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STRUCTURAL, ELECTRONIC, OPTICAL AND MAGNETIC PROPERTIES OF Co_2CrZ (Z= Al, Bi, Ge, Si) HEUSLER COMPOUNDS

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In this paper, we have studied the structural, electronic, optical and magnetic properties of Co_2CrZ (Z= Al, Bi, Ge, Si) compounds by using two different methods one is full potential linearized augmented plane wave (FP-LAPW) method as implemented in WIEN2k and second is pseudo potential method as implemented in Atomistic Tool Kit-Virtual NanoLab (ATK-VNL). The respective band gaps in their minority-spin of Co_2CrZ (Z= Al, Bi, Ge, Si) are 0.696, 0.257, 0.602 and 0.858 eV near the Fermi level, which is implemented in WIEN2k code and showing 100% spin polarization. Further, these compounds have been found to be perfectly half-metallic ferromagnetic (HMF). However, above mentioned compounds shows zero band gaps in ATK-VNL code. The calculated magnetic moment of these compounds Co_2CrZ (Z= Al, Bi, Ge, Si) are 3.06, 4.99, 3.99 and 3.99μ_B respectively in FP-LAPW method. However, the respective magnetic moment of these compounds is found to be 3.14, 5.08, 4.11 and 4.08μ_B in ATK-VNL code. Optical properties play an important role to understand the nature of material whether it can be used as optoelectronics device. From the optical Spectra, complex dielectric functions calculated values are 312.370 and 141.991, 299.812 and 111.368, 288.127 and 106.342, 290.688 and 99.095 for the compounds Co_2CrZ (Z= Al, Bi, Ge, Si) respectively by using WIEN2k. The maximum energy loss is observed between 11.4 to 13eV for above these compounds. The refractive index values for the compounds Co_2CrZ (Z= Al, Bi, Ge, Si) are observed as 18.104, 17.602, 17.252 and 17.289 respectively. In the optical conductivity spectrum a sharp peak is observed at 1.6 - 2.3eV.
KEYWORDS: Half-metallic ferromagnetic, band gap, dielectric constant, magnetic moment

A German mining engineer and chemist Friedrich Heusler discovered the Heusler compounds [1]. The Full Heusler compounds are the ternary compounds of the composition 2:1:1 with chemical formula X_2YZ and having structure of the $L2_1$ formed by four interpenetrating FCC-lattices [2-3]. Heusler alloys shows half metallic ferromagnetism and was first predicted by de Groot [4]. Half metallic ferromagnets (HMFs) having band structure for majority spins is metallic and for minority spin is semiconducting presenting 100% spin polarization at Fermi level. Half metallicity attracted more attention due to its various applications in Spintronics devices, such as nonvolatile magnetic random access memories, magnetic sensors, spin-resonant tunneling diodes, spintronic transistors and spin light emitting diodes and so on [5-10]. Felser et al. [11] have studied the X_2RbCa (X = C, N, O) full-Heusler compounds showing the half-metallicity primarily originate from the spin-polarization of the p-like states of N and O atoms. Bai et al. [12] have presented a comprehensive review of the Heusler family with special focus on its broad applications in the field of magnetic data storage, ranging from CPP-GMR read heads, to MRAM arrays, and emerging SPRAMs. These compounds are outstanding functional building blocks for spintronics devices. Sharma et al**.** [13] have investigated that Fe_2CrAl compound has high density of states and shows a 100% spin polarization in the vicinity of the Fermi level. Rai et al. [14] have also proposed that Full-Heusler compound Co_2CrGe is half-metallic ferrimagnet using Generalized-gradient approximation for the structural and local spin density approximation for electronic calculation. It was found that the Co_2YZ compounds exhibit half-metallic ferromagnetic and an apparently linear dependence of the Curie temperature on the magnetic moment [15]. Among the Heusler compounds, Co-based compounds were investigated by ab initio techniques and most of them are found HMFs [16-17]. Seema et al. [18] had investigated the effect of disorder by using density functional theory on electronic, magnetic and optical properties of Co_2CrZ (Z= Al, Ga, Ge, Si) Heusler compounds. They consider three types of disorders DO_3, A2 and B2 in which B2 disorder retains the spin polarization whereas DO3 and A2 disorder leads decrease in the spin polarization value at Fermi level.

In this paper, we have calculated the structural, electronic, optical and magnetic properties of Co_2CrZ (Z= Al, Bi, Ge, Si) compounds, by using WIEN2k code and Atomistic Tool Kit-Virtual NanoLab (ATK-VNL) code within Generalized-gradient approximation (GGA) for exchange correlation functions.

COMPUTATION DETAILS

Wien2k code based on the full-potential linearized augmented plane wave (FP-LAPW) method [19,20,21] was applied for the fundamental physical properties calculations of Co_2CrZ (Z= Al, Bi, Ge, Si) compounds within

Generalized-gradient approximation (GGA) for exchange correlation functions. Wien2k is one of the most accurate methods for performing electronic structure calculations for solids. Core states are considered relativistically and valence states are considered as semi-relativistic way and energy between these two states was set -6.0Ry. We have used 1000 k-points in the first Brillouin zone for this code. For the calculation of optical properties we used here 10000 k-points. The convergence or cutoff parameter R_{mt} K_{max} is set to 7.0, which is used to control the size of the basis sets. Here plane wave radius is denoted by R_{mt} and maximum modulus for reciprocal lattice vector is denoted by K_{max}. The energy convergence criterion was taken as 0.0001Ry. The angular momentum maximum (l_{max}) value is taken as 10. In the central region the charge density and potential were elaborated as a fourier series with wave vector up to G_{max}=10. For the each atom muffin tin sphere radii (R_{MT}) are tabulated in Table 1.

Table 1

Muffin tin radius (R_{MT}) for Co_2CrZ (Z= Al, Bi, Ge, Si).

R_{MT} (a.u.)	Compound			
	Co_2CrAl	Co_2CrBi	Co_2CrGe	Co_2CrSi
Co	2.38	2.22	2.28	
Cr	2.26	2.12	2.17	
Z	2.15	2.26	2.12	1.89

Pseudo-potential method has been carried out in the framework of density functional theory implemented in the commercially licensed Atomistic Tool Kit-Virtual NanoLab (ATK-VNL) package [22,23]. First-principles calculations was applied to investigate electronic and magnetic properties of Co_2CrZ (Z= Al, Bi, Ge, Si) using Pulay Mixer algorithm. For investigations, we use double-zeta (ζ) polarized basis set for electron wave function expanding and GGA for exchange-correlation functional [20]. For spin polarization, up and down initial state have been selected for the atoms. We used 10 x 10 x 10 Monkhorst-Pack k-mesh [24] for brillouin zone sampling to maintain balance between computational time and results accuracy. Further, for optimisation of structures we do not impose any constrain in x, y and z directions. The structures are permitted to optimized until each atom achieve force convergence criteria of 0.05 eV/Å.

RESULTS AND DISCUSSIONS:

Structural Study

The Full Heusler compounds have the composition 2:1:1 with chemical formula X_2YZ having structure of the $L2_1$ (space group: 225 Fm-3m) 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. The equation of state given by Murnaghan [25] gives the value of total energy & pressure as a function of volume is stated as:

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

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

where

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

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. The structural optimization results are shown in Figure 1. The optimized lattice parameter in WIEN2k for Co_2CrBi is slightly higher than the ATK lattice parameters; but the optimized lattice parameters in WIEN2k for Co_2CrAl, Co_2CrGe and Co_2CrSi are slightly less than the lattice parameters optimized in ATK-VNL. Calculated values of the optimized lattice parameter, equilibrium energy and pressure derivative have been presented in Table 2.

Table 2

Lattice parameter, Bulk modulus, Equilibrium energy and Pressure derivative for Co_2CrZ (Z= Al, Bi, Ge, Si).

Compound	Lattice Constants a_0 (Å)		Bulk modulus (GPa)		Equilibrium	Pressure
	Calculated		Calculated			
	WIEN2k	ATK	WIEN2k	ATK	Energy (Ry)	derivative (GPa)
Co_2CrAl	5.712	5.843	195.42	172.96	-8161.392	4.842
Co_2CrBi	6.151	6.120	195.32	198.36	-50838.608	-0.832
Co_2CrGe	5.740	5.833	218.32	216.10	-11873.869	4.159
Co_2CrSi	5.633	5.794	191.00	215.75	-8255.854	4.054

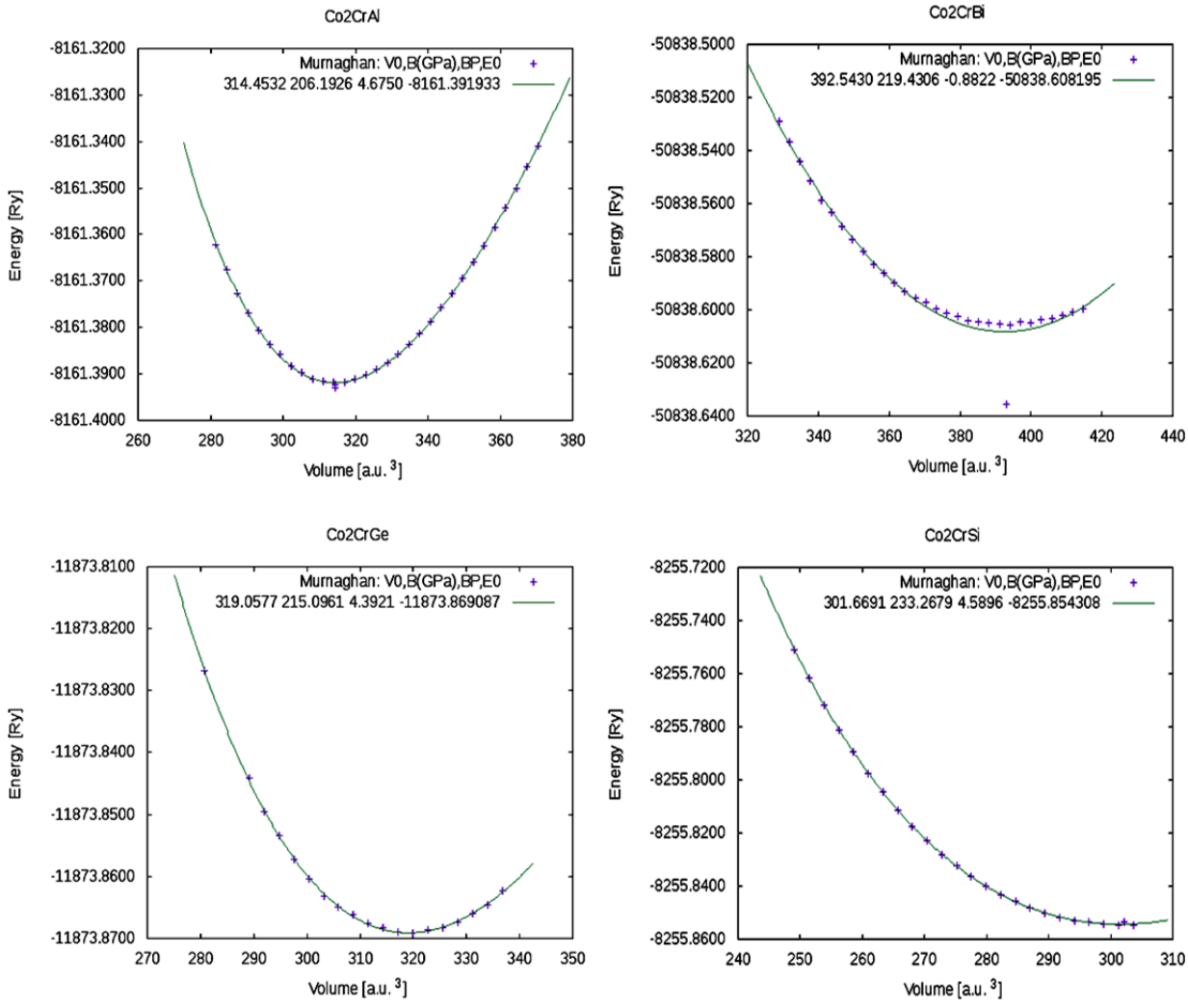

Fig. 1. Volume optimization for the lattice parameters

Electronic and magnetic properties

Spin polarized calculations of Co_2CrZ (Z= Al, Bi, Ge, Si) compounds within Generalized-gradient approximation (GGA) full Heusler have been carried out at the optimized lattice parameters. The calculations revealed a gap in the minority states and zero gaps in the majority states at the Fermi level resulting 100% spin polarized band structure at the Fermi level.

In Spintronics, magnetic moment is associated due to intrinsic spin of electron. By using the given formula the spin polarization has been calculated theoretically.

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

If $n_\uparrow = 0$ or $n_\downarrow = 0$; $P_n = 1$ or -1 in these cases only up or down spins are exist and the spin polarization is 100%. Such materials are known as half metals ferromagnetic or Heusler alloys with 100% spin polarization. If the value of P_n is vanishes then the materials are paramagnetic or anti-ferromagnetic even below the magnetic transition temperature [26]. This impressive category of materials has highly prospective for different application such as spintronics, magneto-electronic devices to increase data processing speed and integration density increasing etc. In Heusler alloy magnetic moment is key point in spintronics and obeys Slater-Pauling rule. This rule correlates the magnetic moment per atom of transition element alloys to the average number of valance electron per atom:

$$m = N_v - 2N_\downarrow$$

Where m is magnetic moment per atom in μ_B, N_v is average number of valence electron per atom & $N_\downarrow$ ($N_\uparrow$) shows the number of minority spin (majority spin) valence electron per atom**.**The component of spin degree of freedom creates non-volatility in materials [27]. The obtained energy gap and spin polarization for the above approximation is summarized as under in Table 3. The detailed results of band structures and density of states are shown in Figures 2-5.

Table 3

Energy gap and spin polarization for Co_2CrZ (Z= Al, Bi, Ge, Si)

Compound	Energy gap E_g (eV)				Spin polarization	
	WIEN2k		ATK		WIEN2k	ATK
	Up spin	Down spin	Up spin	Down spin		
Co_2CrAl	0.0	0.696	0.0	0.0	100%	P_n vanishing
Co_2CrBi	0.0	0.257	0.0	0.0	100%	P_n vanishing
Co_2CrGe	0.0	0.602	0.0	0.0	100%	P_n vanishing
Co_2CrSi	0.0	0.858	0.0	0.0	100%	P_n vanishing

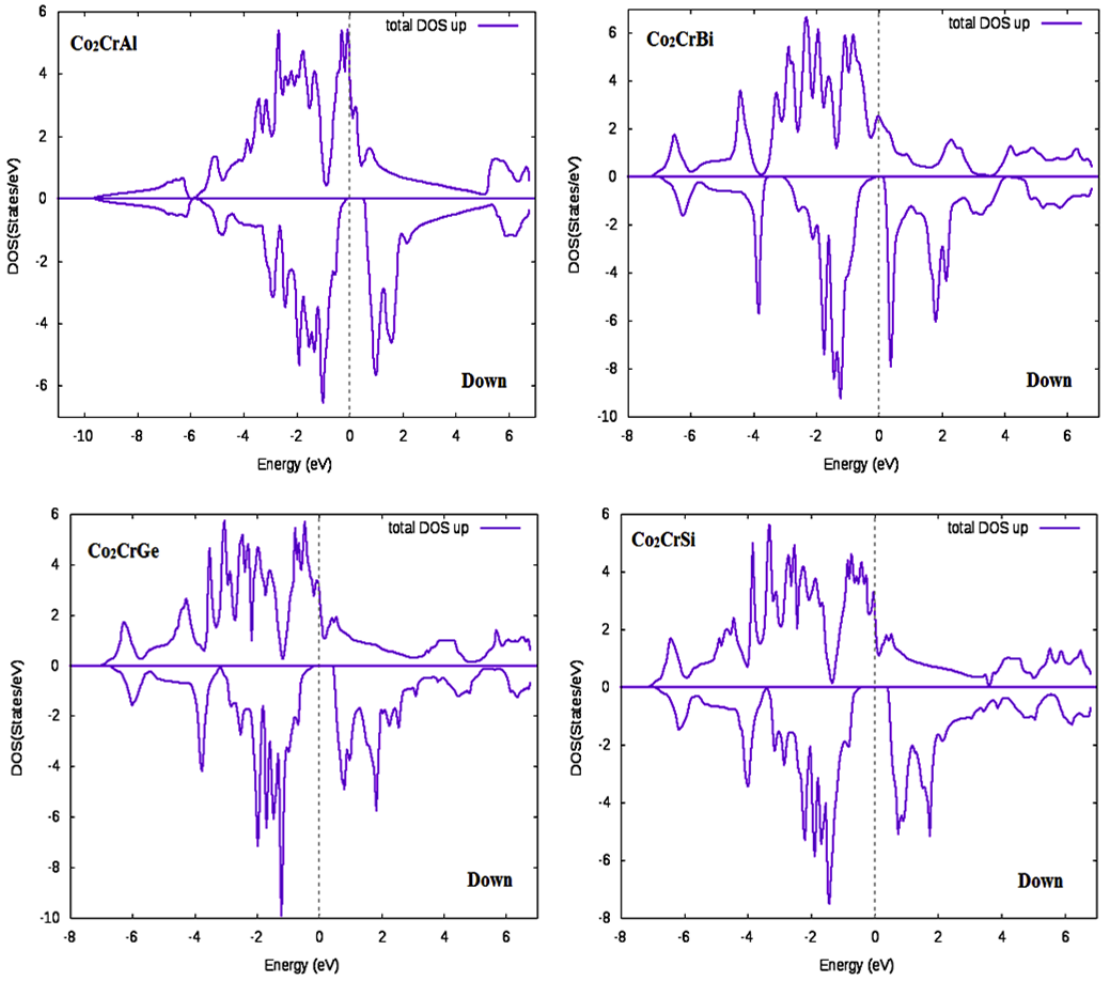

Fig. 2. DOS of Co_2CrZ (Z= Al, Bi, Ge, Si) using WIEN2K Code

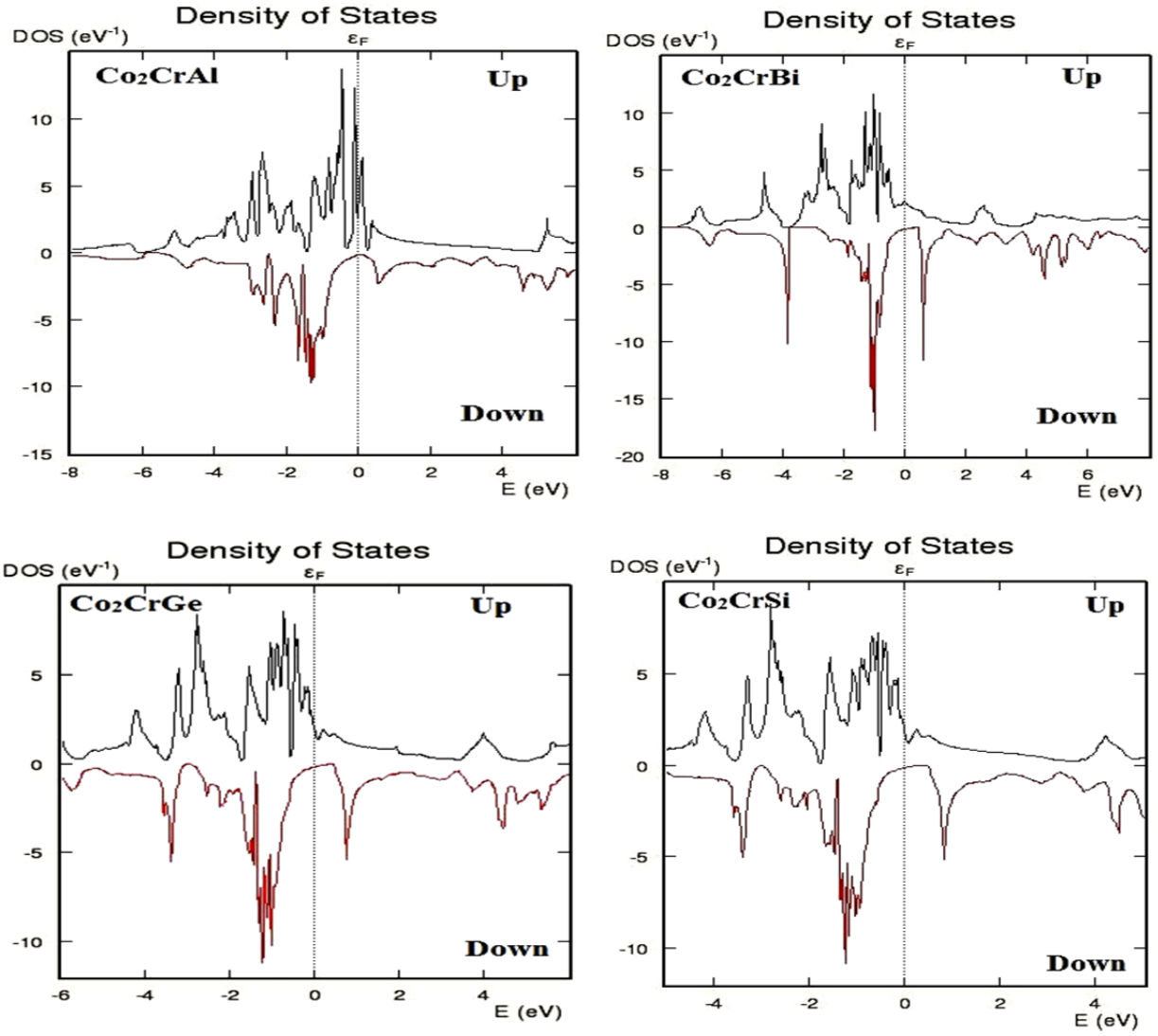

Fig. 3. DOS of Co_2CrZ (Z= Al, Bi, Ge, Si) using ATK-VNL Code.

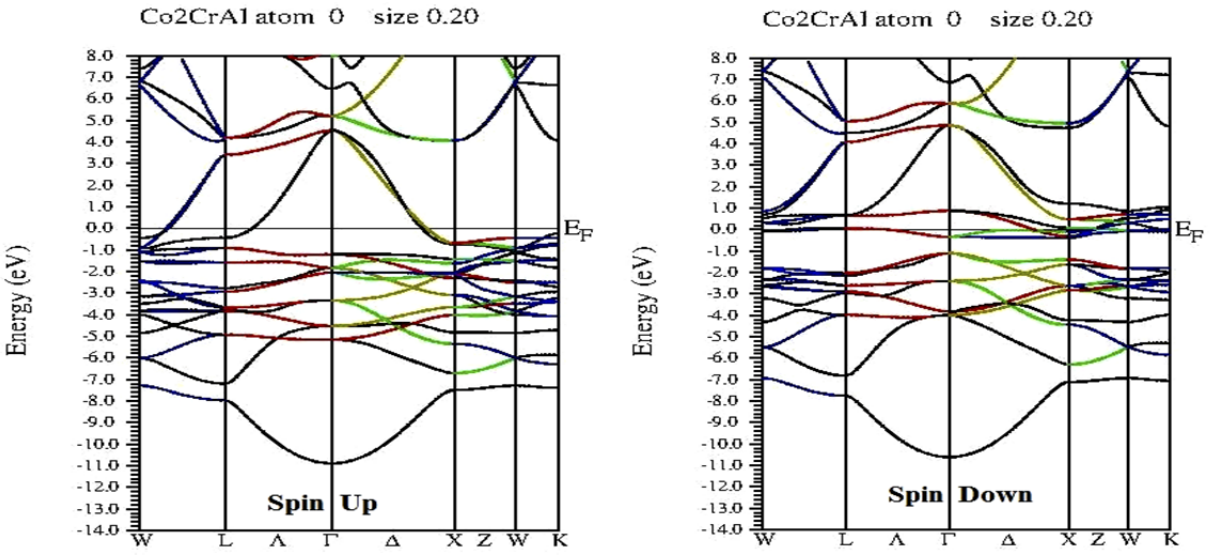

Fig. 4. Band Structure of Co_2CrZ (Z= Al, Bi, Ge, Si) using WIEN2K Code

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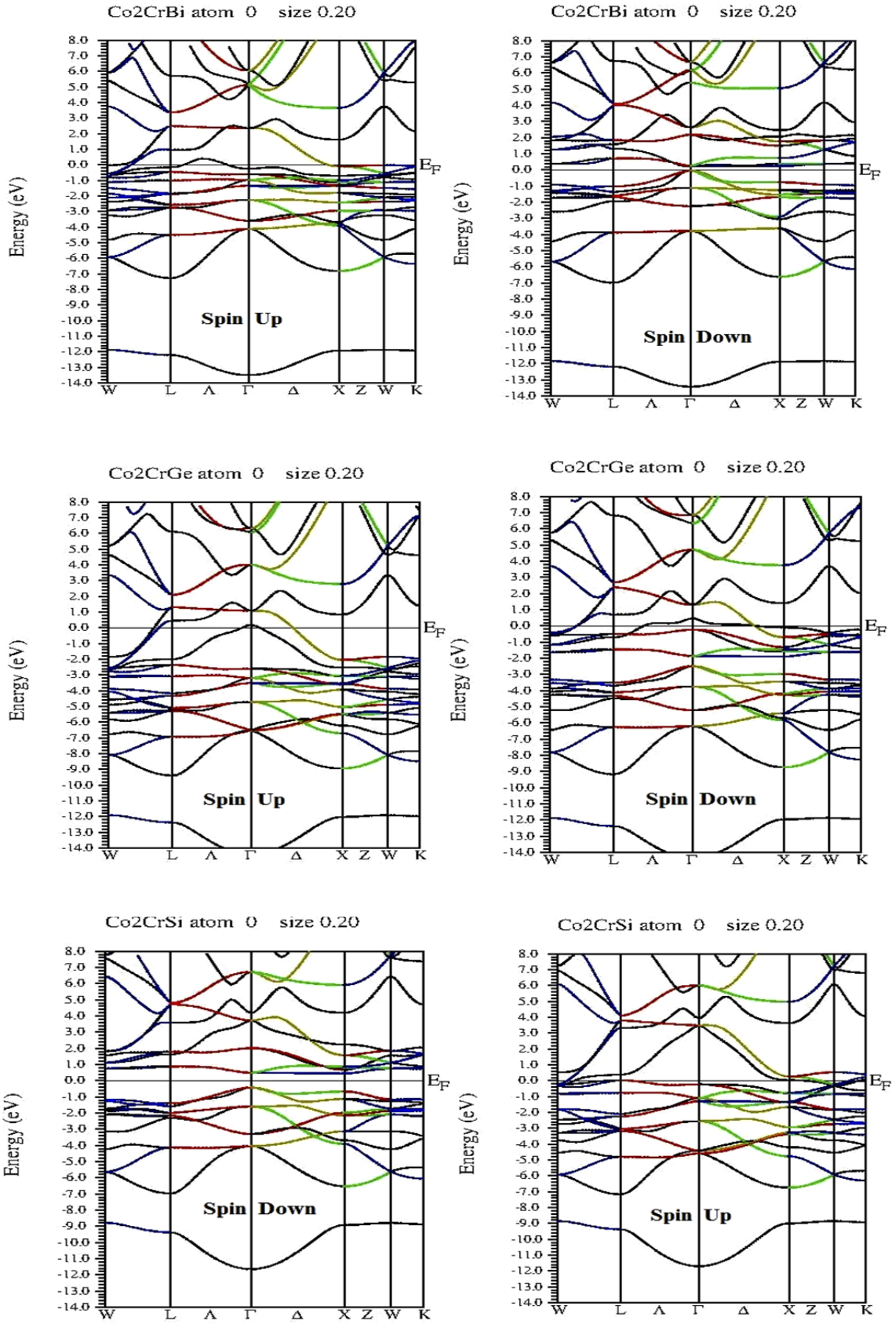

Fig. 4. Band Structure of Co_2CrZ (Z= Al, Bi, Ge, Si) using WIEN2K Code

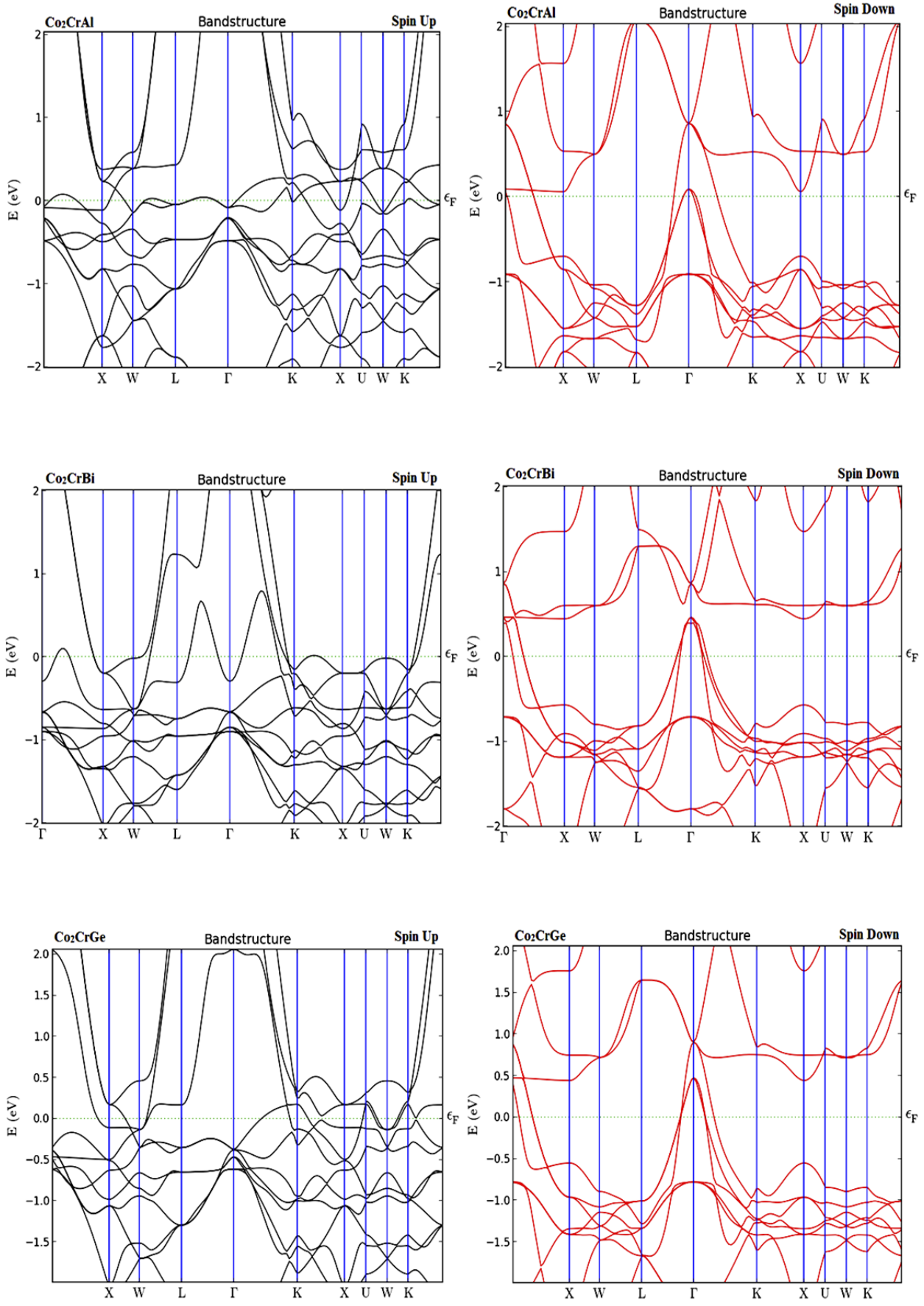

Fig. 5. *(continued)* Band Structure of Co_2CrZ (Z= Al, Bi, Ge, Si) using ATK-VNL Code

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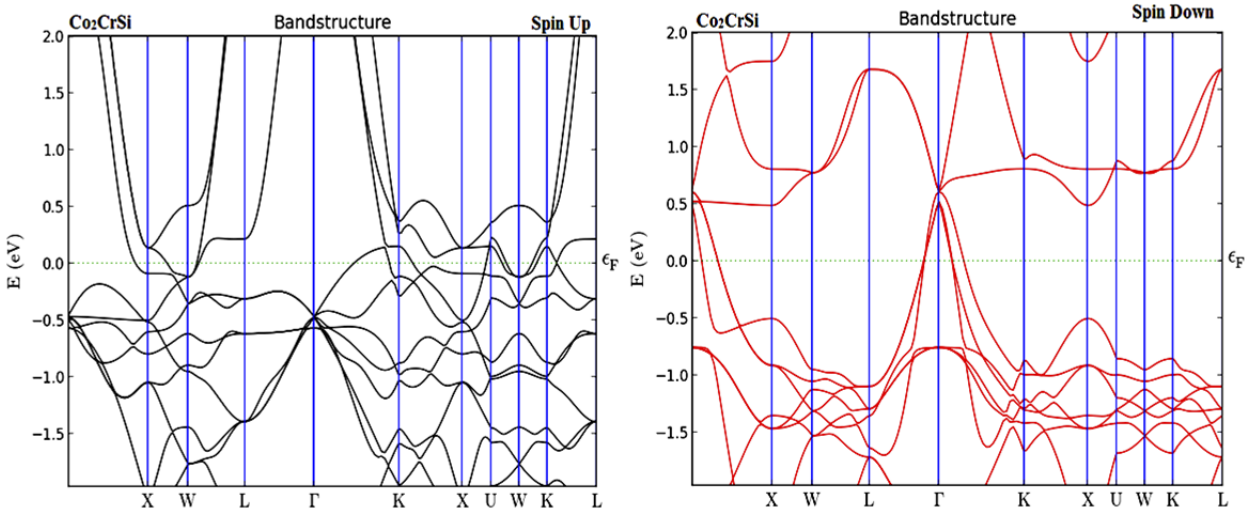

Fig. 5. *(continued)* Band Structure of Co_2CrZ (Z= Al, Bi, Ge, Si) using ATK-VNL Code

By counting the number of valence electrons of the Heusler alloys, it is possible to predict the magnetic properties of the alloys. Even 24 valence electron concentration semiconductors are possible in case of three transition metals per formula unit. For example Fe_2Val is a non magnetic semiconductor with non-magnetic iron. Co_2YZ Heusler compounds have more than 24 valence electron concentration and follow the Slater-Pauling rule. If the numbers of valence electrons are differ from 24, and then these materials are magnetic, where the magnetic moment per formula unit is directly related to the number of valence electrons minus 24 ($M = Z_t - 24$). Here M denotes the total magnetic moment per unit cell and Z_t is the total number of valence electrons. An important distinction from the half Heusler compounds is that the full Heusler compounds have two distinct magnetic sub-lattices [17]. For the ferromagnetic half-metallic Heusler compounds, the Curie temperature increases by ~175 K per added electron. For example Co_2CrAl has 27 valence electrons with a saturation magnetization of 3 μ_B/formula unit is ferromagnetic with a magnetic moment that mainly resides on the Co sites with a Curie temperature of ~525 K [11]. From the results, it was observed that the magnetic moment exists mainly on Co and Cr positions, while the Z position atom has negligible small magnetic. It was observed that Z atom having more valence electrons increases more magnetic moments on both sits at Co and Cr. The results also revealed that when Al replaces by Si or Ge or Bi increases the localized magnetic moments on both sites at Co and Cr due to addition of increased valence electrons. As the electro-negativity increases localized magnetic moments are increases at X and Y site. There is a good agreement with the Slater-Pauling behavior. Here we have observed that there are very slight difference between full potential linearized augmented plane wave (FP-LAPW) method implemented in WIEN2k and pseudo-potentials method implemented in ATK-VNL. There is also good agreement between above these methods. The calculated results for magnetic moments for Co_2CrZ (Z= Al, Bi, Ge, Si) obtained using 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 correlation functions is tabulated in Table 4.

Table 4.

Total magnetic moments of the compounds Co_2CrZ (Z= Al, Bi, Ge, Si).

Compound	Z_t	Magnetic moment (μ_B)		
		WIEN2k	ATK	Slater-Pauling (Z_t - 24)
Co_2CrAl	27	3.07	3.15	3.00
Co_2CrBi	29	5.00	5.08	5.00
Co_2CrGe	28	4.00	4.11	4.00
Co_2CrSi	28	4.00	4.08	4.00

Optical properties

Optical properties play an important role to understand the nature of material whether it can be used as optoelectronics device. In the present section, we discuss the optical properties of the compounds Co_2CrZ (Z= Al, Bi, Ge, Si). For the optical properties, we calculate the dielectric function, optical conductivity, reflectivity, excitation coefficient, absorption coefficient and electron energy loss as a function of photon energy for the above compounds. The complex dielectric function describes the optical response of a material on incident electromagnetic radiation.

$$\varepsilon(\omega)=\varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

where $\varepsilon_1(\omega)$ real represents polarization and anomalous dispersion of medium and $i\varepsilon_2(\omega)$ corresponds imaginary part represents the absorption or loss of energy into the medium [28, 29]. The different optical spectra are shown in Figure 6.

The imaginary part of dielectric function for all four compounds shows the main peak in visible region, after that imaginary part of dielectric function decreases continuously. The zero frequency real (ε_1 (ω)) and imaginary part of complex dielectric functions values are 312.370 and 141.991, 299.812 and 111.368, 288.127 and 106.342, 290.688 and 99.095 for the compounds Co_2CrZ (Z= Al, Bi, Ge, Si) respectively as observed from the figure 6 (a) and 6 (b). Optical conductivity is an important optical parameter for conduction of electron due to an applied electromagnetic field. In the optical conductivity spectrum, several peaks are observed between 5.4 - 8.6eV and a sharp peak is observed at 1.6 - 2.3eV. As the material has high absorption coefficient means that they absorb more photon, which excite electron from valence band to conduction band.

The values of absorption coefficient are an increase along the values of energy is increases towards visible region to ultraviolet region as shown in the figure 6 (d). Electron energy-loss function gives the energy loss of a fast moving electron when passing through the medium. The plasma frequency is the frequency corresponding to plasma resonance at which sharp peaks are associated. As if the frequency is above the plasma frequency then the material showing the dielectric behavior and below which the material shows metallic behavior. The maximum energy loss is observed between 11.4 to 13eV for above these compounds as shown in figure 6 (e) and extinction coefficient spectra is displaced in the above figure 6 (h). A prominent peak is shown in the visible region and then value of extinction coefficient is decreases in the ultraviolet region. The values of zero frequency reflectivity are 0.810, 0.802, 0.799 and 0.798 for the compounds Co_2CrZ (Z= Al, Bi, Ge, Si) respectively as observed from figure 6 (f). Noticeably, from the absorption and reflection spectra relation, if the absorption is maximum then obviously reflectivity will be minimum. The region in which material substantially absorbs light and it cannot effectively reflect light in the same span. The refractive index is the important optical property due to wide applications because it determines the dispersive power of prisms, focusing power of lenses, light guiding, and critical angle for total internal reflection etc. How fast light is traveling through the materials is described by refractive index. The values for zero frequency refractive index for the compounds Co_2CrZ (Z= Al, Bi, Ge, Si) are observed as 18.104, 17.602, 17.252 and 17.289 respectively.

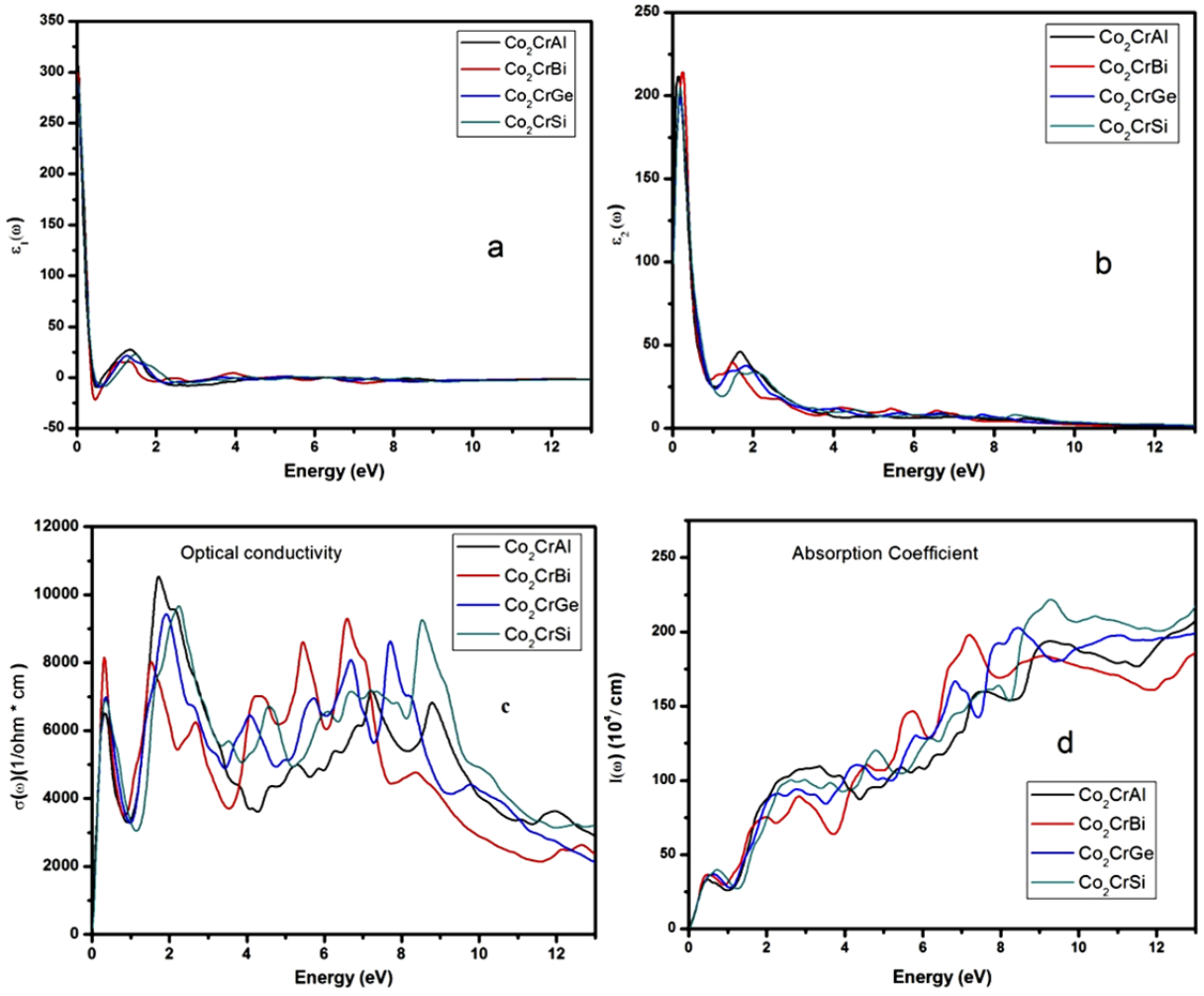

Fig. 6. Calculated optical parameters (a) real part of dielectric function, (b) imaginary part of dielectric function, (c) optical conductivity, (d) absorption coefficient, (e) electron energy-loss function, (f) reflectivity, (g) refractive index and (h) extinction coefficient for Co_2CrZ (Z= Al, Bi, Ge, Si).

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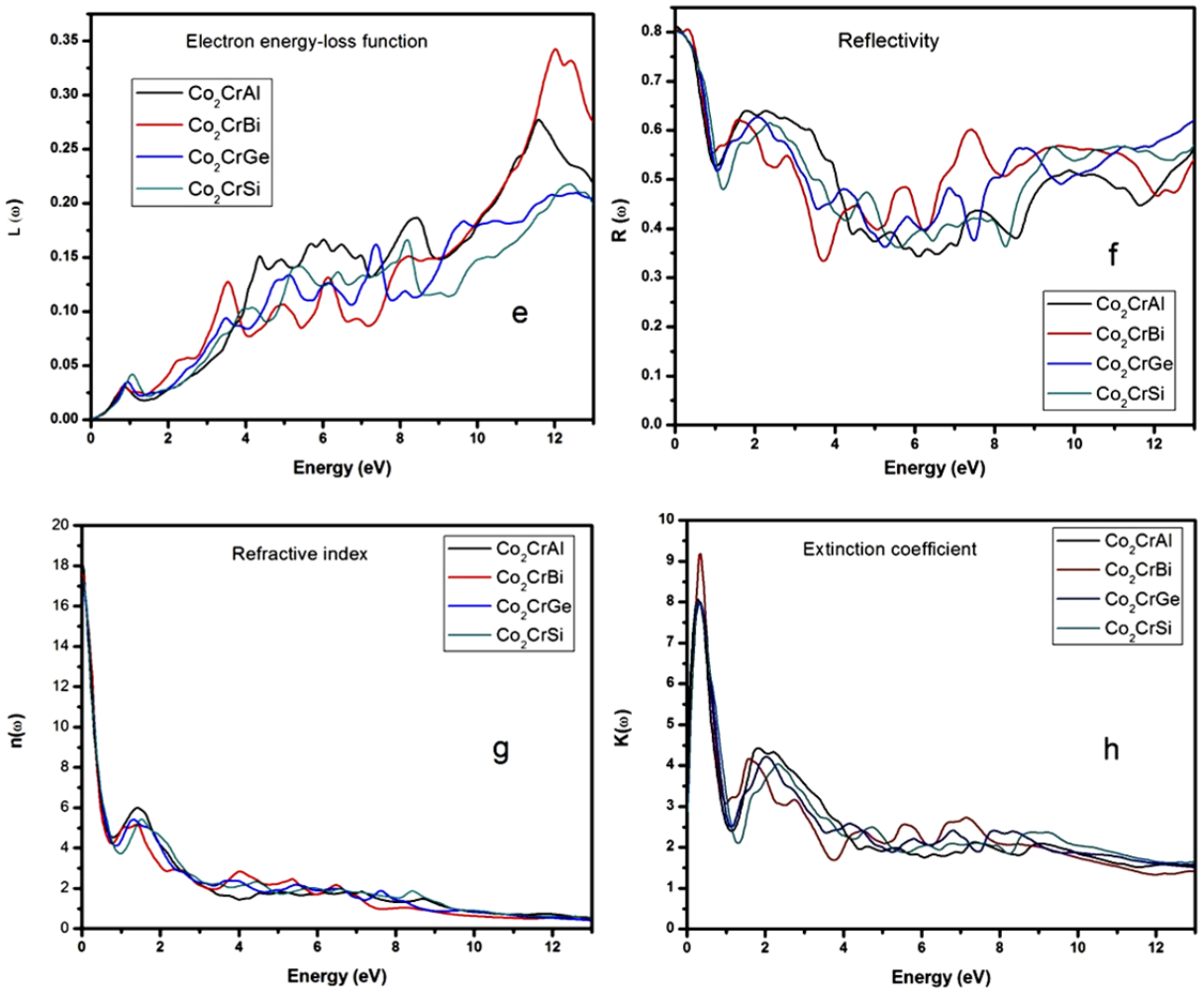

Fig. 6. *(continued)* Calculated optical parameters (a) real part of dielectric function, (b) imaginary part of dielectric function, (c) optical conductivity, (d) absorption coefficient, (e) electron energy-loss function, (f) reflectivity, (g) refractive index and (h) extinction coefficient for Co_2CrZ (Z= Al, Bi, Ge, Si).

CONCLUSIONS

Structural, electronic, optical and magnetic properties of Co_2CrZ (Z= Al, Bi, Ge, Si) compounds have been studied by using 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-correlation functional. From this study we have found that most of the compounds show half metallicity and 100% spin polarization with $L2_1$ ordered stable structures. Calculated magnetic moments have good agreement with the Slater-Pauling behavior. For above listed compounds, the optical properties named as reflectivity, refractive index, excitation coefficient, absorption coefficient, optical conductivity and electron energy loss have been calculated. Also, we have analyzed their optical spectra. The predicted results of Co_2CrZ (Z= Al, Bi, Ge, Si) are suitable for Spintronic applications.

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СТРУКТУРНІ, ЕЛЕКТРОННІ, ОПТИЧНІ ТА МАГНІТНІ ВЛАСТИВОСТІ СПОЛУК ХІСЛЕРА Co_2CrZ (Z = Al, Bi, Ge, Si)

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У цій роботі ми вивчили структурні, електронні, оптичні та магнітні властивості сполук Co_2CrZ (Z = Al, Bi, Ge, Si) за допомогою двох різних методів, один – це метод повноцінної лінеаризованої розширеної плоскої хвилі (FP-LAPW) реалізований у WIEN2k, а другий – псевдопотенційний метод, реалізований у Atomistic Tool Kit-Virtual NanoLab (ATK-VNL). Відповідні заборонені зони для Co_2CrZ (Z = Al, Bi, Ge, Si) знаходяться біля рівня Фермі 0,696, 0,257, 0,602 і 0,858 еВ, що реалізовано в коді WIEN2k і показують 100% спінову поляризацію. Крім того, було виявлено, що ці сполуки є ідеально напівметалічними феромагнітами (HMF). Однак вищезгадані сполуки показують нульові заборонені зони в коді ATK-VNL. Обчислений методом FP-LAPW магнітний момент цих сполук Co_2CrZ (Z = Al, Bi, Ge, Si) становить 3,06, 4,99, 3,99 і 3,99 μ_B відповідно. Однак у коді ATK-VNL відповідний магнітний момент цих сполук становить 3,14, 5,08, 4,11 та 4,08 μ_B. Оптичні властивості відіграють важливу роль для розуміння природи матеріалу, чи можна його використовувати як пристрій оптоелектроніки. Обчислені з оптичних спектрів комплексні діелектричні функції з використанням WIEN2k становлять 312,70 і 141,991, 299,812 і 111,368, 288,127 і 106,342, 290,688 і 99,095 для сполук Co_2CrZ (Z = Al, Bi, Ge, Si) відповідно. Максимальні втрати енергії для вище зазначених сполук спостерігаються між 11,4 до 13еВ. Значення показника заломлення для сполук Co_2CrZ (Z = Al, Bi, Ge, Si) спостерігаються як 18.104, 17.602, 17.252 і 17.289 відповідно. В спектрі оптичної провідності різкий пік спостерігається при 1,6 - 2,3еВ.

КЛЮЧОВІ СЛОВА: напівметалічний феромагнетик, заборонена зона, діелектрична константа, магнітний момент

СТРУКТУРНЫЕ, ЭЛЕКТРОННЫЕ, ОПТИЧЕСКИЕ И МАГНИТНЫЕ СВОЙСТВА СОЕДИНЕНИЙ ХИСЛЕРА Co_2CrZ (Z = Al, Bi, Ge, Si)

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В этой работе мы изучили структурные, электронные, оптические и магнитные свойства соединений Co_2CrZ (Z = Al, Bi, Ge, Si) с помощью двух различных методов, один - это метод полноценной линеаризованной расширенной плоской волны (FP-LAPW) реализован в WIEN2k, а второй - псевдопотенциальный метод, реализованный в Atomistic Tool Kit-Virtual NanoLab

(ATK-VNL). Соответствующие запретные зоны для Co_2CrZ (Z = Al, Bi, Ge, Si) находятся около уровня Ферми 0,696, 0,257, 0,602 и 0,858 эВ, что реализовано в коде WIEN2k и показывают 100% спиновую поляризацию. Кроме того, было обнаружено, что эти соединения являются идеально напивметаличнимы ферромагниты (HMF). Однако вышеупомянутые соединения показывают нулевые запретные зоны в коде ATK-VNL. Исчисленный методом FP-LAPW магнитный момент этих соединений Co_2CrZ (Z = Al, Bi, Ge, Si) составляет 3,06, 4,99, 3,99 и 3,99 μ_B соответственно. Однако в коде ATK-VNL соответствующий магнитный момент этих соединений составляет 3,14, 5,08, 4,11 и 4,08 μ_B. Оптические свойства играют важную роль для понимания природы материала, можно ли его использовать как устройство оптоэлектроники. Вычисленные из оптических спектров комплексные диэлектрические функции с использованием WIEN2k составляют 312,70 и 141,991, 299,812 и 111,368, 288,127 и 106,342, 290,688 и 99,095 для соединений Co_2CrZ (Z = Al, Bi, Ge, Si) соответственно. Максимальные потери энергии для вышеуказанных соединений наблюдаются между 11,4 до 13эВ. Значение показателя преломления для соединений Co_2CrZ (Z = Al, Bi, Ge, Si) наблюдаются как 18.104, 17.602, 17.252 и 17.289 соответственно. В спектре оптической проводимости резкий пик наблюдается при 1,6-2,3эВ.

КЛЮЧЕВЫЕ СЛОВА: полуметаллический ферромагнетик, запретная зона, диэлектрическая постоянная, магнитный момент