ISSN: 2961-1989
Academia Research Journal
Research Management Cell (RMC), Mahemdra Multiple Campus, Nepalgunj
Volume: 5 Issue: 2, Year: 2026

Ab Initio Study on the Electronic Structure of Half-Heusler Compound VPtIn

Laxman Pokhrel[1], Himanshu Joshi[2*]

DOI: https://doi.org/10.3126/academia.v5i2.97493

[1]Department of Physics, Mahendra Multiple Campus, Nepalgunj, Tribhuvan University, Nepal
Email: laxman.pokhrel@mahemc.tu.edu.np ORCID: https://orcid.org/0009-0009-2076-2663
[2]Department of Physics, SRM University Sikkim, Gangtok, Sikkim, India -737102
*Corresponding Author: Email: himanshu.j@srmus.ac.in /himanshuabijoshi09@gmail.com
ORCID: https://orcid.org/0000-0001-8717-0042

Article History: Received: Jan.03, 2026 Revised: May. 08 2026 Accepted: July. 19, 2026

ABSTRACT

We report a novel half-Heusler semiconducting compound, VPtIn, from first-principles Density Functional Theory (DFT) calculations. The electronic structure was obtained from Full Potential-Linearized Augmented Plane Wave method (FP-LAPW) using the Generalized Gradient Approximation (GGA). The compound is a non-magnetic semiconductor with net zero magnetic moment. A direct narrow band gap of 0.3 eV was observed along the X-high symmetry point. The partial density of states plot reveal that 3d-states of V atom dominate the band edges. Furthermore, the highly dispersive nature of conduction band indicates large charge carrier concentration and enhanced mobility. These characteristics of the electronic structure make VPtIn a potential candidate for green energy applications, particularly in thermoelectric and optoelectronic devices.

Keywords: Half-Heusler, Density Functional Theory, Electronic Structure, Density of States, Band Structure, FP-LAPW

,

INTRODUCTION

Half-Heusler (HH) alloys are one of the most actively studied families of intermetallic compounds due to their remarkable structural stability and a wide range of tunable physical properties, including semiconducting, half-metallic and topological behaviour (Oxley et al., 1963; Graf et al., 2011; Parzer et al., 2024; Souza et al., 2023). Heusler compounds were first reported by Friedrich Heusler in 1903, who observed ferromagnetism in Cu_2MnAl despite the absence of intrinsically magnetic elements (de Groot et al., 1983). Subsequent research has since identified over 1500 Heusler systems exhibiting functional properties valuable in spintronics, magneto-electronics and energy conversion devices (Katsnelson et al., 2008; Joshi et al., 2019). The general chemical formula of a HH compound is XYZ, where X and Y are transition metals and Z is a main-group element. They crystallize in the MgAgAs-type structure with space group F-43m (No. 216), consisting of three interpenetrating face-centered cubic sublattices with one Wyckoff site vacant (Ma et al., 2017). The electronic and magnetic character of HH compounds is predicted through the Slater–Pauling (S-P) rule (Galanakis et al., 2002; Abdullah et al., 2025), which relates the magnetic moment M to the total number of valence electrons Z by $M = Z - 18$ for HH compounds. Accordingly, compounds with valence electron count of 18 are therefore expected to be non-magnetic semiconductors with a zero net magnetic moment, a prerequisite for piezoelectric and thermoelectric applications (Sekhar et al., 2021).

ISSN: 2961-1989
Academia Research Journal
Research Management Cell (RMC), Mahemdra Multiple Campus, Nepalgunj
Volume: 5 Issue: 2, Year: 2026

In this work, we report a new vanadium-platinum based HH compound, VPtIn. The present study is a part of broader investigation on the VPtX (X=Al, Ga, In, Tl) HH series, undertaken to understand its electronic and thermoelectric evolution. Among these, VPtIn was particularly found to display promising semiconducting behaviour, motivating the detailed study reported here. To the best of our knowledge, no detailed theoretical or experimental investigation of VPtIn has been reported and therefore no direct study is available for comparision. Motivated by this, herein we perform a rigorous DFT investigation of the structural stability and electronic structure of this previously unexplored HH compound, determining its most stable structural configuration and calculating its electronic structure, including the total and partial density of states and the electronic band structure. The remainder of this paper is organized as follows: Section II describes the computational methodology; Section III presents and discusses and results and Section IV summarizes our conclusions.

METHODOLOGY

The electronic structure calculations were performed using the Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method (Blaha et al., 1990) implemented in the WIEN2k code (Blaha et al., 2020; Singh, 1994), within the DFT framework (Hohenberg & Kohn, 1964; Kohn & Sham, 1965). The exchange-correlation energy was treated using the Generalized Gradient Approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) parametrization (Perdew et al., 1996), which provides reliable structural parameters and band-edge positions for semiconducting HH compounds (Borlido et al., 2020). It should be noted that GGA functionals typically underestimate band gaps of semiconductors; the reported band gap is therefore a lower-bound estimate. The energy cutoff separating core and valence states was set to −8.0 Ry. The plane-wave basis was defined by the cutoff product RMT × K_{max} = 8, where RMT is the smallest muffin-tin sphere radius and K_{max} is the maximum reciprocal-lattice vector. The charge density in the interstitial region was expanded in a Fourier series up to G_{max} = 12 and the maximum angular momentum inside the spheres was l_{max} = 10. Self-consistency was achieved using a dense 20 × 20 × 20 k-point mesh in the irreducible part of the Brillouin zone, with convergence criteria of 10^{-5} Ry for the total energy and 10^{-3} e^- for the charge density. Semi-core states were treated semi-relativistically. A denser k-mesh of 50 × 50 × 50 was employed for the DOS and band structure to ensure super fine resolution around the band edges. All calculations were performed in the non-spin-polarized mode after confirming that the spin-polarized solution converges to zero magnetic moment.

RESULTS AND DISCUSSION

Structural Properties

The compound crystallize in the MgAgAs-type structure with space group F-43m (No. 216), consisting of three interpenetrating face-cantered cubic sublattices with one Wyckoff site vacant (Figure 1a). To find the most stable configuration for VPtIn we choose the structures with minimum total energy, for each combination of Wyckoff positions 4a (0 ,0, 0), 4b (½, ½, ½), 4c (¼, ¼, ¼) & 4d (¾, ¾, ¾), which is 24 configurations. We choose the one among 24 with least total ground state energy. The least ground state energy is obtained for V: 0, 0, 0; Pt: 0.75, 0.75, 0.75; In: 0.5, 0.5, 0.5. Lattice constant a = 6.13 Å is obtained from the energy vs volume plot, using the third-order Birch-Murnaghan equation of state (Angel, 2000), shown in figure 1b and is given by:

$$E = E_0 + \frac{9}{16}\left(\frac{B}{14703.6}\right)V_0[(\eta^2-1)^3B^* + (\eta^2-1)^2(6-4\eta^2)] \quad \text{(i)}$$

The structural parameters are tabulated in Table 1.

Table 1

Structural Parameters of VPtIn. Lattice constants (a) in Å, Bulk modules (B) in GPa and pressure derivative of bulk modules (B') obtained using Brich-Murnaghan's equation of state.

Compound	a	B	B'	Previous Work
VPtIn	6.13	140.85	7.184	-

ISSN: 2961-1989
Academia Research Journal
Research Management Cell (RMC), Mahemdra Multiple Campus, Nepalgunj
Volume: 5 Issue: 2, Year: 2026

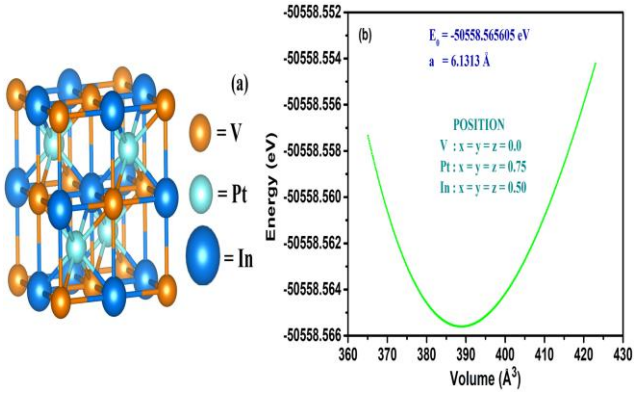

Figure 1: (a) Unit cell structure and **(b)** Volume optimization plot for VPtIn.

Electronic Structure

The total and partial Density of States (DOS) plot is shown in figure 2 a and b. The valence region is shown from -5 eV to 0 eV and the conduction region starts from just above the Fermi level at 0 eV. The missing DOS states around the Fermi level indicate the semiconducting nature of the compound. V atom shows the highest contribution to the DOS around the band edges, in both the valence and the conduction region, with small contribution from Pt atomic states. The In atom has almost negligible contribution to the total DOS. The sharp DOS peaks indicate high density of electronic states near the band edges and would lead to enhanced Seebeck coefficient in these compounds. The lower valence region is dominated by the 5d states of Pt atom, whereas the conduction region remains entirely dominated by 3d states of V atom. The profound DOS peaks near the valence band maximum and the conduction band minimum is a notable feature of the DOS plots. The sharp peaks are due to the localized nature of the V 3d orbitals. Such steep variation in DOS near the band edges is highly favoured for thermoelectric applications.

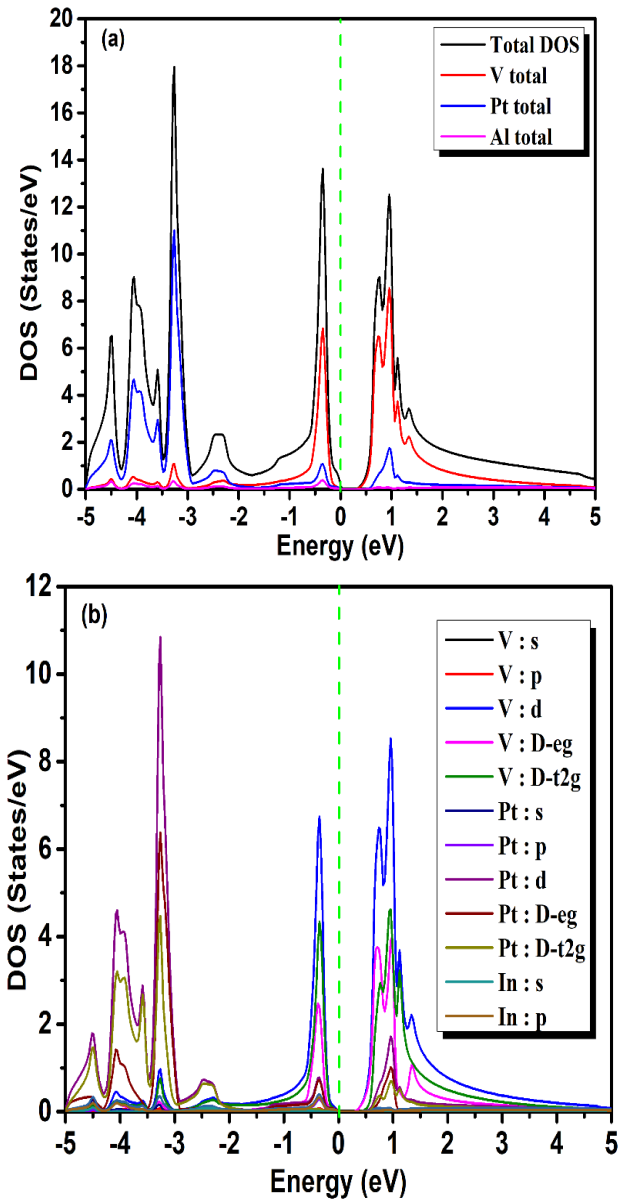

Figure 2: (a) Total Density of States and **(b)** orbital resolved partial Density of States for VPtIn.

The formation of band gap in VPtIn can be understood from the orbital resolved partial density of states shown in figure 2b. The crystal field splitting on the d orbitals of V and Pt atoms give rise to the e_g and t_{2g} components. The valence band edge is dominated by V t_{2g} state and the conduction band shows mixed contribution from V e_g and t_{2g} states. The lower valence region is dominated by Pt e_g states. From the DOS plots it is evident that the d-d-hybridization is responsible for the formation of band gap. The valence band is composed of V 3d states with small contributions from Pt 5d orbitals. The

ISSN: 2961-1989
Academia Research Journal
Research Management Cell (RMC), Mahemdra Multiple Campus, Nepalgunj
Volume: 5 Issue: 2, Year: 2026

conduction band is dominated by the unoccupied V 3d states. The interaction between the occupied bonding states and the unoccupied antibonding states is the primary reason for opening of band gap. The d-d hybridization leads to the splitting of bonding and antibonding d electronic states, shifting the unoccupied antibonding states above the Fermi level. The weak contribution of other electronic states near the band edges makes the band gap to be governed by transition metal d orbitals.

Figure 3 shows the band structure of the compound plotted along the *W-L- Γ-X-W-K* high symmetry direction of the first Brillouin zone. A direct band gap of 0.3 eV is observed along the X symmetry point, confirming the semiconducting nature of the compound. It is well known that GGA underestimates the band gap, therefore hybrid functionals have to be employed for accurate determination of band gap values. The absence of bands near the Fermi level (E_F) is consistent with the zero DOS states at E_F. The valence band maximum and the conduction band minimum is both located at the X symmetry point making it a direct band gap material. Such direct band gap nature is highly favourable for photovoltaic and solar cell applications. The conduction band is observed to be highly dispersive along the *Γ-X* direction, leading to reduced electron effective mass and high carrier mobility. In contrast, several valence bands are relatively flat bands, reflecting high hole effective mass. Such a combination of dispersive conduction band and flat valence bands are favoured for thermoelectric applications. However, a qualitative analysis of figure merit is required to confirm the claim.

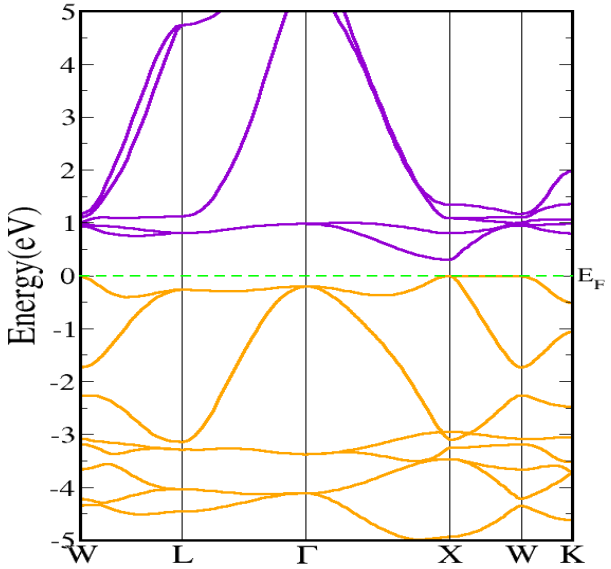

Figure 3: Band structure plots for VPtIn calculated using the GGA exchange-correlation functional.

A notable feature of the band structure plot is the presence of flat valence band along the *X-W* high symmetry direction, just below the Fermi level. The band indicates a relatively large hole effective mass and localized electronic state. As DOS is inversely proportional to band dispersion, this flat band arises from the sharp DOS peaks just at the valence band edge. The coexistence of this flat band along with other dispersed band in the band structure increases the overall electronic conductivity of the material and may be beneficial in achieving high thermoelectric power factor.

CONCLUSION

We have performed a detailed electronic structure calculation of VPtIn half-Heusler compound from first-principles Density Functional Theory. The lattice constant obtained for the compound was 6.13 Å and it crystallizes in cubic symmetry with space group number 216. The sharp DOS peaks near the band edge are transition atom d orbital dominant and the band gap in the compound arises due to d-d hybridization. The band structure revealed the compound to be a narrow direct band gap semiconducting material. An energy gap of 0.3 eV was obtained from GGA functional along the X high symmetry point. The combination of a narrow direct gap, sharp DOS peaks near the band edges, and a dispersive conduction band indicates that VPtIn is a promising candidate for further investigation as a

thermoelectric and optoelectronic material. Quantitative transport and optical calculations, together with stability analyses, will be the subject of future work.

Acknowledgement: H.J. and L.P. acknowledge Prof. R. K. Thapa, former VC, Sikkim Alpine University for providing the computational facility.
Declaration of generative AI: During the preparation of this work, the author(s) used ChatGPT for polishing the text and grammar. The author(s) reviewed and edited the output as needed and take full responsibility for the content of the published article.
Funding: The authors have nothing to report.
Conflicts of Interest: The authors declare no conflicts of interest.
Data Availability Statement: The data that support the findings of this study are available from the corresponding author upon reasonable request.

.

REFERENCES

Abdullah, D., Gautam, S., Seh, A. Q., Mir, S. A., & Gupta, D. C. (2025). Assessing half-Heusler alloys PtNbZ (Z = Al, Ga, In) via DFT: Acceptability for thermoelectric applications. *RSC Advances*, *15*, 47036. https://doi.org/10.1039/D5RA06109A

Angel, R. J. (2000). Equations of state. In R. M. Hazen & R. T. Downs (Eds.), *High-temperature and high-pressure crystal chemistry* (Reviews in Mineralogy and Geochemistry, Vol. 41, pp. 35–60). Mineralogical Society of America. https://doi.org/10.1515/9781501508707-006

Blaha, P., Schwarz, K., Sorantin, P., & Trickey, S. B. (1990). Full-potential, linearized augmented plane wave programs for crystalline systems. *Computer Physics Communications*, *59*(2), 399–415. https://doi.org/10.1016/0010-4655(90)90187-6

Blaha, P., Schwarz, K., Tran, F., Laskowski, R., Madsen, G. K. H., & Marks, L. D. (2020). WIEN2k: An APW+lo program for calculating the properties of solids. *Journal of Chemical Physics*, *152*(7), Article 074101. https://doi.org/10.1063/1.5143061

Borlido, P., Schmidt, J., Huran, A. W., Tran, F., Marques, M. A. L., & Botti, S. (2020). Exchange-correlation functionals for band gaps of solids: Benchmark, reparametrization and machine learning. *npj Computational Materials*, *6*, Article 96. https://doi.org/10.1038/s41524-020-00360-0

de Groot, R. A., Mueller, F. M., van Engen, P. G., & Buschow, K. H. J. (1983). New class of materials: Half-metallic ferromagnets. *Physical Review Letters*, *50*(25), 2024–2027. https://doi.org/10.1103/PhysRevLett.50.2024

Galanakis, I., Dederichs, P. H., & Papanikolaou, N. (2002). Origin and properties of the gap in the half-ferromagnetic Heusler alloys. *Physical Review B*, *66*(13), Article 134428. https://doi.org/10.1103/PhysRevB.66.134428

Graf, T., Felser, C., & Parkin, S. S. P. (2011). Simple rules for the understanding of Heusler compounds. *Progress in Solid State Chemistry*, *39*(1), 1–50. https://doi.org/10.1016/j.progsolidstchem.2011.02.001

Hohenberg, P., & Kohn, W. (1964). Inhomogeneous electron gas. *Physical Review*, *136*(3B), B864–B871. https://doi.org/10.1103/PhysRev.136.B864

Joshi, H., Rai, D. P., Laref, A., & Thapa, R. K. (2019). Electronic and thermoelectric properties of half-Heusler compounds MCoSb (M = Ti, Zr, Hf): A first principles study. *Materials Research Express*, *6*(6), Article 066307. https://doi.org/10.1088/2053-1591/ab0c68

Katsnelson, M. I., Irkhin, V. Y., Chioncel, L., Lichtenstein, A. I., & de Groot, R. A. (2008). Half-metallic ferromagnets: From band structure to many-body effects. *Reviews of Modern Physics*, *80*(2), 315–378. https://doi.org/10.1103/RevModPhys.80.315

Kohn, W., & Sham, L. J. (1965). Self-consistent equations including exchange and correlation effects. *Physical Review*, *140*(4A), A1133–A1138. https://doi.org/10.1103/PhysRev.140.A1133

Ma, J., Hegde, V. I., Munira, K., Xie, Y., Keshavarz, S., Mildebrath, D. T., Wolverton, C., Ghosh, A. W., & Butler, W. H. (2017). Computational investigation of half-Heusler compounds for spintronics applications. *Physical Review B*, *95*(2), Article 024411. https://doi.org/10.1103/PhysRevB.95.024411

Oxley, D. P., Tebble, R. S., & Williams, K. C. (1963). Heusler alloys. *Journal of Applied Physics*,

34(4), 1362–1364. https://doi.org/10.1063/1.1729511

Parzer, M., Garmroudi, F., Riss, A., Reticcioli, M., Podloucky, R., Stöger-Pollach, M., Constable, E., Pustogow, A., Mori, T., & Bauer, E. (2024). Semiconducting Heusler compounds beyond the Slater-Pauling rule. *PRX Energy*, *3*(3), Article 033006. https://doi.org/10.1103/PRXEnergy.3.033006

Perdew, J. P., Burke, K., & Ernzerhof, M. (1996). Generalized gradient approximation made simple. *Physical Review Letters*, *77*(18), 3865–3868. https://doi.org/10.1103/PhysRevLett.77.3865

Sekhar, B. C., Dhanalakshmi, B., Rao, B. S., Ramesh, S., Prasad, K. V., Rao, P. S. V. S., & Rao, B. P. (2021). Piezoelectricity and its applications. In D. Ranjan Sahu (Ed.), *Multifunctional ferroelectric materials* (Chapter). IntechOpen. https://doi.org/10.5772/intechopen.96154

Singh, D. J. (1994). *Planewaves, pseudopotentials and the LAPW method* (pp. 35–43). Springer.

Souza, J. C., Ale Crivillero, M. V., Dawczak-Dębicki, H., Ptok, A., Pagliuso, P. G., & Wirth, S. (2023). Tuning the topological character of half-Heusler systems: A comparative study on *YT*Bi (*T* = Pd, Pt). *Physical Review B*, *108*(16), Article 165154. https://doi.org/10.1103/PhysRevB.108.165154

***