FUDMA Journal of Sciences (FJS)
ISSN online: 2616-1370
ISSN print: 2645 - 2944
Vol. 10 No. 14, July, 2026, pp 299 – 303
DOI: https://doi.org/10.33003/fjs-2026-1014-5432

Structural, Electronic, Mechanical, Vibrational and Superconducting Properties of Pd_2ZrAl: A DFT Study

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Received: 03 Jul. 2026
Accepted: 09 Aug. 2026
Published: 25 Aug. 2026

ABSTRACT
We have applied first-principles density functional theory calculations to investigate the structural, electronic, mechanical vibrational and superconducting properties of Pd_2ZrAl. Our results reveal some interesting properties about the full Heusler alloy we studied. We observed that the compound is energetically stable in the non-magnetic cubic phase. The electronic property of the compound reveal a metallic behaviour with the presence of van Hove singularity around the Fermi energy which indicates that the compound is a superconductor. The mechanical properties show that the full-Heusler alloy is mechanically stable and having a ductile characteristics. The phonon dispersion curve reveals that the compound is dynamically stable due to the absence of negative frequencies. Pd_2ZrAl crystallizes in the Cu_2MnAl-type structure with space group Fm3m (no.225). The mechanical stability of the cubic structure satisfies the stability criteria. The phonon spectrum consists of three acoustic modes and optical modes, with one optical mode within 200-250cm^{-1} and two others within 120-180cm^{-1}. These results demonstrate the structural stability and superconducting potential of Pd_2ZrAl.

Keywords: Full Heusler, van Hove singularity, Electronic band structure, Mechanical properties, Superconductivity

INTRODUCTION

Over the years, Full Heusler alloys with the general formula X_2YZ have attracted the attention of many researchers due to their diverse and multifunctional properties (Graf *et al., 2011;* Webster & Ziebeck, 1988; Babalola *et al.,* 2024; Galanakis *et al*., 2002; Fadila *etl al.,* 2018). Among these multifunctional properties include the half metallic property, (Ishida *et* al., 1995; Babalola & Iyorzor, 2019; Alijani *et al*., 2011; Amudhavalli *et al*., 2018), topological insulator (Chadov *et al*.,2010; Yan&Visser,2014; Lin *et al*., 2010), shape memory effect (Ullakko *et al*., 1996; Yu *et al*.,2015;Planes *et al*.,2007), and superconducting property. (Amano *et al*., 1980; Klimczuk *et al*., 2012; Xiao *et al*., 2018; Hoffmann *et al*., 2023). The superconducting property of a material is when a material experiences zero resistivity below a critical temperature (Mahdjouba *et al*., 2024). Although Ni-based and Pd-based full Heusler superconductors were the earliest discovered superconductors, researchers' interest in this field is still growing especially in Pd-based superconductors due to the role of Pd suppressing magnetism and improving superconductivity in the materals (Mahdjouba *et al*., 2024). There has been a deep dive into experimental and theoretical approach in order to gain insight about this phenomenon. For instance, the experimental work of Kamashev et al., (2018) (Kamashev *et al*., 2018) shows how engineering superconducting property of a Heusler alloy is possible. While for the theoretical approach, first-principles computations are now essential and reliable for understanding superconducting behavior. Important discoveries have been made from research on materials such as Ni_2ZrAl, Ni_2ZrGa highlight the significance of particular electronic properties that increase the density of states at the Fermi level and encourage electron-phonon coupling, such as van Hove singularities and Fermi surface nesting (Mahdjouba *et al*., 2024). Despite superior critical properties of high Tc superconductors over Heusler alloys there is still the challenge of being able to be drawn into wires. Hence Heusler alloys possess the ability of being ductile and superconducting at the same time. In this work, we explore the structural, electronic, mechanical, vibrational and superconducting properties of Pd_2ZrAl using first principles calculation.

MATERIALS AND METHODS

All properties of the Pd_2ZrAl full-Heusler alloy were computed using ab initio calculation based on density functional theory (DFT). The calculation utilized the generalised gradient approximation (GGA) type of exchange correlation functional and with the norm conserving type of pseudopotential which is implemented in QUANTUM ESPRESSO (Giannozzi *et al*., 2024). During optimization a 100Ry kinetic energy cut-off and a k-point grid of 8×8×8 were used and the total energy versus the lattice constants was plotted as shown in Fig. 2. To get the optimized lattice constant, we fitted our curve the the murnaghan equation of state. The thermo_pw code (Dal Corso *et al*., 2016) was used for computing the mechanical and vibrational properties.

RESULTS AND DISCUSSION

Structural Properties

We present the structural property of Pd2ZrAl in this section and the obtained results are shown in Table 1. Since Pd2ZrAl is a full Heusler alloy it crystallizes in the Cu_2MnAl-type structure with Fm3m (no. 225) and it is shown in Fig. 1. The typically Cu_2MnAl-type structure occupies the following Wyckoff positions: 4a (0,0,0), 4b (1/2,1/2,1/2), 8c (1/4,1/4,1/4), 8c (3/4,3/4,3/4). Optimisation was done for two different magnetic states: ferromagnetic (FM), non-magnetic (NM). The obtained total energy-lattice constant curves, shown in Figure 2, were then fitted to the Murnaghan equation of state. Due to the overlap of the curves in Fig. 1 then the non-magnetic state is considered.

Table 1: Computed Lattice Parameters a, Bulk Moduli (B), Pressure Derivatives (B'), Magnetic States M_g, Density of States n (EF) at the Fermi Energy of Pd_2ZrAl

Compound	a(Å)	B(GPa)	B'	M_g	$n(E_F)$ $(eV)^{-1}$
Pd_2ZrAl					
Cu_2MnAl-type	6.459	149.7	4.48	NM	2.70
	6.458	149.4	4.61	FM	
[a]experiment	6.406				2.70
[a]Theory	6.467	151			2.60

[A] (Winter *et al.*, 2009)

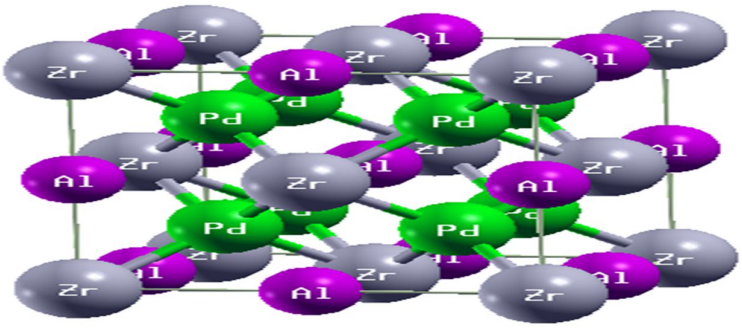

Figure 1: Unit cell of N_2SrRb full-Heusler alloy in Cu_2AlMn-type and Hg_2CuTi-type

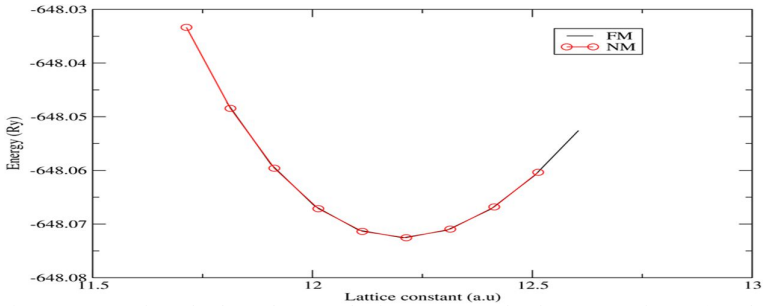

Figure 2: Energies of Pd_2ZrAl versus lattice constants for ferromagnetic (FM) and non-magnetic (NM) states in Cu_2MnAl-type. The non-magnetic states possesses the lowest energy

Electronic Properties

In this section we discuss the electronic properties of Pd2ZrAl. Figs. 3 and 4 are the electronic band structure and Partial density of states (PDOS) of Pd2ZrAl respectively. From Fig. 3 we observed that the conduction band and the valence band overlap which indicate that the compound has a metallic behavior. We also observed a saddle point at the Γ-L-W point near the Fermi energy as indicated by the arrow, this saddle point is also known as the van Hove singularity which is responsible for the unusual high density of states around the Fermi energy as shown in Fig. 4. The presence of the van Hove singularity at the Fermi energy signifies superconducting property. The value of the density of states at the Fermi energy is shown in Table 1. This value when compared to other results shows a good agreement. Fig. 4 (a) represent the total density of state (DOS) while Fig. 4 (b), (c), and (d) are the various Pd, Zr, and Al atomic orbital contribution to the DOS. We observed that the major contributions come from the Pd-3d, Zr-3d, and Al-2p orbitals.

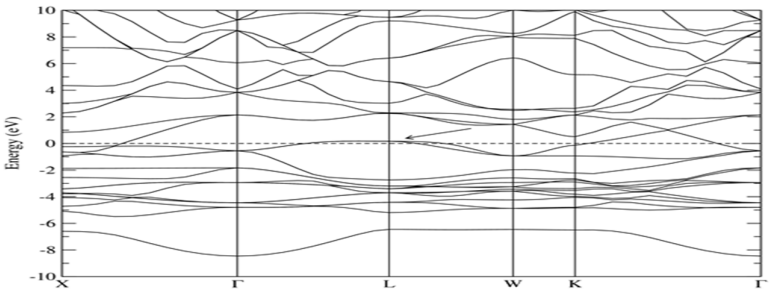

Figure 3: Electronic band structure of Pd_2ZrAl. The arrow shows the presence of the van Hove singularity

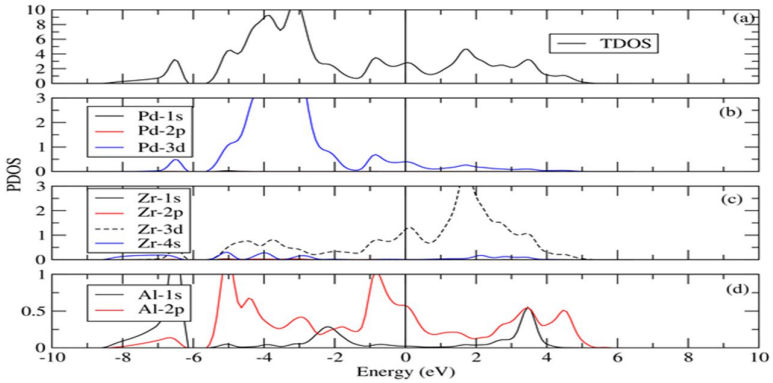

Figure 4: Partial density of states (PDOS) of Pd_2ZrAl (a) Total density of states of Pd_2ZrAl (b) Contribution of Pd atoms to PDOS (c) Contribution of Zr atoms to PDOS (d) Contribution of Al atoms to PDOS

Mechanical Properties

We present the mechanical property of Pd_2ZrAl in this section. The mechanical property includes the elastic constants which explains how various materials respond to external pressures, shear modulus, Young modulus, Poisson's ratio, anisotropic factor, and B/G ratio.

The computed parameters are shown in Table 2. The elastic constants for cubic materials are usually C_{11}, C_{12}, and C_{44}. The mechanical stability of cubic structure is determined by the stability criteria given by equ. 1[Conditi *et al*., 2014]:

$C_{11}>0, C_{44}>0, C_{11}>B>C_{12}$ and $C11+2C_{12}>0, C_{11}-C_{12}>0$ (1)

Table 2: Elastic constants C_{ij}, shear moduli G, Young moduli E, bulk modulus, Poisson's ratio v *from the Voigt, Reuss and Hill's approximation* B/G ratio and anisotropy factor of Pd_2ZrAl

Compound	Pd_2ZrAl
C_{11} *(GPa)*	175.94
C_{12} *(GPa)*	139.81
C_{44} *(GPa)*	0.16
E_V*(GPa)*	21.61
E_R*(GPa)*	0.79
E_H*(GPa)*	11.20
G_V*(GPa)*	7.32
G_R*(GPa)*	0.26
G_H*(GPa)*	3.79
B_V*(GPa)*	151.85
B_R*(GPa)*	151.85
B_H*(GPa)*	151.85
v_V	0.4763
v_R	0.4991
v_H	0.4771
B/G	40.07
A	0.0089

Most of the mechanical parameters computed in this work are based on the Hill's, Voigt's and Reuss models, where the Hill's model ia an average of the Voigt's and Reuss models. The calculated parameters are presented in Table 2. equs. 4 - 11 are used to compute the mechanical properties of Pd_2ZrAl

$$B=\frac{1}{2}(B_R+B_V) \quad (2)$$

$$G=\frac{1}{2}(G_R+G_V) \quad (3)$$

$$B_R=B_V=\frac{1}{3}(C_{11}+2C_{12}) \quad (4)$$

$$G_V=\frac{1}{5}(C_{11}-C_{12}+3C_{44}) \quad (5)$$

$$G_R=\frac{5(C_{11}-C_{12})C_{44}}{4C_{44}+3(C_{11}-C_{12})} \quad (6)$$

$$E=\frac{9GB}{G+3B} \quad (7)$$

$$A=\frac{2C_{44}}{(C_{11}-C_{12})} \quad (8)$$

$$v=0.5\frac{\left(B-\frac{2}{3}G\right)}{\left(B+\frac{1}{3}G\right)} \quad (9)$$

where B_R, G_R, and G_R represent bulk, shear, and Young's modulus for the Reuss model repectively, while B_H, G_H, and G_H represent B_V represents bulk, shear, and Young's modulus for the Voigt's model repectively. From equ. 1 it is evident that the crystal structure of Pd_2ZrAl is mechanically stable. The B/G ratio of the alloy is measure of ductility with value greater than the critical threshold of 1.75, suggesting that Pd_2ZrAl exhibits ductility.

Vibrational Properties

We present the vibrational property of Pd_2ZrAl in this section. Fig.5 shows the phonon dispersion curve of Pd2ZrAl which helps us to understand the vibrational property of the full Heusler compound. From Fig. 5, it is observed that there are no negative frequencies which implies that the compound is dynamically stable. Also it is observed that the four atoms in the unit cell of the compound contribute three phonon each which results to a total of12 phonon modes three of which are the acoustic modes and 9 are the optical modes. The acoustic modes are the ones within the 0 cm^{-1} and about 150 cm^{-1}. The optical modes of the phonon dispersion curve have higher frequencies compared to the acoustic modes. One of the optical mode is clearly seen within the frequency range of 200 to 250 cm^{-1} while the other two optical modes are found within the 120 to 180 cm^{-1} frequency range.

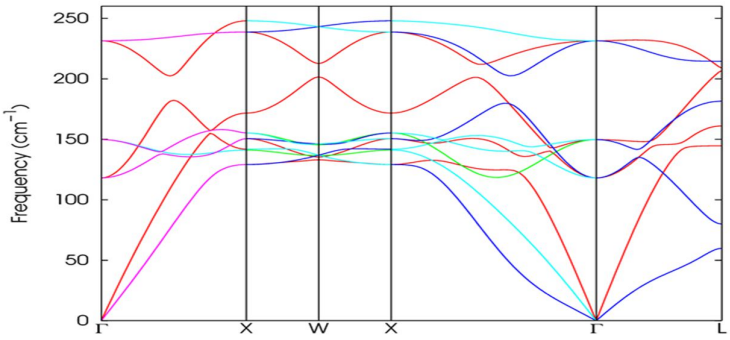

Figure 5: Phonon dispersion curve of Pd2ZrAl

CONCLUSION

In conclusion, our first-principles DFT study of Pd_2ZrAl full Heusler alloy reveals that it is a stable and promising superconducting material. The full Heusler alloy is energetically most stable in a non-magnetic cubic structure. Its electronic structure confirms metallic behavior, with the presence of a van Hove singularity near the Fermi level providing a key mechanism for superconductivity. Further stability is confirmed through mechanical property analysis, which indicates both mechanical stability and ductile character, and through phonon dispersion calculations, which show dynamic stability with no imaginary frequencies.

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