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ELECTRONIC, OPTICAL, ELASTIC AND MAGNETIC PROPERTIES OF Co_2VZ (Z= As, B, In, Sb) FULL HEUSLER COMPOUNDS

Sukhender[a], Lalit Mohan[a], Sudesh Kumar[b], Shiv R. Bhardwaj[c], Ajay Singh Verma[a,*]

[a]*Department of Physics, Banasthali Vidyapith, Banasthali 304022, India*
[b]*Department of Chemistry, Banasthali Vidyapith, Banasthali 304022, India*
[c]*Department of Physics, B. S.A. College, Mathura 282004, India*
**Corresponding Author: ajay_phy@rediffmail.com*
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Here in, we have investigated electronic, optical, elastic and magnetic properties of Co_2VZ (Z= As, B, In, Sb) full Heusler compounds by using two different computational methods. One is full potential linearized augmented plane wave (FP-LAPW) method as implemented in WIEN2k and second one is pseudo potential method as implemented in Atomistic Tool Kit-Virtual NanoLab (ATK-VNL). All these compounds show zero band gaps in majority spin channel in both computational codes and in minority-spin conduction band or valence band crosses the Fermi level. Magnetic moment calculated by these compounds Co_2VZ (Z= As, B, In, Sb) are 3.64 and 3.76, 2.00 and 1.97, 1.99 and 1.99, 3.96 and 3.82μ_B in WIEN2k and ATK-VNL simulation codes respectively. Optical properties of these compounds such as reflectivity, refractive index, excitation coefficient, absorption coefficient, optical conductivity and electron energy loss have been analyzed. Absorption coefficient and electron energy-loss function values are increases as we increase the value of energy. Absorption and reflection are inversely proportional to each other at same instant of time. Pugh's ratio B/G is greater than 1.75 for Co_2VZ (Z= B, In, Sb) compounds showing ductile in nature, but B/G value for Co_2VAs is less than 1.75, so this compound is brittle in nature. Values of Cauchy pressure ($C_P = C_{12} - C_{44}$) derived and these compounds Co_2VZ (Z= As, B, In, Sb) shows metallic nature.
KEYWORDS: band gap, Spintronics, magnetic moment, elastic constants

Half metallic ferromagnetism is those Heusler compounds, which shows zero band gap in spin up form representing metallic nature and a finite gap in spin down form exhibiting semiconducting nature [1-5]. Spin of electron is responsible for such type of dual nature of material and named as Spintronics. The materials which are metallic in majority spin and non-metallic in minority spin reveals 100% spin polarization at Fermi level [6-8]. Heusler alloys represent high magnetic moment and Curie temperature [9]. Due to such type of electronic and magnetic characteristics, half metallic ferromagnetic materials have wide application in Spintronics devices, such as magnetic tunneling junctions with tunnel magneto-resistance (TMR), magnetic sensors, spin torque oscillators (STO), non-volatile magnetic memory, spin light emitting diodes (LED) and so on. These devices increase the data processing speed and decrease the power consummation [10-15]. Ishida et al. [16] have put their results represent that the compounds Co_2MnZ (Z= Ge, Sn) are semi metals and showing 100% spin polarization. Shreder et al. [17] have studied the electronic, optical and magnetic properties of Fe_2TiAl, Fe_2Val and Fe_2CrAl. They observed radical conversion in band spectrum in domain of Fermi energy and when change Y= Ti, V, Al, there are significant changes in optical and electrical properties. Their results have good agreement with experimental results. Seema et al. [18] have studied the electronic, optical and magnetic properties of Co_2CrZ (Z= Al, Ga, Ge, Si). From their study, they have observed three types of disorders, namely DO_3, A_2 and B_2. In these disorders DO_3 and A_2 disorder leads decrease in the spin polarization and B_2 disorder retains the spin polarization at Fermi level. In this paper, we have performed the first principle calculation of the structural, electronic, optical, elastic and magnetic properties of Co_2VZ (Z= As, B, In, Sb) compounds, by using WIEN2k code and Atomistic Tool Kit-Virtual NanoLab (ATK-VNL) code within Generalized-gradient approximation (GGA) for exchange correlation functions.

COMPUTATIONAL DETAILS

We have performed by using full-potential linearized augmented plane wave (FP-LAPW) [19] executed by WIEN2k simulation code [20]. During optimization different parameters need to set, like $R_{mt}K_{max}$, k-point, lattice constant and optimized energy, Generalized-gradient approximation (GGA). Where R_{mt} denote plane wave smallest radius of muffin-tin sphere and K_{max} is used for elaboration of flat wave function by making maximum modulus of reciprocal lattice vector. Here R_{mt} K_{max} (cutoff parameter), which is used for control the basis set size and we set 7.0 values for this. The energy between two states (core states are considered relativistically and valence states are considered as semi-relativistic) was set 6.0Ry. In first Brillouin zone, we fix 1000 k-points. This value of k-points is increased to 10000, when we calculate the optical properties of Heusler compounds. Angular momentum is used to expand the spherical harmonics in the atomic sphere taken as l_{max} = 10. In the central region the charge density and potential were elaborated with wave vector up to G_{max}=10. The value of energy convergence criterion was set to 0.0001Ry. For the each atom muffin tin sphere radii (R_{MT}) are tabulated in Table 1.

Table 1.

Muffin tin radius (R_{MT}) for Co_2VZ (Z= As, B, In, Sb).

R_{MT} (a.u.)	Compound			
	Co_2VAs	Co_2VB	Co_2VIn	Co_2VSb
Co	2.35	2.20	2.37	2.21
V	2.24	2.09	2.31	2.15
Z	2.24	1.82	2.37	2.21

A pseudo-potential method has been carried out in the framework of density functional theory is also apply for study of above physical fundamental properties of full Heusler alloys, used by a code Atomistic Tool Kit-Virtual NanoLab (ATK-VNL) [21]. Electronic and magnetic properties of Co_2VZ (Z= As, B, In, Sb) are calculated by using Pulay Mixer algorithm. Double-zeta (ζ) polarized basis set is applied for expanding the electron wave function and GGA (Generalized-gradient approximation) for exchange-correlation functional. When each atom achieves force convergence criteria 0.05 eV/Å; then we have obtained an optimized structure of a compound having maximum stress is 0.05 eV/Å^3. Maximum 200 numbers of steps are executed with a fix step size 0.2 Å for the optimization. Convergence is achieved by deciding mesh cutoff energy on the ground of convergence principle and for this computation 150 Ryd has been projected all over calculation as the most favorable after several convergence tests. Initial state has been selected up and down for spin polarization purpose in an atom. We used 10 x 10 x 10 Monkhorst-Pack k-mesh [22] for brillouin zone sampling to maintain balance between computational time and for accuracy results. Further, no any constrain in x, y and z directions are applied for structure optimization.

RESULTS AND DISCUSSIONS

Structural parameters

In this study, we have concentrated on the Full Heusler compounds with formula X_2YZ and having atomic composition 2:1:1. They are inter-metallic alloys formed by four penetrating FCC-lattices with atomic positions at X_1 (1/4, 1/4, 1/4), X_2 (3/4, 3/4, 3/4), Y (1/2, 1/2, 1/2) and Z (0, 0, 0). Where X and Y atoms are transition metal and Z is main group metal or semimetal. Their cubic lattice structure is of the $L2_1$ type having space group Fm-3m (no. 225) [23]. The equation of state given by Murnaghan [24] gives the value of total energy and pressure as a function of volume is stated as:

$$E(V) = E_O + \left[\frac{BV}{B_P}\left(\frac{1}{(B_P-1)}\left(\frac{V_O}{V}\right)^{B_P} + 1\right) - \frac{BV_O}{(B_P-1)}\right]$$

$$P(V) = \frac{B}{B_P}\left\{\left(\frac{V_O}{V}\right)^{B_P} - 1\right\}$$

$$\text{Pressure } (P) = -\frac{dE}{dV},\ B_P = -V\frac{dP}{dV} = V\frac{d^2E}{dV^2}$$

In the above equations E_0 is the minimum energy at T = 0K, B is the bulk modulus, B_P is the pressure derivative of the bulk modulus and V_o is the equilibrium volume. Structural optimization curves have been presented in figure 1. Comparison of lattice constants compiled from both the computational codes WIEN2k and ATK-VNL, revels the results that values of lattice constants of ATK-VNL are slightly greater than the lattice constants of WIEN2k. But in case of bulk modulus, there is a significant difference between the values generated by these computational codes. Bulk moduli of WIEN2k are slightly greater than the bulk modulus of ATK-VNL. The compound Co_2VSb have the lowest value of Pressure derivative while Co_2VIn have the highest value of Pressure derivative. Calculated values of the optimized lattice constant, equilibrium energy and pressure derivative have been presented in Table 2.

Table 2.

Lattice parameter, Bulk modulus, Equilibrium energy and Pressure derivative for Co_2VZ (Z= As, B, In, Sb).

Compound	Lattice Constants a_0 (Å)		Bulk modulus (GPa)		Equilibrium Energy (Ry)	Pressure derivative
	Calculated		Calculated			
	WIEN2k	ATK	WIEN2k	ATK		
Co_2VAs	5.814	5.794	170.66	182.91	-11994.720	4.193
Co_2VB	5.431	5.359	263.33	287.67	-7522.265	5.541
Co_2VIn	6.005	5.794	183.19	210.39	-19239.105	6.072
Co_2VSb	6.036	5.957	178.51	234.92	-20439.77	0.662

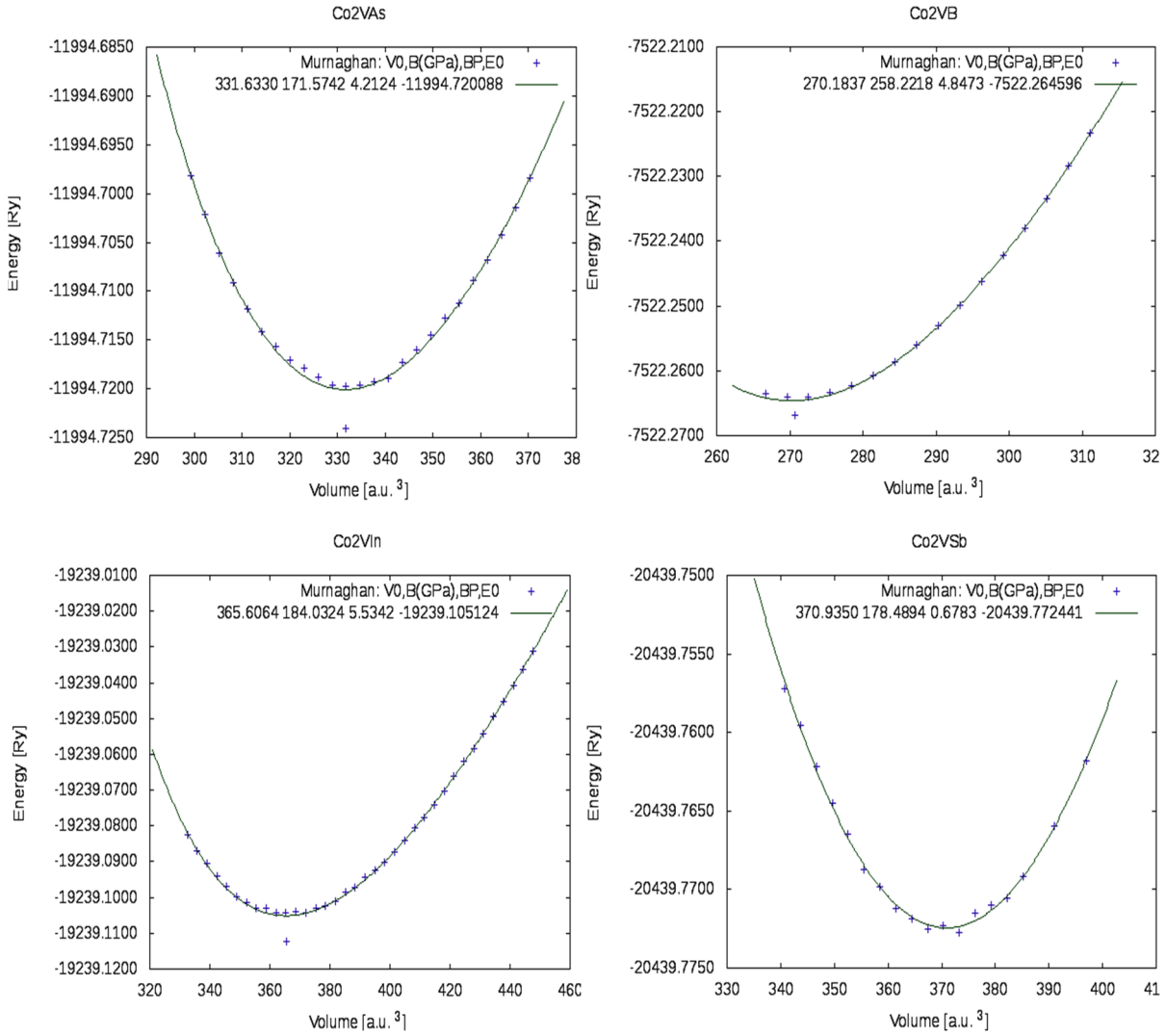

Figure 1. Volume optimization for the lattice parameters

Electronic and magnetic properties

Co-based Heusler alloys attracted researchers due to this trait half metallic ferromagnetic. Co-based Heusler alloys, which does not show any band gaps in up spin, are metallic by nature and down spin have a finite band gap and are semiconducting or insulating by nature. Then these Co-based materials are half metallic ferromagnetic showing 100% spin polarization at Fermi level. Now a day's Spintronics is a new growing field of research with numerous of applications. These materials have high Curie temperature and magnetic moment [25]. Due to such type of electronic and magnetic characteristics, half metallic ferromagnetic materials have wide application in Spintronics devices, such as magnetic tunneling junctions with tunnel magneto-resistance (TMR), magnetic sensors, spin torque oscillators (STO), non volatile magnetic memory, spin light emitting diodes (LED) and so on. These devices increase the data processing speed and decrease the power consummation. Different magneto-electronic and high processing devices are developed using the concept of Spintronics. These devices reduce electric power consummation and there is also decrease in heat dissipation. Spin polarized calculations of Co_2VZ (Z= As, B, In, Sb) compounds within Generalized-gradient approximation (GGA) have been carried out at the optimized lattice parameters. Value of spin polarization can be derived theoretically using the formula as given below.

$$P_n = \frac{n\uparrow - n\downarrow}{n\uparrow + n\downarrow}$$

If either $n_\uparrow = 0$ or $n_\downarrow = 0$, then $P_n = 1$ or -1. It means, if either up or down spin is existing then the spin polarization is 100%. These types of materials are known as half metals ferromagnetic. If the value of P_n is vanishes; then the materials are paramagnetic or anti-ferromagnetic even below the magnetic transition temperature. Study of energy gap from DOS and band structure of the compounds Co_2VZ (Z= As, B, In, Sb) shows that there are valence band extreme and conduction band extreme exists around the Fermi level. It is clear in minority spin that minima of conduction band crosses the Fermi level of compounds Co_2VZ (Z= As, B, Sb) and maxima of valence band touches the Fermi level of

compound. There does exist a significant band gap in WIEN2k code. The study of these graphs for those materials is near to half metallic. Both codes produce the same results with zero band gaps in majority spin representing the material is metallic. Graphical study of ATK-VNL also shows that the compounds Co_2VZ (Z= B, In, Sb) are near to half metallic, because their minima of conduction band crosses the Fermi level. But, the compound Co_2VAs is metallic in nature. The detailed results of band structures and density of states are shown in Figures 2-5.

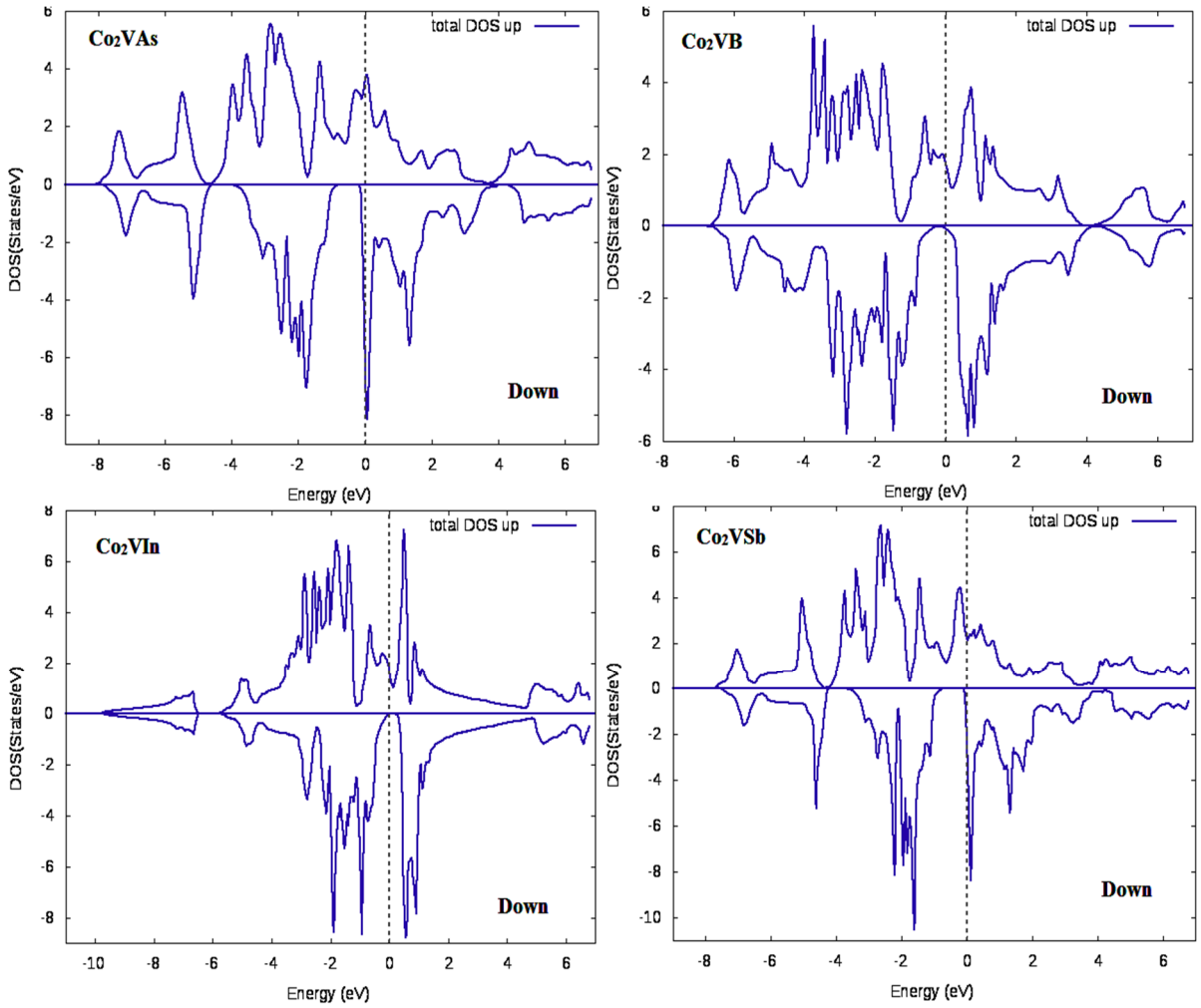

Figure 2. DOS of Co_2VZ (Z= As, B, In, Sb) using WIEN2K Code

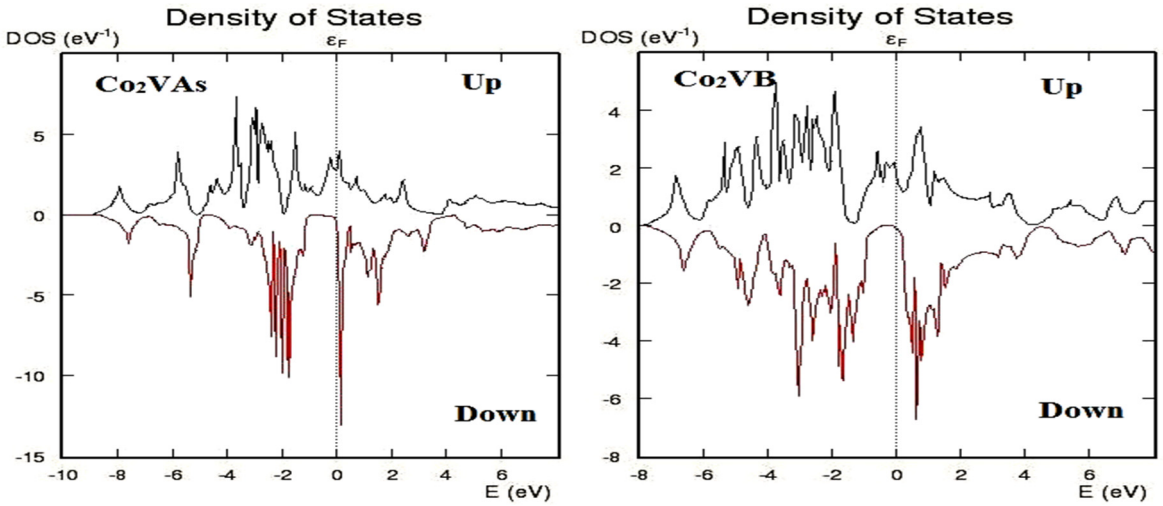

Figure 3. DOS of Co_2VZ (Z= As, B, In, Sb) using ATK-VNL Code

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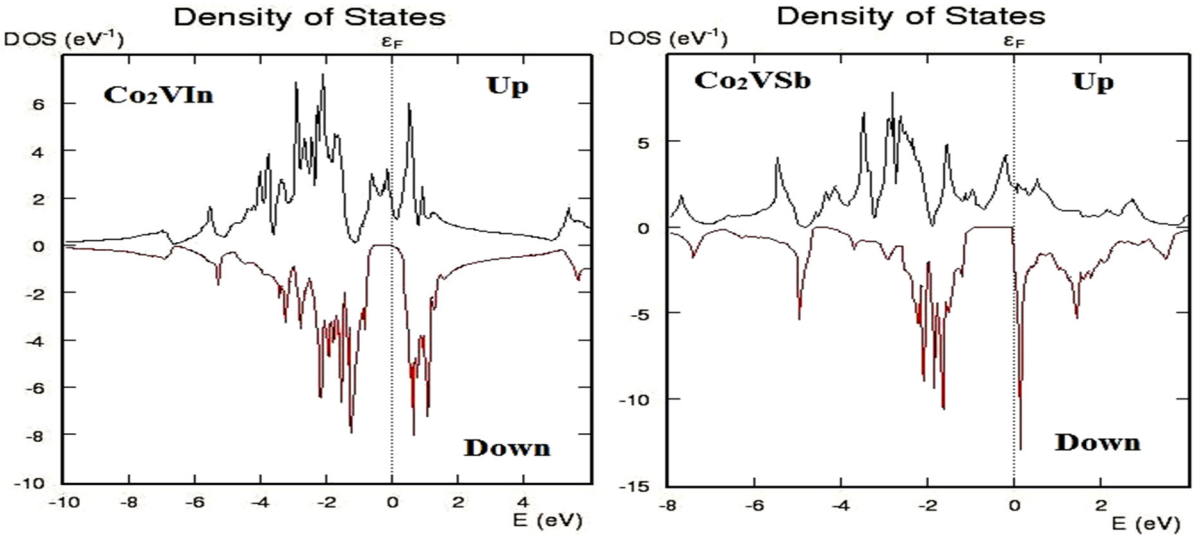

Figure 3. DOS of Co_2VZ (Z= As, B, In, Sb) using ATK-VNL Code.

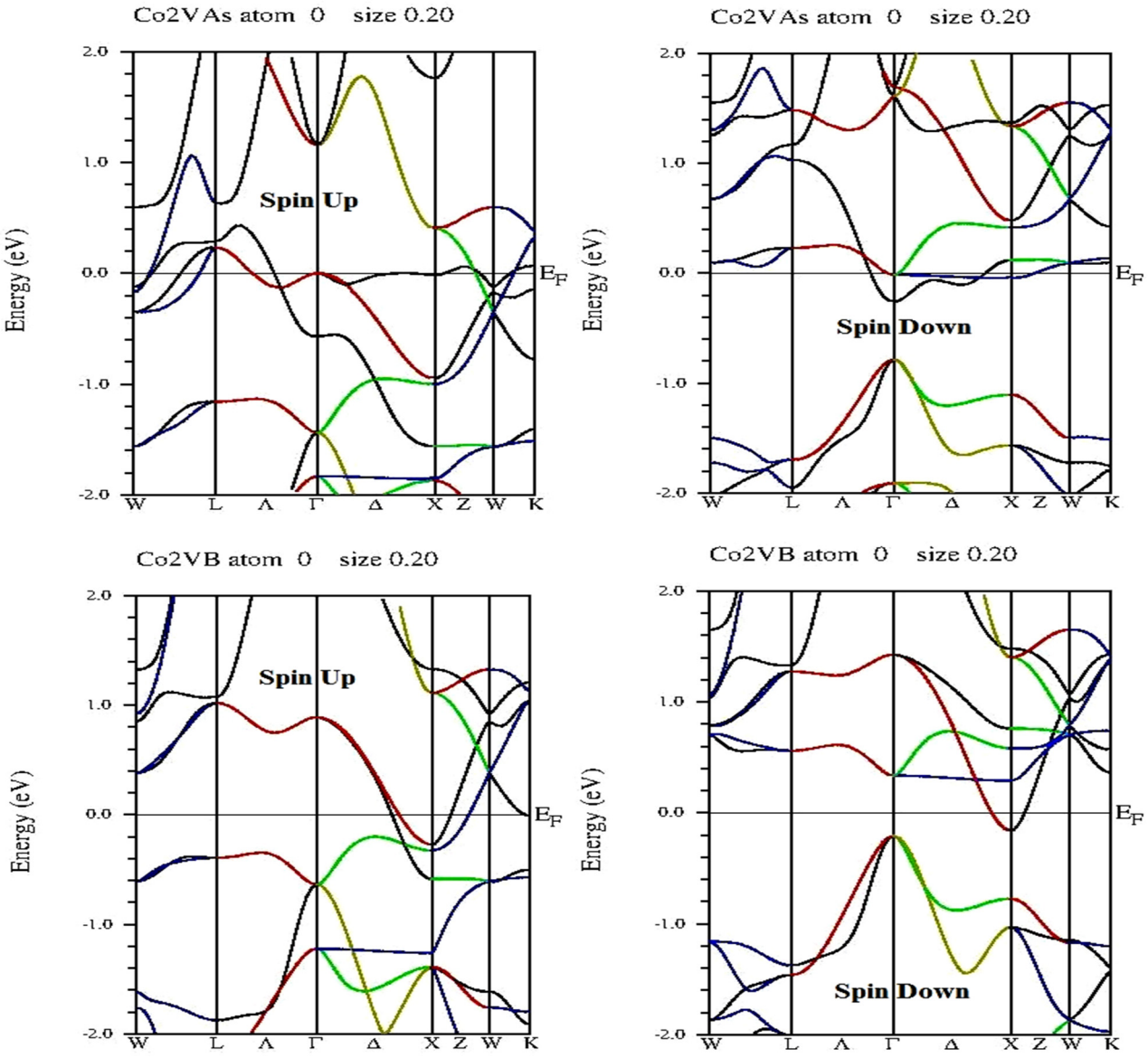

Figure 4. Band Structure of Co_2VZ (Z= As, B, In, Sb) using WIEN2K Code

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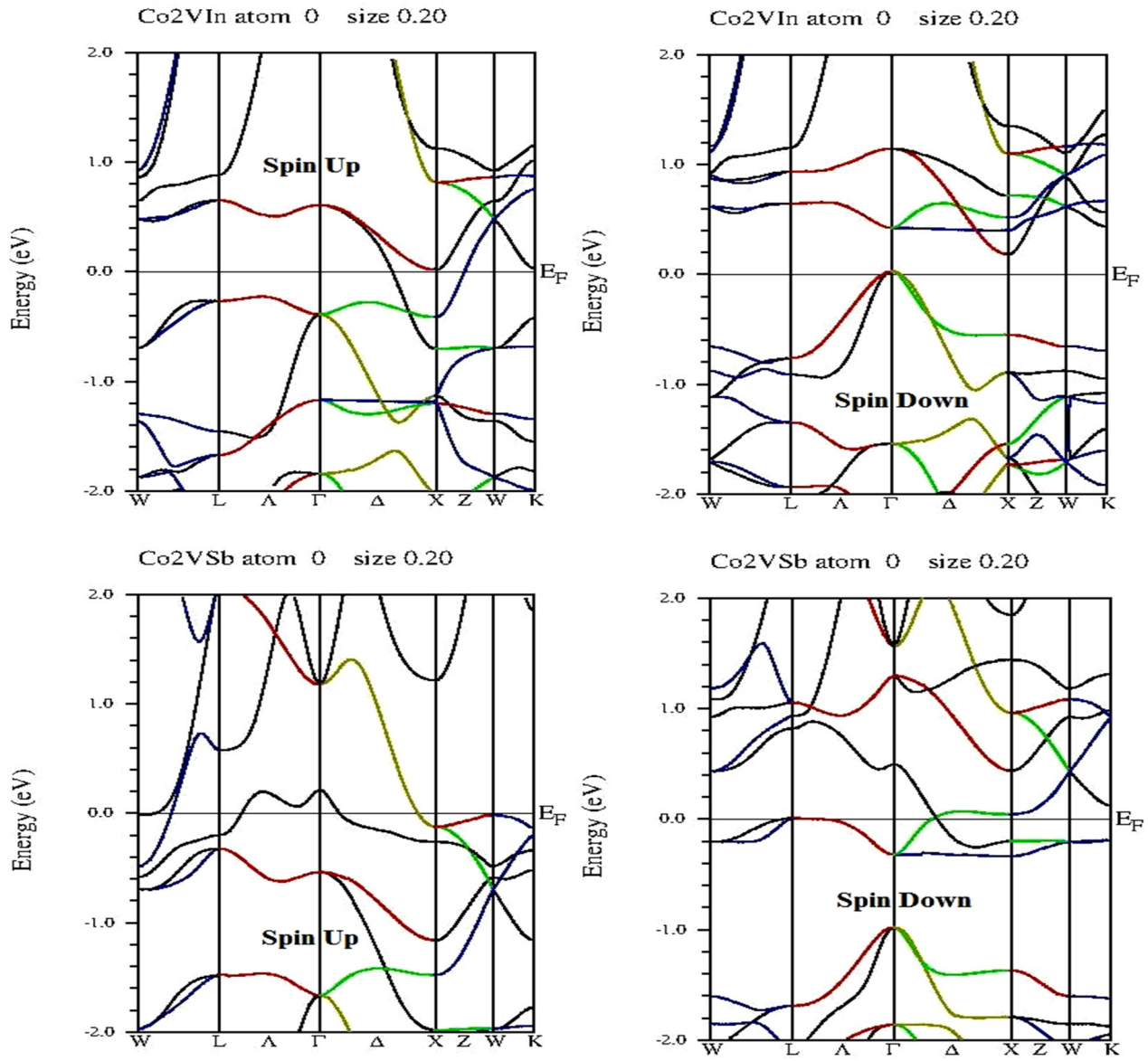

Figure 4. Band Structure of Co_2VZ (Z= As, B, In, Sb) using WIEN2K Code

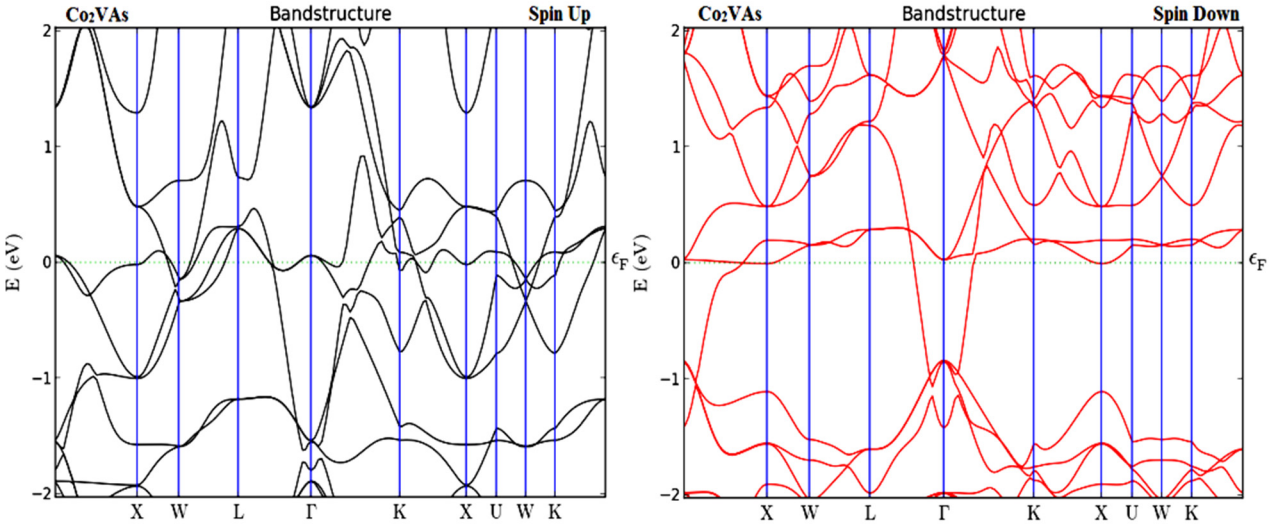

Figure 5. Band Structure of Co_2VZ (Z= As, B, In, Sb) using ATK-VNL Code

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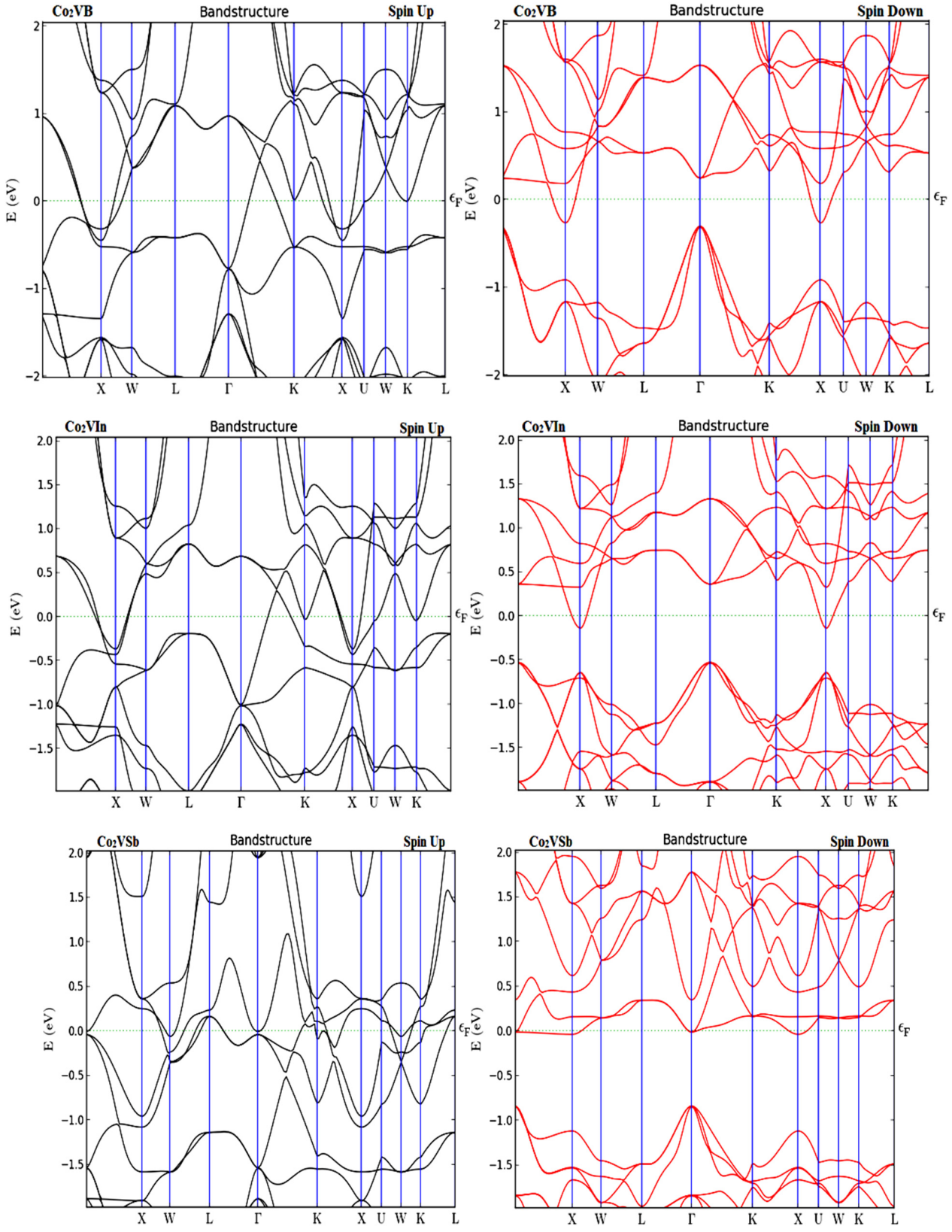

Figure 5. Band Structure of Co_2VZ (Z= As, B, In, Sb) using ATK-VNL Code

These magnetic moments and Curie temperature can be calculated by counting the total number of valence electron present in the compounds. Curie temperature is equal to the integral multiple of 175 K by the difference of total valence electron. In the same manner, magnetic moment per unit cell is equal to the difference between total numbers of valence electron. These theoretical results of magnetic moments are driven by Slater-Pauling rule [26]. Here, total number of valence electron of the compounds Co_2VZ (Z= As, B, In, Sb) are 28, 26, 26 and 28. According to the Slater-

Pauling rule their magnetic moments are 4, 2, 2 and 4 μ_B respectively and Curie temperature of these compounds Co_2VZ (Z= As, B, In, Sb) are 700, 350, 350 and 700 K respectively. We have summarized that these compounds have very good agreement with Slater-Pauling rule. The calculated results for magnetic moments for Co_2VZ (Z= As, B, In, Sb) obtained by full potential linearized augmented plane wave (FP-LAPW) method implemented in WIEN2k and pseudo-potentials method implemented in Atomistic Tool Kit-Virtual NanoLab (ATK-VNL) within Generalized-gradient approximation (GGA) for exchange and correlation functions and is tabulated in Table 3.

Table 3.

Total magnetic moments of the compounds Co_2VZ (Z= As, B, In, Sb).

Compound	Z_t	Magnetic moment (μ_B)		
		WIEN2k	ATK	Slater-Pauling (Z_t - 24)
Co_2VAs	28	3.64	3.76	4.00
Co_2VB	26	2.00	1.97	2.00
Co_2VIn	26	1.99	1.99	2.00
Co_2VSb	28	3.96	3.82	4.00

Optical properties

These optical properties are such as reflectivity, refractive index, excitation coefficient, absorption coefficient, optical conductivity and electron energy loss. The optical spectra for different optical properties are shown in Figure 6 (a-h).

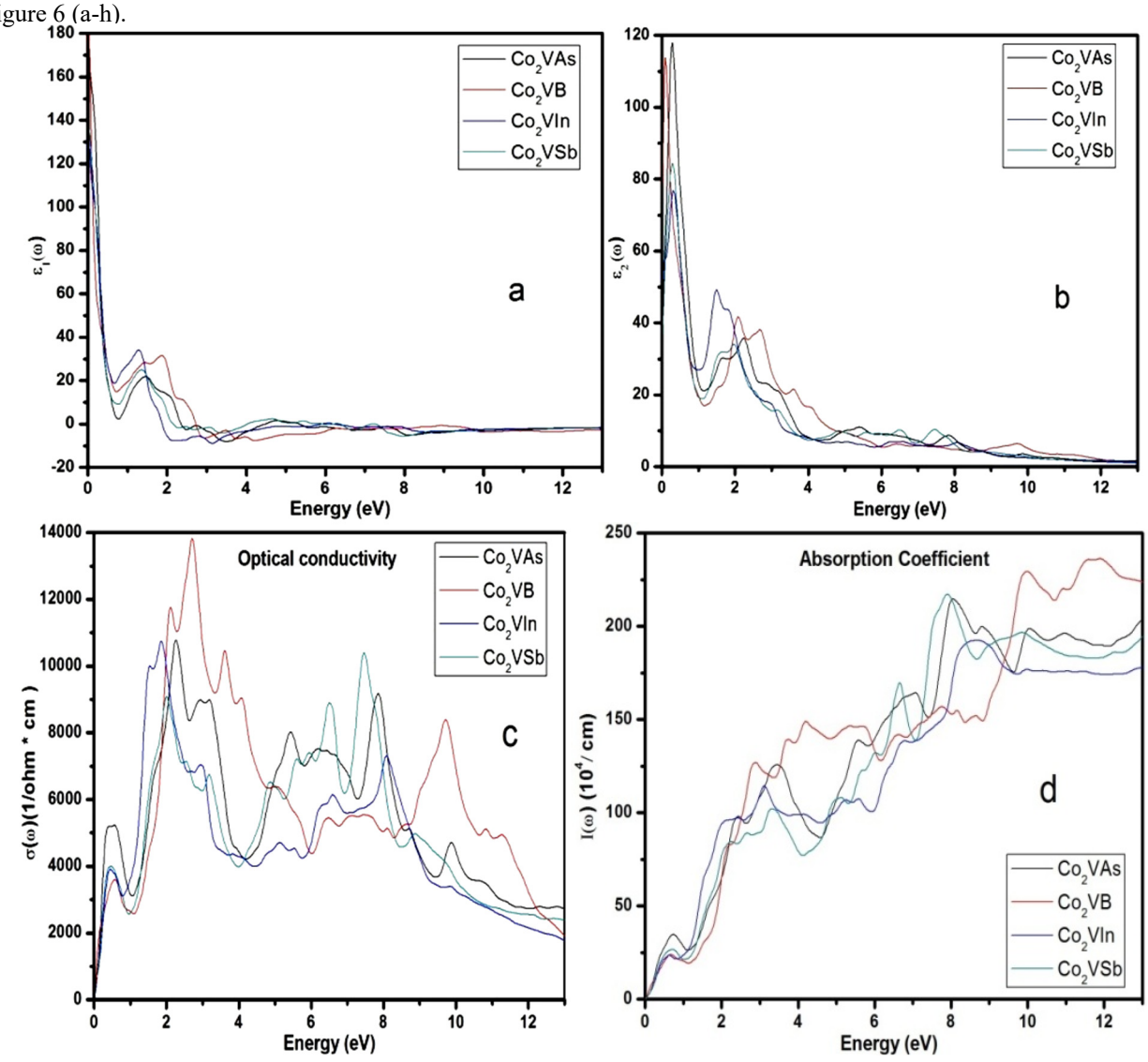

Figure 6. Calculated optical parameters (a) real part of dielectric function, (b) imaginary part of dielectric function, (c) optical conductivity, (d) absorption coefficient, (e) electron energy-loss function, (f) reflectivity, (g) refractive index and (h) extinction coefficient for Co_2VZ (Z= As, B, In, Sb).

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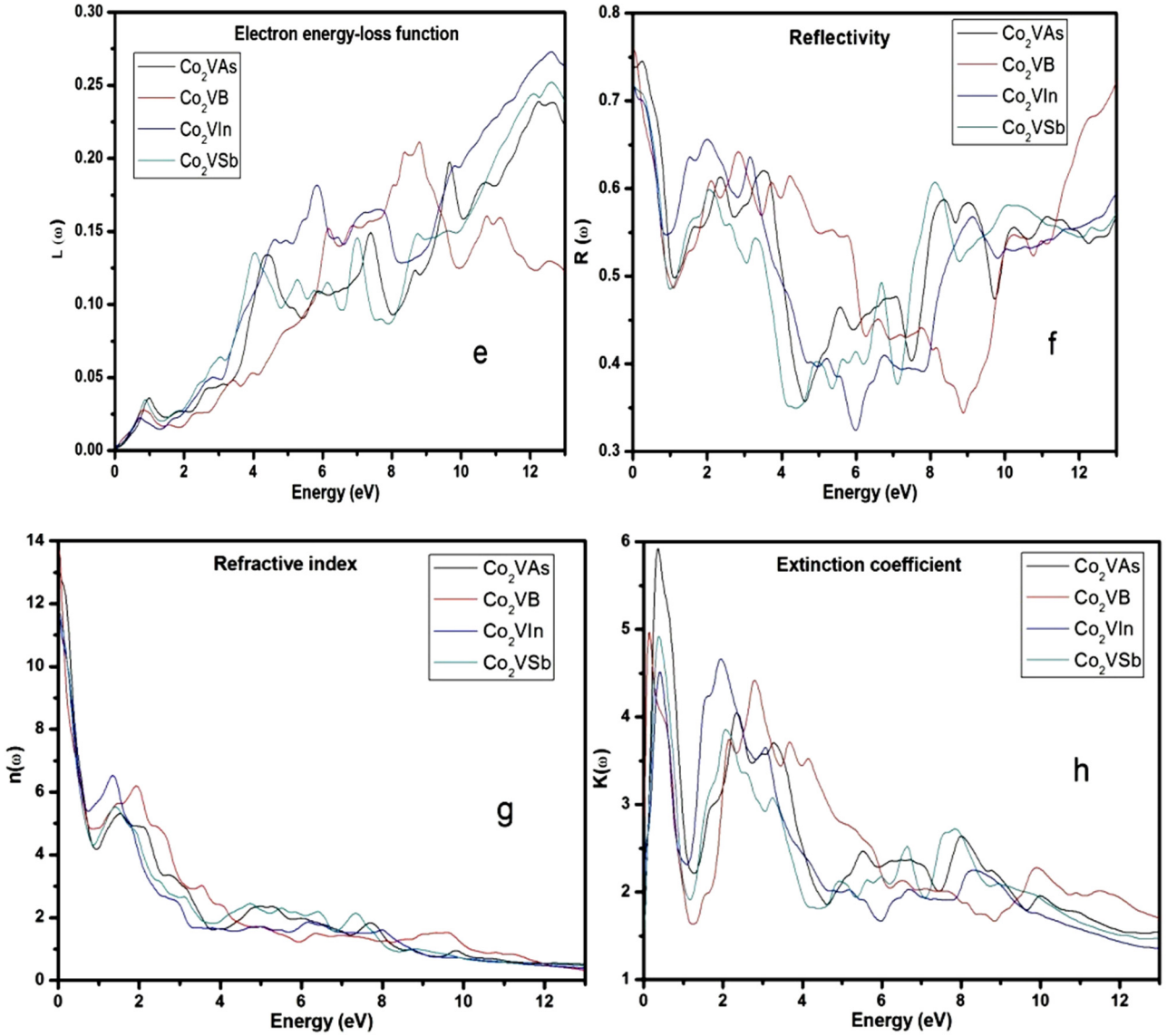

Figure 6. Calculated optical parameters (a) real part of dielectric function, (b) imaginary part of dielectric function, (c) optical conductivity, (d) absorption coefficient, (e) electron energy-loss function, (f) reflectivity, (g) refractive index and (h) extinction coefficient for Co_2VZ (Z= As, B, In, Sb).

From the Figure 6 (d-e), we have observed that along the increase of energy, values of absorption coefficient and electron energy-loss function are increases. The value of energy of fast moving particle is decreases or absorbed, when passes through a medium. Small wave vector optical response of material is described by complex dielectric function. This complex dielectric function can be written as $\varepsilon(m) = \varepsilon_1(m) + i\varepsilon_2(m)$. Where $\varepsilon_1(m)$ is the real part of complex dielectric function and ($\varepsilon_2(m)$) imaginary part of complex dielectric function. Which describe the polarization for material; when electric field is applied and gives the value of absorption in a material or loss of energy into the medium respectively [27-29]. The main peaks of imaginary part of dielectric function are obtained in infrared region from 0.08 to 0.30eV. After that, imaginary part of dielectric function decreases rapidly and some small peaks are observed near visible region. From figure 6 (a-b), we have obtained the zero frequency values of real (ε_1 (ω)) and imaginary part (ε_2 (ω)) of complex dielectric functions are 166.34 and 39.81, 180.54 and 78.45, 130.11 and 51.64, 136.16 and 37.02 for the compounds Co_2VZ (Z= As, B, In, Sb) respectively. Figure 6 (c), sharp peaks of optical conductivity are obtained in visible region and highest sharp peak is observed at 2.73eV by Co_2VB representing more conduction of electron as compared with other compounds. From figure 6 (f), we have determined the ability of material to reflect from material surface responding electromagnetic radiation. Zero frequency reflectivity values of the compounds Co_2VZ (Z= As, B, In, Sb) are 0.738, 0.756, 0.717 and 0.716 respectively. Reflection and absorption are inversely proportional to each other at the same instant of time. Plasma resonance corresponding frequency is known as plasma frequency at which sharp peaks are associated. Above the plasma frequency, material shows the dielectric behavior and below which the material shows metallic behavior. Refractive index has vast area of application such as dispersive power of prisms, focusing power of lenses, light guiding, and

critical angle for total internal reflection etc. Zero frequency value of refractive index from Figure 6 (g) for the compounds Co_2VZ (Z= As, B, In, Sb) were obtained as 12.98, 13.73, 11.62 and 11.77 respectively. Figure 6 (h) shows sharp peak of extinction coefficient infrared region and then some smaller peaks are obtained in visible region. Further, the values of extinction coefficient are decreases in the ultraviolet region.

Elastic properties

These constants provide information about structure stability, mechanical properties, bond indexes and anisotropy of material. The cubic crystal must satisfy the traditional mechanical stability condition of elastic constant, which is as below [27].

$$C_{11} - C_{12} > 0,\ C_{11} > 0,\ C_{11} + 2C_{12} > 0,\ C_{44} > 0,\ C_{12} < B < C_{11}$$

Structural stability is necessary for any material, which is determined by anisotropic factor and denoted by 'A'. The material is anisotropic for the value of 'A' is other than one. A property of material which does not depend on the direction is known as isotropic. Anisotropic is related with reduced elastic constants as.

$$A = \frac{2C_{44}}{C_{11} - C_{12}}$$

Bond index can determine the Stiffness and flexibility of a material by using Cauchy pressure, which is expressed as $CP = C_{12} - C_{44}$. If the value of Cauchy pressure is positive, then the material is metallic and ductile nature in nature, otherwise material is nonmetallic and ductile in nature. Pugh's ratio B/G is used to determine the material is brittle or ductile. If the B/G ratio is less than 1.75 then material is brittle type otherwise it is ductile. Mechanical properties of the compounds are determined by Bulk modulus (B), young modulus (E), Shear modulus (G) and Poisson ratio (v) by Voigt-Reuss-Hill (VRH) averaging method [30]. Formulas for B, E, G and v by using elastic constant can be expressed as.

$$B = B_V = B_R = \frac{C_{11} + 2C_{12}}{3}$$

$$G = \frac{G_V + G_R}{2}$$

$$G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5}$$

$$G_R = \frac{5C_{44}\,(C_{11} - C_{12})}{[4C_{44} + 3(C_{11} - C_{12})]}$$

(V = Voigt and R = Reuss)

Stiffness of material can be determined by Young modulus. This can be calculated in term of B and G.

$$E = \frac{9BG}{3B + G}$$

The value of Poisson ratio can be calculated with the help of B and G. The values of Poisson ratio lie between 0 - 0.5 for most of the material.

$$v = \frac{3B - 2G}{2(3B + G)}$$

Here, we have used Atomistic Tool Kit-Virtual NanoLab (ATK-VNL) package using Pseudo-potential method carried out in the framework of density functional theory (DFT). All the results carried out from this code are assembled in Table 4.

From the Table 4, we observe that traditional mechanical stability condition $C_{11} - C_{12} > 0$, $C_{11} > 0$, $C_{11} + 2C_{12} > 0$, $C_{44} > 0$, $C_{12} < B < C_{11}$ for the compounds Co_2VZ (Z= B, In, Sb) is satisfied but Co_2VAs compound does not show mechanical stability. Results of anisotropic constant 'A' are not equal to one for these compounds showing anisotropic in nature. Values of Poisson are lie between zeros to 0.5 except Co_2VAs. Table 4 revel the result that Pugh's ratio B/G is greater than 1.75 for Co_2VZ (Z= B, In, Sb) compounds showing ductile in nature; but B/G value for Co_2VAs is less than 1.75 and is brittle in nature. Values of Cauchy pressure ($C_P = C_{12} - C_{44}$) derived from the Table 4 and are positive for these compounds Co_2VZ (Z= As, B, In, Sb) and shows metallic nature.

Table 4.
Elastic constants and bulk modulus *B* (GPa), shear modulus *G* (GPa), Young's modulus *E* (GPa), *B/G* values, Poisson's ratio *v* and anisotropy factor *A* of Co_2VZ (Z= As, B, In, Sb) compounds.

Compound	Elastic constant			B (GPa)	G (GPa)	E (GPa)	B/G	v	A
	C_{11}	C_{12}	C_{44}						
Co_2VAs	150.56	199.08	104.21	182.91	-20.19	-76.14	-9.06	0.57	-4.30
Co_2VB	351.34	255.85	104.68	287.68	76.39	135.73	3.77	0.42	2.19
Co_2VIn	242.77	194.20	132.10	210.39	68.28	70.16	3.08	0.44	5.44
Co2VSb	251.04	226.86	112.70	234.92	49.24	35.66	4.77	0.47	9.32

SUMMARY AND CONCLUSIONS

First principle investigations are performed of full Heusler compounds Co_2VZ (Z= As, B, In, Sb). For it we calculate structural, electronic, optical, elastic and magnetic properties of these compounds by using first principle methods. Two computational codes are applied for above properties of Co_2VZ (Z= As, B, In, Sb) compounds. Results obtained by two computational codes are analyzed. First one is full potential linearized augmented plane wave (FP-LAPW) method implemented in WIEN2k and second one is pseudo- potentials method implemented in Atomistic Tool Kit-Virtual NanoLab (ATK-VNL) within Generalized-gradient approximation (GGA) for exchange and correlation function. Band structures in majority spin compounds have zero band gaps and in minority spin conduction or valence band crosses the Fermi level. Calculated magnetic moments per unit cell have good agreement with the Slater-Pauling behavior. Optical properties of these compounds named as reflectivity, refractive index, excitation coefficient, absorption coefficient, optical conductivity and electron energy loss have been observed. With the increase of energy, values of absorption coefficient and electron energy - loss function are increases. Results of elastic properties suggest that Co2VZ (Z= B, In, Sb) compounds are ductile in nature and Co_2VAs is brittle in nature. Compounds are metallic in nature.

ORCID IDs

Sukhender, https://orcid.org/0000-0002-2149-5669; **Lalit Mohan**, https://orcid.org/0000-0003-3323-8296
Sudesh Kumar, https://orcid.org/0000-0002-7507-4712; **Shiv R. Bhardwaj**, https://orcid.org/0000-0002-1895-158X
Ajay Singh Verma, https://orcid.org/0000-0001-8223-7658

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ЕЛЕКТРОННІ, ОПТИЧНІ, ПРУЖНІ ТА МАГНІТНІ ВЛАСТИВОСТІ ПОВНИХ ХЕЙСЛЕРОВИХ СПОЛУК Co_2VZ (Z = As, B, In, Sb)

Сухендер[a], Лаліт Мохан[a], Судеш Кумар[b], Шив Р. Бхардвадж[c], Аджай Сінгх Верма[a]
[a]Фізичний факультет, Банастхалі Від'япіт, Банастхалі 304022, Індія
[b]Хімічний факультет, Банастхалі Від'япіт, Банастхалі 304022, Індія
[c]Фізичний факультет, Коледж Б.С.А., Матхура 282004, Індія

За допомогою двох різних обчислювальних методів досліджені електронні, оптичні, еластичні та магнітні властивості сполук Хейслера Co_2VZ (Z = As, B, In, Sb). Один – це метод повного потенціалу лінеаризованої доповненої плоскої хвилі (FP-LAPW), реалізований у WIEN2k, а другий – метод псевдопотенціалу, реалізований в Atomistic Tool Kit-Virtual NanoLab (ATK VNL). Всі ці сполуки демонструють нульову ширину забороненої зони як в мажоритарному спіновому каналі в обох обчислювальних кодах, так і в зоні провідності з неосновним напрямком спіну, або зоні валентності, що перетинає рівень Фермі. Магнітний момент, розрахований для цих сполук Co_2VZ (Z = As, B, In, Sb), становить 3,64 та 3,76, 2,00 та 1,97, 1,99 та 1,99, 3,96 та 3,82 μ_B відповідно в модельних кодах WIEN2k та ATK-VNL. Проаналізовано оптичні властивості цих сполук, такі як відбивна здатність, показник заломлення, коефіцієнт збудження, коефіцієнт поглинання, оптична провідність та втрати енергії електронів. По мірі збільшення значення енергії коефіцієнт поглинання та значення функції втрат енергії електронами збільшуються. Поглинання і відбиття обернено пропорційні один одному в один і той же момент часу. Співвідношення П'ю – B/G перевищує 1,75 для сполук Co_2VZ (Z = B, In, Sb), які мають пластичну природу, але значення B/G для Co_2VA менше 1,75, отже ця сполука є крихкою за своєю природою. Отримано значення тиску Коші (CP = C12 - C44), що для сполук Co_2VZ (Z = As, B, In, Sb), показує їх металеву природу.

КЛЮЧОВІ СЛОВА: заборонена зона, спінтроніка, магнітний момент, пружні константи

ЭЛЕКТРОННЫЕ, ОПТИЧЕСКИЕ, УПРУГИЕ И МАГНИТНЫЕ СВОЙСТВА ПОЛНЫХ ХЕЙСЛЕРОВИХ СОЕДИНЕНИЙ Co_2VZ (Z = As, B, In, Sb)

Сухендер[a], Лалит Мохан[a], Судеш Кумар[b], Шив Г. Бхардвадж[c], Аджай Сингх Верма[a]
[a]Физический факультет, Банастхали Видьяпит, Банастхали 304022, Индия
[b]Химический факультет, Банастхали Видьяпит, Банастхали 304022, Индия
[c]Физический факультет, Колледж Б.С.А., Матхура 282004, Индия

С помощью двух различных вычислительных методов исследованы электронные, оптические, эластичные и магнитные свойства соединений Хейслера Co_2VZ (Z = As, B, In, Sb). Один – это метод полного потенциала линеаризованной дополненной плоской волны (FP-LAPW), реализованный в WIEN2k, второй – метод псевдопотенциала, реализованный в Atomistic Tool Kit-Virtual NanoLab (ATK VNL). Все эти соединения демонстрируют нулевую ширину запрещенной зоны как в мажоритарном спиновом канале в обоих вычислительных кодах, так и в зоне проводимости с неосновным направлением спина, или зоне валентности, пересекающий уровень Ферми. Магнитный момент, рассчитанный для этих соединений Co_2VZ (Z = As, B, In, Sb), составляет 3,64 и 3,76, 2,00 и 1,97, 1,99 и 1,99, 3,96 и 3 82 μ_B соответствии в модельных кодах WIEN2k и ATK-VNL. Проанализированы оптические свойства этих соединений, такие как отражательная способность, показатель преломления, коэффициент возбуждения, коэффициент поглощения, оптическая проводимость и потери энергии электронов. По мере увеличения значения энергии коэффициент поглощения и значение функции потерь энергии электронами увеличиваются. Поглощения и отражения обратно пропорциональны друг другу в один и тот же момент времени. Соотношение Пью – B/G превышает 1,75 для соединений Co_2VZ (Z = B, In, Sb), которые имеют пластическую природу, но значение B/G для Co_2VA менее 1,75, следовательно это соединение является хрупким по своей природе. Получено значение давления Коши (CP = C12 - C44), что для соединений Co_2VZ (Z = As, B, In, Sb), показывает их металлическую природу.

КЛЮЧЕВЫЕ СЛОВА: запрещенная зона, спинтроника, магнитный момент, упругие константы