EAST EUROPEAN JOURNAL OF PHYSICS
East Eur. J. Phys. **4**. 42-50 (2020) DOI:10.26565/2312-4334-2020-4-06

PACS: 71.15.Mb; 71.20.−b; 71.55.Ak

STRUCTURAL, ELECTRONIC, MECHANICAL AND THERMAL PROPERTIES OF CoVZ (Z= Si, Ge, Sn, Pb) HALF-HEUSLER COMPOUNDS

Lalit Mohan[a], Sukhender[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*
Received August 25, 2020; accepted September 15, 2020

Half-Heusler compounds pose unusual behavior because of their variable band gap and as well as both metallic and semi-metallic nature. These compounds can be used in different applications on the basis of band gap tenability. We have discussed the structural, electronic, elastic and magnetic properties of CoVZ (Z = Pb, Si, Sn, Ge) by using WIEN2k simulation code based on density functional theory (DFT). We have optimized the all-possible structural configuration of each compound and considered which optimized with lowest energy and lowest equilibrium volume. For determination of electronic exchange correlation energy, the generalized gradient approximation (GGA) is used in both platforms. We have also obtained the individual elastic constants, shear modulus, Young's moduli, B/G ratio and Poisson's ratio, which shows that these compounds are ductile except CoVGe shows little ductility. Debye temperatures are calculated by compression wave velocity, shear wave velocity and with their average value.
KEYWORDS: Half-Heusler compounds, structural properties, electronic properties, mechanical properties

The structure of Half Heusler compounds is a combination of rock salt and zinc blend type sublattices. This class of compounds can be represented as XYZ (Pb, Si, Sn, and Ge) type. Half-Heusler compounds, crystallize in the face-centered cubic having structurbericht designation C1b with the space group F-43 m [1]. These compounds can be viewed as Co and V form zinc blend sublattice arranged in a primitive cell at Wyckoff positions (0, 0, 0) and $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ whereas NaCl sublattice is formed by V and Z at $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. We can also mention the ordering by interchanging above said Wyckoff positions, but the preferred atomic arrangements have a dependency on the size of involved atoms and the inter-atomic interaction between them [2-4]. Nevertheless, the size dependence on the transition metal configuration is the predominant influence over the inter-atomic interaction formed by the electronegativity of atoms. One can study the properties of such compounds simply by knowing the number of valence electrons per formula [5]. The properties of these XYZ compounds are highly dependent on the concentration of the number of valence electrons (n_v) in the primary cell, which predict the band structure and physical properties of the compounds [6].

The half Heusler compounds can be used to decrease electric power consumption by using them in photovoltaic devices. The most efficient way to do so is by transforming sunlight into electrical energy using semiconductor-based materials products. It is found that compounds with eight valence electrons are likely to be classic semi-conducting behaviors such as GaAs, Si. As with a K-shell, these valence electrons are tightly bound, as a result of which some gap separates the conduction and valence band. Similarly, the half Heusler compounds demonstrate the same behavior with the composition of the first, second and fifth group elements and can be used as traditional semiconductors to replace classical ones. The same behavior, however, is observed in compounds with 18 and 24 valence electrons.

In this study, we have 18 valence electrons compounds and it has been observed that this particular valence electrons count alloys shows the semiconducting behavior in both majority and minority spin states. The alloy's elastic constants are important mechanical properties, as well as correlated with other thermodynamic properties such as Debye temperature specific heat and heat of expansion. In addition, the elastic constants also provide useful information about the anisotropic bonding as well as mechanical stability. We have obtained the individual elastic constants, shear modulus, Young's moduli, B/G ratio and Poisson's ratio, which shows that these compounds are ductile [7,8]. The Debye temperatures obtained from the average sound velocity and have been discussed. In this paper, we have used the first-principles calculations to systematically examine structural, mechanical, electronic and magnetic stability to explore the potential properties of these compounds.

COMPUTATIONAL DETAIL

In order to explain the interaction between atomic core and valence electrons, the first principles calculations are made using the full potential linearized augumated plane wave (FP-LAPW) method implemented in the WIEN2k simulation code [9,10]. The electronic wave function is extended keeping in mind the valance electrons. Generalized gradient approximation (GGA) is used at Perdew-Burke-Ernzerhof (PBE) to define the energy of exchange-correlation [11-13]. To optimize the geometry of the electronic structure; we have used the FP-LAPW method, which is the part of the spin-polarized density functional theory (SDFT). The value of l_{max} is taken as 4 to extend the spherical harmonics in the atomic sphere. In the central region, the charge density and the potential were developed as Fourier series

with a wave vector up to G_{max} = 12. The muffin-Tin radii of a particular atomic sphere as per the alloys studied and are listed in Table 1 [14]. The RK_{max} value are 6.68, 6.85, 6.84, 6.86 for CoVZ (Z= Si, Ge, Sn, Pb). Core states are considered relativistic and valence states are considered semi-relativistic, and the energy between these two states has been set -6.0 Ry. The SCF cycle are considered to be converged; when the energy difference and the integration of absolute charge density difference between subsequent iterations is less than 10^{-5} Ry and 0.001 Coulomb/formula unit respectively. Total numbers of K - point are kept 1000 for irreducible Brillouin zones in Wien2k. ElaStic_1.0 based on ab initio total-energy and/or stress calculations is used to calculate the full second-order elastic stiffness tensor for crystal structures. The maximum absolute value for Lagrangian strain is considered to be 0.5 with number of distorted strain structure are set to value 11.

Table 1.

For the prevention of overlapping spheres during the SCF process, the muffin-Tin radii of the specific atomic sphere for optimized lattice parameter of the individual alloy are shown.

Compounds / **Atom**	**CoVSi**	**CoVGe**	**CoVSn**	**CoVPb**
Co	2.2	2.30	2.36	2.35
V	2.09	2.19	2.30	2.35
Z	1.82	2.19	2.36	2.47

RESULT AND DISCUSSION

The lattice constants were determined in the first step. The total energies are measured as a function of the lattice constant for the said compounds with a half-Heusler structure. The constants for the equilibrium lattice were obtained by minimizing the total energy.

Structural Properties

Half-Heusler compounds, crystallize in the face-centered cubic having structurbericht designation C1b with the space group F-43 m. These compounds can be viewed as V and Co form zinc blend sublattice arranged in a primitive cell at Wyckoff positions (0, 0, 0) and $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$; whereas NaCl sublattice is formed by V and Z at $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. Volume optimization has been performed for all possible arrangements of each compounds based on the Murnaghan equation of state. The volume vs. energy curves is shown in Figure1 and which has minimum energy and electronegativity order is to be considered [15-17].

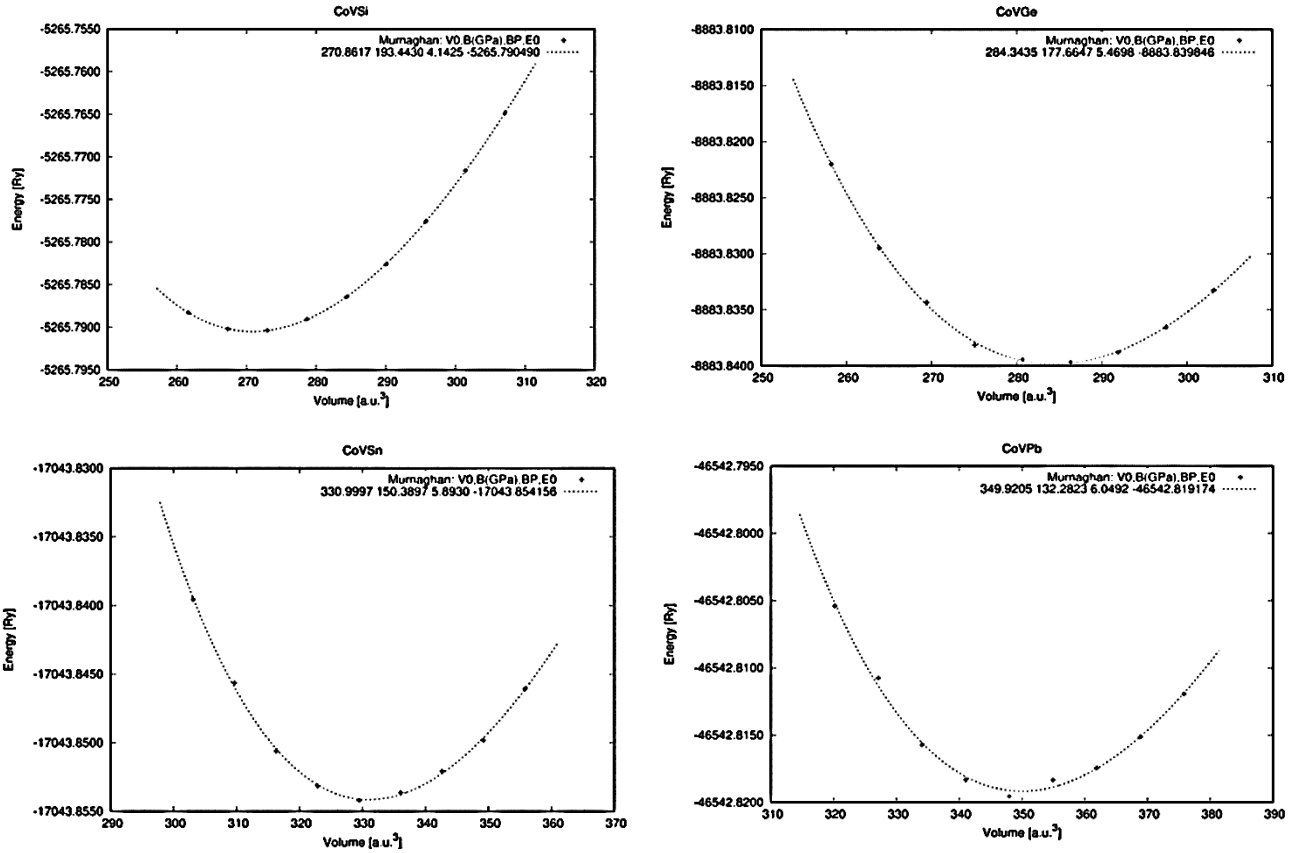

Figure 1. Total energy as a function of volume per formula unit corresponding to CoVSi, CoVGe, CoVSn and CoVPb alloys.

For the each arrangement electronegativity and energy for CoVPb are tabulated in Table 2.

Table 2.

We displayed the measured values of the equilibrium lattice constant a_0, equilibrium volume, the bulk modulus B (GPa), the bulk modulus pressure derivative and minimum energy during optimization.

	Co	**V**	**Pb**	**Energy (Ry)**	**Equilibrium Volume (a.u.^{3})**	**Band Gap (eV)**
Electronegativity	1.88	1.63	2.33			
Type a	$(\frac{1}{4},\frac{1}{4},\frac{1}{4})$	(0, 0, 0)	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	-46542.82	349.97	0.69
Type b	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$(\frac{1}{4},\frac{1}{4},\frac{1}{4})$	(0, 0, 0)	-46542.73	389.50	0
Type c	(0, 0, 0)	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$(\frac{1}{4},\frac{1}{4},\frac{1}{4})$	-46542.67	415.20	0

Murnaghan's state equation [18] provides the total energy and pressure value as a function of volume and is described as:

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

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

The structural parameters values have been presented in Table 3. To predict the electronic and magnetic properties of compounds, the optimized value of the lattice constant was used for the DOS, band structures and magnetic moment calculations.

Table 3.

Calculated values of the equilibrium lattice constant a_o, equilibrium volume, the bulk modulus B (GPa), the pressure derivative of bulk modulus B_P and minimum energy during optimization.

Compound	Lattice Parameter (A^0)	Equilibrium Volume (V_0)	Bulk Modulus (GPa)	B_P	Energy
CoVSi	5.44	270.85	193.97	4.42	-5265.79
CoVGe	6.30	283.89	176.87	10.77	-8883.84
CoVSn	5.81	330.99	150.23	5.89	-17043.85
CoVPb	5.92	349.97	131.67	5.82	-46542.82

Electronic Properties

To get an in-depth analysis of the electronic structure for the CoVZ alloys (Z = Si, Ge, Sn, Pb), which have 18 valence electrons respectively, we first analysis their complete DOS configuration. Because the half-metallic band gap is an important factor in these materials partial DOS are also shown in Fig. 2 for all the four compounds.

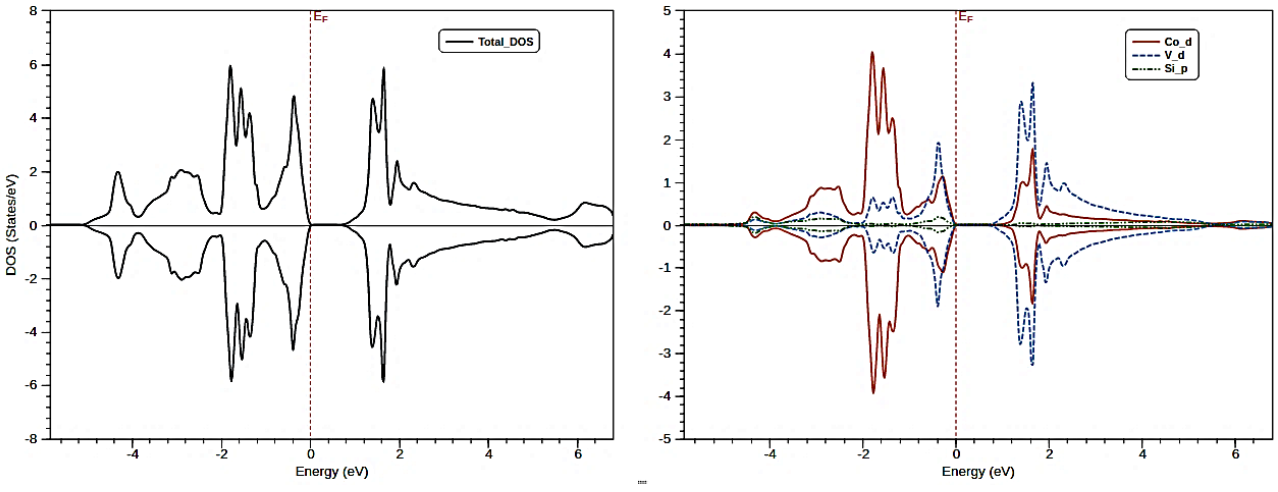

Figure 2. Total and atomic spin- density of states of all the compounds at their equilibrium lattice constant. Negative of DOS axis represents the minority spin (*Continued on next page*)

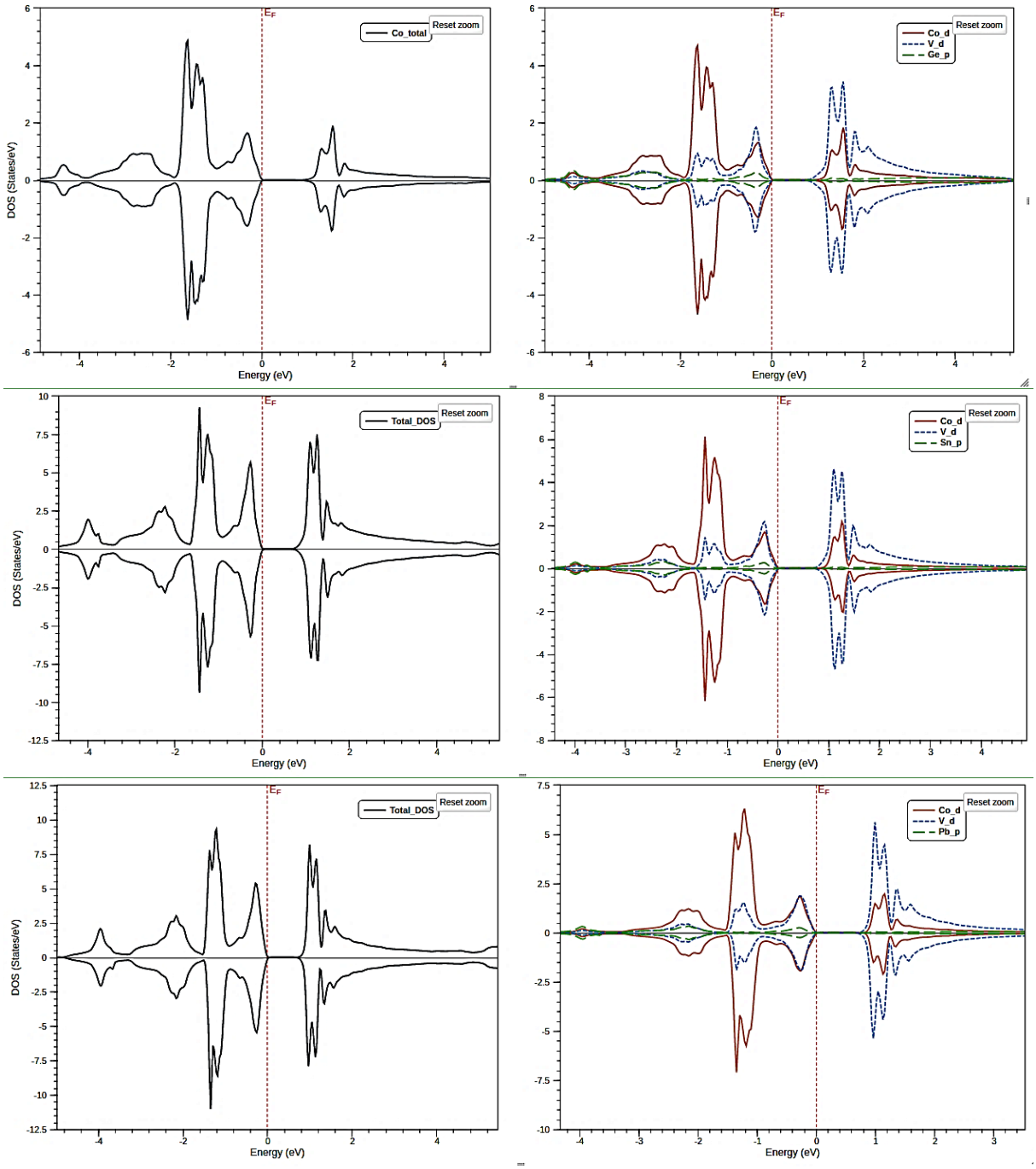

Figure 2. Total and atomic spin-density of states of all the compounds at their equilibrium lattice constant
Negative of DOS axis represents the minority spin

As illustrated in Fig. 2, their shapes are similar and the characters can be defined as follows: the low-energy component below -4.5eV, -3.7 eV, -4 eV, -3.5 eV is primarily the p states of the Si, Ge, Sn, Pb atom in the occupied valence states, which hybridize the Co atoms with and d electrons and decide the degree of occupation of the p – d orbitals. 3d metal atom states range from -0.5 to + 5.3eV, and hybridize with each other. CoVZ chemical bonding character can be studied from the density of State. It is evident from the partial densities of the figure below that the key mechanism of the chemical bond is the hybridization between the Co and V's d- states. Chemical bond has a covalent and ionic character at the same time, covalent since the d states of both transition elements are strongly hybridized and degenerate over much of their extension and ionic because the relative quantity of the 3d states of Co and V is different below and above Fermi point, the 3d states of V dominate.

To determine the band gap, we have also calculated the band structures of Half-Heusler compounds as shown in Figure 4. In the band structure of all half Heusler compounds, the valence band maximum (VBM) is at the W-point and the conduction band minimum (CBM) at the X-point. Thus, the band structure shows semiconducting behavior with an indirect energy gap. The origin of the gap is mainly attributed to the covalent hybridization between the d-states of the Co and V atoms, leading to the formation of bonding and anti-bonding bands with a gap in between [19].

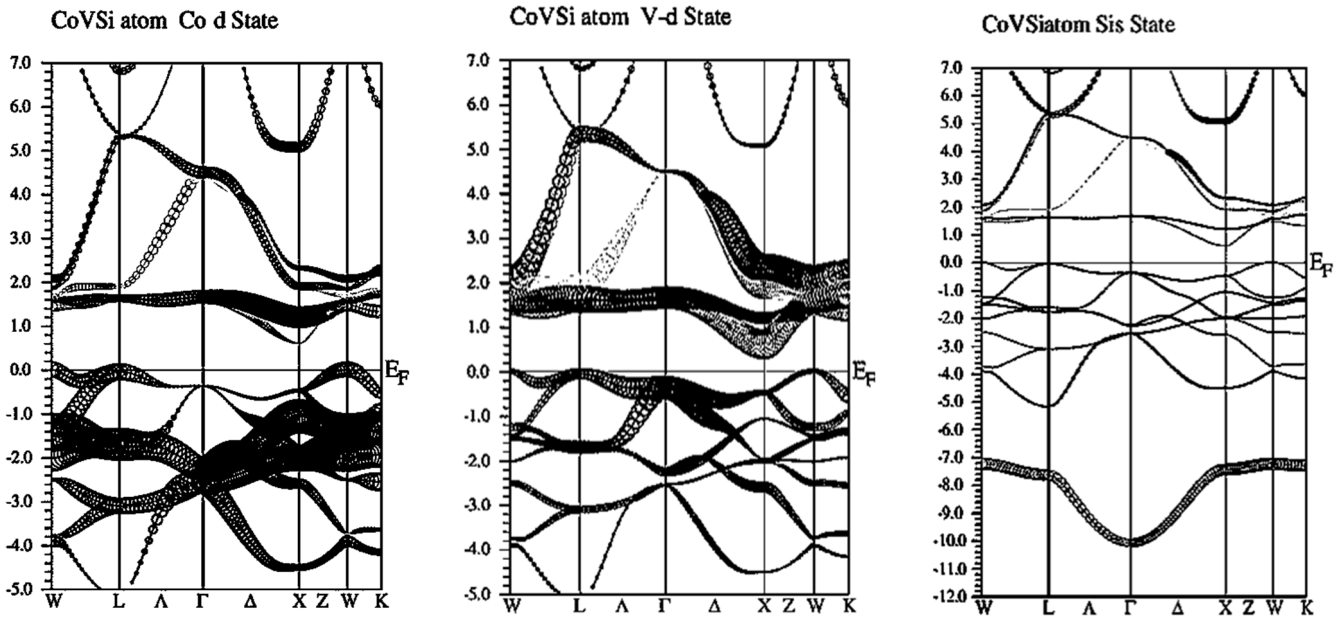

Figure 3. Orbital projected band structure of CoVSi for Co-d, V-d & Si-p states.

The orbital projected band structures (wide bands) of CoVSi as shown in Figure 3. The nearest V coordinating neighbors are 4 Co and 4 Si atoms. Analogous to the binaries, we have obtained in Figure 3 that the lowest bands below -5 eV are Si - p bands, separated by a pseudo gap from seven primarily V - d bands, which in turn are separated by an indirect gap from relatively wide Co-d bands. The relative positions of the Fe d and V d levels with respect to the Sb p levels are summarized in Table 4. The characteristic feature of all half-Heusler compounds is a d–d gap close to the Fermi level. All the states below this gap are occupied for the 18 valance electrons compounds; due to this the compound with 18 valence electrons doesn't have half metallic nature as shown by compounds with more than 18 valence electrons.

Table 4.

Indirect band gaps for hybridized d states and total energy band gaps

Compound	Co			V			E_g	Band Transition
	E_d	E_{eg}	E_{t2g}	E_d	E_{eg}	E_{t2g}		
CoVSi	0.44	0.45	0.61	0.23	0.28	0.56	0.59	W→X
CoVGe	0.51	0.53	0.71	0.28	0.29	0.64	0.69	L→X
CoVSn	0.45	0.5	0.64	0.21	0.57	0.55	0.66	L→X
CoVPb	0.47	0.48	0.71	0.16	0.28	0.49	0.69	L→X

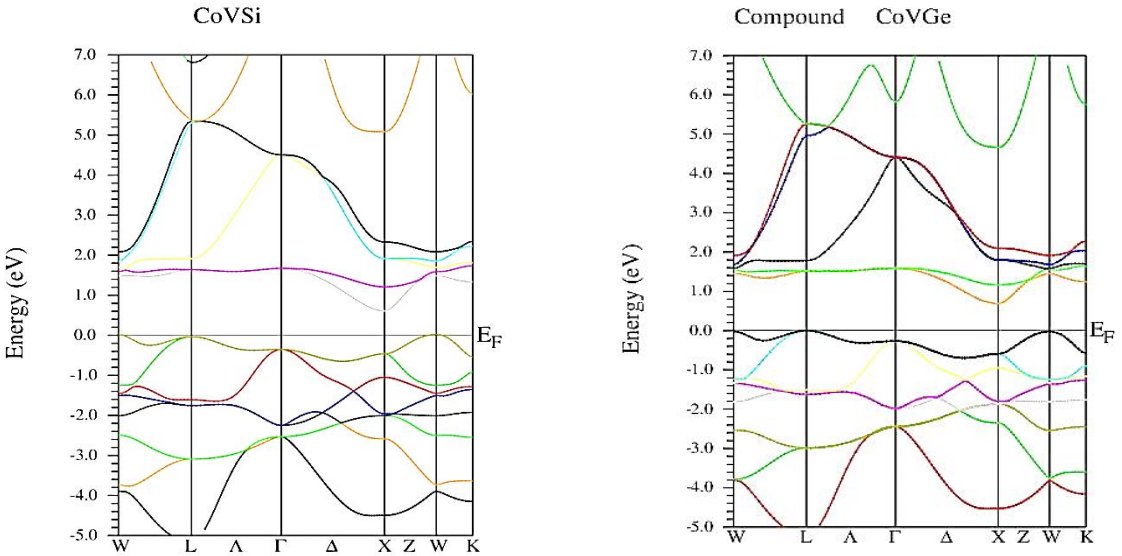

Figure 4. Band structure diagram of compounds corresponding to their equilibrium lattice constant.
(*Continued on next page*)

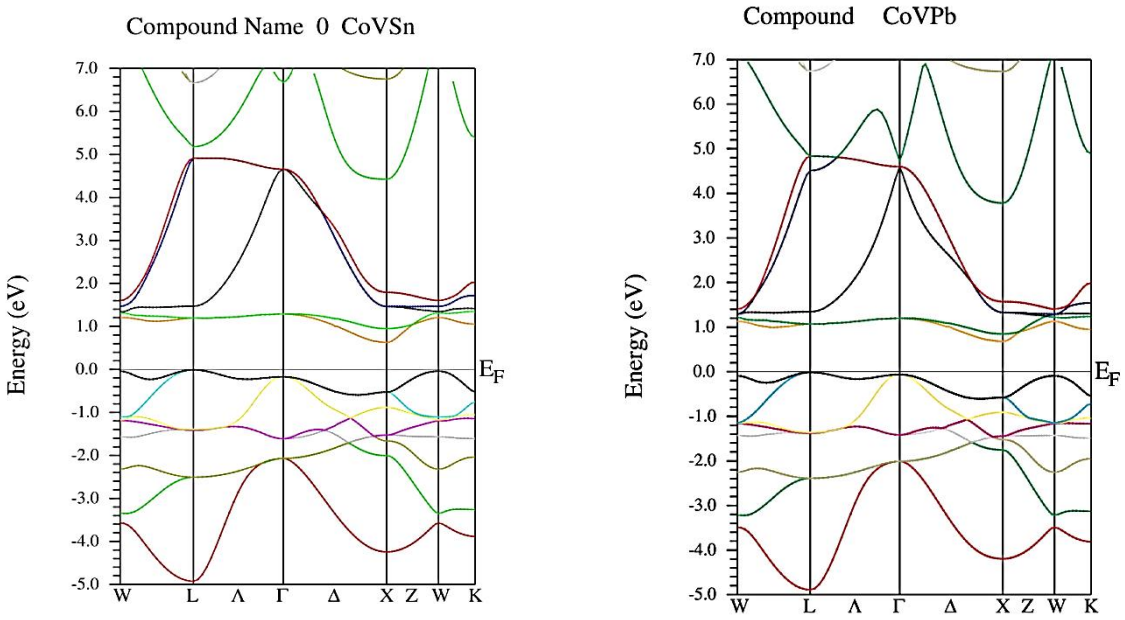

Figure 4. Band structure diagram of compounds corresponding to their equilibrium lattice constant.

Elastic properties

Hardness, stress and other structural deformations caused by pressure have been examined with the help of elastic constant. These constants play an important role in studying the Poisson ration effect, Young's modulus, Shear modulus, Debye temperature, and melting temperature of solid. They have three distinct elastic constants for cubic crystal namely C_{11}, C_{12} and C_{44}. Here the C_{ij} are the elastic constant tensors (in Voigt notation) resulting from the change in internal energy deformation [20,21]. The bulk modulus B defines the resistance of the solid to volume change and the shear modulus takes into account its resistance to shear deformation preserving volume.

Mechanical stability. Elastic structures play a significant role in the research and development of materials. Elastic tensors of any order are characterized by Taylor's expansion of the elastic energy or stress in terms of the applied strain. To define the dynamic and mechanical behavior of studied alloys there are three second – order elastic constants (SOEC) C_{11}, C_{12} and C_{44} need to be determined. According to Hooke's law, for cubic crystal structures, there are only three distinct elastic constants C_{11}, C_{12} and C_{44}. From the symmetry of the second – order elastic constant matrix in Voigt notation

$$C_{11}=C_{22}=C_{33}; \qquad C_{12}=C_{13}=C_{23}; \qquad C_{44}=C_{55}=C_{66}.$$

None of the eigen value of elastic constant matrix is zero confirms the stability of compound.
Apart from this condition, the stability criteria based on Born's theory given below [22]

$$C_{11}>0; \qquad C_{44}>0; \qquad C_{11}>|C_{12}|; \qquad (C_{11}+2C_{12})>0.$$

Computation of elastic properties. The elastic constants of the cubic crystals are assumed to be compatible with the above stability conditions, so studied XYZ compounds are mechanically stable. Different elastic properties based on SOEC's have shown in Table 5, 6 and 7 in Voigt, Reuss and Hill averaging scheme from elastic constants [23, 24]. The Shear constant C_S and elastic stiffness constant C_L are expressed in terms of SOECs as

$$C_s = \frac{C_{11}-C_{12}}{2}, \; C_L = \frac{C_{11}+C_{12}+2C_{44}}{2}$$

Bulk modulus (B), the measure of compressibility resistance have measured using the expression

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

The bulk modulus for a cubic structure is same for Voigt, Reuss and Hill averages [25].Shear modulus (G) is the deformation caused by force applied on any parallel face by keeping opposite face fixed by applying opposite forces,

$$G_V = \frac{C_{11}-C_{12}+3C_{44}}{5} \qquad \text{and} \qquad G_R = \frac{5C_{44}(C_{11}-C_{12})}{4C_{44}+3(C_{11}-C_{12})}$$

The Young's modulus (E) and Poisson's ratio (η) are calculated by the following relation [26]

$$E = \frac{9BG}{3B+G} \qquad \text{and} \qquad \eta = \frac{3B-E}{6B}$$

To quantify the anisotropy of these cubic crystals Zener's anisotropy index (A) can be calculated as

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

The degree of elastic anisotropy (A^*) has some practical importance. If A^* has value zero or A=1 crystal represent elastic isotropy and A^* gives relative magnitude of the actual elastic anisotropy possessed by crystal.

$$A^* = \frac{3(A-1)^2}{\{3(A-1)^2 + 25A\}}$$

Kleinman parameter (ζ) and Lame's coefficient (λ) for cubic crystals can be obtained as:

$$\zeta = \frac{C_{11}+8C_{12}}{7C_{11}+2C_{12}}; \qquad \lambda = C_{12} - \frac{A}{5}$$

Hardness of a material is determined by Vickers hardness factor (H_V) followed by relation [27]

$$H_V = 2[(K^2G)^{0.585} - 3]$$

Where K is the Pugh ratio define as [28]; $K = \frac{B}{G}$

Table 5.

Elastic constants of CoVSi,CoVGe,CoVSn and CoVPb in the units of GPa.

Compounds	**CoVSi**	**CoVGe**	**CoVSn**	**CoVPb**
C_{11}	295.10	294.20	223.60	204.60
C_{12}	135.70	113.30	108.80	106.90
C_{44}	89.00	119.30	92.70	82.60

Table 6.

Voigt bulk modulus(B_V), shear modulus(G_V), Young modulus (E_V), Poisson ratio(η_V), Reuss bulk modulus(B_R), shear modulus(G_R), Young modulus (E_H), Poisson ratio(η_V), Hill bulk modulus(B_H), shear modulus(G_H), Young modulus (E_H), Poisson ratio(η_H) and B/G ratio calculated from ElaStic_1.0.

Compounds	**CoVSi**	**CoVGe**	**CoVSn**	**CoVPb**
B_V= B_R= B_H	188.84	173.60	147.07	139.47
G_V	85.25	107.78	78.58	69.09
G_R	85	105.83	74.39	64.72
G_H	85.13	106.81	76.48	66.90
E_V	222.30	267.91	200.11	177.89
E_R	221.73	263.87	190.96	168.14
E_H	222.02	265.89	195.55	173.04
η_V	0.30	0.24	0.27	0.29
η_R	0.30	0.25	0.28	0.30
η_H	0.30	0.24	0.28	0.29
B_H/G_H	2.22	1.63	1.92	2.09

Table 7.

Values of Zener anisotropy index (A), degree of elastic anisotropy in percentage (A^*), Kleinman parameter (ζ), Lame's coefficient (λ), Pugh ratio (K) and Vickers hardness of material.

Compounds	**CoVSi**	**CoVGe**	**CoVSn**	**CoVPb**
A	1.12	1.32	1.62	1.69
A^*(%)	0.15	0.92	2.75	3.27
ζ	0.59	0.53	0.61	0.64
λ	-0.05	-0.14	-0.13	-0.12
K	0.45	0.62	0.52	0.48
H_V	4.61	11.4	5.77	3.9

Thermodynamic Properties

Many physical properties of solids such that acoustic velocity, specific heat capacity, thermal expansion coefficient, elastic constants and melting temperature are related to Debye's temperature [29]. At low temperature, the vibrational excitation is induced solely by the acoustic vibrations, so that Debye temperature derived from elastic constants is the same as that determined by specific heat measurements. From the data of elastic properties of the materials, we have calculated the wave velocity V_S, longitudinal wave velocity V_P and average wave velocity V_m and obtained from Navier's equation given below listed in Table 8 [30, 31]

$$V_S = \left[\frac{G_H}{\rho}\right]^{\frac{1}{2}};\quad V_P = \left[\frac{B_H + \frac{4}{3}G_H}{\rho}\right]^{\frac{1}{2}};\quad V_m = \left[\frac{\frac{2}{V_S{}^3} + \frac{1}{V_P{}^3}}{3}\right]^{\frac{-1}{3}}$$

Another method to calculate Debye temperature is to estimate it from average elastic wave velocity V_m is represented as

$$\theta_D = \frac{\hbar}{k}\left[\frac{3n}{4\pi}\left(\frac{N\rho}{M}\right)\right]^{1/3} \nu_m$$

here *h*, K, N, n, M are plank's constant, Boltzmann's constant, Avogadro's number, number of atoms per formula unit, molecular mass per formula unit respectively, ρ=M/V is the density of compound.

Table 8.

Thermodynamic parameters shear wave velocity (V_S), compression wave velocity (V_p), average wave velocity (V_m), molecular mass (M), crystal volume (V), density (ρ).

Compounds	**CoVSi**	**CoVGe**	**CoVSn**	**CoVPb**
M(g/mol)	137.96	182.51	228.58	317.07
V(a.u^3)	160.99	250.05	367.06	543.34
ρ(g/cc)	5.69	4.85	7.74	10.15
V_S	3867.99	4692.83	3143.43	2567.32
V_P	7289.48	8072	5672.40	4746.48
V_m	4322.68	5206.73	4787.94	4634.16
θ_D	565	588	586	556

SUMMARY AND CONCLUSIONS

In this paper, we have presented first-principles calculations on cubic CoVZ (Z = Pb, Si, Sn, Ge) half Heusler compounds including structural parameters, structural stability, band structure, density of state, elastic constants, Debye temperature and velocity of the acoustic wave in different directions. We have observed that for structure stabilities of these Heusler compounds, the electronegativity is an important factor to select the suitable structural arrangement. These compounds have indirect band gap and can be used in solar cell applications over the similar compounds obey Nowotny–Juza phase. Apart from this, these compounds also have useful aspects towards thermoelectric devices and topological insulators. Elastic properties of these compounds show that they have ductile nature except CoVGe, which is close to ductility. The Poisson ratio of CoVGe represent covalent character and others have metal character; which have predicted by their narrow band gaps. The hardness of materials can be compared by arranging them in decreasing order i.e. CoVGe>CoVSn>CoVSi>CoVPb. Debye's temperature is also calculated with the help of compressed, strained, average wave velocities.

ORCID IDs

Lalit Mohan, https://orcid.org/0000-0003-3323-8296; **Sukhender**, https://orcid.org/0000-0002-2149-5669
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

REFERENCES:

[1] G.E Bacon, and J.S Plant, J. Phys. F: Metal. Phys. **1,** 524-532 (1971), https://doi.org/10.1088/0305-4608/1/4/325.
[2] A. Zakutayev, X. Zhang, A. Nagaraja, L. Yu, S. Lany, T. O. Mason, D. S. Ginley, and A. Zunger, J. Am. Chem. Soc. **135** (2013) 10048-10054, https://doi.org/10.1021/ja311599g.
[3] P. Villars, and L.D Calvert, *Pearson's handbook of crystallographic data for intermetallic phases*, (ASM International, Materials Park, OH, 1991).
[4] J. Nuss, and M. Jansen, Z. Anorg. Allg. Chem. **628**, 1152-1157 (2002), https://doi.org/10.1002/1521-3749(200206)628:5%3C1152::AID-ZAAC1152%3E3.0.CO;2-1.
[5] C. Felser, G. H Fecher, and B. Balke, Ang. Chem. Int. Ed. Engl. **46**, 668-699 **(**2007), https://doi.org/10.1002/anie.200601815.
[6] J. Pierre, R.V. Skolozdra, J. Tobola, S. Kaprzyk, C. Hordequin, M.A. Kouacou, I. Karla, R. Currat, and E. Leliévre-Berna, Properties on request in semi-Heusler phases, J. Alloys & Comp. **262**, 101-107 (1997), https://doi.org/10.1016/S0925-8388(97)00337-X.
[7] K. Chen, and L.R. Zhao, J. App. Phy. **93**, 2414 (2003), https://doi.org/10.1063/1.1540742.
[8] K. Chen, L.R. Zhao, J.S. Tse, and J.R. Rodgers, Phys. Lett. A. **31**, 400-403 (2004), https://dx.doi.org/10.1016/j.physleta.2004.09.034.
[9] P. Blaha, K. Schwarz, F. Tran, R. Laskowski, G.K.H Madsen, and D.L. Marks, J. Chem. Phys. **152**, 074101 (2020), https://doi.org/10.1063/1.5143061.
[10] K. Schwarz, P.G.K. Blaha, and H. Madsen, Comput. Phys. Commun. **147**, 71 (2002), http://sciold.ui.ac.ir/~sjalali/jalali/paper/LAPW/compu_phys_commu147_71_02.pdf.
[11] Z. Wu, and R.E. Cohen, Phys. Rev. B **73**, 235116 (2006), https://doi.org/10.1103/PhysRevB.73.235116.
[12] F. Tran, R. Laskowski, P. Blaha, and K Schwarz, Phys. Rev. B **75**, 115131 (2006), https://doi.org/10.1103/PhysRevB.75.115131.
[13] J. P Perdew, K Burke, and M Ernzerhof, Generalized gradient approximation made simple, Phys. Rev. Lett. **77**, 3865 (1996).

[14] B.M. Wong, and J.G. Cordaro, J. Phys. Chem. C **115**, 18333-18341 (2011), https://doi.org/10.1021/jp204849e.
[15] H.U. Schuster, H.W. Hinterkeuser, W. Schäfer, and G. Will, Z. Naturforsch. B, **31**, 1540-1541 (1976).
[16] H. Hohl, A. P. Ramirez, C. Goldmann, G. Ernst, B. Wolfling, and E. Bucher, J. Phys. Condens. Matter. **11**, 1697–1709 (1999), https://doi.org/10.1088/0953-8984/11/7/004.
[17] C.P. Sebastian, H. Eckert, S. Rayaprol, R.D. Hoffmann, and R. Pöttgen, Solid State Sciences, **8**(5), 560-566 (2006), https://doi.org/10.1016/j.solidstatesciences.2006.01.005.
[18] F.D. Murnaghan, Proc. Natl. Acad. Sci. **30**, 244–247 **(**1944), https://dx.doi.org/10.1073%2Fpnas.30.9.244.
[19] J. Toboła, and J. Pierre, J. Alloys and Comp. **296**, 243-252 (2000), https://doi.org/10.1016/S0925-8388(99)00549-6.
[20] M. Catti, Acta Cryst. A, **45**, 20-25 (1989), https://doi.org/10.1107/S0108767388008748.
[21] P. Dobson, Physics Bulletin, **36**, 506-506 (1985), https://doi.org/10.1088/0031-9112/36/12/027.
[22] M. Born, and K. Huang, Acta Cryst. **9**, 837-838 (1956), https://doi.org/10.1107/S0365110X56002370.
[23] W. Voigt, *Lehrbook der Kristallphysik*, (Teubner, Leipsig, 1928).
[24] I.R. Shein, and A.L. Ivanovskii, Scr. Mater. **59**, 1099-1102 (2008), https://doi.org/10.1016/j.scriptamat.2008.07.028.
[25] R. Hill, Proc. Phys. Soc. Lond. A, **65**, 349 (1952), https://doi.org/10.1088/0370-1298/65/5/307.
[26] A.M. Blanco, E. Francisco, and V. Luana, Comput. Phys. Commun. **158**, 57 (2004), https://doi.org/10.1016/j.comphy.2003.12.001.
[27] A.S. Verma, and S.R. Bhardwaj, J. Phys. Condens. Matter, **19**, 026213 (2006), https://doi.org/10.1088/0953-8984/19/2/026213.
[28] S.F. Pugh, Philos. Mag. **45**, 823 (1953), https://doi.org/10.1080/14786440808520496.
[29] E. Schreiber, O.L. Anderson, and N. Soga, *Elastic Constants and Their Measurements*, (McGraw-Hill, New York, 1973), pp. 196.
[30] T. Ichitsubo, H. Ogi, S. Nishimura, T. Seto, M. Hirao, and H. Inui, Phys. Rev. B, **66**, 052514 (2002), https://doi.org/10.1103/PhysRevB.66.052514.
[31] E. Franciso, M.A. Blanco, and G. Sanjurjo, Phys. Rev. B, **63**, 094107-094115 (2001), https://doi.org/10.1103/PhysRevB.63.094107.

СТРУКТУРНІ, ЕЛЕКТРОННІ, МЕХАНІЧНІ І ТЕПЛОВІ ВЛАСТИВОСТІ НАПІВХЕЙСЛЕРОВИХ СПОЛУК CoVZ (Z = Si, Ge, Sn, Pb)

Лаліт Мохан[a], Сукхендер[a], Судеш Кумар[b], Шив Р. Бхардвадж[c], Аджай Сингх Верма[a]
[a]Фізичний факультет, Банастхалі Відьяпітх, Банастхалі 304022, Індія
[b]Хімічний факультет, Банастхалі Відьяпітх, Банастхалі 304022, Індія
[c]Фізичний факультет, Коледж Б.С.А., Матхура 282004, Індія

Напівхейслерові сполуки демонструють незвичайну поведінку через їх змінну ширину забороненої зони, а також через їх металеву, і напівметалеву природу. Ці сполуки можуть використовуватися в різних застосуваннях залежно від ширини забороненої зони. Ми обговорили структурні, електронні, пружні і магнітні властивості CoVZ (Z = Pb, Si, Sn, Ge) використовуючи код моделювання WIEN2k, який заснований на теорії функціонала щільності (DFT). Ми оптимізували всю можливу структурну конфігурацію кожного з'єднання і розглянули, яка з них оптимізована з найменшою енергією і найменшим рівноважним об'ємом. Для визначення енергії кореляції електронного обміну в обох платформах використовується наближення узагальненого градієнта (GGA). Ми також отримали індивідуальні пружні постійні, модуль зсуву, модулі Юнга, відношення B/G і коефіцієнт Пуассона, які показують, що ці сполуки пластичні, за винятком сполук CoVGe, які показують низьку пластичність. Температури Дебая розраховані по швидкості хвилі стиснення, швидкості зсувної хвилі та їх середнього значення.

КЛЮЧОВІ СЛОВА: напівхейслерові сполуки, структурні властивості, електронні властивості, механічні властивості

СТРУКТУРНЫЕ, ЭЛЕКТРОННЫЕ, МЕХАНИЧЕСКИЕ И ТЕПЛОВЫЕ СВОЙСТВА ПОЛУХЕЙСЛЕРОВЫХ СОЕДИНЕНИЙ CoVZ (Z = Si, Ge, Sn, Pb)

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

Полухейслеровы соединения демонстрируют необычное поведение из-за их переменной ширины запрещенной зоны, а также как металлической, так и полуметаллической природы. Эти соединения могут использоваться в различных приложениях в зависимости от ширины запрещенной зоны. Мы обсудили структурные, электронные, упругие и магнитные свойства CoVZ (Z = Pb, Si, Sn, Ge) с помощью кода моделирования WIEN2k, основанного на теории функционала плотности (DFT). Мы оптимизировали всю возможную структурную конфигурацию каждого соединения и рассмотрели, какая из них оптимизирована с наименьшей энергией и наименьшим равновесным объемом. Для определения энергии корреляции электронного обмена в обеих платформах используется приближение обобщенного градиента (GGA). Мы также получили индивидуальные упругие постоянные, модуль сдвига, модули Юнга, отношение B/G и коэффициент Пуассона, которые показывают, что эти соединения пластичны, за исключением CoVGe которые показывают низкую пластичность. Температуры Дебая рассчитаны по скорости волны сжатия, скорости волны сдвига и их среднему значению.

КЛЮЧЕВЫЕ СЛОВА: полухейслеровы соединения, структурные свойства, электронные свойства, механические свойства