. The n-type Fe$_2$ScP has $ZT$ in the range 0.07–0.43, while p-type Fe$_2$ScP has 0.03–0.34 which is the highest among p-type Fe$_2$ScX compounds. The doped Fe$_2$ScAs is showing intermediate $ZT$ among the optimal doped Fe$_2$ScX compounds. The $ZT$ range for n-type and p-type Fe$_2$ScAs are 0.09–0.48 and 0.03–0.28 in 300–1200 K, respectively. For last compound in the family, n-type Fe$_2$ScSb, the highest $ZT$ is observed in the range of 0.11–0.52. In case of its p-type counterpart of $\sim 5 \times 10^{21}$ cm$^{-3}$ doped, $ZT$ at 300 K is 0.03 and it is reaching 0.26 at 1200 K. Higher $ZT$ values are observed in the high temperature region for both type of doping, which hints at the possible applicability in high temperature power generation. The 900–1200 K range $ZT$ for $\sim 1 \times 10^{21}$ cm$^{-3}$ doping of Fe$_2$ScX compounds are, 0.34–0.43, 0.40–0.48 and 0.45–0.52, respectively. For the hole doping of $\sim 5 \times 10^{21}$ cm$^{-3}$, the $ZT$ values in the same temperature range are 0.25–0.34, 0.20–0.28 and 0.18–0.26, respectively.

The higher $ZT$ observed at temperatures $>900$ K, indicates that for the high temperature thermoelectric power generation, doped Fe$_2$ScX full-Heuslers could be one of the suitable candidates. Currently, doped Si–Ge alloys are one of thermoelectric materials in use for power generation in high temperature region (673–1273 K) with $ZT$ ranges of $\sim 0.5–0.8$ and $\sim 0.4–0.6$ for n-type and p-type Si–Ge, respectively [4]. The simultaneous increase in thermopower and electrical conductivity with moderate decrease in thermal conductivity was observed in the work of Makongo et al [33] leading to $\sim 2.5$ times $ZT$ enhancement for the bulk nanostructured (Zr, Hf) NiSn half-Heusler alloys. In the TE area of research, with the considerable interest in enhancement of $ZT$ by complex nanostructuring [4, 34], we anticipate that Fe$_2$ScX family of full-Heuslers could be worth considering next to Si–Ge alloys. Also, the $ZT$ plot, hints that, with both electron and hole doped compounds showing good $ZT$ number, they can be used as n-type and p-type thermoelements in constructing TEGs. Therefore, an attempt by experimental community to synthesize and study the thermoelectric properties are highly desired.

4. Conclusions

In the present work, electronic structure and dependent thermoelectric coefficients of Fe$_2$ScX (X = P, As, Sb) compounds are studied using two functionals viz. SCAN and mBJ. The differences in the features of the electronic bands obtained from mBJ and SCAN are brought out by comparison. The effective mass values are calculated at the bands extrema of SCAN. The indirect band gaps for Fe$_2$ScP, Fe$_2$ScAs and Fe$_2$ScSb, obtained from mBJ are 0.81, 0.69 and 0.60 eV, respectively. $S$, $\sigma/\tau$, PF and $\kappa_e/\tau$ are calculated for various values of electron and hole doping by introducing band gaps from mBJ into

![Figure 8. Temperature dependent $ZT$ plot of Fe$_2$ScX (X = P, As, Sb) compounds for electron doping of $\sim 1 \times 10^{21}$ cm$^{-3}$ shown in solid (green) lines and hole doping of $\sim 5 \times 10^{21}$ cm$^{-3}$ in dashed (red) lines.](image-url)
suggests that Fe$_2$ScX compounds could be worth considering. The PF obtained at the temperature of 800 K for electron doping of $\sim 1 \times 10^{21}$ cm$^{-3}$ are $\sim 121$, $\sim 125$ and $\sim 131$ 10$^{14}$ $\mu$W K$^{-2}$ cm$^{-1}$ s$^{-1}$ for Fe$_2$ScX where X = P, As, Sb, respectively. While, at the same temperature, highest PF values is obtained for hole doping of $\sim 5 \times 10^{21}$ cm$^{-3}$ which are $\sim 118$, $\sim 83$ and $\sim 63$ 10$^{14}$ $\mu$W K$^{-2}$ cm$^{-1}$ s$^{-1}$ for Fe$_2$ScX, respectively. The phonon dispersion and density of states are calculated for the three compounds which supported the structural stability. The calculated lattice contribution to $\kappa_c$ shows at any temperature $\kappa_c$ are in order Fe$_2$ScSb > Fe$_2$ScAs > Fe$_2$ScP. The maximum phonon energy (or frequency) for Fe$_2$ScX are $\sim 55$, $\sim 48$ and $\sim 43$ meV, respectively. The Debye temperatures are calculated for three compounds which are $\sim 637$ K, $\sim 556$ K and $\sim 498$ K, respectively. Based on the calculation of slopes of acoustic branches in the linear region and estimated $\tau_{\text{ph}}$ of Fe$_2$ScX compounds at 300 K are calculated. The $\tau_{\text{ph}}$ for three compounds are 18.2, 13.6 and 10.3 Wm$^{-1}$ K$^{-1}$, respectively. For three compounds, the $ZT$ values in the temperature range 900–1200 K, for the hole doping of $\sim 5 \times 10^{21}$ cm$^{-3}$ are 0.25–0.34, 0.20–0.28 and 0.18–0.26, respectively. In the same temperature range, $ZT$ for $\sim 1 \times 10^{21}$ cm$^{-3}$ electron doping are 0.34–0.43, 0.40–0.48 and 0.45–0.52, respectively. The work suggests that Fe$_2$ScX compounds could be worth considering for high temperature thermoelectric applications with both n-type and p-type compounds showing good $ZT$ values.

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ORCID IDs

Shivprasad S Shastri @ https://orcid.org/0000-0002-4979-0985

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