

Investigations of Structural, Elastic, Electronic, Magnetic and Transport Properties of the Heusler Compounds Zr_2PdZ ($Z = Al, Ga, \text{ and } In$): FP-LAPW Method

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Structural, elastic, electronic, magnetic and thermoelectric properties of the Heusler compounds: Zr_2PdAl , Zr_2PdGa , and Zr_2PdIn are performed using generalized gradient approximation with exchange-correlation function of the Perdew–Burke–Ernzerhof. The elastic constants are calculated at $P = 0$ GPa. From the obtained elastic parameters, it is inferred that these compounds, with the Hg_2TiCu -type structure, are elastically stable and ductile in nature. The calculated density of states, magnetic moments and band structure are also given. The band structures of these compounds reveal that all of them have almost half metallic character with the narrow indirect band gap in the minority spin channel that amounts to 0.36, 0.46, and 0.40 eV for Zr_2PdAl , Zr_2PdGa , and Zr_2PdIn , respectively. The total spin magnetic moments (M_{tot}) of the considered compounds are very close to integer value 3, which satisfies a Slater–Pauling type rule for localized magnetic moment systems $M_{tot} = Z_T - 18$, where $Z_T = 21$ is the number of valence electrons in the primitive cell. The thermoelectric properties of these materials are discussed on the basis of the Seebeck coefficients, electrical and thermal conductivity relative to relaxation time as a function of temperature, at the Fermi level, using the Boltzmann transport theory. After several browse in the literature, the obtained results are the first predictions of the physical properties for the inverse full-Heusler compounds Zr_2PdZ ($Z = Al, Ga \text{ and } In$).

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1. Introduction

In the last years, the full-Heusler compounds have extensive attention of researchers, due to their interesting properties in spintronic applications [1–3]. They are characterized as magnetic materials and most of them have a half-metallic character due to the different behavior of the two spin bands. As a rule, the minority state density has a band gap around the Fermi level (E_F), whereas the majority state density has a metallic behavior. Hence, the electrons with only one direction of spin contribute to the conduction current. This makes the Heusler alloys very interesting for the spintronic applications.

Theoretical researches focused their interest to this kind of materials using *ab initio* magnetic exchange parameters and/or MC calculations of magnetic and magnetocaloric properties in some example of full-Heusler alloys have been reported in Refs. [4–8]. The electronic structure, magnetic and thermal properties of Rh_2MnZ

($Z = Ge, Sn, \text{ and } Pb$) compounds under pressure from *ab initio* quasi-harmonic method have been presented by Benkhelifa et al. [9]. In addition, Esteki et al. have been found that the new Heusler alloys $CoYO_2$ ($Y = Sc, Ti, V, Cr, Mn, Fe, Ni, Cu, \text{ and } Zn$) presented half-metallic behavior [10].

Ricci reports a joint theoretical and experimental study focused on understanding the optical and magneto-optical properties of Co-based full-Heusler compounds [11]. They show that magneto-optical spectra calculated within *ab initio* density functional theory are able to uniquely identify the features of the experimental spectra in terms of spin resolved electronic transitions. The full potential linearized augmented plane wave method with the generalized gradient approximation (FP-LAPW-GGA) has been used to understand the electronic, magnetic, optical and elastic properties of Cu_2MnAl a gapless full-Heusler compound [12].

The first synthesized compounds of these materials are the ingots Co_2MnAl , Co_2MnSi , Co_2MnGa , Co_2MnGe , Co_2MnSn , and Co_2MnSb which have the general formulae X_2YZ [13, 14]. Their half-metallicity has been predicted by Japanese research groups, using *ab initio* electronic structure calculations [15, 16]. They have two

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structural types, which consist of four interpenetrated fcc sublattices: the first one, known as the full-Heusler compounds (Cu_2MnAl -type structure), crystallized in $L2_1$ structure wherein the both X atom positions are equivalent. The second, so-called inverse full-Heusler, in which the valence of the X transition-metal atom is smaller than the valence of the Y transition metal atom, crystallizes in XA structure, where the sequence of the atoms is X–X–Y–Z and the prototype is Hg_2TiCu [17]. Due to robust half metallic properties, reported in Zr₂-based Heusler-type alloys by Xie et al., the study on the half-metallic states and magnetic properties versus the lattice constant of newly designed Zr₂-based HM materials would be necessary [18, 19]. The study of the magnetic properties of the inverse full-Heusler compounds Zr_2RhZ ($Z = \text{Al}, \text{Ga}$ and In) was performed, the compounds are crystallized in Hg_2CuTi -type structure [20].

In this paper, we have investigate the structural, elastic, electronic and magnetic properties of Zr_2PdZ ($Z = \text{Al}, \text{Ga}$ and In) in their structure-type Hg_2CuTi -type. The calculations have been performed with the generalized-gradient approximation using the Perdew–Burke–Ernzerhof functional (GGA96-PBE) implemented in the WIEN2k code [21]. From the calculated electronic structures and magnetic properties of the Zr_2PdZ ($Z = \text{Al}, \text{Ga}$ and In), it is found that the later are magnetic materials with a near half-metallic behavior. Furthermore, we present also the theoretical investigation of the transport properties (of studied compounds) calculated using the Boltzmann theory implemented in the BoltzTrap code [22].

2. Crystal structure and method of calculation

The inverse full-Heusler Zr_2PdZ ($Z = \text{Al}, \text{Ga}$ and In) crystallize in XA structure (fcc, space group No. 216) with four inequivalent atoms: $\text{Zr}_1(0,0,0)$, $\text{Zr}_2(0.25, 0.25, 0.25)$, $\text{Pd}(0.5,0.5,0.5)$ and $\text{Z}(0.75, 0.75, 0.75)$. In order to study the structural, elastic, electronic and magnetic properties, we use *ab initio* full-potential linear augmented plane wave (FP-LAPW) approximation, implemented in the WIEN2k computer code [21]. The first-principles density functional theory (DFT) calculations are performed within the GGA approximation using the exchange-correlation (XC) function PBE [23]. In this method, the space is divided into an interstitial regions (IR) and non-overlapping (MT) spheres centered on the atomic sites. In the IR regions, the Fourier series represents the basic functions. Inside MT spheres, the basic set is treated as a linear combination of radial functions times spherical harmonics. In order to achieve a satisfactory degree of convergence on energy eigenvalues, the wave functions in the interstitial regions were expanded in plane waves with an energy cut-off equal to -6.0 Ry. The values of muffin-tin sphere radius (MTS) are taken to be 2.5, 2.5, and 2.45 a.u. for Zr, Pd, and Z ($Z = \text{Al}, \text{Ga}$ and In) atoms, respectively. The valence wave functions inside spheres are expanded in terms of the multiplication of spherical harmonics and the radial eigenfunctions

up to $L_{max} = 10$. The K integrations over the Brillouin zone (BZ) are performed up to (14, 14, 14) grid (yielding 3000 k -points in the irreducible BZ).

For the thermoelectric properties of Zr_2PdZ ($Z = \text{Al}, \text{Ga},$ and In) compounds, we apply the Boltzmann theory as implemented in the Boltztrap program [22] using the results of the electronic properties, obtained by GGA96-PBE approximation, as input data. The electrical and thermal conductivity might be only calculated with respect to relaxation time τ . In order to obtain the converged results of the thermoelectric properties, we used dense 100000 k points in the irreducible Brillouin zone (IBZ) with k -mesh $46 \times 46 \times 46$.

3. Results and discussion

3.1. Structural and elastic properties

The Heusler compounds X_2YZ crystallize in two face cubic centered (fcc) type-structures [24–26], XA, and $L2_1$ structures. In the first one, so-called inverse full-Heusler (Hg_2CuTi -type structure), X atoms occupy $4a(0, 0, 0)$ and $4c(0.25, 0.25, 0.25)$ sites, Y atom occupies $4b(0.5, 0.5, 0.5)$ sites, and the Z atom occupies $4d(0.75, 0.75, 0.75)$ sites, whereas in Cu_2MnAl -type ($L2_1$ structure) X atoms occupy ($4a(0, 0, 0)$, $4b(0.5, 0.5, 0.5)$) sites and Y atom occupies $4c(0.25, 0.25, 0.25)$ site, and Z atom occupies $4d(0.75, 0.75, 0.75)$, as shown in Fig. 1.

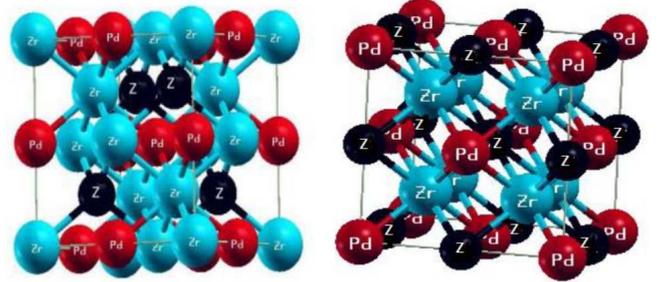


Fig. 1. Crystal structures of the Heusler compounds Zr_2PdZ ($Z = \text{Al}, \text{Ga}$ and In): (a) the inverse full-Heusler (Hg_2TiCu -type structure), (b) the full-Heusler (Cu_2MnAl -type structure).

In order to determine the stable structure and the equilibrium structural parameters of the Zr_2PdZ ($Z = \text{Al}, \text{Ga}$ and In) compounds, we optimized these alloys for magnetic and paramagnetic states in their two-type structures. The total energy-volume curves are shown in Fig. 2.

One can be seen from these curves that the Cu_2MnAl -type structure in its magnetic phase is most stable, energetically, for the compounds Zr_2PdZ ($Z = \text{Al}, \text{Ga}$ and In) at the equilibrium volume. Based on the fitting of these results to the Murnaghan equation of state [27], we obtain, for all compounds, the ground-state parameters (a_0 , B_0 and B'), quoted in Table I.

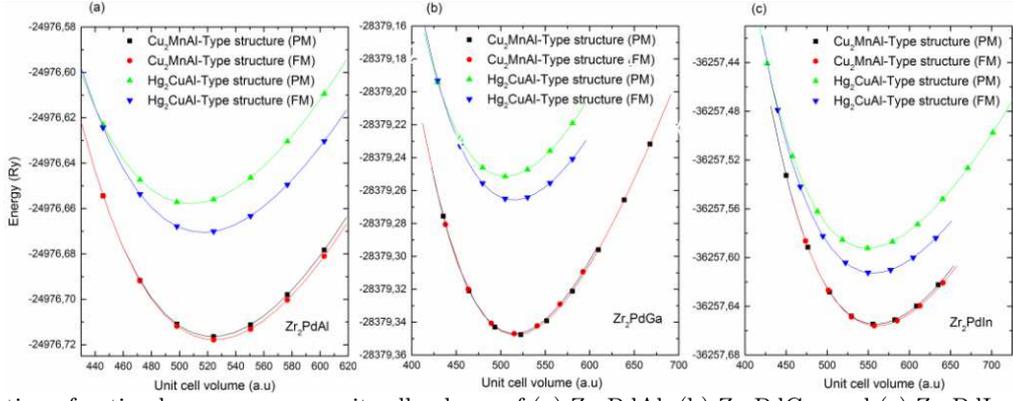


Fig. 2. Variation of optimal energy versus unit cell volume of (a) Zr_2PdAl , (b) Zr_2PdGa , and (c) Zr_2PdIn compounds in their FM and PM phases.

TABLE I

The calculated values of the lattice parameter a_0 [\AA], bulk modulus B_0 and its pressure derivative [GPa], ground state energy E_{\min} [Ry] for Zr_2PdZ ($Z = Al, Ga$ and In).

Comp.	Phase	a_0	B	B'	E_{\min}
Hg ₂ CuTi-type structure					
Zr_2PdAl	FM	6.7415	106.4681	4.1275	-24976.670433
	PM	6.7013	106.5902	4.2135	-24976.657800
Zr_2PdGa	FM	6.7339	107.7041	4.1204	-28379.265682
	PM	6.6908	107.9378	4.4066	-28379.251320
Zr_2PdIn	FM	6.9126	104.1811	4.1318	-36257.612704
	PM	6.8812	100.9407	4.3775	-36257.591893
Cu ₂ MnAl-type structure					
Zr_2PdAl	FM	6.7766	117.3660	4.0111	-24976.717776
	PM	6.7708	118.1554	4.1103	-24976.716384
Zr_2PdGa	FM	6.7402	120.5406	4.4743	-28379.347590
	PM	6.7373	123.2809	4.2024	-28379.346960
Zr_2PdIn	FM	6.9254	112.4693	4.2599	-36257.655841
	PM	6.9204	114.0042	4.1830	-36257.654653

TABLE II

Elastic constants [GPa]: bulk modulus B , C_{11} , C_{12} , C_{44} .

Comp.	Phase	B	C_{11}	C_{12}	C_{44}
Hg ₂ CuTi-type structure					
Zr_2PdAl	FM	123.762	111.88	129.70	28.50
	PM	120.11	79.43	140.45	13.64
Zr_2PdGa	FM	123.76	111.88	129.70	28.50
	PM	124.95	103.75	135.55	9.53
Zr_2PdIn	FM	114.29	102.51	120.18	41.20
	PM	115.23	89.27	128.22	21.87
Cu ₂ MnAl-type structure					
Zr_2PdAl	FM	107.91	137.89	92.92	59.00
Zr_2PdGa	FM	108.65	125.57	100.20	67.58
Zr_2PdIn	FM	103.72	117.48	96.90	68.48

To confirm more stability of these compounds, the elastic constants are calculated, using the method developed by Charpin, integrated in WIEN2k code [21] and based on direct calculation of macroscopic strain on atoms, for

more stable energetically until we obtain results verifying the mechanical stability criteria, for a cubic structure which is: ($C_{11} - C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$, $C_{12} < B < C_{11}$), as shown in Table II. Therefore, we demonstrate that the Hg₂CuTi-type structure in FM phase, for all studied compounds Zr_2PdZ ($Z = Al, Ga$ and In) is most stable among the mechanically stable structures.

For the Hg₂CuTi-type structure and FM phase of the studied compounds Zr_2PdZ ($Z = Al, Ga$ and In), the lattice constants of 6.7415, 6.7339, and 6.9126 \AA , respectively, are obtained, using GGA96 approximation with the exchange-correlation functional of PBE. To the best of our knowledge, no comparable studies have been done on Zr_2PdZ ($Z = Al, Ga$ and In) compounds. However, our results await experimental confirmation. The formation energy indicates the stability of the alloys in regard of decomposition into its bulk constituents. The formation energy is calculated using the formula

$$E_f = E_{Zr_2PdZ}^{total} - (2E_{Zr}^{bulk} + E_{Pd}^{bulk} + E_Z^{bulk}), \quad (1)$$

where E_{Zr}^{bulk} , E_{Pd}^{bulk} , and E_Z^{bulk} ($Z = Al, Ga$ and In), correspond to the total energy per atom for Zr, Pd, and Z atoms, respectively, obtained by the same approximation used in the calculation of $E_{Zr_2PdZ}^{total}$. We found that the calculated formation energies are -0.18 , -0.21 and -0.16 Ry for Zr_2PdAl , Zr_2PdGa , and Zr_2PdIn , respectively, which indicate that the Zr_2PdZ ($Z = Al, Ga$ and In) alloys are thermodynamically stable due to their negative formation energies.

Shear modulus G , the Young modulus E , anisotropic parameters $A, B/G$ ratios and the Poisson ratios ν for the Hg₂CuTi-type structure of Zr_2PdZ ($Z = Al, Ga$ and In) compounds are summarized in Table III. The study, carried out by Born and Huang [28], expressed in terms of the elastic constants for cubic structure, predict that: $C_{11} - C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$, $C_{12} < B < C_{11}$ at $P = 0$ GPa. According to this study, the condition of the mechanical stability criteria of this cubic structure is satisfied for the inverse full-Heusler Zr_2PdZ ($Z = Al, Ga$ and In). The high values of B/G ratios ($B/G > 1.75$) indicate the ductility proposed by Pugh [29] of all studied compounds.

TABLE III

Shear modulus G , the Young modulus E , anisotropic parameter A , B/G ratio and the Poisson ratio ν for Zr_2PdZ ($Z = Al, Ga$ and In) in the Hg_2CuTi -type structure at $P = 0$ GPa

	Zr_2PdAl	Zr_2PdGa	Zr_2PdIn
G	44.39	45.62	45.20
E	117.12	120.07	118.41
A	2.62	5.33	6.65
B/G	2.43	2.38	2.29
ν	0.43	0.43	0.43

3.2. Electronic and magnetic properties

The calculated band structures and densities of state of the inverse full-Heusler Zr_2PdZ ($Z = Al, Ga$ and In) were calculated and plotted, in their stable magnetic structures, as shown in Figs. 3 and 4, yielding an indication of the valence band (VB) and conduction band (CB) separated by the Fermi levels indicated by red dashed lines for all figures. The band structures of the inverse full-Heusler Zr_2PdZ ($Z = Al, Ga$ and In) that appear around the E_F at Γ point are mainly formed by valence d -electrons states of two Zr atoms, in the spin-up channel (Fig. 3), whereas the total densities of states, for all studied compounds, are almost equal zero, for spin-down channels (Fig. 4). Hence, the spin-up polarizations come to 98.29, 97.79 and 98.67% for Zr_2PdAl , Zr_2PdGa and Zr_2PdIn respectively, which are mainly due to the large exchange splitting between the spin-up and spin-down states of Zr atoms at E_F . To understand the electronic properties of Zr_2PdZ ($Z = Al, Ga$ and In), using GGA96-PBE the calculations of the electronic band structures along high-symmetry directions in the Brillouin zone are shown in Fig. 3. We notice that, in the majority-spin channels, there are overlaps between the conduction and valence bands, which mean that these channels have metallic character. In the minority-spin channels, we see forbidden indirect bands, below and very close to the E_F , around the energy ranges 0.3831, 0.46323 and 0.40543 eV along the Γ - X symmetry for the compounds Zr_2PdAl , Zr_2PdGa , and Zr_2PdIn , respectively. These results mean that the studied inverse full-Heusler Zr_2PdZ ($Z = Al, Ga$ and In) are almost half-metallic materials. Further, we can see the almost flat covalent bands along Γ to X direction in the band structures of the spin-down channels of these inverse full-Heusler alloys.

The magnetic character is originated mainly from d -electron of the Zr atoms (Fig. 4). It is seen that the main contribution to the magnetic character in the resulting DOS, obtained by GGA (PBE) method around the Fermi level, is due to both Zr atoms. It is found that Zr1 at the position (0.25, 0.25, 0.25) has a magnetic momentum larger than that of Zr2(0, 0, 0). This result is confirmed by the outcomes of the DOS of both atoms Zr1 and Zr2 (Fig. 4) in which there is a large difference of DOS between up and down channels around Fermi level for Zr2 atom compared to Zr1.

They are close to integer value 3. Therefore, the compounds Zr_2PdZ ($Z = Al, Ga$ and In) are near half-metallic materials and almost obey the rule for half metallic full-Heusler: $M_{tot} = (Z_T - 18) \mu_B$ where M_{tot} stands for the total magnetic momentum (in μ_B) per formula unit and Z_T represents the total number of valence electrons.

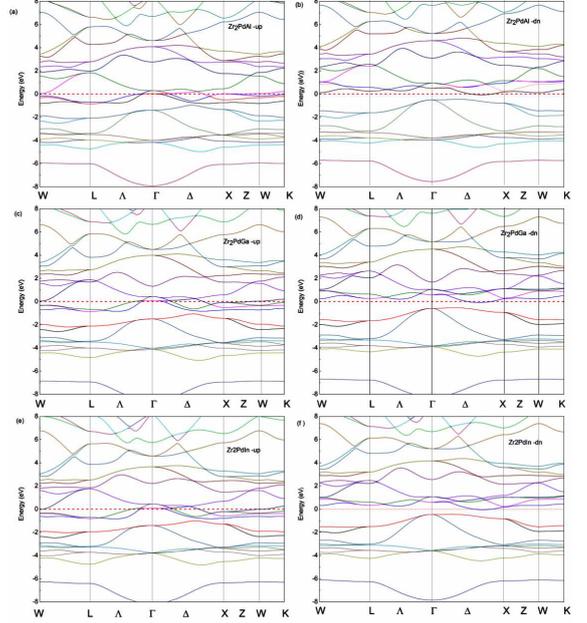


Fig. 3. Band structures for the inverse full-Heusler compounds: (a) the majority spin channel of Zr_2PdAl , (b) the minority spin channel of Zr_2PdAl , (c) the majority spin channel of Zr_2PdGa , (d) the minority spin channel of Zr_2PdGa , (e) the majority spin channel of Zr_2PdIn , and (f) the minority spin channel of Zr_2PdIn .

The calculated total and partial magnetic moments using GGA (PBE) are summarized in Table IV. We notice that the total spin magnetic momenta are 2.99441, 2.99853, and 3.00046 μ_B of the inverse full-Heusler Zr_2PdAl , Zr_2PdGa , and Zr_2PdIn , respectively.

TABLE IV

The calculated magnetic momentum in the unit of μ_B , the Zr atom moment (M_{Zr}), Pd atom moment (M_{Pd}), Z atoms moment (M_Z), interstitial moment (M_{int}) and the unit cell total magnetic moment (M_{tot}) for Zr_2PdZ ($Z = Al, Ga$ and In).

Zr_2PdZ	Zr_2PdAl	Zr_2PdGa	Zr_2PdIn
M_{Zr1}	0.69040	0.75599	0.75459
M_{Zr2}	1.11920	1.10263	1.07006
M_{Pd}	0.16436	0.16461	0.14916
M_Z	0.04119	0.02319	0.01120
M_{int}	0.97926	0.95211	1.01545
M_{tot}	2.99441	2.99853	3.00046

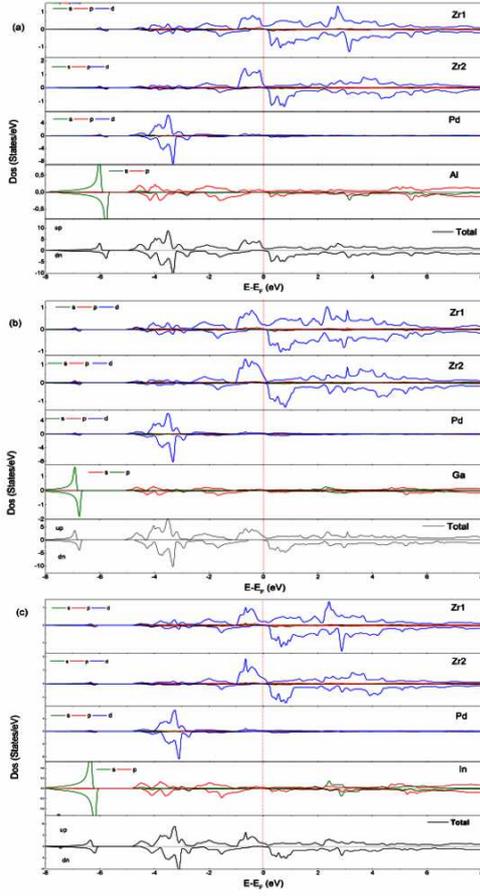


Fig. 4. Total and partial densities of states of the inverse full-Heusler alloys: (a) Zr_2PdAl , (b) Zr_2PdGa , and (c) Zr_2PdIn .

3.3. Transport properties

In order to study the thermoelectric properties of the inverse full-Heusler compounds Zr_2PdZ ($Z = Al, Ga$ and In), we used semi-classical Boltzmann transport theories, based on a smoothed Fourier interpolation of the bands, as implemented in the BoltzTraP code. The Seebeck coefficient S , electrical σ/τ and thermal conductivity κ/τ are calculated as function of temperature (at E_F) for all studied compounds. We have predicted above that our studied compounds are magnetic materials, so we can use the two-current model [30, 31] in which the Seebeck coefficient is formulated by

$$S = \{[S(\uparrow) \times \sigma(\uparrow) + S(\downarrow) \times \sigma(\downarrow)] / [\sigma(\uparrow) + \sigma(\downarrow)]\}, \quad (2)$$

where $S(\uparrow), S(\downarrow), \sigma(\uparrow)$ and $\sigma(\downarrow)$ are the Seebeck coefficients and electrical conductivity for *up* (\uparrow) and *down* (\downarrow) spin channels. In addition, it is important to note that the value of S for semiconductors is found to be about 100 times larger than that of the metals [32]. The studied compounds Zr_2PdZ ($Z = Al, Ga$ and In) have been found that they do not exhibit pure semiconductor behavior in both spin-channels, so we have to perform the calculations of the transport coefficients for both spin channels.

The Seebeck coefficient, which jointed thermal and electrical conductivity, is an important thermoelectric (TE) property for estimating the potential performance of novel thermoelectric materials performance [33]. Figure 5a–f shows dependence temperature of the Seebeck coefficient of the inverse full-Heusler compounds Zr_2PdAl , Zr_2PdGa , and Zr_2PdIn , respectively, for both spin-channels (up and down). It is seen that the absolute values of thermopower S of the three compounds increase with increase of the temperature. Moving $Al \rightarrow Ga \rightarrow In$ causes decreases in the Seebeck coefficient, and Zr_2PdAl compound shows the highest Seebeck coefficient along whole temperature scale. At this value of the chemical potential, the three compounds represent only *p*-type conduction for spin-up channel, whereas they have *n*-type conduction for spin-down channel.

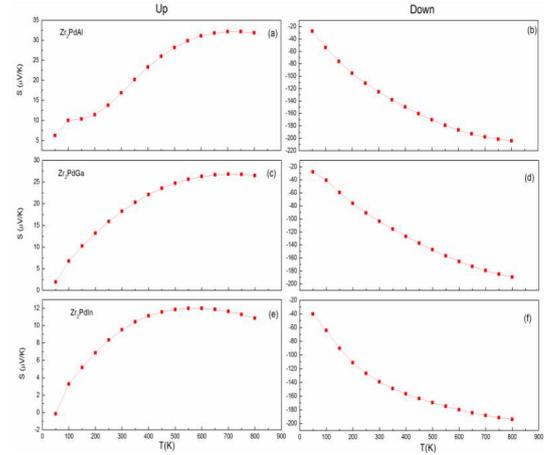


Fig. 5. Temperature dependence of the Seebeck coefficient of: (a) the majority spin channel of Zr_2PdAl , (b) the minority spin channel of Zr_2PdAl , (c) the majority spin channel of Zr_2PdGa , (d) the minority spin channel of Zr_2PdGa , (e) the majority spin channel of Zr_2PdIn , and (f) the minority spin channel of Zr_2PdIn .

We see obviously in Fig. 5 that the Seebeck coefficients show almost the same behavior for Zr_2PdAl , Zr_2PdGa , and Zr_2PdIn compounds. They have the maximum values of 32.12, 26.8 and 12 $\mu V/K$ at 750, 700, and 600 K, respectively, at the Fermi level in the spin-up channel. Further, the spin-down channel for all studied compounds shows negative values of thermopower S , these mean that they have *n*-type conduction for this channel. The room temperature values of ($S \uparrow, S \downarrow$) are (16.87, -125.36), (18.23, -103.9) and (9.52, -139.3) ($\mu V/K$) for the inverse full-Heusler compounds Zr_2PdAl , Zr_2PdGa , and Zr_2PdIn , respectively.

The electrical conductivities of the compound Zr_2PdZ ($Z = Al, Ga$, and In) as function of the temperature, for both the spin channels, have been plotted in Fig. 6 at the Fermi level. Due to the negative value of thermopower S and metallic behavior of the majority spin channel, we can see obviously that the electronic conductivity (σ/τ) decreases with increasing temperature. The room tem-

perature ($T = 300$ K) values of $\sigma(\uparrow)/\tau(\uparrow)$ are about 0.5427×10^{20} , 1.2284×10^{20} and $1.7 \times 10^{20} \Omega^{-1}\text{m}^{-1}\text{S}^{-1}$ for the compounds Zr_2PdAl , Zr_2PdGa , and Zr_2PdIn , respectively. For minority spin channel, the electrical conductivity values are less than of those of the majority spin channel because of the lower values of DOS at Fermi level.

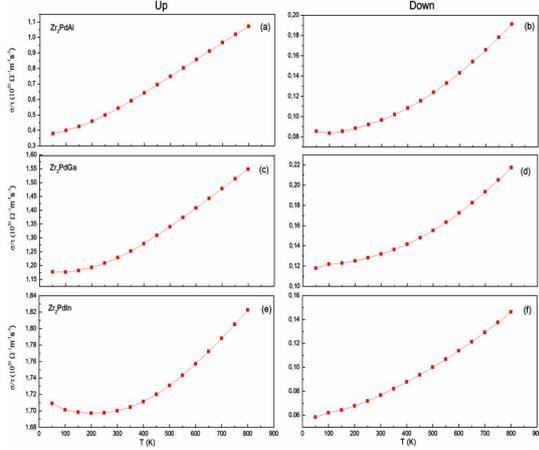


Fig. 6. Temperature dependence of electrical conductivity of: (a) the majority spin channel of Zr_2PdAl , (b) the minority spin channel of Zr_2PdAl , (c) the majority spin channel of Zr_2PdGa , (d) the minority spin channel of Zr_2PdGa , (e) the majority spin channel of Zr_2PdIn , and (f) the minority spin channel of Zr_2PdIn .

Figure 7 shows the electronic thermal conductivity with the temperature for spin-up and spin-down channels. In the majority spin channel (up), we can see that the κ/τ increases almost linearly with temperature for all these studied compounds and their values are 6, 10.54 and $12.8 (10^{14} \text{ W}/(\text{mK s}))$ for Zr_2PdAl , Zr_2PdGa , and Zr_2PdIn , respectively, whereas the minority spin channel shows an increase with curvature of κ/τ for all studied compounds Zr_2PdZ ($Z = \text{Al, Ga, and In}$). In this channel, the room temperature thermal conductivities are almost 6, 8, and 10 times smaller than those of the spin-up channel that have the 1.06, 1.26, and 1.26 ($10^{14} \text{ W}/(\text{mK s}))$, respectively.

4. Conclusion

The structural, elastic, electronic and magnetic properties of the Heusler compounds Zr_2PdZ ($Z = \text{Al, Ga and In}$) are studied using the first-principle (FP-LAPW+lo) method based on DFT within the GGA approximation. We have predicted that the structural and magnetic ground state is ferromagnetic phase of Cu_2MnAl -type structure, for all studied compounds. However, the study of the mechanical stability, investigated by performing the calculations of the elastic constants (C_{11}, C_{12}, C_{44} , shear modulus G , the Young modulus E , anisotropic parameters A , B/G ratios and the Poisson ratios) of these compounds using Charpin method, show that the

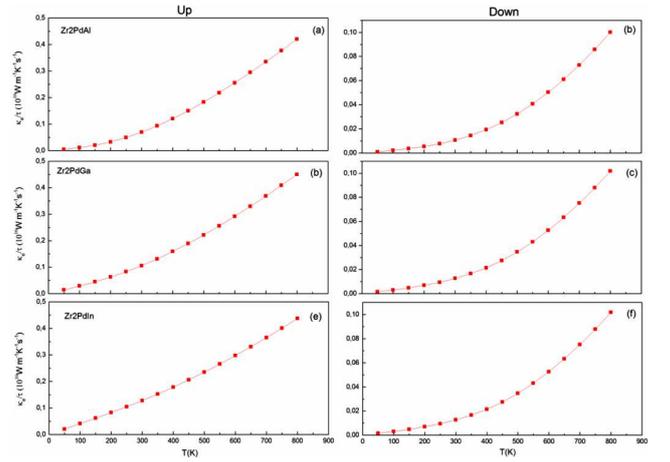


Fig. 7. Temperature dependence of thermal conductivity of: (a) the majority spin channel of Zr_2PdAl , (b) the minority spin channel of Zr_2PdAl , (c) the majority spin channel of Zr_2PdGa , (d) the minority spin channel of Zr_2PdGa , (e) the majority spin channel of Zr_2PdIn , and (f) the minority spin channel of Zr_2PdIn .

Cu_2MnAl -type structure of these compounds is not mechanically stable, whereas their Hg_2CuTi -type structure is mechanically stable. We have predicted, from the DOS and band structure calculations, that these compounds are magnetic materials. The majority spin channel (up) is found to be metallic, whereas there is almost half-metallic character in the minority spin channel (down). Therefore, the inverse full-Heusler Zr_2PdZ ($Z = \text{Al, Ga, and In}$) are all near half metallic materials. Hence, the calculated total magnetic moment of Zr_2PdAl , Zr_2PdGa , and Zr_2PdIn are near the integer number $3\mu_B$ per formula unit which follow the Slater–Pauling rule as $M_{tot} = (Z_T - 24) \mu_B$. Both Zr atoms for all studied compounds show large exchange splitting and contribute largely to the total magnetic moment.

The transport coefficients, thermopower, electrical conductivity, and electronic thermal conductivity of the compounds Zr_2PdZ ($Z = \text{Al, Ga and In}$) have been calculated, as a function of temperature at the Fermi level, by combining the electronic band structure calculations with the Boltzmann transport theory. We have predicted that the near half metallic materials Zr_2PdAl , Zr_2PdGa , and Zr_2PdIn could be prospective magnetic materials for spintronic applications and they are also thermoelectric materials. Furthermore, we expect that the experimental efforts will be motivated by this present study toward fabrication of these compounds.

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