Electronic Structure and Thermoelectric Properties of Half-Heusler Alloys \(\text{NiTZ}\)

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We have investigated the electronic and thermoelectric properties of half-Heusler alloys \(\text{NiTZ} (T = \text{Sc, and Ti}; Z = \text{P, As, Sn, and Sb})\) having 18 valence electron. Calculations are performed by means of density functional theory and Boltzmann transport equation with constant relaxation time approximation, validated by NiTiSn. The chosen half-Heuslers are found to be an indirect band gap semiconductor, and the lattice thermal conductivity is comparable with the state-of-the-art thermoelectric materials. The estimated power factor for NiScP, NiScAs, and NiScSb reveals that their thermoelectric performance can be enhanced by appropriate doping rate. The value of \(ZT\) found for NiScP, NiScAs, and NiScSb are 0.46, 0.35, and 0.29, respectively at 1200 K.

I. INTRODUCTION

In the past few decades, researchers have been focused on the investigation of the multi-functional materials, which can be used as various applications such as in spintronics, optoelectronics, thermoelectrics (TE), etc. With the surge in demand for green energy sources, TE materials are extensively taken into consideration for their ability to convert relatively small and waste heat into useful energy at the time of energy consumption. Wide range of materials has been explored for the potential half-metals and TE devices such as organic1–3, chalcogenides4–6, skutterudites7–21 oxides22–24, hybrid perovskites25–28, triple-point metals29, ternary compound30, and half-Heusler (hH) alloy14,32–34. Among them, Heusler compounds have gained much more attention since their discovery in 1903 due to their simple crystalline structure with fascinating properties that includes magnetism, half metallicity, superconductivity, optoelectronic, piezoelectric semiconductors, thermoelectricity, topological insulators and semimetals30–33.

Thermoelectric materials are found applicable in day-to-day lives to fulfill the increasing demand of energy of the globalized society. The highly efficient TE devices (cooler, power generator, temperature sensors, etc) can utilize a large amount of wasted thermal energy to generate electricity and vice-versa30–32. For this, the device needs a larger figure of merit (\(ZT\)), which depends on the transport properties33–35 defined by

\[
ZT = \frac{\alpha^2 \sigma T}{\kappa} 
\tag{1}
\]

where \(\alpha (V \text{K}^{-1})\) is the Seebeck coefficient, \(\sigma (S \text{ m}^{-1})\) is the electrical conductivity, \(\kappa=\kappa_e+\kappa_l\) (W m\(^{-1}\)K\(^{-1}\)) is thermal conductivity, and \(T(\text{K})\) is the absolute temperature. \(\alpha^2 \sigma\) is defined as the power factor (PF). The symbol \(\kappa_e\) and \(\kappa_l\) represents the electronic and lattice thermal conductivity, respectively. The materials having a high value of PF along with the low value of \(\kappa\) are suitable for the efficient TE devices33.

Among others, most of the cubic hH alloys with 18 valence electron count (VEC) exhibits high Seebeck coefficients and are reported as promising materials for TE application due to high electrical conductivity and narrow band gap semiconductors with novel electrical and mechanical properties even at high-temperature34,35. In addition to it, hH alloys contain non-toxic and readily available elements, making them environmentally friendly and more cost effective.

Recent experimental and theoretical investigations on hH alloys are mainly focused on improving their thermoelectric efficiency \(ZT\) by tuning the power factor and thermal conductivity. Band gap engineering and fluctuation of carrier concentration around the Fermi level \((E_F)\) in \(Z\) position is a widely used method to enhance the power factor, whereas, thermal conductivity can be decreased by alloying or by doping on \(X\) or \(Y\) site to fluctuate the mass of the carriers introducing impurities and nanostructuring35–48.

From the literatures, we noticed that Ni-based hH alloys with 18-VEC are less investigated. Following the Slater-Pauling’s rule, the total magnetic moment for these type of hH alloys should be zero. Thus, the zero moment on Ti or Sc at \(Y\) site and P or As or Sb at \(Z\) site will give rise to zero moment for the Ni atom at the \(X\) site resulting in a non-magnetic system49–50. This motivates us to explore the electronic, TE, and other related properties to confirm if these groups of materials could be suitable for TE devices.

II. COMPUTATIONAL DETAILS

The cubic hH alloys \(\text{NiTZ} (T=\text{Sc, and Ti}; Z=\text{P, As, Sn, and Sb})\) belongs to \(\text{C}\text{i}_6\) structure with space group \(F\text{4}3\text{m}\). It contains three in-equivalent atoms forming inter-penetrating fcc sublattices with the Wyckoff positions Ni (1/4, 1/4, 1/4), T (1/2, 1/2, 1/2) and Z (0, 0, 0), respectively as shown in Figure 1. The iso-structural NiTiSn is used here to validate our calculations based on the earlier reported results (both theoretical
and experimental).

The density functional (DF) calculations has been performed using the full-potential linear augmented plane wave (FP-LAPW) method as implemented in the WIEN2k code\textsuperscript{51}. We double checked some parts of our calculations using the plane-wave based pseudopotentials Quantum Espresso (QE) package\textsuperscript{52}. The standard generalized-gradient approximation (GGA) in the parameterization of Perdew, Burke, and Ernzerhof (PBE)\textsuperscript{53} was used in scalar-relativistic mode. The modified Becke-Johnson (mBJ) potential\textsuperscript{54} was further included to check the accuracy of the band gaps. The self-consistency convergence criteria for charge was set to $10^{-4}$ e, and energy to $10^{-5}$ Ry.

In the plane-wave pseudopotential approach, we used the norm-conserving pseudopotentials with plane wave cut-off energy for wave function set to 90 Ry. The full Brillouin Zone (BZ) was sampled with an optimized $10 \times 10 \times 10$ mesh of Monkhorst-Pack $k$–points. To check the dynamical stability, phonon spectrum calculations have been performed with $4 \times 4 \times 4$ $q$–mesh in phonon BZ, which is based on the DF perturbation theory (DFPT) implemented in the QE package\textsuperscript{52}.

The TE properties were calculated using the Boltzmann semi-classical transport equation and constant relaxation time approximation based on a smoothed Fourier interpolation of the bands implemented on BoltzTraP code\textsuperscript{55}. The full BZ was sampled with $50 \times 50 \times 50$ $k$–mesh for the calculation of the transport properties. The electrical conductivity and PF were calculated under constant relaxation time approximation ($\tau$) using the BoltzTraP code based on Boltzmann theory. $\tau$ is approximated by fitting the experimental data from Kim \textit{et al}\textsuperscript{18}.

The lattice thermal conductivity was obtained by solving linearized Boltzmann transport equation (BTE) within the single-mode relaxation time approximation (SMA) using thermal2 code implemented in QE package\textsuperscript{52}.

### III. RESULTS AND DISCUSSION

#### A. Structure Optimization and Phonon Stability

We started our calculations by optimizing the cubic hH alloys with $F\bar{4}3m$ symmetry. Our calculated values of lattice parameters and the band gap within GGA and GGA + mBJ are listed in Table I. These values are found to be in fair agreement with the earlier reports of Ma \textit{et al}\textsuperscript{49} for the GGA case.

| System  | GGA $a$ (Å) | GGA $E_g$ (eV) | GGA+mBJ $E_g$ (eV) |
|---------|-------------|----------------|-------------------|
| NiScP   | 5.69        | 0.54           | 0.62              |
| NiScAs  | 5.84        | 0.48           | 0.52              |
| NiScSb  | 6.12        | 0.28           | 0.32              |
| NiTiSn  | 5.95        | 0.46           | 0.45              |

The calculated phonon dispersion curves along the high-symmetry points shown in Figure 2 depicts that the proposed hH alloys are thermally stable. This is evidenced by the absence of imaginary phonon frequencies throughout the whole BZ, as expected for dynamic stability\textsuperscript{56}. We observed three acoustic (low-frequency region) and six optical phonon (high-frequency region) branches due to three atoms per unit cell.

![FIG. 2. Phonon band structures for finding the dynamic stability of](image)
The majority of the lattice contribution to the thermal conductivity arises from the acoustic part as it has high group velocity compared to the optical part. We found that the acoustical phonon branches of NiScP and NiScAs extends nearly to 200 cm$^{-1}$ while NiScSb and NiTiSn lies within 150 cm$^{-1}$ in frequency. The observation of dynamical stability and preferable energy gap in our proposed hH alloys motivate us to explore the electronic and transport properties for their potential application as TE materials.

### B. Electronic Properties

To understand the ground state electronic properties of the material, the total and partial density of states (DOS) are shown in Figure 3. The proposed systems are found to be semiconducting with an energy gap lying within $\sim 0.32 - 0.62$ eV, in fair agreement with the earlier reports. As seen in the PDOS the main contribution to the total DOS at and around $E_F$ are from the 3$d$-orbitals of Ni and Sc atoms while the contributions from atom on the Z site is negligible (see in Figure 3). This is an indication that doping onto the Z site may improve the carrier concentration.

![Figure 3: Total and Partial density of states](image)

**FIG. 3.** Total and Partial density of states of a) NiScP, b) NiScAs, c) NiScSb, and d) NiTiSn within GGA + mBJ. Vertical dotted line represent $E_F$.

It is interesting to note that with increase in the atomic radius of atoms at Z site, say, from P to Sb, the band gap reduces gradually which further leads to the decrease in the hybridization of Ni-3$d$ and Sc-3$d$ states. An indirect band gap is observed in the band structures for hH alloys (see Figure 4) with their valence band maximum (VBM) lying at $\Gamma$ and conduction band minimum (CBM) at $X$ in the BZ. The VBM for the hH alloys are 3-fold degenerate comprising of heavy and light bands. From the observed band structure in Figure 4, the scenario of heavy bands can enhance the Seebeck coefficient, whereas, the light band can facilitate the mobility of charge carriers. Thus, the combination of heavy and light bands are preferable for increasing the TE performance. The band structure shown in Figure 4 (a), (b), and (c) dictates the effective mass to be more at $X - \Gamma$ in CBM than that of VBM at $\Gamma$ (i.e., the effective mass of electron at CBM is greater than that of the hole at VBM), which play an significant role in TE properties. As seen in NiTiSn (Figure 4 (d)), the VBM (at $\Gamma$) is flatter than the CBM (at $X$) indicating that the effective mass of holes at VBM is more than that of electrons on CBM.

![Figure 4: Electronic band structure](image)

**FIG. 4.** Electronic band structure of a) NiScP, b) NiScAs, c) NiScSb, and d) NiTiSn within GGA + mBJ.

### C. Transport Properties

For an efficient TE material, a high value of $\alpha$ and $\sigma$ with a low $\kappa$ is expected, as depicted in equation (1). The dimensionless figure of merit $ZT$ can be optimized when these parameters are optimum. But these parameters are inter-related with themselves. Thus, to obtain high value of $ZT$ is in-sufficient just by tuning one or two parameters. To get insight into the TE properties of hH alloys, we calculate the Seebeck coefficient $\alpha$, electrical conductivity $\sigma$, thermal conductivity $\kappa$, power factor (PF), and the $ZT$ by using constant relaxation time approximation and rigid band approximation.

We first initiate our calculations for NiTiSn by validating...
the theoretical results, such as PF and thermal conductivity with the reported experimental measurements. From the comparison of the calculated and experimental electrical conductivity, we approximated the relaxation time \( \tau \approx 2 \times 10^{-15} \) s. In the whole process, we use the constant relaxation time, even though it depends on doping level and temperature, obtained for NiTiSn to implement for all the iso-electronic systems.

The PF of NiTiSn was reported to be \( \sim 16 \mu \text{Wcm}^{-1}\text{K}^{-2} \) at 700 K, which upon electron doping (by 1% of Sb atom to Sn site), PF rises to \( \sim 30 \mu \text{Wcm}^{-1}\text{K}^{-2} \). When temperature rises above 700 K, PF is found to decrease in both cases. Comparing these values, we estimate that PF may range between \( 10 - 15 \mu \text{Wcm}^{-1}\text{K}^{-2} \) at 0.04–0.06 doping level of electron per unit cell in the same temperature range. In case of hole doping, PF lies within \( 17 - 23 \mu \text{Wcm}^{-1}\text{K}^{-2} \) at the same temperature range when dopants is \( 0.1 - 0.2 \) hole per unit cell. This indicates that hole doping is more appropriate than the electrons for PF. The calculated total thermal conductivity \( 21 - 10 \text{Wm}^{-1}\text{K}^{-1} \) (see Figure 5(b)) was slightly higher than the earlier report (i.e., \( 7 - 10 \text{Wm}^{-1}\text{K}^{-1} \)), which is mainly due to the electronic contribution found prominent at higher temperature. Our calculated results are comparable with the experimental measurements.

The Seebeck coefficient (a, c, e) and the PF (b, d, f) for different level of doping are shown in Figure 6 for NiScP, NiScAs, and NiScSb, respectively. Around \( E_F \) (i.e., \( \mu = 0 \)), the Seebeck coefficient is large (\( > \pm 150 \mu \text{V/K} \)), which on doping to either side, falls-off significantly. This is evident from its inverse relation with the carrier concentration.

The optimum values of the doping levels and corresponding TE parameters for 1200 K are listed in Table II

PF is another parameter to check the reliability of TE materials. As observed in Figure 5, the PF value for \( p \) or \( n \)-type is significant within the doping range of \( \pm 0.3 \). To be specific, at 1000 K the calculated values are approximately 15, 12 and 13 \( \mu \text{Wcm}^{-1}\text{K}^{-2} \) for NiScP, NiScAs, and NiScSb within 0.02–0.04 hole per unit cell reaching its maximum value at 1200 K. Similarly, for doping range 0.06–0.07 electron per unit cell, PF rises to \( \sim 27, 25, \) and \( 20 \mu \text{Wcm}^{-1}\text{K}^{-2} \) at 1000 K, respectively. The sizable value of PF within the doping range 0.07–0.08 electron per unit cell suggests that these material could be a good TE materials.

We further show the variation of PF with the chemical potential, \( \mu \), in Figure 7. The peak values of PF noted in the chemical potential ranges between 0.4 – 0.7 eV for NiScP, NiScAs and NiScSb. In contrast, the peak value of PF are around –0.2 eV for NiTiSn. From the above scenario, electron doping is found to be more suitable for NiScP, NiScAs, and NiScSb due to larger effective mass of electrons to get better TE performance. This indicates the presence of larger electron pockets resulting in the dense carriers which are confined on the CBM along \( \Gamma - X \) (Fig. 4a-c). On the other hand, in NiTiSn, hole doping is much more favorable due to the higher effective mass of holes resulting from the nearly flatter band in the VBM and CBM along \( \Gamma - X \) (see band structure in Fig. 4d).

Figure 8 shows the calculated thermal conductivity as a function of temperature for NiScP, NiScAs, NiScSb, and NiTiSn, respectively. The total thermal conductivity consists of two components \( \text{viz.} \) electronic (\( \kappa_e \)) and lattice (\( \kappa_l \)) parts. At low temperature (say 300 K), the lattice part was found dominant over the electronic part, and with rise in temperature (say upto \( \sim 900 \) K, except NiScP), the lattice thermal conductivity and the overall conductivity decreases uniformly.
FIG. 7. The power factor vs chemical potential (µ) at 1200 K temperature. The values of chemical potential in negative (positive) represents the hole (electron) doping.

FIG. 8. Total thermal conductivity (κ) as a function of temperature, inset dictates lattice contribution to thermal conductivity (κl) of NiScP, NiScAs, NiScSb, and NiTiSn.

To note is, with an increase in temperature starting from 300 K, the carrier concentration increases resulting in higher electrical conductivity, and hence the overall thermal conductivity. Similar features was observed in the recent report of CoMnSb. The calculated lattice conductivity are 10.6, 19, and 18.5 Wm\(^{-1}\)K\(^{-1}\) at 300 K which reduces abruptly to 2.5, 4.7, and 4.5 Wm\(^{-1}\)K\(^{-1}\) at 1200 K for NiScP, NiScAs, and NiScSb, respectively.

The figure of merit ZT for hH alloys is as shown in Figure 9. With low value (say, 0.05) of ZT at 300 K, it is found to rise linearly with the increase in temperature. At 1200 K, the calculated values are 0.30, 0.45, 0.35 and 0.29, respectively for NiTiSn, NiScP, NiScAs, and NiScSb alloys. On the otherhand, the values of total thermal conductivity is found minimum at ~ 700 K for NiScP and ~ 900 K for the remaining systems which starts increases afterwards due to the dominance of electronic part. The variation of ZT with temperature shows linear nature. PF is dominant at higher temperature range due to the increase in carrier concentration along with the electrical conductivity. The observed ZT is low mainly due to a higher value of κ. Even if our ZT values are lower than the commercialized TE materials such as Bi\(_2\)Te\(_3\) and PbTe but can be enhanced by means of doping to any of the three atomic sites. Though the ZT value is low (~ 0.05) for the pristine systems compared to the widely used doped Bi-based alloys, say, Bi\(_2\)S\(_2\)Te\(_3\) (~ 0.01 – 0.05)\(^{61}\), Bi\(_2\)S\(_2\)Te\(_3\) at Bi\(_2\)Te\(_3\) (~ 0.7)\(^{62}\), and Bi-Sb alloys (~ 0.4)\(^{63}\), it can be enhanced by electron doping\(^{64}\).

As observed from the calculations above, ZT value can increase when PF is enhanced while minimizing the thermal conductivity. The possible route to tune this from DF is by...

Table II. Calculated optimal doping levels and the corresponding Seebeck coefficient, electrical conductivity, power factor, and ZT of NiTZ (T= Sc, and Ti; Z= P, As, Sn, and Sb) in cubic symmetry F\(_{43m}\) at 1200 K. Negative (−) sign indicates the n−type characteristics.

| System   | n | α   | σ   | α²σ | ZT  |
|----------|---|-----|-----|-----|-----|
| NiTiSn   | 0.20 | 154 | 1.15 | 27.61 | 0.30 |
| NiScP    | -0.08 | -177 | 1.05 | 33.16 | 0.46 |
| NiScAs   | -0.08 | -168 | 1.12 | 31.50 | 0.35 |
| NiScSb   | -0.07 | -163 | 0.90 | 24.20 | 0.29 |

FIG. 9. The ZT as a function of temperature.
proper tuning of the band gap with appropriate electron/hole doping as discussed.

IV. CONCLUSIONS

On the basis on density functional calculations, we investigate the half-Heuslers NiTiSn, NiScP, NiScAs, and NiScSb, respectively. Electronic properties reveal that these materials are semiconductor with an indirect band gap. The narrow-band gap marks them as suitable candidate for TE performance. The calculated power factor shows large value in both the electron and hole doping case. Electron doping is found more preferable than hole for NiScP, NiScAs, and NiScSb, while hole doping is preferable for NiTiSn. Based on the constant relaxation time approximation and rigid band approximation with sizable $ZT$, these compounds are predicted as a possible TE materials.

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DATA AVAILABILITY

The data that support the findings of this study are available with the corresponding author and can be obtained upon reasonable request.

DECLARATION OF COMPETING INTEREST

There is no conflict of interest.

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