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Research Article

INVESTIGATING STRUCTURAL, MECHANICAL, ELECTRONIC AND MAGNETIC PROPERTIES OF SPIN-GAPLESS QUATERNARY HEUSLER ALLOY CrMnVAl

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Abstract

Utilizing density functional theory (DFT), the study thoroughly investigates the equiatomic quaternary Heusler compound CrMnVAl, revealing its promising properties across multiple domains. The energy minimization curve shows its structural stability with lattice parameter 5.91Å in ferromagnetic phase. The negative values of formation and cohesive energy indicate its chemical stability, while electronic structure analysis demonstrates spin gapless semiconducting behavior. The total spin magnetic moment of this compound is almost 3.00 μ_B obeying the Slater-Pauling 18 electron rule($M_t = Z_t - 18$). The 100% spin polarisation and the Curie temperature higher than ambient temperature indicate that this compound acts as a promising material for spin dependent applications. Furthermore, exploring its mechanical properties complements these findings, offering insights into its structural integrity and suitability for diverse applications. Overall, the study underscores CrMnVAl's potential as a versatile material for spintronics and beyond.

Keywords: *DFT, Spin-gapless semiconductor, Slater-Pauling rule, Curie temperarure.*

I. INTRODUCTION

Heusler alloys encompass a vast range of ternary and quaternary intermetallic compounds. Extensive theoretical and experimental studies have focused on uncovering their half-metallic (HM) and spin gapless semiconducting behavior, particularly with advancement in computer engineering (Felser, Fecher, Balke, 2007; Kübler, Williams, Sommers, 1983). In a half-metal, the compound exhibits semiconducting behavior in one spin channel while being metallic in the other. Conversely, in a spin gapless semiconductor (SGS), one spin channel resembles a semiconductor with a small band gap, while the other spin channel has the valence and conduction bands touching at the Fermi energy level, resulting in a zero band gap or gapless contact.

SGSs possess unique band structures, leading to remarkable properties such as high Curie temperature, minimal energy required for electron excitation due to the zero energy gap, 100% spin polarization of both electrons and holes, and very high electron mobility (Dhakal *et al.*, 2020). Similar to ternary Heusler alloys, quaternary Heusler alloys offer an excellent platform for developing new materials with HM and spin gapless semiconducting behavior.

Half Heusler compounds with the stoichiometric structure XYZ adopt the $C1_b$ configuration with space group F-43m (Ozdemir, Merdan, 2019;

Yadav, Bhandari & Kaphle, 2020; Paudel, Kaphle, & Batouche, 2020) while full Heusler compounds (X_2YZ) crystallize in the $L2_1$ configuration with space group Fm-3m (Liu *et al.,* 2008; Dhakal *et al.,* 2020; Hongzhi, *et al.,* 2007; Cherid *et al*., 2017). Similarly, equiatomic quaternary Heusler compounds of the form XX'YZ crystallize in the Y-type structure, with space group F-43m. These structures are achieved by replacing one of the transition metal elements X with another transition metal element X' in the full Heusler compound X_2YZ (Zhang, Wang, Cheng, 2017, Bainsla & Suresh, 2016, Regmi *et al.,* 2022, Ray *et al.,* 2021). Here, X, X', and Y represents transition metal elements, while Z is derived from the main group (III, IV, or V group) elements of the periodic table.

Theoretical and experimental studies have revealed intriguing properties in various Zr and Co based quaternary Heusler compounds exhibits a spin gapless semiconducting nature that transforms into a half-metal under pressure, adhering to the Slater-Pauling rule with a Curie temperature exceeding ambient levels (Gao *et al.,* 2015, Bainsla *et al.,* 2014 & 2015). Similarly, TiZrMnAl displays spin gapless semiconducting behavior with a zero net magnetic moment, consistent with the Slater-Pauling rule (Hao *et al.,* 2020). Recent research has expanded this understanding to other compounds like CoFeCrAl, CoFeMnGe, CoFeMnSi, CoFeMnSn, NiFeMnGa, NiCoMnGa, and CuCoMnGa, highlighting ongoing exploration in Heusler compounds and their potential for advancements in materials science and technology.

Theoretical and experimental study proved that the spin gapless semiconducting nature of CoFeCrGa, transferred into a half-metal under pressure and obeys the Slater-Pauling rule with a Curie temperature of more than ambient temperature (400 K) (Bainsla,*et al,* 2015). In 2020, Hao *et al.,* investigated two potential structural configurations of the quaternary Heusler compound TiZrMnAl, revealing that both configurations exhibit spin gapless semiconducting behavior with a zero total magnetic moment. Their findings are in accordance with the Slater-Pauling rule, $Z_t = M_t - 18$, where Z_t and M_t respectively represents the total magnetic moment and total number of valence electrons of the compound. Recent studies have identified spin gapless semiconducting behavior in a variety of unique quaternary Heusler compounds, including CoFeCrAl, CoFeCrGa, CoFeMnGe, CoFeMnSi, CoFeMnSn, NiFeMnGa, NiCoMnGa, and CuCoMnGa (Bainsla *et al.,* 2014, 2015, Dia *et al.,* 2009, Gupta *et al*., 2023, Alijani *et al.,*2011). These discoveries highlight the continuous exploration of novel Heusler compounds and their fascinating properties, driving further advancements in material science and technology.

Motivated by the theoretical and experimental investigations into quaternary Heusler alloys, here, we conduct a comprehensive investigation of the quaternary Heusler compound CrMnVAl through first-principles calculations.

II. METHODOLOGY

The investigation of the CrMnVAl compound is performed using density functional theory (DFT) implemented in WIEN2k (Hohenberg & Kohn, 1964, Schwarz *et al.,* 2018), we utilized the full potential linearized augmented plane wave (FP-LAPW) method alongwith various exchange-correlation functionals : the generalized gradient approximation (GGA), modified Becke-Johnson (mBJ) potential, and GGA+U(Hubbard) method (Perdew *et al.,* 1996, Koller *et al.,* 2012, Becke *et al.,* 2006). These methods were chosen to accurately evaluate structural, chemical, mechanical, electronic structure, and magnetic properties of the considered compound. Computational parameters included a 17x17x17 Monkhorst-Pack k-point mesh (approximately 5000 k points), an energy cutoff of -6 Ry. The

self consistent field (SCF) computations are executed until the energy change is less than 10^{-7} eV and the charge convergence is 10^{-4} e. The Hubbard U parameters (0.21 eV for Cr, 0.64 eV for Mn, and 0.61 eV for V) were employed to account for on-site Coulomb interactions (Sasioglu *et al.*, 2013). Mechanical stability was assessed through elastic constants computed using the Elastic 1.1.0 patching software embbeded in the code. This comprehensive approach allowed for a thorough examination of the compound's properties, accounting for electronic correlations and accurately predicting band gaps.

III. RESULTS AND DISCUSSION

A: Structural Properties and Phase Stability

In the present calculation, we focused on the equiatomic quaternary Heusler compound, CrMnVAl (1 : 1 : 1 : 1 composition), which follows the typical XX'YZ chemical formula. Here, X, X', and Y represents transition metals, while Z denotes a main group (III, IV or V group of periodic table) element. This compound crystallizes in the Y-type (LiMgPdSn-type) cubic structure (space group F-43m) and can take on different arrangements (Ray *et al.*, 2021, Paudel *et al.*, 2019), labeled as Structures I, II, and III via Structure I : Al (0, 0, 0), Cr (¼, ¼, ¼), V (½, ½, ½), Mn (¾, ¾, ¾), structure II : Al (0, 0, 0), V (¼, ¼, ¼), Cr (½, ½, ½), Mn (¾, ¾, ¾), and structure III: V (0, 0, 0), Al (¼, ¼, ¼), Cr (½, ½, ½), Mn (¾, ¾, ¾). Through volume optimization calculations in both ferromagnetic (FM) and non-magnetic (NM) states for these structures, we found that structure I in the FM state has the lowest energy than NM state, indicating its stability. Therefore,

we selected structure I in the FM state for further investigation. Analyzing the energy-volume plot provided valuable insights, and applying the Birch-Murnaghan equation of state (Murnaghan, 1944), we determined an optimized equilibrium lattice constant of 5.906 Å for CrMnVAl, which serves as a foundational parameter for subsequent analyses of the present study. This is comparable with the results obtained from OQMD.

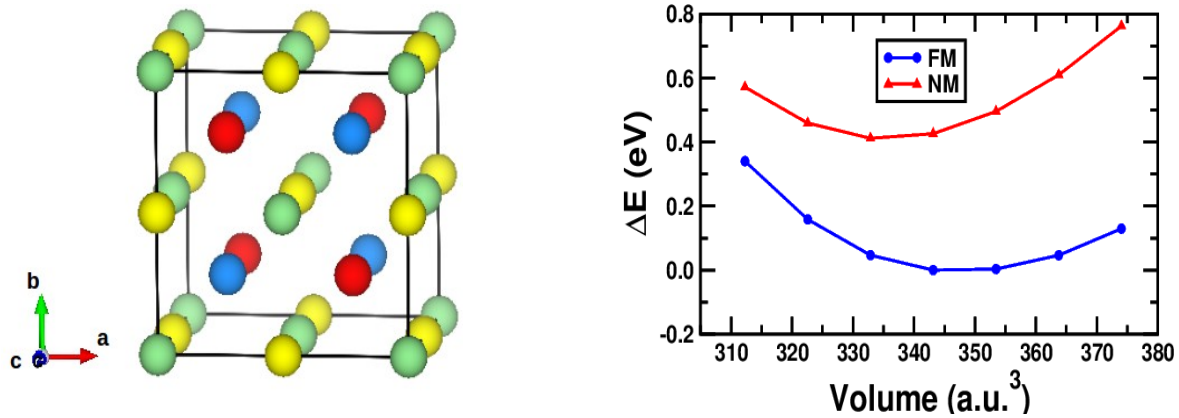


Fig. 1. (Color online) Schematic crystal structure (Cr = red, Mn = blue, V = yellow, Al = green) (left) and Energy optimization curve (Right) of CrMnVAl.

The chemical stability of the compound is analyzed through the calculation of its formation energy (E_f) and cohesive energy (E_c) (Ray *et al.*, 2021, Paudel *et al.*, 2019) :

$$E_f = E^{tot}_{CrMnVAl} - \left(E^{bulk}_{Cr} + E^{bulk}_{Mn} + E^{bulk}_{V} + E^{bulk}_{Al} \right) \quad (1)$$

$$E_c = E^{tot}_{CrMnVAl} - \left(E^{iso}_{Cr} + E^{iso}_{Mn} + E^{iso}_{V} + E^{iso}_{Al} \right) \quad (2)$$

Here, $E^{tot}_{CrMnVAl}$ is the total energy of the compound, E^{bulk}_{Cr}, E^{bulk}_{Mn}, E^{bulk}_{V}, E^{bulk}_{Al} are the total energies of the atoms in the most stable

bulk form of Cr, Mn, V and Al; and E_{Cr}^{iso}, E_{Mn}^{iso}, E_{V}^{iso}, E_{Al}^{iso} are the total energies of the corresponding atoms in the isolated form respectively. The computed values of E_f and E_c of CrMnVAl are -0.459 eV and -5.441 eV respectively. The negative values of formation and cohesive energies predict that the compound CrMnVAl is chemically stable and can probably be synthesized experimentally.

The mechanical behavior of a solid can be analyzed by computing its elastic constants C_{ij}. The Born-Huang stability requirements are given by (Born & Huang, 1954, Wu *et al.,* 2007),

$C_{11} > 0$, $C_{44} > 0$, $C_{12} < B < C_{11}$, $C_{11} - C_{12} > 0$, $C_{11} + 2C_{12} > 0$ (3)

Similarly, the calculation of resistance to volume change of a material (Bulk modulus B), shear modulus (G), Young's Modulus (Y), Poisons ratio (*v*), Pugh's ratio (B/G) and Cauchy's pressure parameters are used for checking brittleness and ductile nature of materials. These parameters are obtained through relations (Zuo *et al.*, 1992, Jain *et al.,* 2018),

$$B=\frac{1}{3}\left(C_{11}+2C_{12}\right) \quad (4)$$

$$G=\frac{1}{2}\left(G_R+G_V\right) \quad (5)$$

Where

$$G_V=\frac{1}{5}\left(C_{11}-C_{12}+3C_{44}\right) \quad (6)$$

$$G_R=\frac{5}{3}\frac{\left(C_{11}-C_{12}\right)C_{44}}{\left(C_{11}-C_{12}\right)+4C_{44}} \quad (7)$$

Here, in G_V and G_R, the subscripts V and R stands Voigt and Reuss bounds respectively.

$$E=\frac{9BG}{\left(3B+G\right)} \quad (8)$$

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

The investigated values of elastic constants are listed in table 1. Our investigation shows that all the cubic elastic constants have positive values and fulfilled all the stability criteria, confirming the compound CrMnVAl is mechanically stable and brittle in nature (ν > 0.26; B/G > 1.75; CP = Negative) (Jain *et al.*, 2018).

Table 1. The calculated elastic constants C_{11}, C_{12}, C_{44} (GPa) and moduli in GPa of compound CrMnVAl.

Compound	**C_{11}**	**C_{12}**	**C_{44}**	**B**	**G**	**E**	**B/G**	**ν**
CrMnVAl	210.80	173.90	318.90	186.19	120.65	297.65	1.54	0.23

B: Electronic properties

In Fig. 3, the band structure plot of CrMnVAl using the GGA method is depicted. It is evident that the valence band maxima (VBM) crosses the Fermi energy level (E_F) at the Γ symmetric point in the spin-up channel, resulting in a small band gap of 0.156 eV whereas in the spin-down channel, the energy bands touch the E_F at various symmetric points, indicating a gapless (zero-gap) behavior. This suggests nearly semiconducting behavior in the spin-up channel and gapless behavior in the spin-down channel, pointing towards CrMnVAl's nearly spin gapless semiconductor (SGS) nature. Fig. 4, illustrates the band structure plot using the mBJ method, revealing a clear energy gap of 0.213 eV in the spin-up channel, while the spin-down channel exhibits nearly gapless behavior. Similarly, Fig. 5, employing the GGA+U method, confirms the nearly spin gapless semiconducting nature of CrMnVAl. Total and partial density of states

(DOS) computations further support these findings.

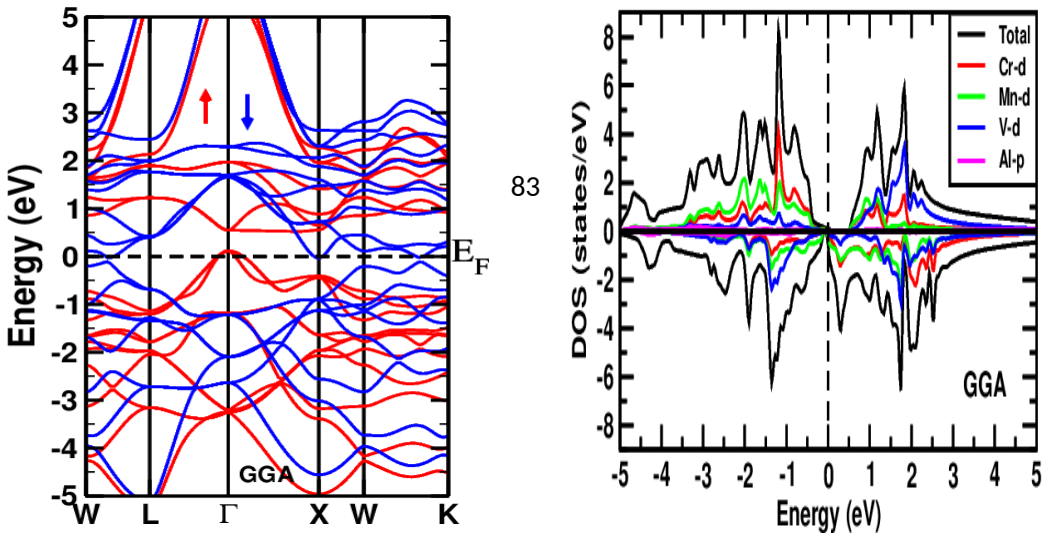


Fig. 3. (Color online) Electronic band structure showing spin-up (red) and spin-down (blue) channels (left) and DOS (right) of CrMnVAl with GGA technique.

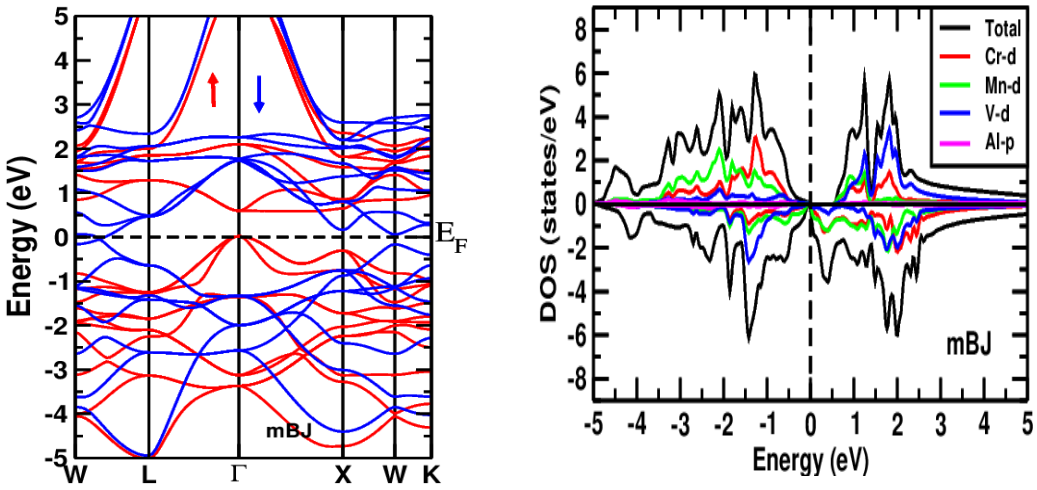
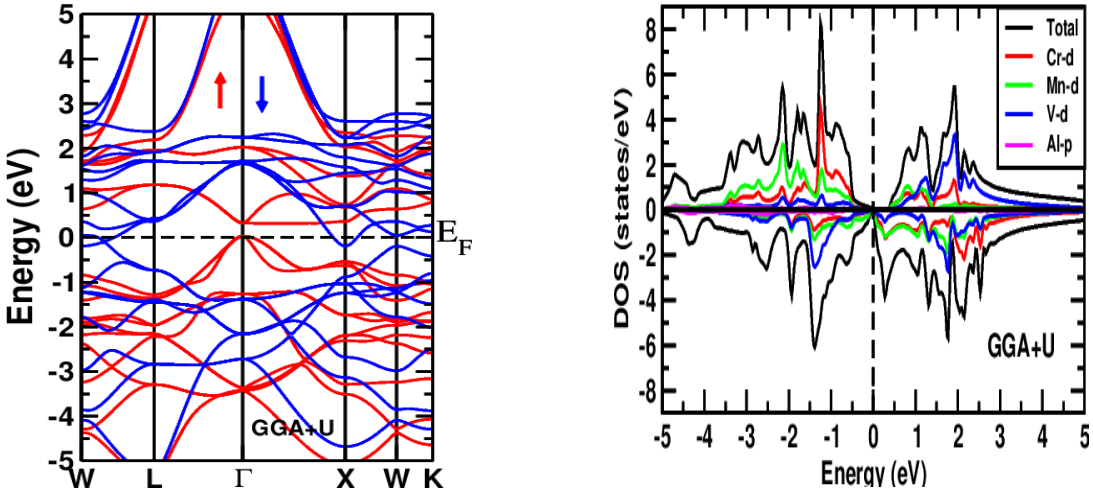


Fig. 4. (Color online) Electronic band structure showing spin-up (red) and spin-down (blue)) channels (left) and DOS (right) of CrMnVAl with mBJ technique.



Fg. 5. (Color online) Electronic band structure showing spin-up (red) and spin-down (blue) channels (left) and DOS

(right) of CrMnVAl with GGA+U technique.

The contribution wise analysis show that the contribution of up spin channels are due to Cr-d, Mn-d and V-d respectively. The gap mainly due to the contribution of Cr-d and Mn-d orbitals. Similarly there is no gap at the minority channels, arise from mixed contributions of 3d-bands of Cr, Mn and V of CrMnVAl.

C: Magnetic properties

The asymmetrical type of density of states (DOS) in the majority (↑) and minority (↓) spin channels clearly indicate that the material under study is magnetic in nature. Table 2 displays the total, atomic, interstitial magnetic moments, VBM, CBM, and band gap of CrMnVAl with GGA, mBJ and GGA+U functionals. Moreover, the investigated total magnetic moment per formula unit of CrMnVAl has almost an integer value 3.00 μ_B in all methods. The integer value of total magnetic moment 3.0 μ_B is a unique property of CrMnVAl which obeys the linear Slater-Pauling rule, Mt = Zt -18, where Mt stands for total magnetic moment and Zt refers to the total number of valence electrons per formula unit of the compound. The investigated atomic magnetic moments of Cr and Mn have positive values indicating FM ground state of the compound (Slater, 1936, Galanakis 2023).

Table 2. The calculated total μ_{total} (μ_B), atomic μ_{atomic} (μ_B), interstitial (μ_B) magnetic moments per formula unit, VBM, CBM and band gap in eV of CrMnVAl with GGA, mBJ and GGA+U functionals.

Compound	μ_{total}	μ_{Cr}	μ_{Mn}	μ_{V}	μ_{Al}	Int. MM	VBM	CBM	E_{bg}
CrMnVAl ^{GGA}	2.990	2.075	1.795	-0.911	-0.010	0.010	-0.123	0.033	0.156
CrMnVAl ^{mBJ}	2.999	2.038	2.024	-1.031	-0.027	-0.003	-0.151	0.062	0.213
CrMnVAl $^{GGA+U}$	3.000	2.116	2.226	-1.253	-0.031	-0.056	-0.142	0.003	0.145

The spin polarization (P) which is the ratio of density of states (DOS) of majority (↑) and minority (↓) spin electrons at the Fermi level and can be expressed as:

$$P = \frac{n\uparrow(E_F) - n\downarrow(E_F)}{n\uparrow(E_F) + n\downarrow(E_F)} \quad (10)$$

Where $n\uparrow(E_F)$ and $n\downarrow(E_F)$ refers the spin-dependent DOS at the Fermi level for spin up and spin down states respectively. The electrons are completely polarized, when $n\uparrow(E_F)$ or $n\downarrow(E_F)$ is equal to zero. The results indicate that CrMnVAl is 100 % spin polarized.

The Curie temperature (T_C) of the considered compound have been determined by utilizing the linear relation $T_C = 23 + 181M_t$, where M_t is the total magnetic moment of the compound, (Paudel *et al.,* 2019). The investigated Curie temperature of CrMnVAl is 566 K.

IV. CONCLUSIONS

First-principles calculations were employed to investigate the structural, mechanical, electronic, and magnetic properties of the quaternary Heusler compound CrMnVAl. The study revealed that CrMnVAl exhibits ferromagnetic behavior in its ground state. Negative values of formation and cohesive energies suggest the chemical stability of the compound and feasibility of experimental synthesis. Analysis of computed elastic constants indicates the compound has brittle nature. Electronic properties indicate that CrMnVAl is nearly spin gapless semiconductor (SGS) with 100% spin polarization of electrons at the Fermi energy level. The calculated total spin magnetic moment aligns closely with the Slater-Pauling 18 electron rule. Moreover, the investigated Curie temperature of CrMnVAl, determined to be

566K, positions it as a highly promising material for spintronic and magnetoelectronic-based devices.

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