

Calculation of Half-Metal, Debye and Curie Temperatures of Co₂VAl Compound: First Principles Study*

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Abstract By FP-LAPW calculations, the structural, elastic, Debye and Curie temperatures, electronic and magnetic properties of Co₂VAl are investigated. The results indicate that Ferromagnetic (FM) phase is more stable than Anti-Ferromagnetic (AFM) and Non-magnetic (NM) ones. In addition, $C_{11}-C_{12} > 0$, $C_{44} > 0$, and $B > 0$ so Co₂VAl is an elastically stable material with high Debye temperature. Also, the B/G ratio exhibits a ductility behavior. The relatively high Curie temperature provides it as a favorable material for spintronic application. It's electronic and magnetic properties are studied by GGA+U approach leading to a 100% spin polarization at Fermi level.

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Key words: exchange energy, Debye temperature, Curie temperature, Co₂VAl, GGA+U

1 Introduction

Spin transport of electrons (spintronics) has attracted a lot of interest due to its applications in FM half-metals with binary structures such as MnX, CrX (X= Sb, Te, As, P)^[1–4] and Heusler alloys.^[5–7]

Heusler alloys are classified as half-Heusler and full-Heusler, mostly possessing half-metallic behavior with different electronic states of the majority and minority spins at the Fermi level, so that some of these compounds exhibit metallic property in the majority state but semiconducting behavior in minority case, and therefore perform, in the ideal form of course, as perfect half-metals with 100% spin polarization at Fermi level.

The full-Heusler alloys have an X₂YZ structure where X and Y are transition metals and Z is an sp element.^[8] In recent decades, some theoretical and experimental investigations have been carried out on Heusler alloys eventually applied in spintronic industry like TMR and GMR effects.^[9–11] Two main advantages of these compounds are their high amount of magnetic momentum and Curie temperature which both have significant roles for magnetic materials.^[12–13] Remarkably, Co-based Heusler alloys,^[14–17] especially the Co₂VAl, have widely been considered both in theoretical and experimental aspects because of their extensive application in spintronics.^[18–23]

Experiments on Co₂VAl have revealed the Curie temperature and lattice constant of 342.7 K and 5.756 Å respectively.^[24] Also, the magnetic moments of

1.4 (μ_B /cell)^[25] and 1.86 (μ_B /cell)^[24] have been reported by experiments performed at 5 K. Li *et al.* have calculated the structural, magnetic and electronic properties of Co₂VAl using GGA calculation method which concluded to the 5.71 Å lattice constant and total magnetic momentum of 2.0 (μ_B /cell). Reported for the Heusler compounds are fully polarization at Fermi level for Co₂VAl based on the density of states (DOS),^[26] and the elastic stability for Co₂FeAl and Fe₂VAl as well.^[27–28]

According to Han *et al.*'s investigation on half-metallic properties of Co₂VAl in $\langle 111 \rangle$ direction, through the GGA approximation, the FM phase is more stable than AFM and NM ones.^[29] It is very important that the transition metals Co and V have half-full *d* orbitals which the electronic and magnetic properties are greatly affected by.

In this effort, we have made use of the on-site Coulomb potential and GGA + U approximation to reach more reasonable results of magnetic and electronic properties. The first section consists of structural properties of Co₂VAl. In the next, the elastic property is discussed, and thence the exchange energy and Curie temperature are calculated. Finally, within the supercell method, we have optimized the U parameter for better electronic studies forward. It is novel, applying GGA+U approximation to calculate the electronic and magnetic properties as well as the Debye & Curie temperature of Co₂VAl which all exhibit acceptable compatibility with experimental and theoretical data in the literature.

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2 Calculation Method

Employing Wien2k code, a self-consistent manner is applied through the FP-LAPW method.^[30–31] The GGA and GGA+U approximations are used to determine the exchange-correlation term,^[32] being called the Monkhorstrst–Pack (mesh) approximation for calculations in the reciprocal lattice.^[33] The separation energy between the core and valance states is taken as -6 Ry. Muffin tin radii for Co, V and Al are set to 2.5 (Bohr), 2.2 (Bohr) and 1.9 (Bohr), while RKmax, KPoint and Lmax parameters are elected as 8.50, 1500, and 10 respectively.^[34]

3 Results and Discussion

3.1 Structural Properties of Co_2VAl

Figure 1 depicts the energy-volume diagram of the bulk Co_2VAl for NM, FM and AFM states obtained from GGA approximation. Regarding the equilibrium volume (zero pressure), it turns out that the FM phase is of more stability than other phases because of its lowest minimum point in the energy-volume curve. Using the graphs to find the common tangent of the intersected curves of the corresponding phases, followed by the relation, $p = -\Delta E/\Delta V$, the transition pressure from FM to AFM and to NM phase has been obtained as 5.49 (GPa) and 26.58 (GPa) respectively. Remarkably, applying pressure to the crystals leads to the mentioned phase transitions, because in less volume (higher pressure) the total energy of the crystal in the NM and AFM phase is lower in comparison with the FM phase. Concerning the most stable phase (FM), Table 1 lists the lattice constant (a), cohesive energy (E_C) and total magnetic momentum (M) calculated by GGA and GGA+U approximations to be compared with other works.

Table 1 Lattice constant $a/\text{\AA}$, bulk module $B(\text{GPa})$, magnetic momentum $M(\mu_B/\text{cell})$ and cohesive energy $E_C(\text{eV})$ of Co_2VAl in the FM phase (stable phase).

	a	M	B	E_C
GGA	5.742	1.92	204.14	$-1.56/\text{Ry}$
GGA+U	5.863	2.00	184.80	$-1.02/\text{Ry}$
Other Works	5.71 ^a	2.05 ^a		
	5.89 ^b	1.4 ^e		
	5.74 ^c	1.86 ^f		
	5.7798 ^d			

^a[26]; ^b[35]; ^c[36]; ^d[37]; ^e[38]; ^f[24].

Obviously, GGA gives a better result for the lattice constant (obtained from Fig. 1) than GGA+U, but GGA+U yields a total magnetic moment of more compatibility with Slater–Pauling rule^[18] as well as the theoretical^[26,29] and newly experimental reports.^[24] In an

FM half-metallic full-Heusler compound such as Co_2VAl , regarding the band gap around the Fermi level for minority states, and compatible with Slater–Pauling rule,^[18] the total magnetic momentum would be an integer:

$$M_{\text{tot}} = Z_{\text{tot}} - 24, \quad (1)$$

in which, Z_{tot} remakes the valance electrons, keeping in mind that in Heusler compound 24 electrons with p-d bound are taking part. Co_2VAl has 26 valance electrons, therefore M_{tot} would be gained as $M_{\text{tot}} = 2 (\mu_B/\text{cell})$.

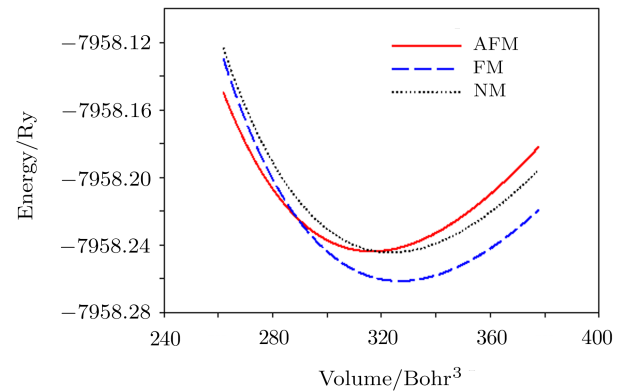


Fig. 1 Energy-Volume diagram of Co_2VAl for non-magnetic (NM), ferromagnetic (FM) and anti ferromagnetic (AFM) phases by GGA approximation.

3.2 Calculation of Elastic Properties

One of the main tools for characterization of the mechanical property of solids is elastic constants, describing the media response to the macroscopic stress. Generally speaking, the stress, does not have to be hydrostatic, since there may be unequally applied stresses in all directions and therefore the stress would be tensorial:

$$\begin{pmatrix} \delta_{11} & \delta_{12} & \delta_{13} \\ \delta_{21} & \delta_{22} & \delta_{23} \\ \delta_{31} & \delta_{32} & \delta_{33} \end{pmatrix}, \quad (2)$$

where δ_{ij} is the stress acting in the x_i direction on the plane perpendicular to the x_j direction; δ_{ij} (or $\delta_{i=j}$) are the axial stresses while $\delta_{i \neq j}$ are the shear stresses.

The strain ε_{ij} is also a second order tensor, therefore the elastic moduli, or elastic constants, are fourth order tensors:

$$\delta_{ij} = \sum c_{ijkl} \varepsilon_{kl}. \quad (3)$$

The stress δ , and the strain ε , must be symmetric, and the nature of c_{ijkl} depends on the symmetry of the crystal. It is customary to use a contracted notation, generally expressed as:

$$\begin{aligned} 11 &\rightarrow 1; & 22 &\rightarrow 2; & 33 &\rightarrow 3; & 23 = 32 &\rightarrow 4; \\ 13 = 31 &\rightarrow 5; & 12 = 21 &\rightarrow 6. \end{aligned}$$

According to the above-noted rule, we reach to these exemplified more compact symbols: $C_{1111} \rightarrow C_{11}$ relating

δ_{11} to ε_{11} , $C_{1122} \rightarrow C_{12}$ relating δ_{11} to ε_{22} , $C_{2323} \rightarrow C_{44}$ relating δ_{23} to ε_{23} . There are a maximum of 21 elastic constants for a crystalline body, but for cubic crystals the elastic constants C_{ij} , may be reduced to just three independent constants: $C_{11} = C_{22} = C_{33} \rightarrow$ modulus for axial compression, i.e. a stress δ_{11} results in a strain ε_{11} along an axis; $C_{44} = C_{55} = C_{66} \rightarrow$ shear modulus, i.e. a shear stress δ_{23} results in a shear strain ε_{23} across a face; $C_{12} = C_{13} = C_{23} \rightarrow$ modulus for dilation on compression, i.e., an axial stress δ_{11} results in a shear strain ε_{22} along a perpendicular axis. And all other $C_{ij} = 0$.

Hence, a set of three equations is required to determine all these constants. The first equation involves calculating the bulk modulus (B), given by

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

The second equation involves performing volume-conservative tetragonal strain tensor ε .

Applying this tetragonal strain changes the total energy from its initial value to

$$E(\varepsilon) = (C_{12} - c_{12})3V_0\varepsilon^2 + o(\varepsilon^2), \quad (5)$$

where V_0 is the volume of the unit cell.

In the last, we use the volume-conserving rhombohedral strain tensor and transform the total energy to

$$E(\varepsilon) = (C_{11} + 2C_{12} + 4C_{44})\frac{V_0}{6}\varepsilon^2 + o(\varepsilon^2). \quad (6)$$

In cubic Co_2VAl we have a tern C_{11} , C_{12} , and C_{44} . The Tables 2 and 3 contain elastic constants and some concerning parameters as well as a comparison between the results of the two methods (GGA & GGA+U).

Table 2 Calculated elastic constants C_{ij} (GPa), Shear module G (GPa), Young's module E (GPa), Elastic Anisotropy A and Poisson's ratio ν by GGA and GGA+U approximations.

	C_{11}	C_{12}	C_{44}	G	Y	A	ν
GGA	299.18	156.62	134.81	104.39	267.56	0.426	0.281
GGA+U	270.68	141.87	128.94	97.58	248.94	0.476	0.268

An important parameter in elastic anisotropy of crystals is the elastic wave velocity defined as follow for cubic lattices, being zero for isotropic materials:[39]

$$A = \frac{2C_{44} + C_{12}}{C_{11}} - 1. \quad (7)$$

The non-zero amounts for A along with the quantities $C_{11} - C_{12} > 0$, $C_{44} > 0$ and $B > 0$ imply a stable elasticity as well as a low anisotropy of Co_2VAl (see Table 2). Another parameter considered is Kleinman Parameter ξ which presents the relative positions of the cation and anion sublattices under volume-conserving strain distortions, so that the positions will not be fixed by symmetry.

This parameter shows a significant resistance against bond bending or bond-angle distortions^[40–41] and relates to the elastic constant as:^[42]

$$\xi = \frac{C_{11} + 8C_{12}}{7C_{11} + 2C_{12}}. \quad (8)$$

Young's module E and Poisson's ratio ν have also been calculated by following equations related to the bulk module and shear module:^[43]

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

$$\nu = \frac{3B - E}{6B}. \quad (10)$$

Also, the Debye temperature has been determined in terms of the mean velocity of the electrons in crystal:^[44]

$$T_D = \frac{h}{K_B} \left(\frac{3n}{4\pi V_a} \right)^{1/3} v_m, \quad (11)$$

wherein V_a , h and K_B are unit cell volume, Planck and Boltzmann constants respectively and V_m is defined as:^[45]

$$v_m = \left[\frac{1}{3} \left(\frac{2}{v_l^2} + \frac{2}{v_t^2} \right) \right]^{-1/3}. \quad (12)$$

In which v_l and v_t are the longitudinal and transverse velocity components of the homogenous crystal and are related to the bulk and shear modules via:

$$v_l = \left(\frac{3B + 4G}{3\rho} \right)^{1/2} \quad v_t = \left(\frac{G}{\rho} \right)^{1/2}. \quad (13)$$

The ratio of bulk to shear module (B/G) that was presented initially by Pugh^[45] indicates the relation between plastic properties and elastic modules. B is the resistance of material against destruction and G presents that versus Plastic deformation. Using GGA and GGA+U approximations beside the parameters of Table 2, we have calculated the elastic constants and other parameters. The small values of (B/G) indicate the ductility, while its large amounts display brittleness of the material. The critical value 1.75 denotes a separation region between ductile and brittle.^[46] So, it is deducible from Table 3 that the bulk Co_2VAl should be a ductile material with relatively large Debye temperature.

Table 3 Kleinman Parameter, Mean velocity V (m/s), Debye Temperature (K) and B/G by GGA and GGA+U approximations.

	ξ	V	T_D	B/G
GGA	0.644	4.34×10^3	567.81	1.95
GGA+U	0.645	2.90×10^3	380.02	1.89

3.3 Calculation of Exchange Interaction

The Kurtulus *et al.*'s theory is based on the coupling of localized magnetic momentums in the Heusler Co-based compounds.^[47–48] In Co_2VAl the interaction between near neighbors of Co and V makes the FM phase more stable. Localized magnetic momentums of Co and V atoms

are ferromagnetically coupled together, in other words there exists FM interaction between Co-V, V-V and Co-Co atoms, with a decreasing behavior versus the inter-atomic distances (r), among which the Co-Co coupling has the largest value with negative sign (for nearest neighbor atoms), while the Co-V case is a positive amount, and the V-V interaction is quantitatively much less to come into account (Fig. 2).

Compared with other Heusler compounds, the Co-based alloys have generally a high curie temperature owing to the strong interaction between their atoms. According to Fig. 2 the coupling of Co and V has an RKKY behavior since the characteristic oscillations of the exchange term depend on the inter-atomic parameters. As obvious from the figure, the exchange interaction J_{ij} , exhibits a damping oscillatory sensitivity to the inter-atomic distance and vanishes at large distances. The sign of the J_{ij} is negative for alike neighbors (Co-Co) but positive for the different ones (Co-V) implying an FM behavior, which actually disappears at the limit of the lattice constant 5.74 \AA ($r = a$).

To calculate the exchange interaction J_{ij} , call the following definition:

$$J_{ij} = \frac{E_{\text{FM}} - E_{\text{AFM}}}{2}, \quad (14)$$

in which E_{FM} is the total energy of the ferromagnetic state (parallel spins), but E_{AFM} is that for the anti-ferromagnetic state (anti-parallel adjacent spins). In con-

tinue, inserting this result as JRKKY in the Heisenberg relation the Curie temperature T_C would be obtained (method 1):^[50]

$$K_B T_C = \frac{2}{3} \sum_{i \neq j} J_{ij}, \quad (15)$$

where J_{ij} is the exchange interaction and K_B is the Boltzmann constant. Besides the abovementioned Heisenberg method, it is also possible to determine T_C by means of the next equation, having in hand the total magnetic momentum μ_B calculated in the last section (method 2):^[51–52]

$$T_C = 23 + 181\mu_B. \quad (16)$$

Comparatively, in Table 4 there are listed the Curie temperature of some Co-based Heusler alloys resulted from some approaches including ours. Considering the results of the two manners for T_C of the Co_2VAL listed in Table 4, it is clear that the Heisenberg approach is in good adoption with others' theoretical achievements, but with a meaningful difference from the experimental data, while the other technique,^[51–52] which has been recommended in the literature for Heusler compounds and we have followed here, reveals much better accordance with experiments. Our results indicate that Co-based Heusler compounds by V atom have low Curie temperature, which could be referred to the lower interaction between Co-V and V-V atoms. Co_2VAL appears to be a suitable material for spintronic devices at room temperature.

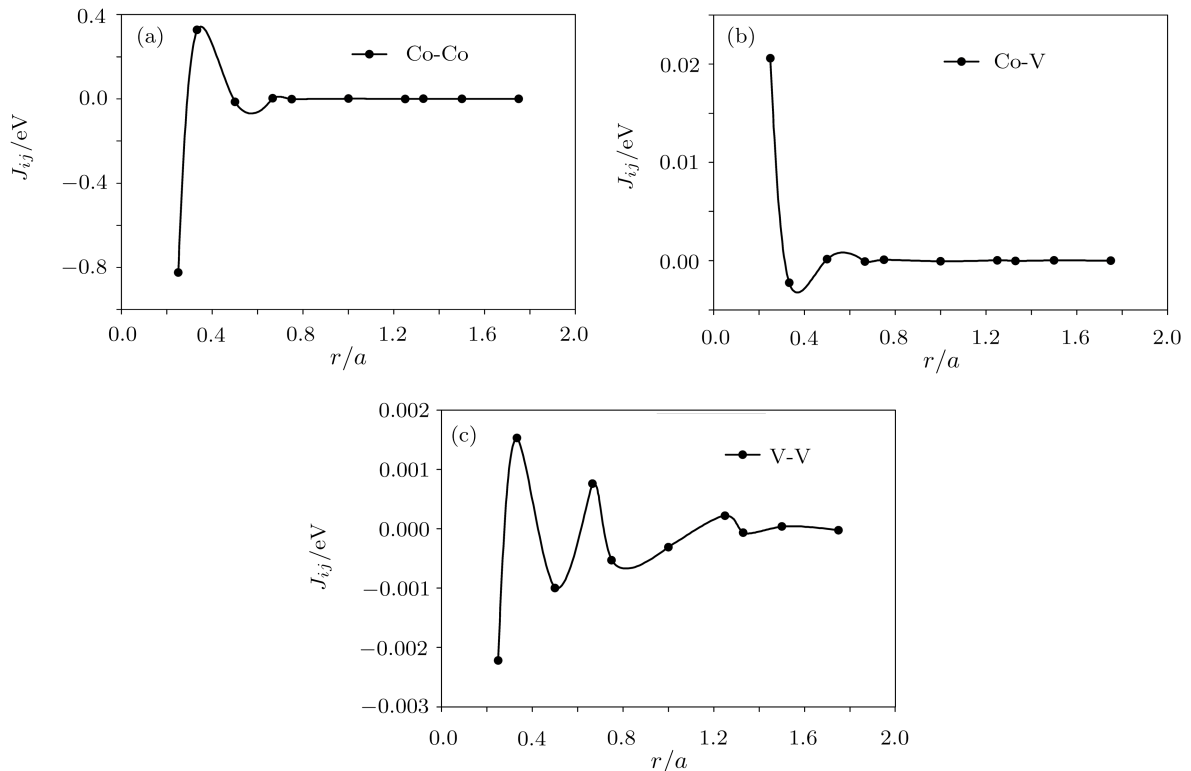


Fig. 2 Variation of J_{ij} in Co_2VAL crystal for Co-Co, Co-V and V-V pairs versus the inter-atomic distance “ r ” gauged by lattice constant “ a ”.

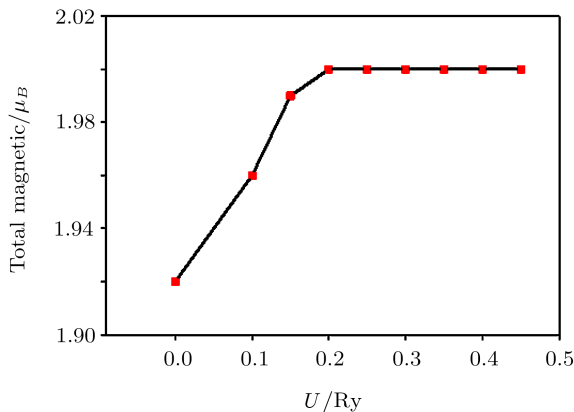
Table 4 Curie Temperature (by two methods) of Co₂VAl in comparison with other Co-based Heusler compounds.

	Co ₂ VAl	Co ₂ FeAl	Co ₂ MnAl	Co ₂ VGa
T_C	342.7 K ^a (experiment) 800 K (method 1) 384.81 K (method 2)	1000 K ^b (theory)	693 K ^c (theory)	357.3 K ^a (experiment)

^a[24]; ^b[49]; ^c[16].

3.4 Calculation of Electronic and Magnetic Properties of Bulk Co₂VAl

The electronic and magnetic calculations of Co₂VAl have already been carried out by other researchers using GGA and LDA approximations^[24–25,28] but here, these properties are to be studied through a GGA+U approach. First the structural parameter of Co₂VAl is optimized by GGA approximation, and then the electronic and magnetic properties are calculated. In comparison with others in Table 1, it is shown that in theoretical efforts magnetic moment is equal to 2 (μ_B /cell)^[26,29] and in the recently experiments at 5 K it is measured by 1.86 (μ_B /cell).^[24] A little deviation of our result with experiment originate that our calculation in 0 K but the experiment reported at 5 K.

**Fig. 3** Variation of the total magnetic moment per formula unit as a function of effective U parameter.

The electronic and magnetic properties of the system have been calculated for different amounts of U for all magnetic atoms. Figure 3 indicates that the magnetic momentum increases with extending effective U from zero to 0.2 Ry and reaches to a fixed integer value of 2(μ_B /cell), which thenceforth all Coulomb exchange interactions indicate a fully half-metallic behavior of Co₂VAl with fully spin polarization, which is compatible with experimental data^[24] along with this suggestion that the optimum value of U is greater than 0.2 Ry (selected common U for both magnetic atoms to show the sensitive total magnetic moment by U). In continue, the density of states (DOS) is shown in Fig. 4 indicating that by increasing U , the minority DOS shift towards higher energies above the Fermi

level and at 0.2 Ry to the greater amount exist the 100% spin-polarization at Fermi level and the spin-Flip gap is increased.

This shifting is related to the d orbitals of Co and V neighbor atoms ending up to a half-metallic energy gap around the Fermi level. Hence the shift of the minority DOS in the range of $U = 0$ –0.2 Ry has slight effects on the total number of the d electrons and causes an on-site charge transfer from minority to majority orbitals for both Co and V ions. In the $U = 0.2$ –0.4 Ry range where the number of the occupied orbitals and their related magnetic moments are equal to $2\mu_B$, the Fermi level lies into the half-metallic gap as expected from the experiments (Fig. 3).^[18,24] Applying greater values of this range leads to larger changes in the electronic structure (Fig. 4) which requires larger modification in GGA results. Also using the supercell method,^[53–54] resulted the amounts of 3.79 eV and 2.35 eV for the U parameter of Co and V respectively, which seem compatible with other works,^[55–57] which is precise enough to calculate the magnetic momentum.

These calculations are consistent with first-principles Hartree–Fock estimated values of the effective U parameter (taking into account the screening effects) for transition-metal elements.^[58] Figure 4 indicates that by increasing the U parameter in GGA+U approximation, the occupied states are shifted towards energies lower than Fermi level. It is obvious that in minority states the upper valance states are due to the Co d -t_{2g} orbitals (d orbital triple degeneracy) while the lower ones are formed by V d -eg orbitals (d orbital double degeneracy). Other d orbitals of Co and V atoms have small contribution to the low-energy conduction states beginning from slightly below the Fermi level. Furthermore, this figure displays that in $U = 0$ Ry the V d -eg orbitals cut the Fermi level and Co states have small spin-Flip gap which gets wider as the U parameter increases.

Comparing the DOS of Co₂VAl with other theoretical efforts,^[26,29] it is clearly deduced that for calculating the spin-polarization and magnetic moment, GGA+U approximation leads to better results of more agreement with Slater–Pauling rule, besides arising a spin-Flip gap of about 0.7 eV. Finally, in the case of $U = 0$ our DOS of Co₂VAl (top of Fig. 4) is well consistent with the others'.^[26,29]

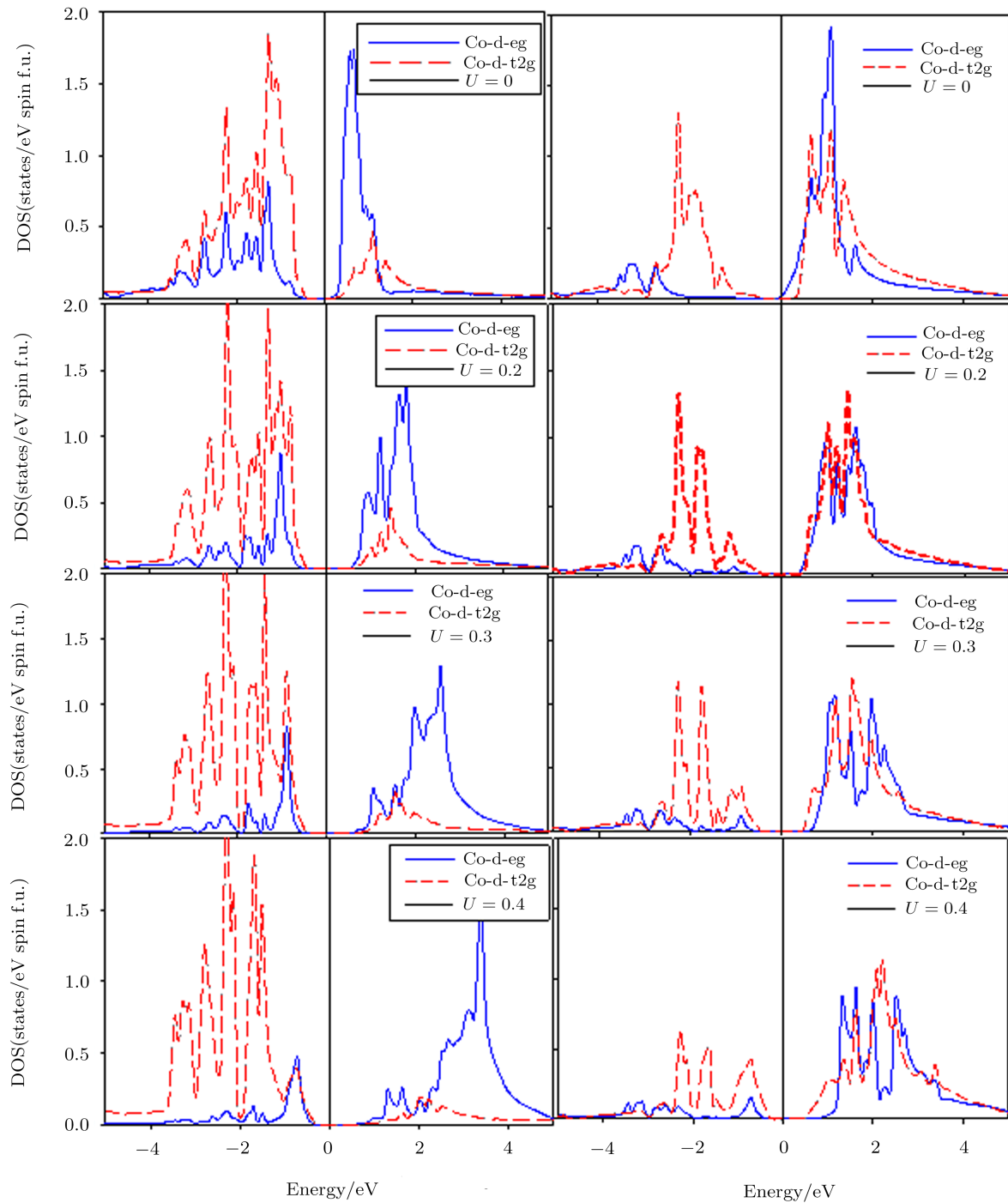


Fig. 4 DOS diagrams of Co d-eg, Co d-t2g, V d-eg and V dt2g by GGA+U ($U = 0-0.4$ Ry) for down spin.

4 Conclusion

The results of this work suggest that the FM phase of the bulk Co_2VAl is more stable than AFM and NM phases. The GGA+U approach confirms a fully spin polarization along with an integer amount for magnetic moment ($2.00\mu_B$), implying a fully half-metallic property. Concluding from elastic calculations, it has elastic stability with a ductile behavior besides a high Debye temperature as well as a relatively high Curie temperature obtained from the exchange parameter (J_{ij}). Conclusively, Co_2VAl is a suitable candidate for spintronic devices.

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