

Elastic and Transport Properties of Half-Heusler Alloy: First Principles Calculation of ZrYSn (Y = Ni, Pd, Pt) Alloys

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Abstract: The density functional theory was used to investigate the structural, electronic, elastic, and thermoelectric properties of ZrNiSn, ZrPdSn, and ZrPtSn Half-Heusler (HH) alloys. For these three alloys, the minimum lattice constants were calculated to be 6.1672, 6.4614, and 6.4550 Å, respectively. Moreover, our calculated band gaps were 0.61, 0.54, and 1.02 eV, respectively. At 300 K, the maximum and minimum Seebeck coefficients for p-type and n-type doping were 900 $\mu\text{V/K}$ and -900 $\mu\text{V/K}$ for ZrNiSn, 800 $\mu\text{V/K}$ and -790 $\mu\text{V/K}$ for ZrPdSn, and 1700 $\mu\text{V/K}$ and -1700 $\mu\text{V/K}$ for ZrPtSn. Maximum high power factors for n-type and p-type doping were found to be $13 \times 10^{11} \mu\text{W/cm}\cdot\text{K}^2\cdot\text{s}$ and $9.5 \times 10^{11} \mu\text{W/cm}\cdot\text{K}^2\cdot\text{s}$ for ZrNiSn, $11 \times 10^{11} \mu\text{W/cm}\cdot\text{K}^2\cdot\text{s}$ and $9 \times 10^{11} \mu\text{W/cm}\cdot\text{K}^2\cdot\text{s}$ for ZrPdSn, and $13 \times 10^{11} \mu\text{W/cm}\cdot\text{K}^2\cdot\text{s}$ and $9.5 \times 10^{11} \mu\text{W/cm}\cdot\text{K}^2\cdot\text{s}$ for ZrPtSn. These alloys exhibit a promising dimensionless Figure of merit (ZT) at room temperature, making them suitable for thermoelectric applications. Our results revealed that both ZrPdSn and ZrPtSn are ductile materials, while ZrNiSn is brittle in nature. This study shows that all these alloys can be applicable to thermoelectricity.

Keywords: Lattice Constant; Bandgap, Poisson Ratio; Anisotropic Factor; Ther-Moelectric Alloys; Power Factor; Seebeck Coefficient.

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I. INTRODUCTION

The global demand for energy has increased significantly over the past century. Climate change is a factor contributing to the worldwide growth in energy demand, exacerbating the energy crisis and accelerating the depletion of fossil fuels. To address the issue of excessive energy demand, researchers are working to improve the effectiveness of environmentally friendly technologies such as solar photovoltaics, biomass, thermoelectric, and wind turbines. As a potential solution to the world's growing energy demand, thermoelectric technology, which uses thermoelectric materials (TE) to convert heat into electricity and vice versa, is gaining popularity. In an attempt to satisfy the demand for this technology in recent years, these materials have attracted considerable research [1, 2, 3]. A dimensionless Figure of merit is typically used to assess a material's TE performance. Heusler alloys relatively high Seebeck coefficient of Heusler

alloys makes them one of the most promising thermoelectric materials [4, 5, 6].

Fritz Heusler created the large family of Heusler alloys in 1903, of which half-Heusler (HH) alloys are a well-known member. The properties of these alloys can be tailored to meet technological requirements across a variety of scientific and technical fields [6]. These Half-Heusler alloys usually differ from other types of Heusler alloys in a few key ways. One characteristic is that they typically have a narrowband gap and 18 valence electrons. By substituting at various crystal locations, it is achievable to improve the thermoelectric efficiency of half-Heusler compounds and reach the optimal equilibrium of Seebeck, electric resistivity, and thermal conductivity [7, 8, 9, 10, 11]. This could make these alloys ideal for thermoelectric applications by increasing their power factor and decreasing their lattice thermal conductivity.

Historically and currently, numerous researchers have employed both theoretical and experimental methods to study the thermoelectric properties of various half-Heusler compounds. For instance, due to their Figure of Merit of 0.7 [12, 13], the half-Heusler alloys MNiSn ($M = \text{Ti, Zr, and Hf}$) are among the most promising materials for thermoelectric technology. In this instance, they carefully replace Ni with Pd to enable fabrication via solid-state processes. In an argon atmosphere, the powdered premium component is heated to 1173 K for 96–168 hours. FeXSb ($X = \text{V, Nb}$) has a high Seebeck coefficient and power factor at room temperature, according to reports [14, 15, 16, 17]. The semi-conducting materials ZrNiSn and FeNbSb show considerable promise as thermoelectric materials. The phase structures of these materials were determined using X-ray diffraction (XRD) on a Rigaku D/MAX-2550PC diffractometer. No impurity phases are present in the samples, as indicated by XRD analysis.

Recently, Kaur and Rai employed density functional theory, coupled with semi-classical Boltzmann transport equations within the constant-relaxation-time approximation, to calculate the structural, electronic, elastic, and thermoelectric properties of novel HfPtPb HH alloys. Their research states that this alloy is both dynamically and mechanically stable. Furthermore, n-type doping yielded the highest Seebeck coefficient in this material. Using first-principles simulations within an enhanced TB-mBJ potential, Wang and Wang examined the electrical structure and thermoelectric characteristics of Half-Heusler semiconductors ABPb ($A = \text{Hf, Zr; B} = \text{Ni, Pd}$) [18]. They projected the band structures of both p- and n-type-doped compounds and computed their Seebeck and power factors under a constant relaxation time using Boltzmann transport theory. They discovered that all compounds are semiconductors with narrowband gaps. They also reported that their power factors were nearly consistent with the research findings and offered recommendations to enhance the thermoelectric properties.

The stoichiometric compositions of the ternary intermetallic full- and half-Heusler alloys are X_2YZ and XYZ , respectively. These classifications assign the Z elements to the semiconductor or sp category, whereas the X and Y elements are transition metals. However, our choice of ZrNiSn, ZrPdSn, and ZrPtSn alloy conforms to this arrangement. Nevertheless, these alloys have received very little research. Another reason to investigate HH compounds further is the outstanding thermoelectric qualities that often characterize undoped HH alloys. To the best of our understanding, ZrNiSn, ZrPdSn, and ZrPtSn alloys are examples of such compounds for which comprehensive research, including the computation of thermoelectric, electrical, elastic, dynamic, and structural properties, is not adequate. Thus, we have investigated the structural, mechanical, electronic, and thermoelectric properties of ZrNiSn, ZrPdSn, and ZrPtSn alloys using density functional theory and semi-classical Boltzmann transport theory under the constant rigid band assumption.

II. COMPUTATIONAL PROCEDURES

The First-Principles total energy was computed using the Plane-Waves Pseudo-Potential (PWPP) method in the ab initio Quantum Espresso Simulation Package [19]. The electronic exchange and correlation functions within the Perdew–Burke–Ernzerhof (PBE) parameterization, the Generalized Gradient Approximation (GGA), were evaluated using density functional theory (DFT) [20]. Troullier and Martins' approach was utilized to produce the pseudopotentials of all the atoms employed to produce scalar-relativistic pseudopotentials. For Ni, Pd, and Pt, the valence electronic configurations are $4d^8 4s^2$, $4d^{10}$, and $5d^9 6s^1$ states, respectively. In contrast, those of Zr and Sn are $4d^2 5s^2$ and $5s^2 5p^2$, respectively. The Brillouin zone integration was replaced by discrete summations over a distinct set of k-points utilizing the conventional k-points approach in order to get dependable results in all computations [21, 22], where $(10 \times 10 \times 10)$ to $(16 \times 16 \times 16)$ is the range of k-points mesh utilized for the whole alloy. A plane-wave cutoff of around 30–70 Ry is used to increase the wave function. For the ground state's total energy, precise convergence tests were carried out.

According to Hooke's law, a mechanical property, like the elastic constant, is a collection of values that measure a material's response to deformation caused by the stress-strain tensor. This value describes the material's center force, nature, and stability. The stress, σ , at equilibrium when a material is treated to a little strain is associated with the following stress-strain tensor:

$$\sigma_{ij} = \sum_{j=1}^6 C_{ij} \epsilon_j \quad (1)$$

The coefficients provide an elastic stiffness tensor of fourth rank, which is represented by a matrix using:

$$11 \rightarrow 1, 22 \rightarrow 2, 33 \rightarrow 3, 23, 32 \rightarrow 4, 13, 31 \rightarrow 5, 21, 12 \rightarrow 6.$$

In Voigt notation, the cubic elastic stiffness tensor is:

$$\begin{bmatrix} \square & C_{11} & & & & \\ & C_{12} & C_{12} & 0 & 0 & 0 \\ \square & C_{12} & \epsilon_{11} & \epsilon_{12} & 0 & 0 \\ \square & 0 & 0 & 0 & C_{44} & 0 \\ \square & 0 & 0 & 0 & C_{44} & 0 \\ \square & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix}$$

There is a maximum for a crystalline material; there are 21 elastic constants; however, three separate elastic constants apply to a cubic structure: $C_{11} = C_{22} = C_{33}$ (axial compression modulus), $C_{12} = C_{13} = C_{21}$ (dilation compression modulus), and $C_{44} = C_{55} = C_{66}$ (shear modulus) [23].

The mechanical characteristics of the structure create the link between the material's mechanical and dynamic behavior ZrYSn (Y=Ni, Pd, Pt), such as the structure of elastic constant is minimized into C_{11} , C_{12} , and C_{44} , Shear modulus (G), bulk modulus (B), and Young's modulus (E). Usually, the stress-strain method is used to obtain these and, correspondingly, to describe the rigidity under significant stresses and the ability to re-sist shear deformation. The Born–Huang stability criterion determines every material's mechanical stability. For a cubic structure, the Born–Huang stability criteria are:

$$C_{11} > 0, C_{44} > 0, C_{11} - C_{12} > 0, \text{ and } C_{11} + 2C_{12} > 0. \quad (2)$$

Equations (1–3) of the Hill technique [24, 25] are used to get mechanical properties like bulk modulus B and shear modulus G , and shear anisotropy A at hydrostatic pressure. Other properties such as Young's modulus E , Pugh's ratio, and the Poisson's ratio ν can be calculated from equations (4–8) as:

$$B = \frac{C_{11} + 2C_{12}}{3}, \quad (3)$$

$$G = \frac{C_{11} - C_{12} + 3C_{44}}{5}, \quad (4)$$

$$A = \frac{2C_{44}}{C_{11} - C_{12}}, \quad (5)$$

$$E = \frac{9BG}{3B + G}, \quad (6)$$

$$\nu = \frac{3B - 2G}{2(3B + G)}. \quad (7)$$

The Boltzmann Transport Theory underpins the thermoelectric properties using Boltz-TraP software code. The figure of merit obtained using a combination of power factor, $S^2\sigma$; temperature, T ; and the lattice and phonon thermal conductivity, κ . This gives:

$$zT = \frac{S^2\sigma T}{\kappa} \quad (8)$$

Where

$$\sigma_{ab}(T, \mu) = \frac{1}{\Omega} \int \sigma_{ab}(\epsilon) \left(-\frac{\partial f_{\mu}(T, \epsilon)}{\partial \epsilon} \right) d\epsilon, \quad (9)$$

$$S(T, \mu) = \frac{1}{eT\Omega\sigma_{ab}(T, \mu)} \int \sigma_{ab}(\epsilon) (\epsilon - \mu) \left(-\frac{\partial f_{\mu}(T, \epsilon)}{\partial \epsilon} \right) d\epsilon, \quad (10)$$

$$\kappa_{ab}(T, \mu) = \frac{1}{e^2 T \Omega} \int \sigma_{ab}(\epsilon) (\epsilon - \mu)^2 \left(-\frac{\partial f_{\mu}(T, \epsilon)}{\partial \epsilon} \right) d\epsilon. \quad (11)$$

III. RESULTS AND DISCUSSION

➤ Structural Properties

Determining the equilibrium lattice constant of the HH alloy ZrYSn (Y=Ni, Pt, Pd) taking into consideration of the two desirable site arrangements of X and Y atoms is shown in Figure 1. The crystal structures of ZrNiSn, ZrPdSn and ZrPtSn are visualized using Xcrysden and are shown in Fig. 1. Crystallization occurs in these alloys in the $C1_b$ structure using the general compounds of XYZ in Fig. 1a–c, Y atoms represent Ni, Pd and Pt, X atoms represent Zr, and Z atoms represent Sn. Considering the lattice parameter for ZrPtSn alloys, the LDA calculation yields a result that is approximately 1.89% greater than what was experimentally observed. The experiment at lattice constant are 6.16 Å, 6.16 Å and 6.31 Å [26]. Based on this observation, all subsequent calculations in this study used GGA due to discrepancies noted in the LDA results, which are attributed to LDA's tendency to overestimate lattice parameters and to the inherent simplifications in the estimate for homogeneous systems.

The lattice parameters for ZrNiSn, ZrPdSn, and ZrPtSn are 6.167 Å, 6.46 Å, and 6.461 Å, respectively. To find the ground state characteristics of these alloys, the fourth-order Murnaghan's equation of state was used to modify the total energies based on the lattice parameters [27]. This approach facilitated the determination of the minimum lattice parameter a , the bulk modulus B , and its pressure derivative B' , which are summarized in Table 2.

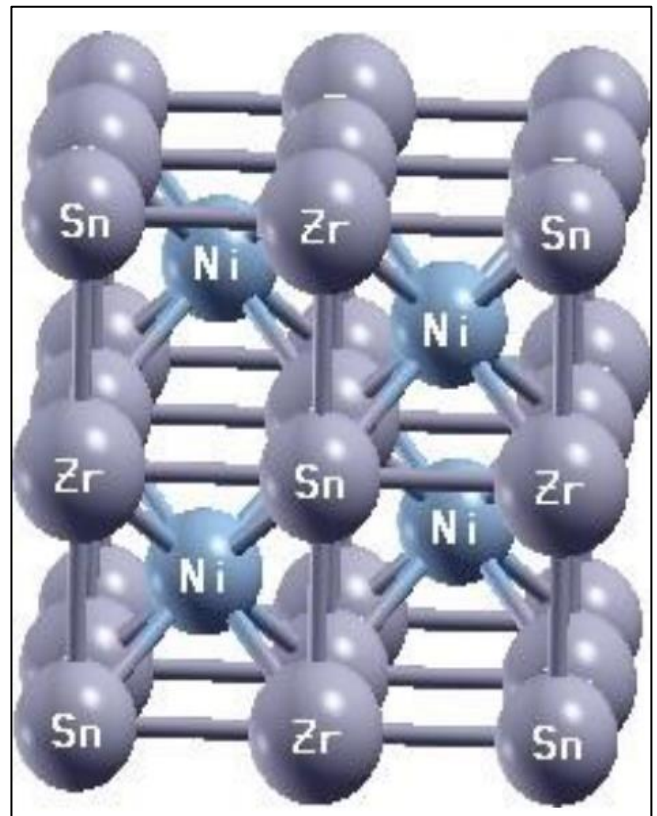


Fig 1 The Optimized Crystal Structure of ZrNiSn Half-Heusler Alloys.

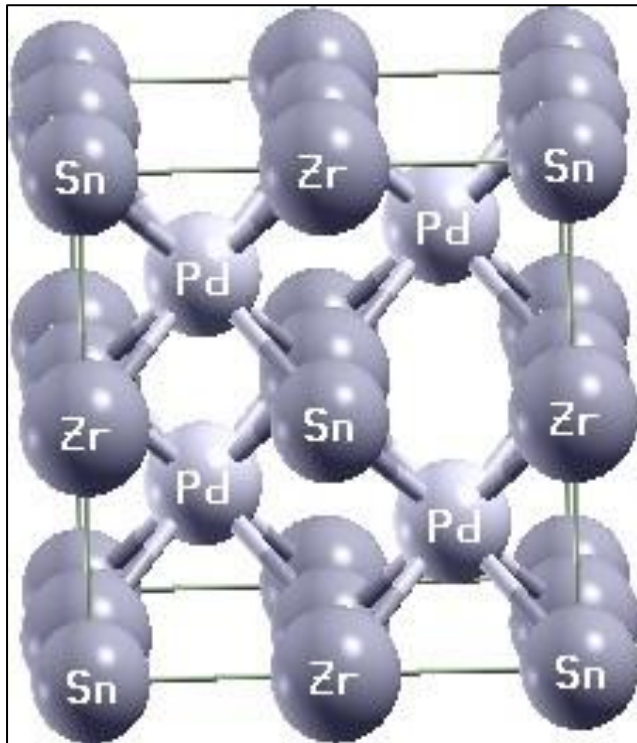


Fig 2 The Optimized Crystal Structure of ZrPdSn Half-Heusler Alloys.

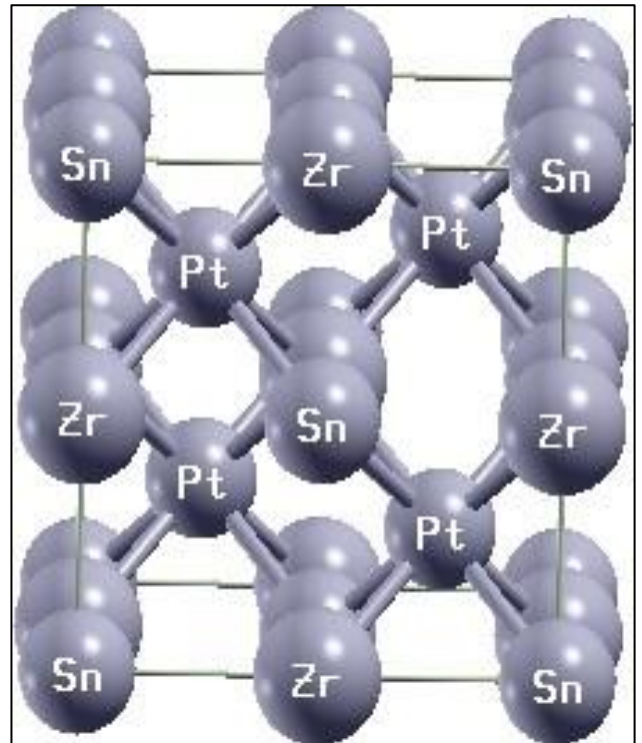


Fig 3 The Optimized Crystal Structure of ZrPtSn Half-Heusler Alloys.

Table 1 The Three Atoms Respective Wyckoff Positions are as follows: 4a= (0, 0, 0), 4b = (0.50, 0.50, 0.50), and 4c = (0.25, 0.25, 0.25), where a is the Lattice Parameter. ZrYSn (Y= Ni, Pd, and Pt)

Structural phase	X	Y	Z
NiZrSn	4c	4b	4a
PdZrSn	4c	4b	4a
PtZrSn	4a	4b	4a

Table 2 The Optimized Lattice Constant, a_o (Å), Energies Equilibrium, $E_{\min}$ (Ry), Bulk Modulus B (GPa), and Pressure Derivative for the Bulk Modulus B' for ZrYSn (Y= Ni, Pd, and Pt), for the Possible Structural Phase.

Alloys	a_o (Å)	B (GPa)	B'	$E_{\min}$ (Ry)
NiZrSn (this work)	6.167	122.5	3.78	-935.12
Other experimental work [26]	6.16	–	–	–
PdZrSn (this work)	6.461	119.5	3.74	-783.13
ZrPtSn (this work)	6.455	155.1	3.51	-1199.36
Other theoretical work	–	–	–	–
Experimental [26]	6.336	–	–	–

Figures 4 to 6 show the optimized parameters of the Half-Heusler alloys of ZrYSn (Y=Ni, Pd, Pt). The calculation of the bulk modulus provides insight into the change in the materials' total energy due to the compressor. Lattice constant is equilibrium stable; the system is stable or parabolic shape.

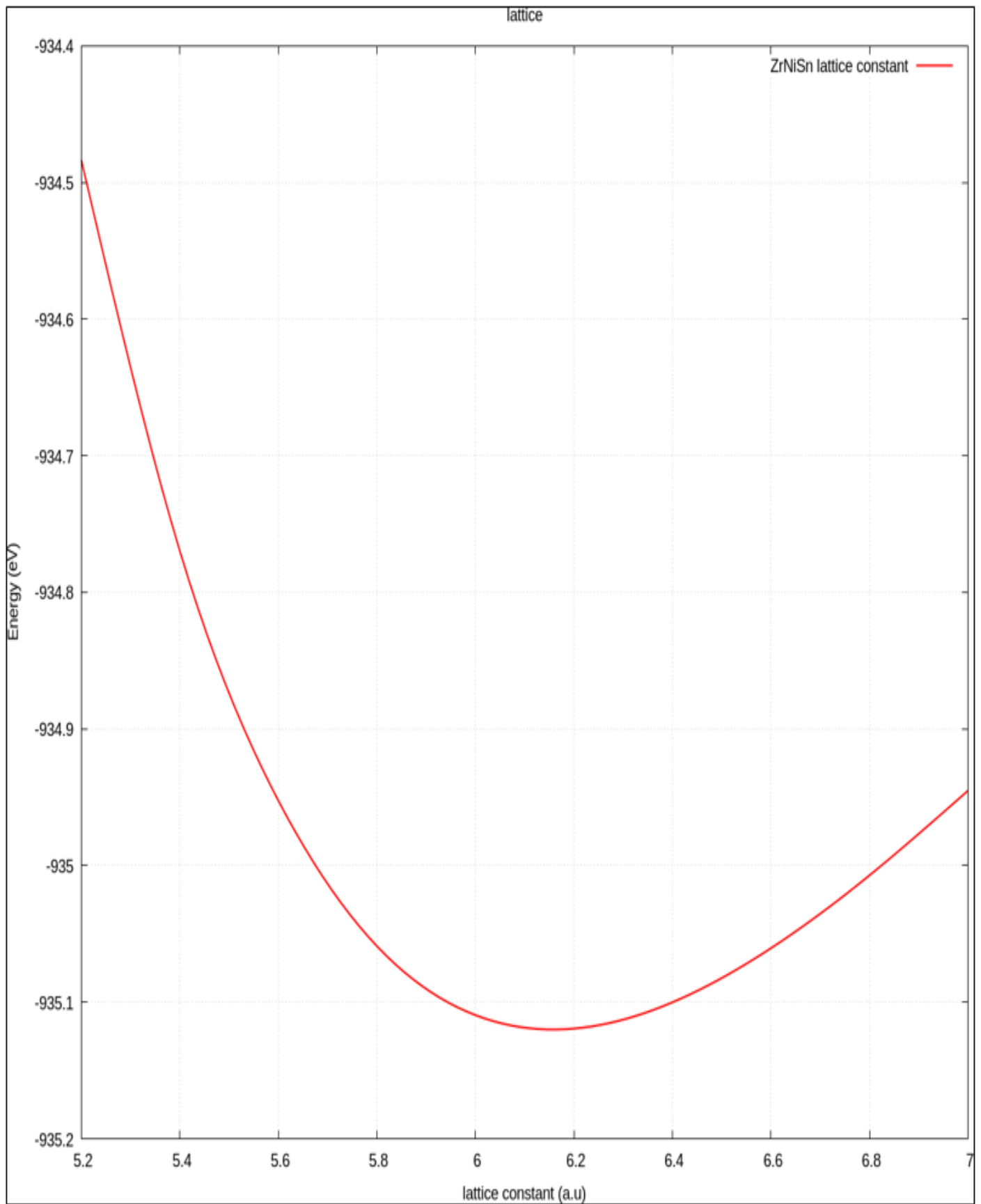


Fig 4 Equilibrium Lattice Constant of ZrNiSn Half-Heusler Alloy.

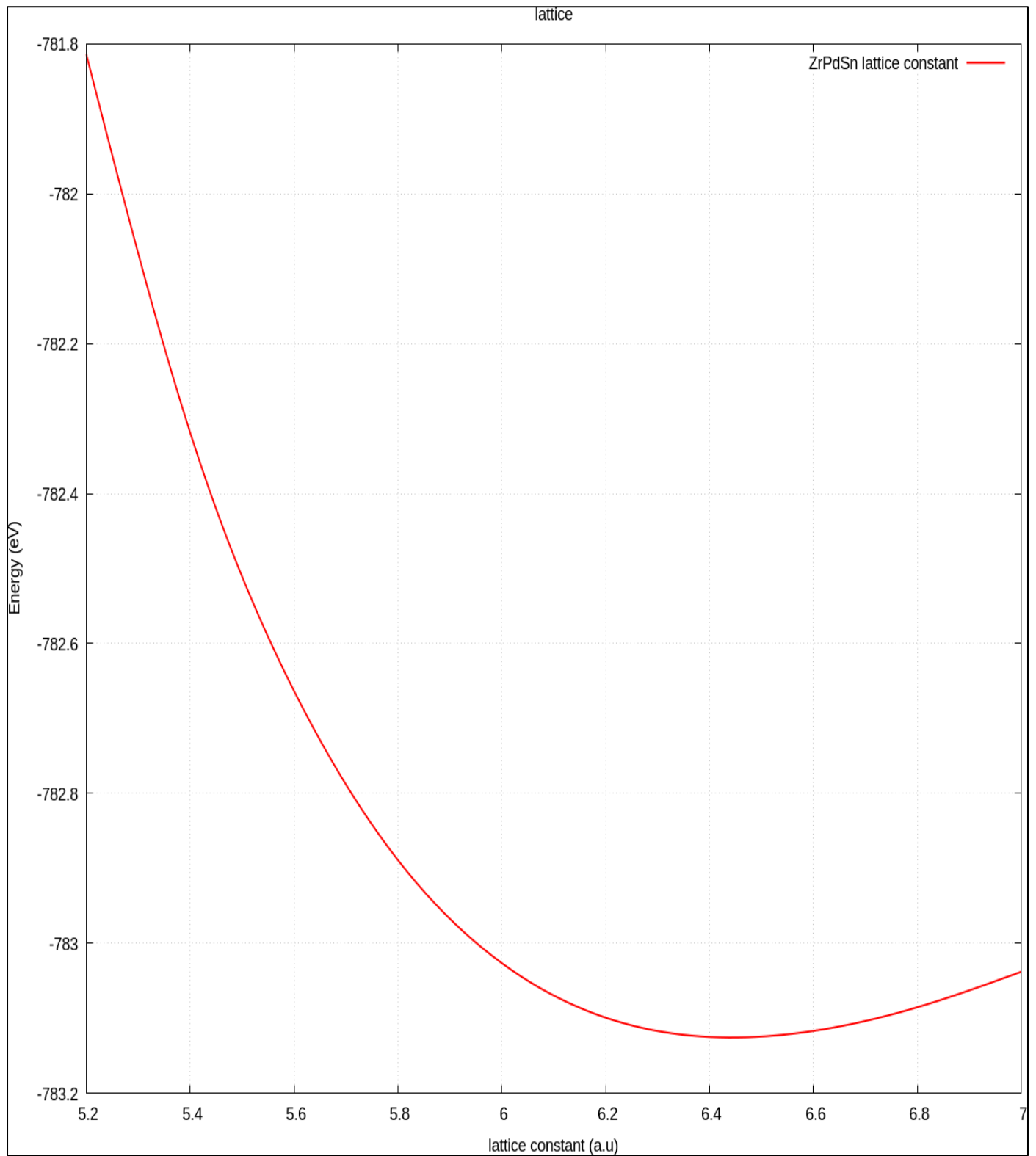


Fig 5 Equilibrium Lattice Constant of ZrPdSn Half-Heusler Alloy.

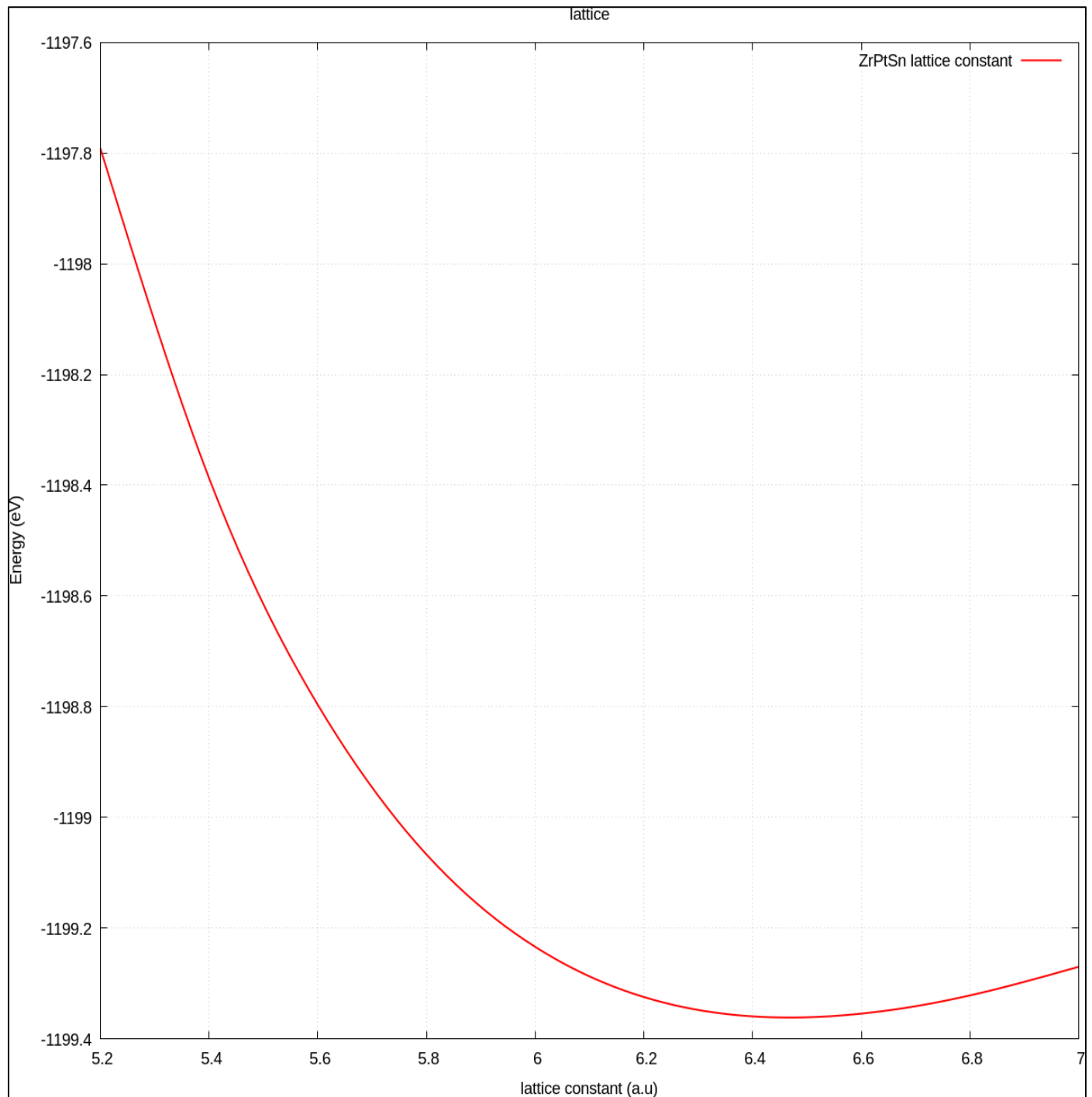


Fig 6 Equilibrium Lattice Constant of ZrPtSn Half-Heusler Alloy.

➤ Electronic Properties

Figure 7-9 shows the density of state and electronics band structure of ZrYSn (Y = Ni, Pd, and Pt) alloys. The alloys are expected to be semiconductors with an indirect bandgap based on our findings. The location of the Maximum Valence Band (VBM) for every alloy under consideration, point X of high symmetry is where the Conductor Band Minimum (CBM) is situated. The dashed line near the valence band displays the Fermi level for each alloy. Moreover, the computed density of states further confirms the semiconducting nature of the alloys. The difference between CBM and VBM revealed the indirect band gap. Furthermore, we have shifted the Fermi energy

level, i.e., E_F , to zero. The Density of State (DOS) distribution around the Fermi level provides information about the electronic behaviour of these alloys and as shown in Figure 5. Consequently, we predicted the energy band gap of 0.61, 0.54, and 1.02 eV for ZrNiSn, ZrPdSn, and ZrPtSn, respectively. The report on the electronic behaviour is to examine the semiconductor properties of the alloy and the spin-polarized band structure computation that shows the semiconductor's minority states. In the first Brillouin zone, Figure 5 shows the minority spin band structure of semiconductors with a bandgap of 0.61, 0.54, and 1.02 eV for ZrNiSn, ZrPdSn, and ZrPtSn Half Heusler alloys, respectively.

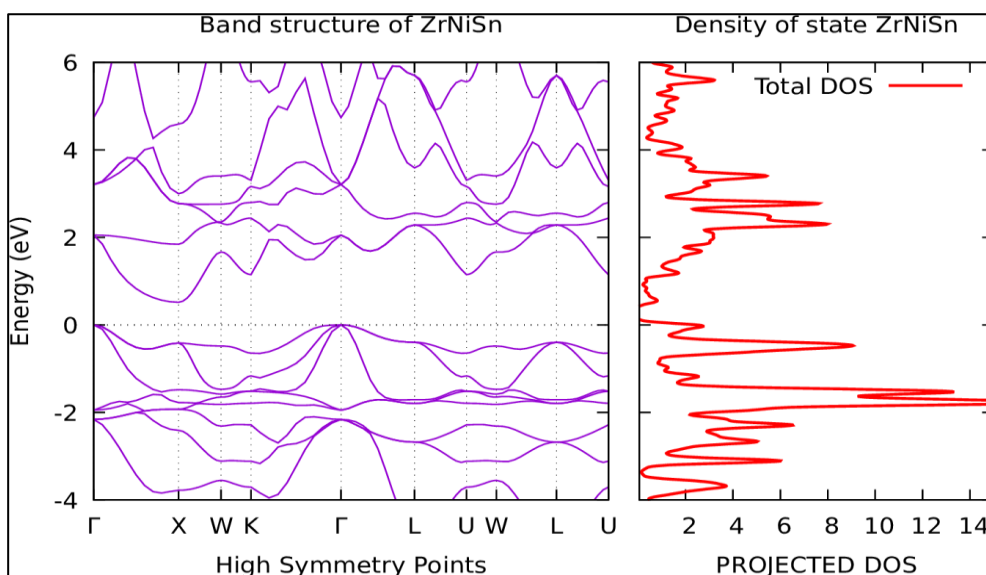


Fig 7 Band Structure and Density of State of ZrNiSn Half-Heusler Alloys.

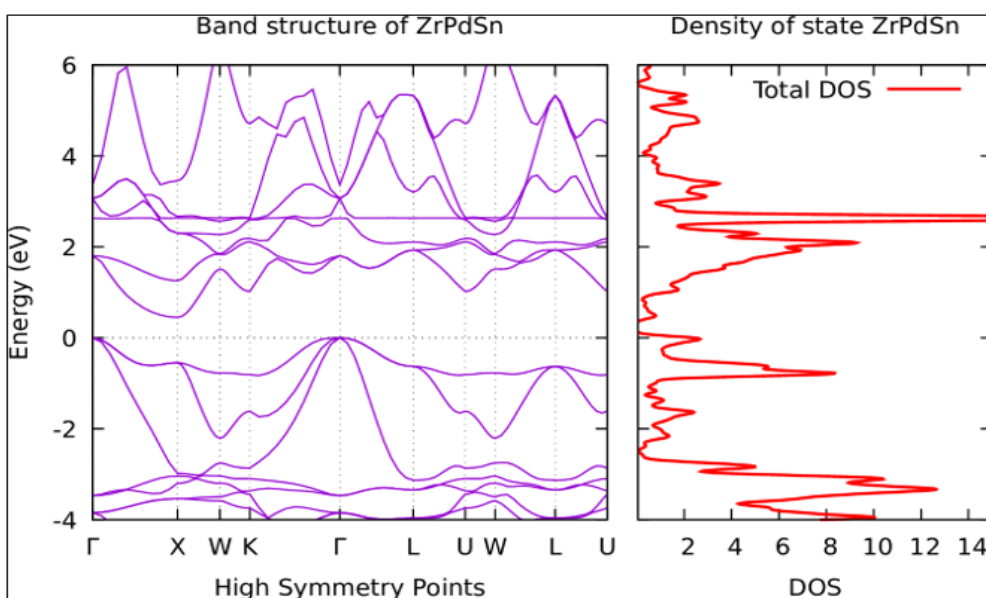


Fig 8 Band Structure and Density of State of ZrPdSn Half-Heusler Alloys.

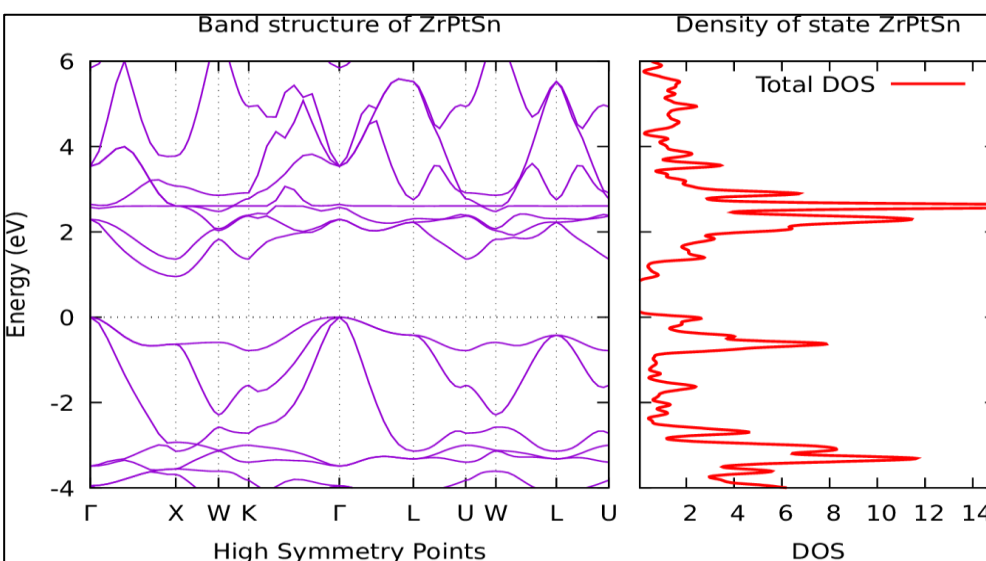


Fig 9 Band Structure and Density of State of ZrPtSn Half-Heusler Alloys.

Table 3 The Results of the Bandgap of ZrYSn (Y= Ni, Pd, Pt) Alloy are Semiconductor.

Alloys	VEC	Calculations	Bandgap(eV)	
ZrNiSn	18	This work	0.61	
		Other calculations	–	–
ZrPdSn	18	This work	0.54	
		Other calculation	–	–
ZrPtSn	18	This work	1.02	
		Other calculation[28]	1.10	

➤ Elastic Properties of ZrYSn (Y= Ni, Pd, Pt)

Shear modulus, bulk modulus, and Young's modulus (G, B, E), as well as the cubic structure of the elastic constants, can all be split down. These values, which are usually discovered using the stress-strain method, establish the relationship between the material's dynamic and mechanical behavior. Whereas C_{11} and C_{44} , respectively, characterize the resistance against shear deformation and stiffness against main strains. Table 4 is a list of the mechanical properties that were calculated.

Table 4 Voigt Reuss Hill Approximation Moduli and Mechanical Properties of ZrYSn (Y= Ni, Pd, Pt) were Calculated. Shear Modulus (G), Bulk Modulus (B), Young Modulus (E), and Poisson's Ratio (ν). Pugh's Ratio and Shear Anisotropy, and Frantsevich's Ratio were Computed Using the Estimated Value.

Properties	ZrNiSn	ZrPdSn	ZrPtSn
C_{11} (GPa)	228.20	180.60	206.70
C_{12} (GPa)	62.81	87.54	98.30
C_{44} (GPa)	67.92	65.71	72.10
$C_{11} - C_{12}$ (GPa)	165.39	93.06	108.50
$C_{11} + 2C_{12}$ (GPa)	353.82	355.68	403.3
B (GPa)	117.9	118.56	134.44
B (GPa) [29]	–	–	139.00
G (GPa)	73.8	58.04	64.95
G (GPa) [29]	–	–	67.00
E (GPa)	183.2	149.6	167.80
E (GPa) [29]	–	–	167.50
A (Anisotropy factor)	0.82	1.41	1.33
A [29]	–	1.087	1.30
ν (Poisson ratio)	0.24	0.29	0.29
Pugh's ratio	1.60	2.04	2.07
Pugh's ratio [29]	–	–	2.10
Frantsevich's ratio	0.63	0.49	0.48
Frantsevich's ratio [29]	–	–	0.48

Based on the results, ZrNiSn, ZrPdSn, and ZrPtSn are mechanically stable, as shown in Table 4. The results for the elastic constants clearly met the Born–Huang criterion, confirming the mechanical stability of a cubic crystal. Poisson's ratio (ν), bulk modulus (B), shear modulus (G), and Young's modulus (E) are all calculated using the Voigt–Reuss–Hill approximation. Frantsevich's ratio and Pugh's ratio B/G were constructed using the computed values. ZrPtSn and ZrPdSn have Pugh's ratio values of 2.04 and 2.07, respectively, which are larger than 1.75. This indicates that the alloys are more ductile than brittle ($B/G > 1.75$), while ZrNiSn is more brittle than ductile ($B/G < 1.75$). In alloy applications, the bulk (B) and shear moduli (G) are essential. In general, resistance to fracture is denoted by B, and resistance to plastic deformation by G. As B increases, resistance to deformation under pressure also increases. Table 4 shows that ZrPtSn has a exhibits higher pressure resistance than the other Half-Heuslers examined, with ZrNiSn having the lowest. The resistance to deformation carried on by shear stress was determined by the shear modulus G. With an

increase in G, it becomes more resistant to shear stress. ZrPtSn $>$ ZrPdSn $>$ ZrNiSn is consequently the least. Young's modulus the stiffness of a material is measured by E; a higher value of E indicates a stiffer material. ZrNiSn is consequently more rigid than the other materials, whereas ZrPtSn and ZrPdSn are the least rigid. If the shear anisotropy is one, the degree of anisotropy is revealed by any fluctuation that is less than or greater than one. However, the crystal's isotropy is demonstrated by a cubic shear anisotropy (A) factor. However, the computed result displays that ZrNiSn, ZrPdSn, and ZrPtSn are all anisotropic. The Pugh ratio indicates an alloy's degree of ductility. As the Pugh's ratio rises, the crystal becomes more ductile and if it is more than 1.75 ($G/B > 0.57$), it is ductile. ZrPdSn and ZrPtSn are ductile since their values are greater than 1.75, while ZrNiSn is brittle ($B/G < 1.75$).

➤ *Thermoelectric Properties*• *Thermoelectric Properties of ZrYSn (Y= Ni, Pd, Pt)*

As shown in Figure 10a, the power factor varies with energy at different temperatures. This power factor illustrates the performance of ZrNiSn thermoelectric materials. The power factor for n-type doping reaches its

highest value of $13 \times 10^{11} \text{ W/cm} \cdot \text{K}^2 \cdot \text{s}$ at 1200 K

K. Meanwhile, the p-type doping has a maximum power factor of $9.5 \times 10^{11} \text{ W/cm} \cdot \text{K}^2 \cdot \text{s}$. It is also discovered that it is at 1200 K. Meanwhile, the maximum power factors for the n-type and p-type were $8.5 \times 10^{11} \text{ W/cm} \cdot \text{K}^2 \cdot \text{s}$ and $6.5 \times 10^{11} \text{ W/cm} \cdot \text{K}^2 \cdot \text{s}$, respectively, at 900 K.

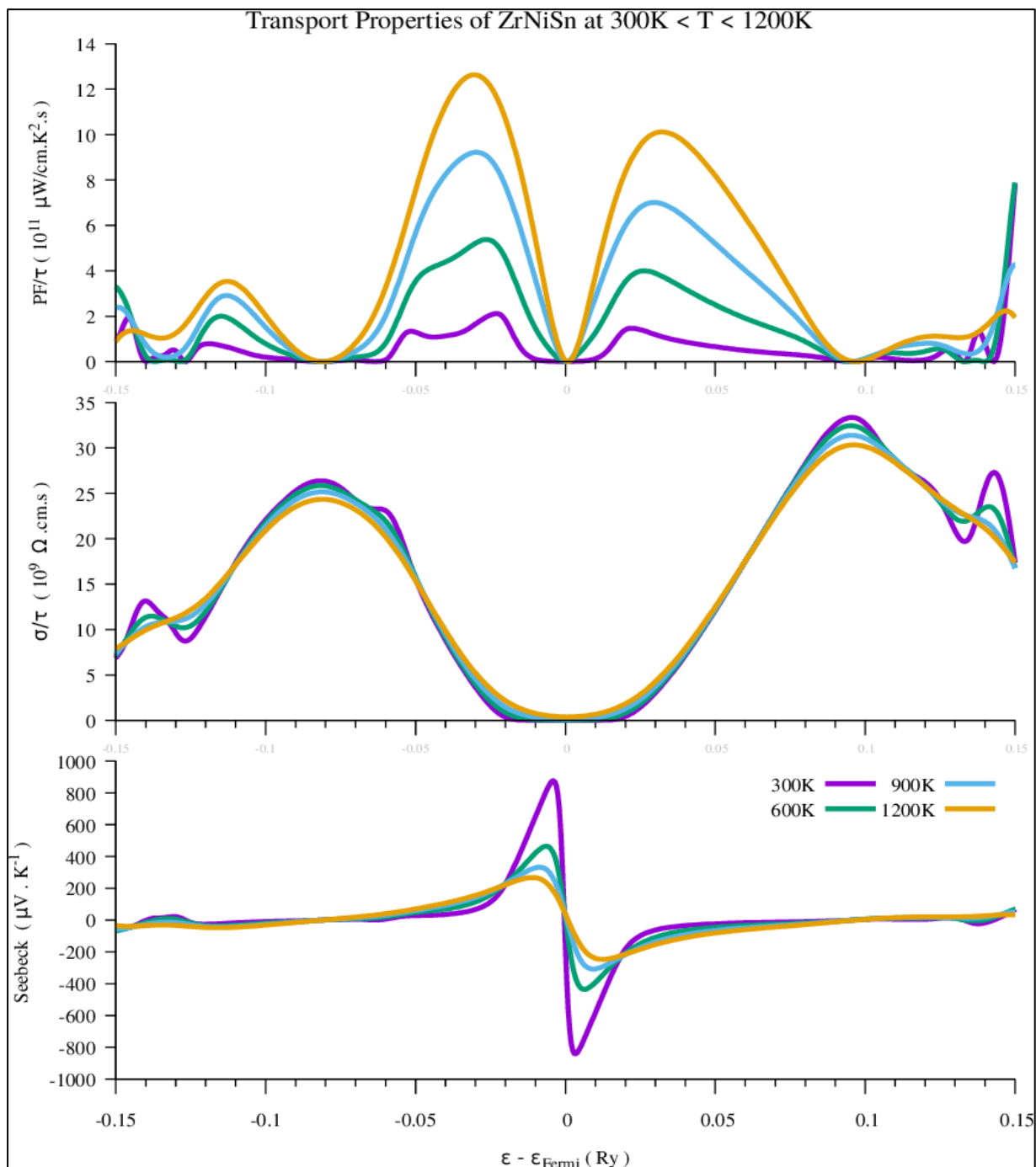


Fig 10 (a) Power Factor, (b) Electrical Conductivity, and (c) Seebeck Coefficient of ZrNiSn Half-Heusler Alloys.

Figure 10b shown how temperature and energy affect electrical conductivity per relaxation time. The electrical conductivity per relaxation time shows a constant pattern at all temperatures. For positively increasing energies, the gradient of electrical conductivity per relaxation period is

larger than for higher negative energies. As a result, n-type compositions are less electrically conductive than p-type compositions. In the energy range of -0.05 to +0.05, there is no electrical conductivity per relaxation period. Beyond this range, nevertheless, the value increases.

The peaks in the energy range of -0.05 and +0.05 show that the Seebeck coefficient at the doping of p-type and n-type materials first increasing as the energy increased before reaching a maximum value and rapidly decreasing in Figure 10c. The curves should be at zero outside of this range. The ZrNiSn alloy's p-type doping peak maximum is located at $900 \mu\text{V}\cdot\text{K}^{-1}$, whereas the n-type doping peak maximum is found at $-900 \mu\text{V}\cdot\text{K}^{-1}$. The excellent

thermoelectric property of ZrNiSn alloy is demonstrated by the peaks detected at normal temperature. As the temperature increases, the peak heights typically decrease. ZrNiSn alloys' present Seebeck coefficient values at 300 K were compared to those of other Half-Heusler alloys [30]. In this context, we conclude that ZrNiSn exhibits the highest Seebeck coefficient.

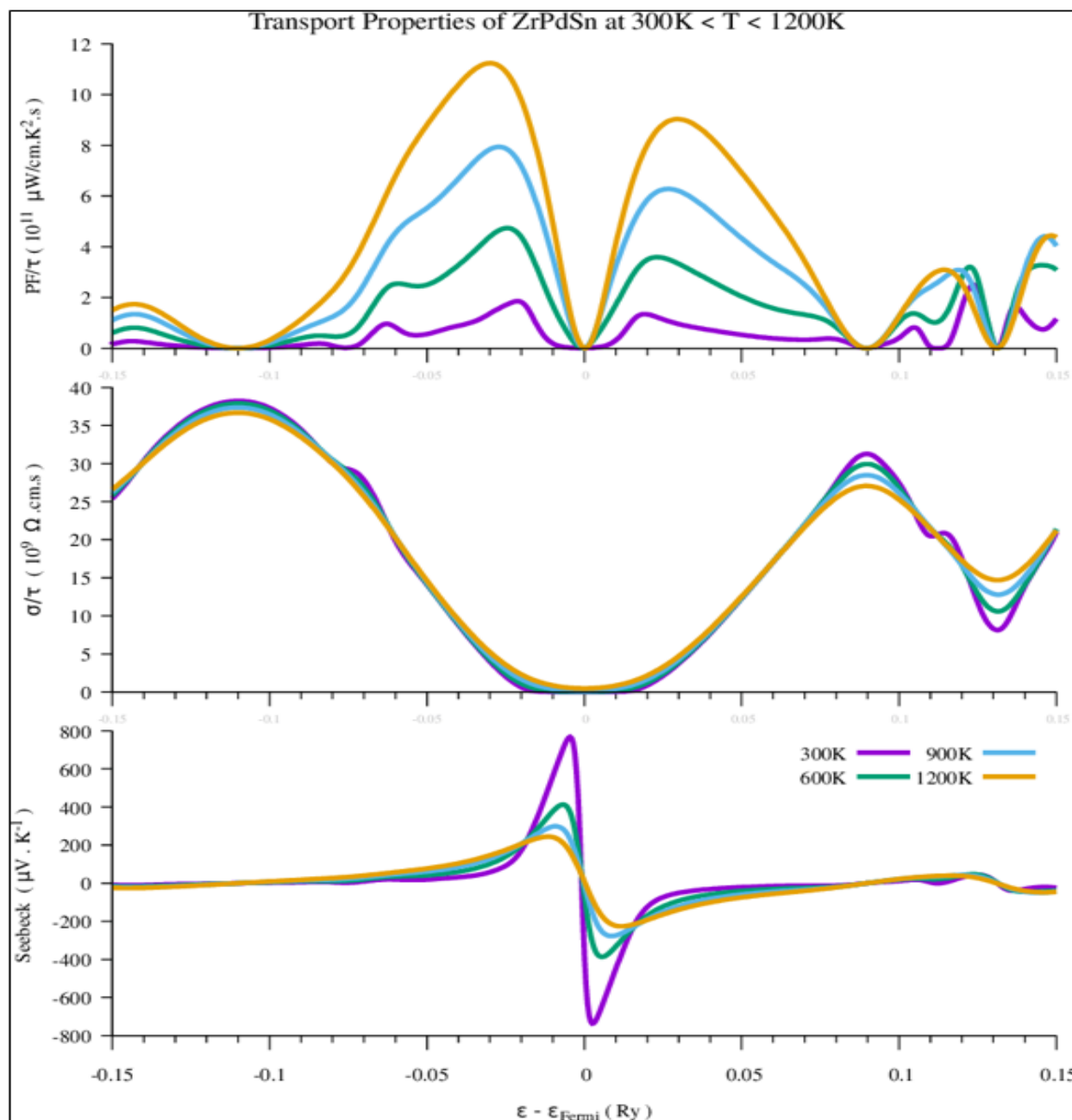


Fig 11 (a) Power Factor, (b) Electrical Conductivity, and (c) Seebeck Coefficient of ZrPdSn Half-Heusler Alloys.

As shown in Figure 11a, the power factor varies with energy at different temperatures. This power factor illustrates the performance of ZrPtSn thermoelectric materials. The power factor for n-type doping reaches its highest value of $12.5 \times 10^{11} \text{ W/cm}\cdot\text{K}^2\cdot\text{s}$ at 1200

K. Meanwhile, the p-type doping has a maximum power factor of $10 \times 10^{11} \text{ W/cm}\cdot\text{K}^2\cdot\text{s}$. It is also discovered

that it is at 1200 K. Meanwhile, the maximum power factors for the n-type and p-type were $9.5 \times 10^{11} \text{ W/cm}\cdot\text{K}^2\cdot\text{s}$ and $8.5 \times 10^{11} \text{ W/cm}\cdot\text{K}^2\cdot\text{s}$, respectively, at 900 K.

Figure 11b-11c demonstrated the consequences of energy and temperature on electrical conductivity per relaxation time. The electrical conductivity per relaxation

time shows a constant manner at all temperatures. In comparison to higher negative energies, the gradient of electrical conductivity per relaxation period is larger for positively increasing energies. As a result, n-type compositions are less electrically conductive than p-type compositions. In the energy range of -0.05 to +0.05, there is no electrical conductivity per relaxation period. But regardless of this range, the value increases. It is demonstrated by the peaks in the energy range of -0.05 and +0.05 in Figure 11c, prior to attaining a maximum value and sharply declining, when p-type and n-type materials were doped, the Seebeck coefficient initially rose as the energy increased. The curves should be at zero outside of this range. The ZrPdSn alloy's p-type doping peak maximum is at $800 \mu\text{V}\cdot\text{K}^{-1}$, whereas the n-type doping peak maximum is at $-780 \mu\text{V}\cdot\text{K}^{-1}$. The peaks found at room temperature show the ZrPdSn alloy's excellent

thermoelectric capability. As the temperature rises, the peak altitudes typically decrease. ZrPdSn alloys' current Seebeck coefficient values at 300 K were contrasted with those of other Half-Heusler alloys. In this sense, ZrPdSn has the highest Seebeck coefficient value.

Figure 12a, at various temperatures, the power factor changes with energy, as can be seen. ZrPtSn thermoelectric material performance is demonstrated by this power factor. The power factor reaches a maximum of $13 \times 10^{11} \text{ W/cm}\cdot\text{K}^2\cdot\text{s}$ for the n-type doping at 1200 K. Meanwhile, 1200 K is also discovered to be the maximum power factor for the p-type doping $10 \times 10^{11} \text{ W/cm}\cdot\text{K}^2\cdot\text{s}$. Meanwhile, at 900 K, the maximum power factors for the n-type and p-type were $9 \times 10^{11} \text{ W/cm}\cdot\text{K}^2\cdot\text{s}$ and $6.5 \times 10^{11} \text{ W/cm}\cdot\text{K}^2\cdot\text{s}$, respectively.

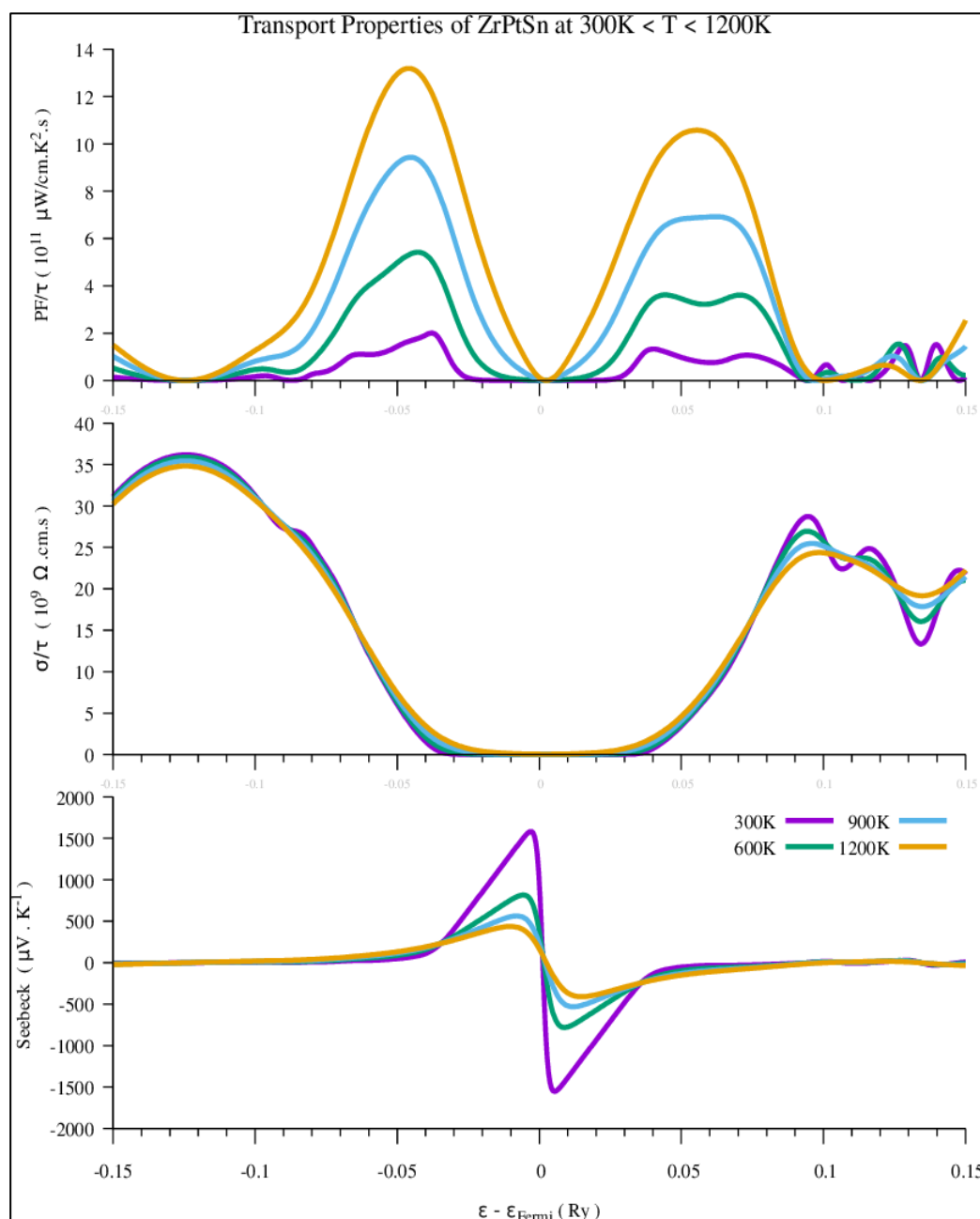


Fig 12 (a) Power Factor, (b) Electrical Conductivity, and (c) Seebeck Coefficient of ZrPtSn Half-Heusler Alloys.

Figure 12b-12c. It is evident that at different temperatures, the power factor varies with energy. The performance of ZrPtSn thermoelectric materials is demonstrated by this power factor. The greatest power factor for the n-type doping is $13 \times 10^{11} \text{ W/cm}\cdot\text{K}^2\cdot\text{s}$ at 1200 K. The p-type doping has a maximum power factor of $10 \times 10^{11} \text{ W/cm}\cdot\text{K}^2\cdot\text{s}$. Additionally, is determined to be 1200 K. At 900 K, the maximum power factors for the n-type and p-type were $9 \times 10^{11} \text{ W/cm}\cdot\text{K}^2\cdot\text{s}$ and $6.5 \times 10^{11} \text{ W/cm}\cdot\text{K}^2\cdot\text{s}$, respectively. Before reaching a maximum value, the Seebeck coefficient at the doping of p-type and n-type materials first increased as the energy increased and dramatically reducing, as demonstrated by the peaks in Figure 10c, energy range of -0.05 and +0.05. The curves should be at zero outside of this range. The ZrPtSn alloy has a p-type doping peak maximum at $1700 \mu\text{V}\cdot\text{K}^{-1}$ and an n-type doping peak

maximum at $-1700 \mu\text{V}\cdot\text{K}^{-1}$. The peaks found at room temperature show the greater thermoelectric property of ZrPtS alloy. The peak heights usually decrease with increasing temperature. ZrPtSn alloys' current Seebeck coefficient values at 300 K were compared to those of other Half-Heusler alloys [30]. ZrPtSn has the greatest Seebeck coefficient value in this respect.

Figures 13 and 14 show the dimensionless Figure of Merit in relation to the chemical potential at each temperature. Even at room temperature, ZrNiSn has a high Figure of Merit, $ZT = 0.95$ in the n-type compound and $ZT \approx 0.93$ in the p-type compound, which is perplexing. The observed decrease in ZT as the temperature increases is caused by the significant effects of phonon contribution to the thermal conductivity κ .

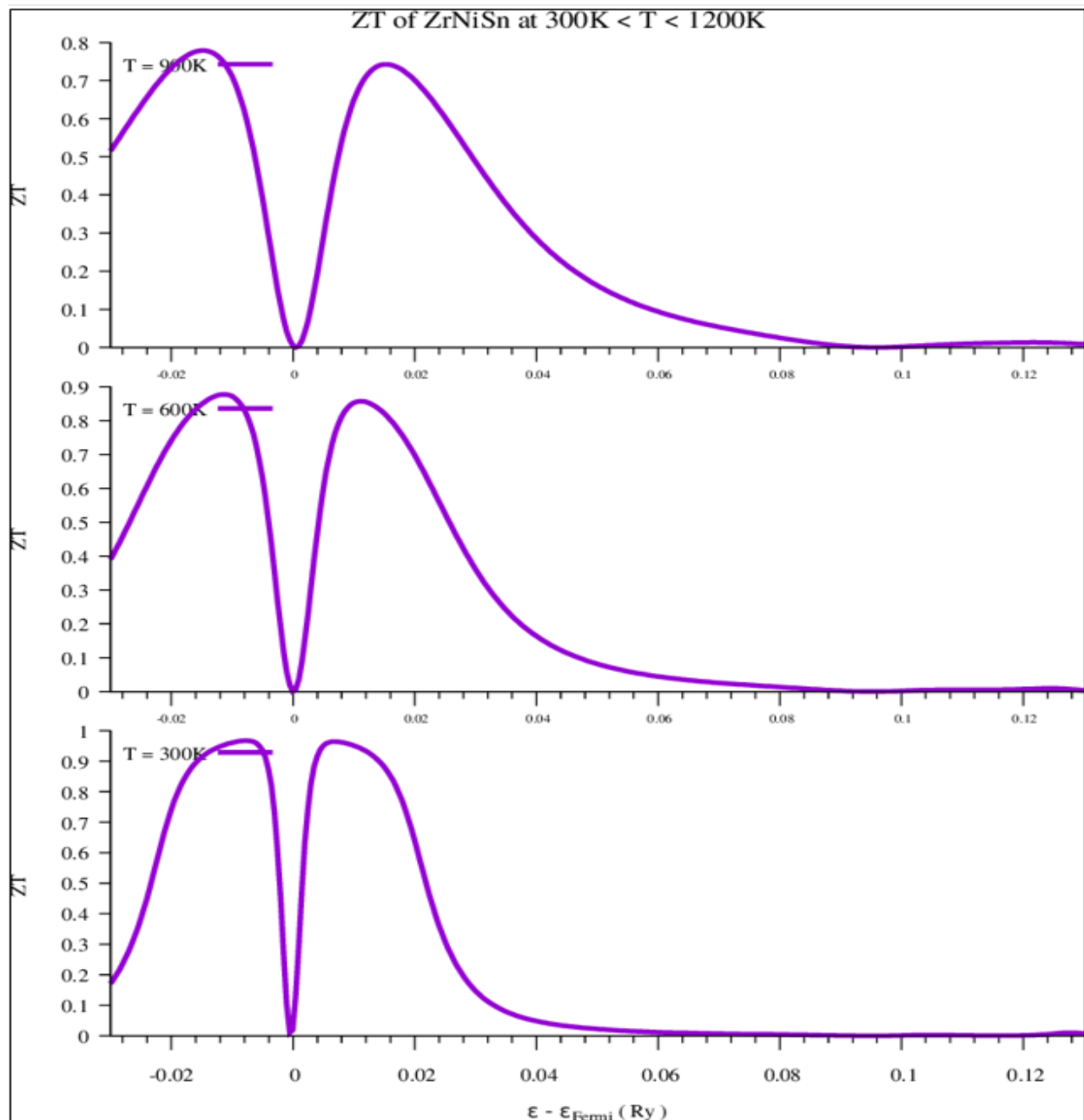


Fig 13 Dimensionless Figure of Merit ZrNiSn.

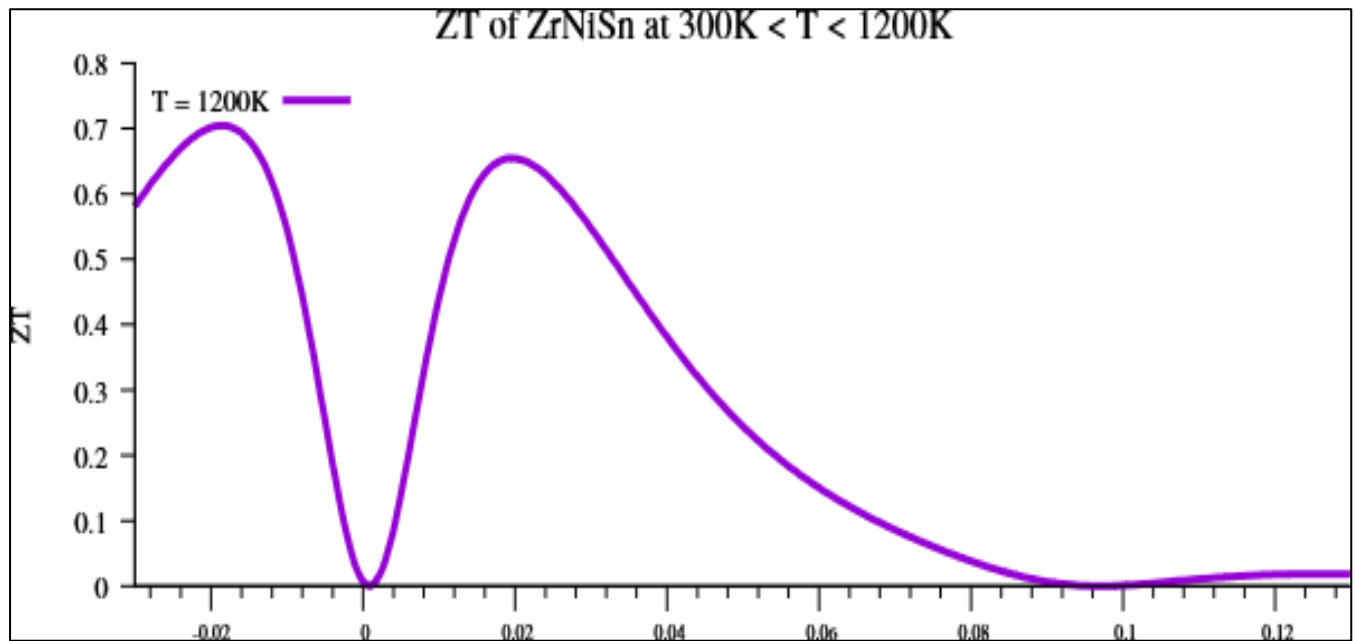


Fig 14 Dimensionless Figure of Merit ZrNiSn.

Figures 15 and 16 show the dimensionless Figure of Merit in relation to the chemical potential at each temperature. Even at room temperature, ZrPdSn has a high Figure of Merit, $ZT = 0.95$ in the n-type compound and $ZT \approx 0.94$ in the p-type compound, which is confusing. The observed decrease in ZT as the temperature increases is caused by the significant effects of phonon contribution to the thermal conductivity κ .

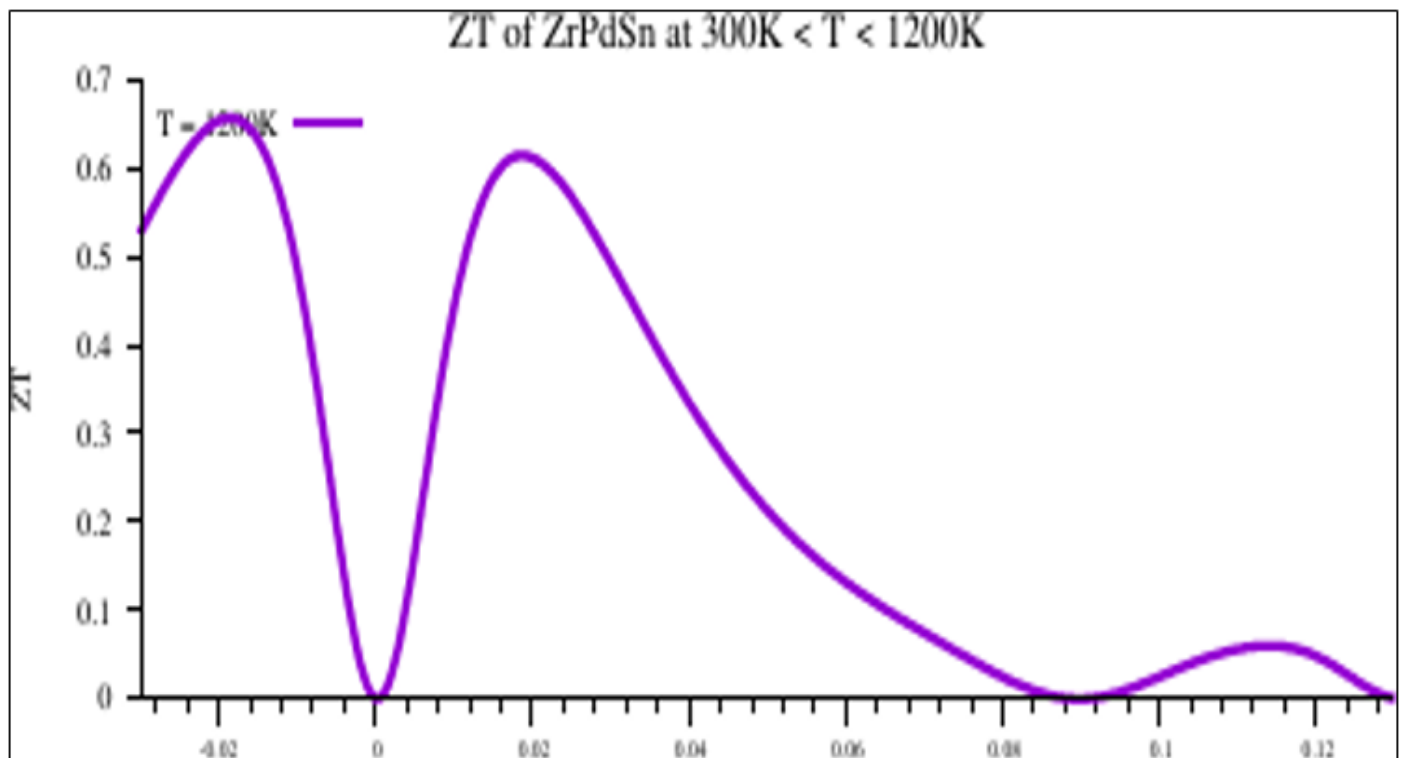


Fig 15 Dimensionless Figure of Merit ZrPdSn.

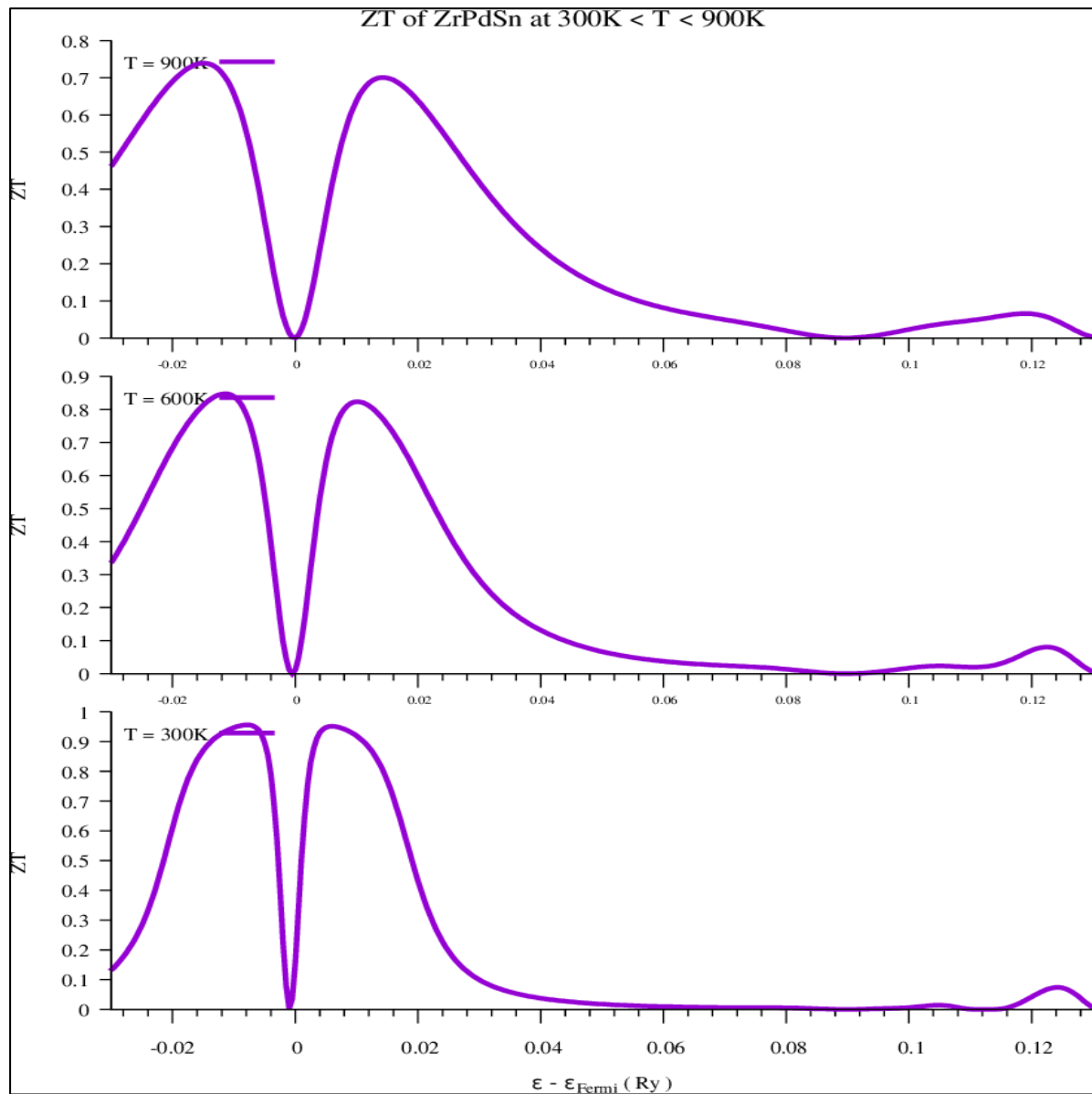


Fig 16 Dimensionless Figure of Merit ZrPdSn.

Figures 17 and 18 display the dimensionless Figure of Merit at each temperature in relationship with the chemical potential. Even at room temperature, ZrPtSn has a high Figure of Merit ($ZT = 1.00$ in the n-type compound and $ZT \approx 1.00$ in the p-type compound), which is perplexing. The observed decrease in ZT as the temperature increases is caused by the significant effects of phonon contribution to the thermal conductivity κ .

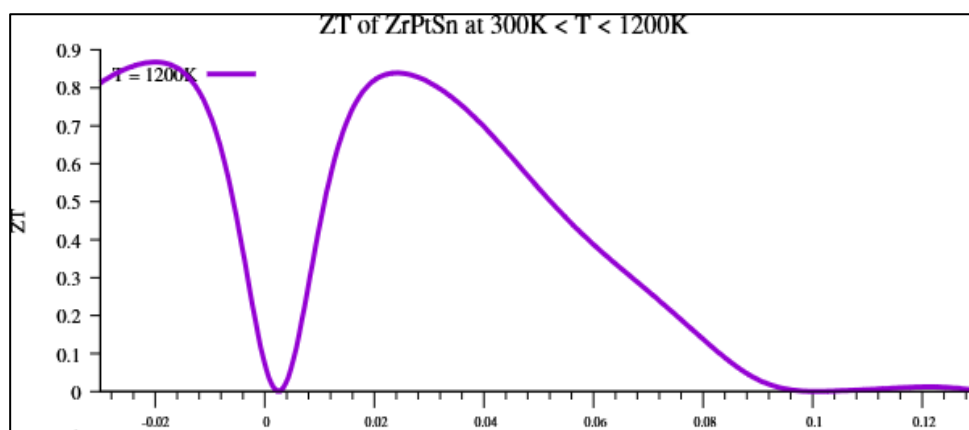


Fig 17 Dimensionless Figure of Merit ZrPtSn.

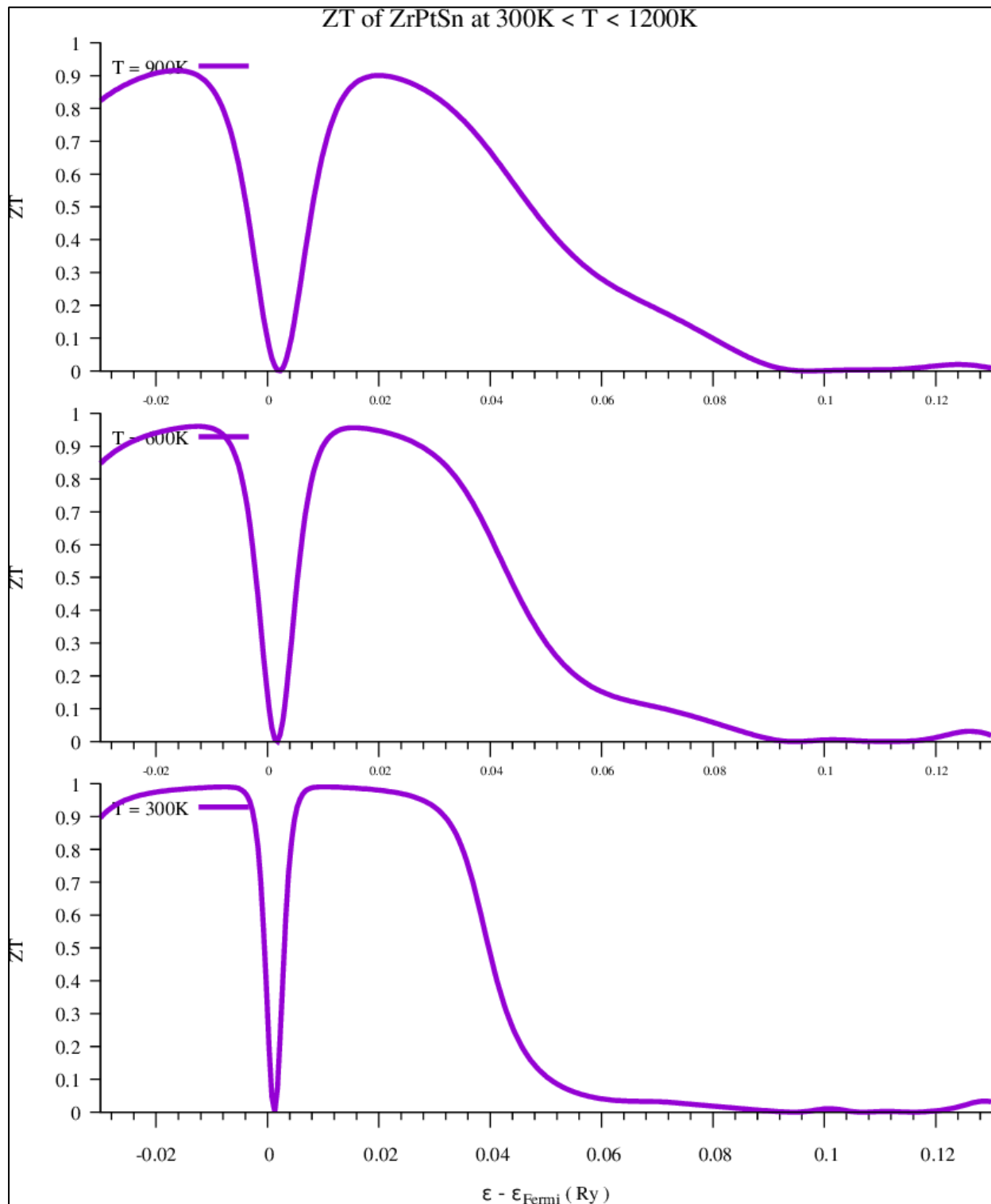


Fig 18 Dimensionless figure of merit ZrPdSn.

IV. CONCLUSIONS

We studied the ZrYSn (Y=Ni, Pd, Pt) alloys' structural, electronic, elastic, and ther-moelectric properties. The atomic configuration of these alloys conforms to the F 43m space group. We discovered and recorded these alloys' stable atomic positions. Electronic band structure analysis shows that ZrNiSn, ZrPdSn, and ZrPtSn are semiconduc-tors, respectively in

nature. Furthermore we predicted their anisotropy and confirmed their mechanical stability. The elastic constant is mechanically stable, and ZrPdSn, and ZrPtSn HH alloys are ductile materials because the Pugh's ratio are greater than 1.75, ZrNiSn is brittle in nature. The thermoelectric materials of the three alloys are high in dimensionless figure of merit with their low thermal conductivities, power factor of the three alloys are very high to improve the thermoelectric materials.

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