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Investigating the Structural, Elastic, Electrical, and Thermodynamic Characteristics of NbCoSn and VRhSn Half-Heusler Compounds Using First-Principles Calculations

*[1]Aigbekaen Eddy Enorense and [2]Ighrakpata Fidelia Chukwudumebi

[1]Department of Physics, University of Benin, Benin City, Nigeria.
[2]Department of Physics, College of Education, Warri, Delta State.

*Corresponding Author's Email: eddy.aigbekaen@uniben.edu

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ABSTRACT

In this work, we used first-principles calculations utilising density functional theory (DFT) to examine the structural, elastic, electrical, and thermodynamic features of NbCoSn and VRhSn HH compounds. It was discovered that the calculated lattice constants of the NbCoSn and VRhSn compounds agreed with both the existing theoretical and experimental data. Because the compounds' elastic constants meet the Born-Huang requirements for cubic system stability, they are mechanically stable. VRhSn and NbCoSn are dynamically stable because there are no imaginary phonons. Because NbCoSn has a higher shear modulus and Vicker's hardness than VRhSn HH, it is harder. The presence of band gaps in both compounds indicates that they are semiconductors. VRhSn has a smaller band gap than the NbCoSn HH combounds. Additionally, thermodynamic properties are calculated and investigated in detail. The results show that NbCoSn and VRhSn HH compounds are promising thermoelectric materials; however, VRhSn HH compound stability might be improved by doping and alloying.

INTRODUCTION

XYZ compounds that crystallise in a cubic shape are known as Half-Heusler compounds (F43m, C 1b, space group no. 216). Eight valence electron HH compounds are semiconductors with a wide bandgap energy interval. I-II-V, I-III-IV, II-II-IV, and III-II-III type compounds are typically Half-Heusler materials having eight valence electrons (Saim*et al.*, 2022). Thethermoelectric materials are used in thermoelectric generators to convert heat to electricity and vice versa, Half-Heuslercompounds have become materials of interest in the thermoelectric industry because energy generation based on thermoelectric (TM) materials offers a potential solution to the twenty-first-century energy dilemma because this method does not rely on fossil fuels and is therefore ecologically beneficial (Mori and Priya, 2018). Thermoelectric technology reduces thermal pollution formed as a result of excess heat in the environment in addition to generating electricity. The kind of thermoelectric materials used has a significant impact on how well energy is converted. The majority of Half-Heusler (HH) compounds are perfect for thermoelectric materials meant for thermoelectric generator (TEG) due to their low band gaps (Caballero-Calero et al., 2021). However, thermal and mechanical compatibility is one of the issues with HH compounds.

The NbCoSn HH compound has been suggested for use as a thermoelectric material and for optoelectronic applications because prior research has demonstrated its mechanical stability (Aigbekaen and Ighrakpata, 2022). However, its thermodynamic stability was not investigated. The VRhSn compound has been found to be a desirable choice to investigate even though it has a lower chance of forming a half-Heusler (HH) structure (Gzyl et al., 2020). Additionally, it is discovered that the VRhSn HH compound has a relatively poor lattice thermal conductivity of 7.11 W/mK at a high temperature of about 700 KKhelfaoui et al., 2018). Therefore, the goal of the current work was to gain a deeper understanding of the mechanical and thermal properties of the VRhSn HH compounds. This study used density functional theory (DFT) as implemented in the quantum ESPRESSO code to examine the structural, elastic, electronic, and thermodynamic views of NbCoSn and VRhSn HH compounds.

MATERIALS AND METHODS

Computational details in this work, which includes the structural, mechanical, electrical, and thermodynamic

features of NbCoSn and VRhSn were investigated using density functional theory. Quantum Espresso Pslibrary 1.0.0 projector augmented wave (PAW) pseudo-potentials were used to study interactions between core and valence electrons (Giannozzi et al., 2017). The exchange-correlation energies were computed using Perdew-Burke-Ernzerhof (PBE) with generalised gradient approximations (GGA) (Perdew and Wang, 1992). For both NbCoSn and VRhSn, the plane wave cu-toff energies were fixed at 120 Ry. For elastic properties of NbCoSn and VRhSn HH compounds, the Monkhorst-Pack special k-point system (Monkhorst and Pack, 1976) with 8×8×8 k-points in the Brillouin zone were utilized while dense k-points of 32×32×32 were used to compute DOS and band structures. The equilibrium lattice constants of NbCoSn and VRhSn compounds were found by interpolating the total energy (Etot) as a function of the unit cell volume (V) using Murnaghan's equation of state (Murnaghan, 1944), as shown in equation (1).

$$E(V) = E(V) + \frac{B_O}{B_O+(B_O-1)}\left[V\left(\frac{V_O}{V}\right)B_O - V_O\right] + \frac{B_O}{B_O}(V - V_O) \quad (1)$$

Where V_O is the volume of a unit cell at zero pressure, B_O and B are the modulus of compressibility and its derivative, respectively, and E(v) is the ground state energy with a volume of cell (V). Using elastic tensors and Voigt-Reuss-average, the thermo thermal algorithm calculated elastic constants as well as other auxiliary elastic characteristics including bulk moduli, shear moduli, Young's moduli, and poison's ratios. Sound velocities are calculated using Hill's averages of bulk and shear moduli. An accurate approach that solves the Christoffel wave equation using the angular average of the sound velocities computed for each propagation direction yields the Debye temperature. In the Debye model, the vibrational energy, free energy, entropy, and constant strain heat capacity are calculated using the precise Debye temperature (Palumbo and Dal Corso, 2017). The density functional perturbation theory (DFPT), as applied in the thermos-pw code, was used to calculate the phonon dispersions at the equilibrium structures of NbCoSn and VRhSn compounds (http://qeforge.qeforge.org/gf/project/thermow/).
Phonon frequencies were obtained using a 2 × 2 × 2 grid of q-points, and additional points in the BZ were interpolated using Fourie (These calculatios are carried out after the optimisation of the ecut , k-points and the lattice parameter).

RESULTS AND DISCUSSION

Structural properties

Table 1: Calculated ground state structural and elastic properties of NbCoSn and VRhSn HH compounds using GGA-PBE and exchange correlation functional

	a(Å)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)	G (GPa)	E (GPa)	v	A
NbCoSn	6.3234	182.20	40.65	48.78	87.83	57.58	141.76	0.231	0.689
	6.018[9]	336.37	107.80	75.85	183.99	89.43	230.88	0.663	
	5.952 expt.								
VRhSn	6.0502	204.99	118.90	36.93	147.60	39.26	108.20	0.377	0.857

Table 1 illustrated the characteristics of NbCoSn and VRhSn HH compounds, 6.3234 Åand 6.0502 Å functional, respectively, and agree well with previous theoretical and experimental data (Ferluccio et al., 2018), demonstrating the validity of the work.

Elastic properties

The elastic characteristics of a compound determine most of its mechanical, thermal, and structural behaviors. Additionally, elastic characteristics offer more details about how a specific material reacts to external forces that are applied to the crystal. Cubic crystals have three distinct elastic constants: C_{11}, C_{12}, and C_{44}(Jamal et al., 2014). The strains were applied to the primitive vectors of the unstrained structures and the elastic constants were computed using the thermo thermal algorithm (Okunzuwa and Aigbekaen, 2021). The volume-conserving tetragonal strain determines the elastic constants C_{11} and C_{12}, whereas orthorhombic strain can be used to calculate C_{44}(Aouimer et al., 2019). The Equations C_{11}>0, C_{44}>0, C_{11}-C_{12}>0, (C_{11} +2C_{12}>0)(Aigbekaen et al., 2023) offer the Born-Huang stability requirement for all cubic systems, suggesting that NbCoSn and VRhSn crystals are mechanically stable. The NbCoSn and VRhSn HH compounds require more external force to compress along the a-axes than along the b- and c-axes, as evidenced by the fact that the elastic constants C_{11} are larger than C_{12} and C_{44}. Additionally, the compounds under study have larger elastic constants C_{11} than C_{44}, which accounts for the poorer resistance to shear deformation in comparison to resistance to unidirectional compression. In order to assess the hardness of polycrystalline materials, other important mechanical parameters including shear modulus (G), Young's modulus (E), and Poisson's ratio (v) are frequently calculated (Aigbekaen and Ighrakpata, (2025). The following equations ((2)–(8)) are used to derive them from the estimated elastic constants (Hill, 2014);

$$B = \frac{B_v+B_R}{2} \quad (2)$$

B indicates a material's ability to resist volume change. Equations (2) determine the Voigt bulk modulus (B_V) and the Reuss bulk modulus (B_R).

$$B_V = B_R = \frac{C_{11}+2C_{12}}{3} \quad (3)$$

$$G = \frac{G_V+G_R}{2} \quad (4)$$

The resistance to plastic deformation is influenced by the shear modulus, or G. The Voigt shear modulus (GV) and the Reuss shear modulus (GR) are given by equations (4) and (5).

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

$$G_R = \frac{5(C_{11}-C_{12})C_{44}}{4C_{44}+3(C_{11}-C_{12})} \quad (6)$$

$$E = \frac{(C_{11}-C_{12})(C_{11}-2C_{12})}{C_{11}+C_{12}} \quad (7)$$

Young's modulus, or E, is a measure of a material's stiffness in response to length change.

$$v = \frac{2B-2G}{6B+2G} \quad (8)$$

The bulk moduli (B), shear moduli (G) and Young's moduli (E) of NbCoSn and VRhSn HH compounds obtained by this study are shown in Table 1. Table 1 indicates that the calculated values of bulk moduli (B)ofNbCoSn compound are larger than those of VRhSn, suggests NbCoSn has a higher volumechange resistance in addition to relativelystrong bond strength. Their findings suggested that the shear moduli are more important for predicting material the shear modulus of the NbCoSn HH compound is higher than the VRhSn, which shows that the NbCoSn is tougher than the VRhSn. Furthermore, we predicted the Vicker's hardness of the NbCoSn and VRhSn HH compounds by using the empirical formula suggested by Chen-Niu model presented in equation (9) (Gruhn, 2010) hardness than the bulk moduli (Kittel, 2021).

$$H_V = 2\left(\frac{G^3}{B^2}\right)5^{0.585} \quad -3 \quad (9)$$

In view of the calculated hardness values, we found that NbCoSn crystal is tougher than VRhSn because its Vicker's hardness was 10.06796GPa, and VRhSn's was 0.3828GPa respectively. According to Table 1, the poison's ratio values for the NbCoSn and VRhSn HH compounds are 0.231 and 0.377, respectively (Greaves et al., 2011), and the ratios were >2/7, indicating that the materials under consideration are ductile (Okunzuwa and Aigbekaen, (2020). The crystal is isotropic if the elastic anisotropy factor $A = \frac{2C_{44}}{C_{11}-C_{12}}$ is equal to 1, but any value less or greater than 1 indicates anisotropy (Iyorzor et al., 2018). The materials examined in this study are anisotropic because the anisotropy factors of NbCoSn and VRhSn HH compounds are less than one from calculations.

Electronic properties

The phonon dispersion curves and phonon DOS for both materials were calculated along the high symmetry points (r-X-K-T-L-W-X) of Brillouin zone, which are shown in Fig. 6 (a) and (b). The NbCoSn and VRhSn HH compound is dynamically stable with no imaginary phonon frequencies. The electronic energy band structures and total density of states of compounds were computed at the ground state conditions along the high symmetry points (r-X-K-r-L-W-X) in the first BZ as shown in Fig. 3, Fig. 4 and Fig. 5 respectively. At Fermi level EF (E =0 eV), we obtained an indirect band gap (Gamma-X) between valence band and conduction band, which confirms that NbCoSn and VRhSn HH compounds are semiconductors. The valence band maximum (VBM) of NbCoSn is located at the L and W points while the conduction band minimum (CBM) is at the X point. The conduction band minimum (CBM) is at the X point, whereas the valence band maximum (VBM) is at the r and W points in VRhSn(Job et al, 2022). As shown in Table 2, the calculated band gaps of NbCoSn and VRhSn HH com pounds are well consistent with previous experimental and theoretical studies (Xi et al., 2016). Moreover, the band gap of the VRhSn HH compound is smaller than that of the NbCoSn compound, indicating that VRhSn may be a promising thermoelectric material if the dynamical stability is improved. The distribution of the electronic states of a system with energy is given by the density of states of a solid (Togo and Tanaka, 2015). The spin-polarized total density of states (DOS) of NbCoSn and VRhSn compounds are shown in the Fig. 5 and Fig. 6 respectively. The upper section of each curve of density of states represents the plot of spin majorities, and the lower part represents the plot of spin minorities (Moussali et al., 2020). The symmetry of the two curves indicates that the two alloys are nonmagnetic(Li et al., 2010). Moreover, the total magnetization of both the compounds from spin-polarized calculations is 0.00 μB/f.u indicating that the materials are non-magnetic.

Thermodynamic properties

The analysis of thermodynamic properties at a certain temperature provides important information on chemical stability that is needed for the identification of these compounds to be used efficiently in the industrial sector (Mentefa et al., 2021). Fig. 7 shows the harmonic thermodynamic parameters of NbCoSn and VRhSn compounds at ground state conditions. The thermodynamic properties were evaluated at zero pressures. Benaddi et al. Pressure does not affect the temperature dependence of the entropy and heat capacity, as reported previously. Figure 7 (a) shows that the Debye vibrational energy for NbCoSn and VRhSn HH compounds remains constant below 100 K. Above 100 K, the vibrational energy increases linearly with temperature. However, for the temperature above 100 K, the vibrational free energy decreases with increasing temperature as the entropy (S) increases, according to the

equation F = U-TS (Ighrakpata and Aigbekaen, (2025), as shown in Figs. 7(b) and (c). As shown in Fig. 7(c), the entropy of VRhSn HH compound is greater than that of NbCoSn, which shows that the VRhSn system is more disordered than NbCoSn with increasing temperature. In Fig. 7(c) and (d) the values of entropy and heat capacity for NbCoSn and VRhSn compounds are essentially zero for temperatures below 100 K. However, for temperatures above 100 K entropy increases almost linearly to the highest temperatures. The heat capacity of the HH compounds of NbCoSn and VRHSn is described by the formula C = AT3 at low temperatures below 200 K, which is due to anharmonic approximations, which corresponds to the lattice contribution to heat capacity. Another important observation is that the heat capacity CV is temperature independent at high temperatures of 500 K and above, which indicates the neglect of the anharmonic effect on heat capacity and its value tends to the Dulong-Petit limit (Dulong and Petit, 1819. The Debye temperature is an important thermophysical parameter, which is the temperature for which all the phonon modes are excited. Thus it is closely related to thermophysical properties such as heat capacity, thermal expansion, Gruneisen parameter and melting point. The value of the Debye temperature can be obtained from the average sound wave velocities as shown in the equations ((11) – (14)); (Ameri et al, 2016)

$$\Theta_D = \frac{h}{k_B}\left[\frac{3n}{4\pi}\left(\frac{N_A\rho}{M}\right)\right]^{\frac{1}{3}} \upsilon_m \quad (10)$$

where h is Planck's constant, k_B is Boltzmann's constant, N_A is Avogadro's number, p is the density, M is molecular weight, n is the number of atoms in the molecule, and v_m is the averaged wave velocity summed over several crystal directions

$$\upsilon_m = \left[\frac{1}{3}\left(\frac{2}{\upsilon_t^3} + \frac{1}{\upsilon_l^3}\right)\right]^{-\frac{1}{3}} \quad (11)$$

Whereυ_t and $\upsilon_l$are the transverse and longitudinal sound velocity determined from the bulk modulus (B) and shear modulus (G) applying Navier's equation:

$$\upsilon_t = \left(\frac{B+\frac{4G}{3}}{\rho}\right) \quad (12)$$

$$\upsilon_l = \left(\frac{G}{\rho}\right)^{\frac{1}{2}} \quad (13)$$

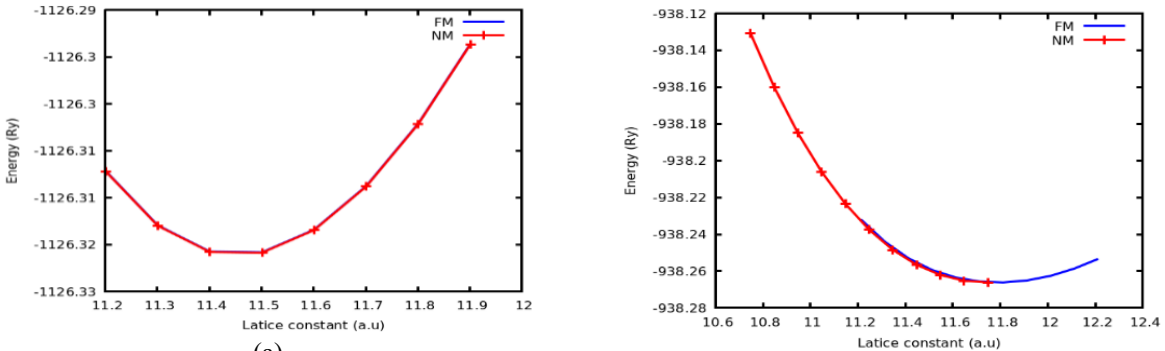
It is proved that the higher the Debye temperature, the higher the thermal conductivity, and conversely. On the other hand minimum thermal conductivity (k_{min}) is exactly proportional to average sound velocity in crystals as given by equation (11) (Clarke, 2003);

$$kB_m \frac{nN_A\rho}{M}_{min} \quad (14)$$

Table 2 summarizes the Debye temperature and average sound velocity of NbCoSn and VRhSn compounds. VRhSn HH compound has lower Debye temperature and average sound velocity values, indicating that VRhSn has reduced thermal conductivity and might be a viable thermoelectric material

Table 2: Calculated band gaps, debye temperatures (ΘD), average sound velocities (Vm) and melting temperatures (Tm) for NbCoSn and VRhSn crystal structures respectively

Compounds	XC	Band gap (eV)	(Θ_D) (k)	V_m(m/s)	$T_m \pm 300$(K)
NaCoSn	GGA	0.331	332.878	3028.103	1929.792
	GGA [39]	0.91	278.94	2479.33	1764.49
VRhSn	GGA	0.507	272.443	2422.411	2045.460
	GGA [10]	0.532			



(a) (b)

Figure 1: The total energies per unit cell as a function of lattice constants for the ferromagnetic (FM) and non-magnetic (NM) states of NbCoSn (a) and VRhSn (b) half-Heusley alloys

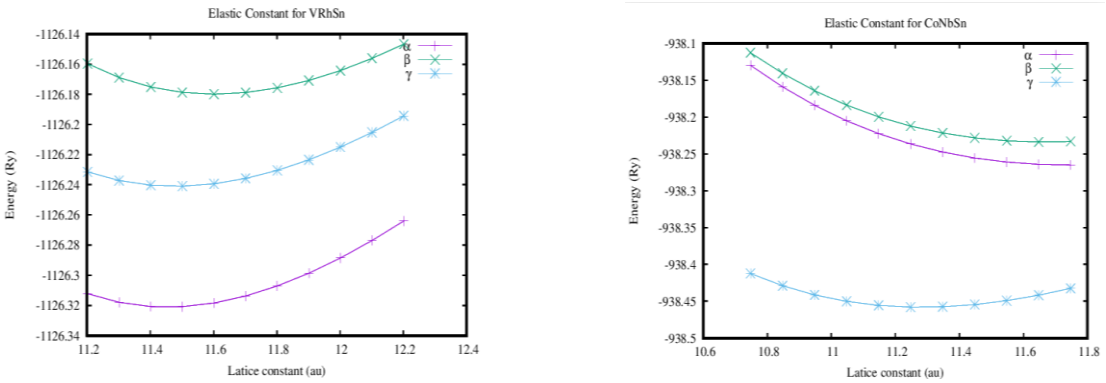


Figure 2: Energy versus Lattice parameter of the α, β, ϒ phases of NbCoSn and VRhSn half-Heusley alloys

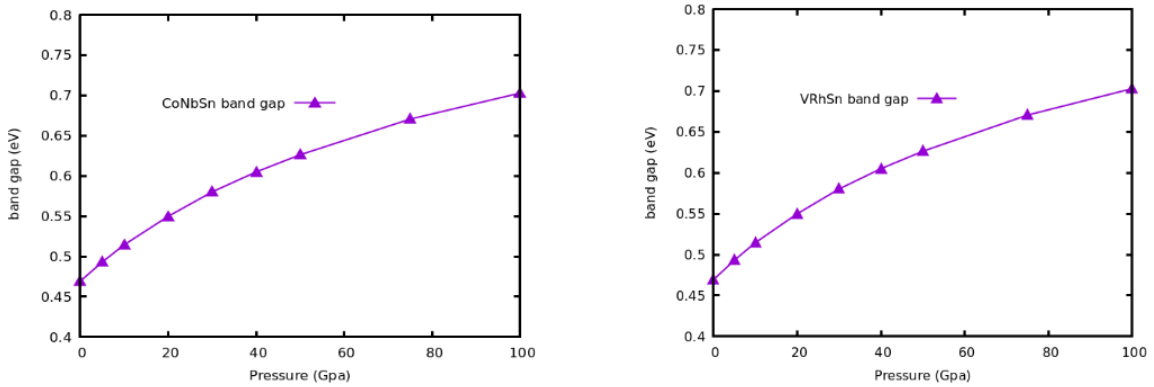
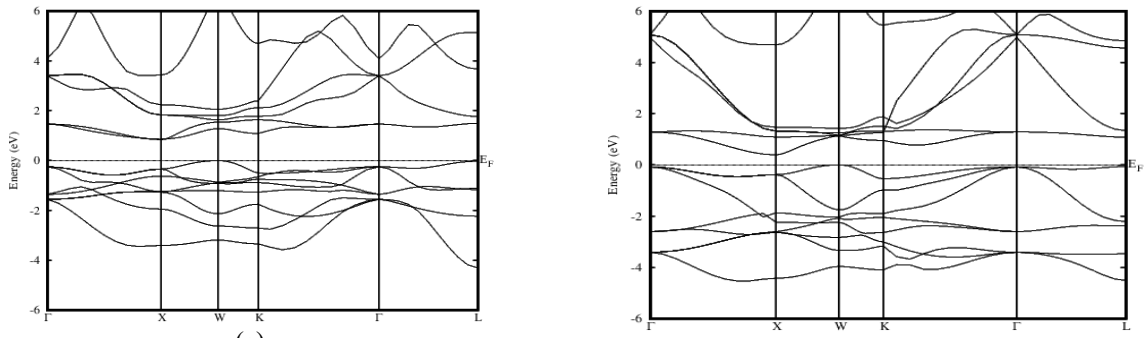


Figure 3: Band gap versus Pressure of NbCoSn and VRhSn half-Heusley alloys



(a) (b)

Figure 4: Electronic band structures of NbCoSb (a) and VRhSn (b) HH half-Heusler alloys

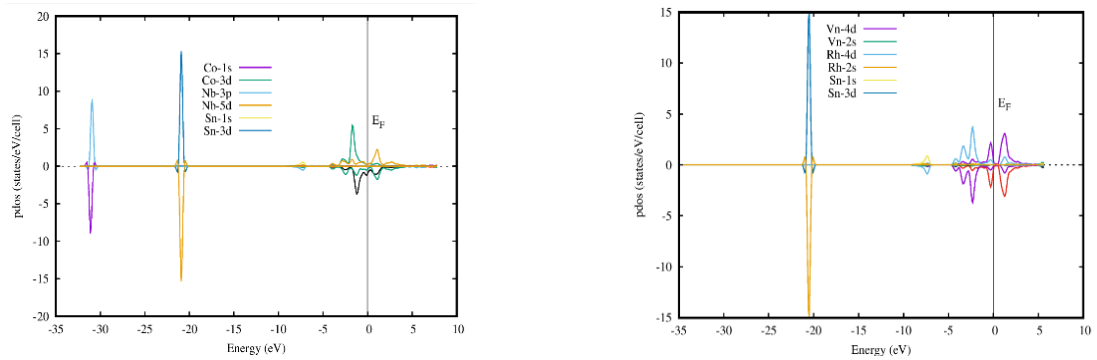


Figure 5: Spin-polarized total density of states of NbCoSn and VRhSn HH compounds

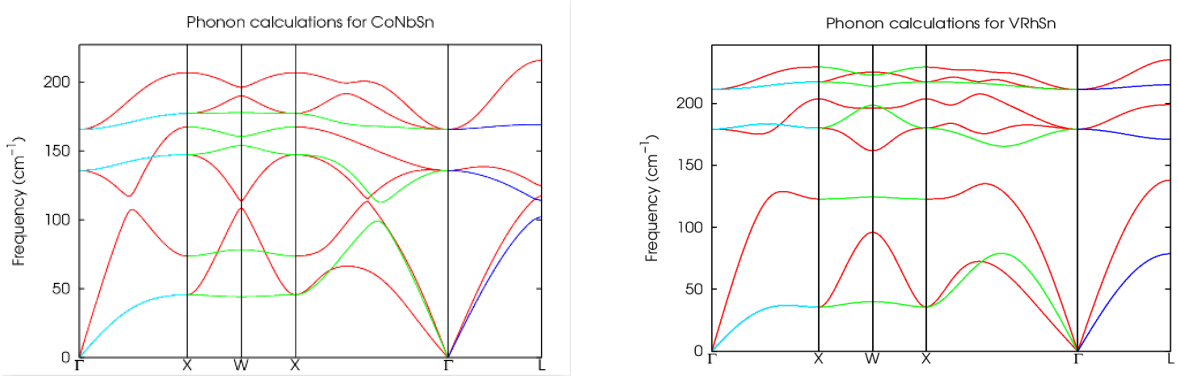


Figure 6: Phonon dispersion curves along symmetry directions of NbCoSn and VRhSn half-Heusley alloy

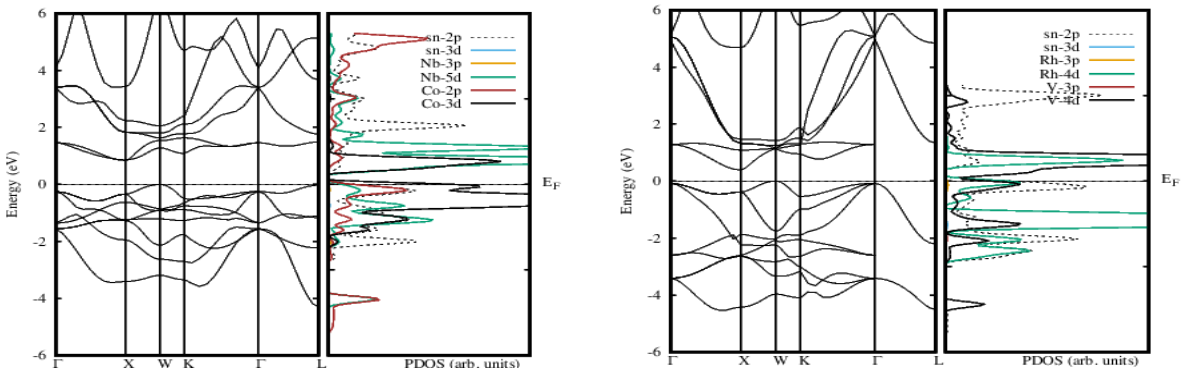


Figure 7: Calculated electronic band structure and density of states of HH compounds

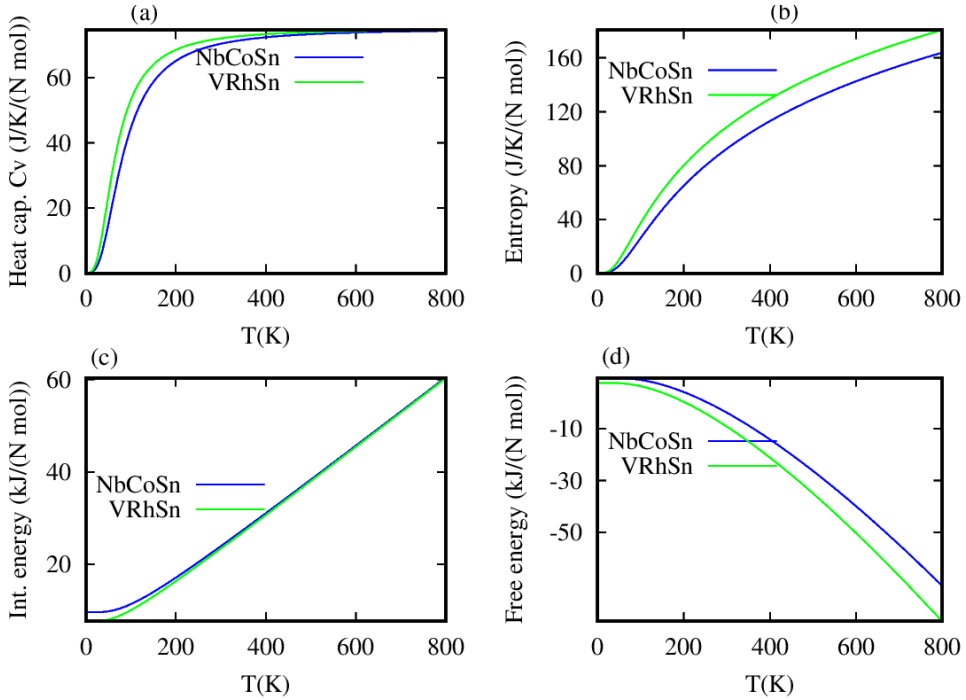


Figure 8: (a, b, c and d) indicating thermodynamic properties of NbCoSn and VRhSn HH compounds as function of temperature

Melting temperature

The empirical formula for prediction of melting temperatures (Tm) of cubic crystals from elastic constant data is given by equation (15) (Chami et al., 2020).

$T_m = [553K + (5.91K/GPa)C_{11}] + 300K$ (15)

The predicted melting temperatures of NbCoSn, andVRhSn compounds are listed in Table 2. The high melting temperatures show that the compounds in this work, particularly the NbCoSn HH compounds, are appropriate for high temperature applications.

CONCLUSION

The structural, elastic, electronic and thermodynamic properties of NbCoSn and VRhSn HH compounds have been calculated by first-principles computations. The calculated ground state lattice parameters of this study are in good agreement with the previous theoretical and experimental data, indicating the reliability of the current study. The HH compound NbCoSn is both mechanically and dynamically stable, while VRhSn is dynamically unstable but mechanically stable. Higher Vicker's hardness of NbCoSn than VRhSn HH was observed which indicated that NbCoSn was tougher than VRhSn material. Moreover, the existence of the band gap at the femi level indicated that the compounds studied in this work are semiconductors. Finally, while both materials are promising for thermoelectric applications, the stability of the VRhSn HH compound can be improved by doping or alloying or nano structuring.

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