First-Principles Studies on the Physical Properties of the Half Heusler RbNbCd and RbNbZn Compounds: A Promising Material for Thermoelectric Applications

Debidatta Behera, Ahmed Azzouz-Rached, Abdessalem Bouhenna, Mostafa M. Salah, Ahmed Shaker, and Sanat Kumar Mukherjee

1. Introduction

Researchers have recently concentrated on the investigation of smart and multifunctional materials. Applications for these materials include sensors, thermoelectricity, optoelectronics, and various forms of renewable energy [1–3]. It is quite concerning that the global ecology is in an alarming state due to continuously rising carbon emission rates. The need to find effective, clean and environmentally friendly renewable energy sources has therefore intensified in order to stop the destruction of our environment. Biodiesel, biomass, wind power, solar power and thermoelectric power are considered potential resources in this regard [4–6]. Therefore, we require such materials that can function as thermoelectric and photovoltaic generators. In contrast to thermoelectric generators, which utilize heat that has been dissipated to produce electricity, photovoltaics can absorb and transform the tremendous quantity of solar energy that the sun emits continually into useful electrical energy [5,7–9].

Numerous substances have been investigated as prospective components for solar and thermoelectric systems, including chalcogenides, triple point metals, oxide perovskites, skutterudites, and Half Heusler compounds [10–14]. Some of the peculiar properties of
these mentioned materials include a simple crystal structure, magnetism, half metallicity, a topological insulator, optoelectronics, and thermoelectricity, etc. [15–17]. In 1903, Friedrich Heusler made the discovery of the Cu$_2$MnAl prototype Heusler compound [18]. The Heusler compound received significant attention only after its first principles calculations revealed its unique property, the half metal ferromagnet (HMF), which revolutionized the developing field of thermoelectrics and spintronics. The many forms of Heusler compounds have been the subject of several studies, and they have a variety of properties that can be exploited in a number of new technological devices. A half-Heusler compound, which has a total of 18 valence electron counts, is a novel prospective thermoelectric material, with higher electrical conductivity than other members of the Heusler compound family.

Numerous Half Heusler compounds have been developed recently for use in thermoelectric applications [16,19–23]. The effectiveness of thermoelectric materials are quantified through Figure of merit (ZT), computed as $ZT = S^2\sigma T/\kappa$, where $S$, $\sigma$, $\kappa$, and $T$ stand for the Seebeck coefficient, electrical conductivity, thermal conductivity, and temperature, respectively [24,25]. The high-power factor ($S^2\sigma$) and ZT value quantifies the performance of the thermoelectric devices.

With the search of novel compounds for the thermoelectric applications, CrVZ ($Z = S$, Se, and Te) were investigated by Javed et al., and they reported their mechanical as well as dynamic stability [26]. Furthermore, NbCoSn and NbFeSb HHs that were reported by Zerrouki et al. were found to be mechanically stable, elastically anisotropic, and brittle by nature [27]. The potential use of these materials in solar and thermoelectric applications was also addressed. The half metallicity of RbSrX ($X = C$, Si, and Ge) was reported by Ahmad et al. [28]. The computed magnetic moment of these compounds was found to be 1 $\mu$B. A literature survey indicated that the structural, electronic, magnetic and thermoelectric properties of RbNbCd and RbNbZn materials have not received significant attention. This motivates us to analyze the structural, electronic, elastic, thermodynamic and thermoelectric properties of RbNbCd and RbNbZn. We believe that the findings of this work will be beneficial in future theoretical and experimental studies of additional HHs.

The first section of the manuscript is an introduction, while the second section introduces the computing strategy. The results are then presented together with an analysis and discussion of them in the third section. The conclusion and the key successes are included in the final section.

2. Computational Method

To analyze the structural as well as the dynamic stabilities of the RbNbCd and RbNbZn including the electronic, magnetic and thermoelectric properties, we employed the full-potential linearized augmented plane wave approach (FP-LAPW) [29], and relied on the density functional theory (DFT), as embedded in Wien2K [30]. The FP-LAPW technique was used to expand the Kohn Sham orbitals in the muffin-tin (MT) atomic spheres into atomic-like orbitals and plane waves in the interstitial space [29,31]. The analysis of the physical characteristics of the RbNbCd and RbNbZn Perdew-Burke Ernzerhof generalized gradient approximation (PBE-GGA) [32] was taken into consideration for structure optimization.

For computation of the electronic properties, the modified Becke-Johnson potential (mBJ) [33,34] was utilized, as it precisely predicts the ground state electronic properties. Inside the atomic spheres, the valence wave functions were enlarged to $l = 10$ partial waves. In this computation, the plane wave expansion $R_{MT}K_{\text{max}} = 7$ was used, where $K_{\text{max}}$ is the magnitude of the largest K vector and $R_{MT}$ is the size of the smallest muffin tin sphere. A muffin-tin (MT) model was used to predict the crystal potential, and the assumed $R_{MT}$ values for Rb, Nb, Cd and Zn were set at 2.5, 1.80, and 1.63, respectively [35]. The potential and charge density were extended up to $G_{\text{max}} = 12$ a.u$.^{-1}$. Using the modified tetrahedron approach, a dense mesh of $10 \times 10 \times 10$ uniformly distributed k-points (equivalent to 405 in irreducible BZ) was used inside the Brillouin zone (BZ), where the total energy concentration was set up to $10^{-6}$ Ry.
The elastic constants were calculated using the IRELAST method [36], which was employed in the WIEN2k. Furthermore, the Gibbs2 code was utilized to compute the thermodynamic properties of RbNbCd and RbNbZn [37]. The thermoelectric properties of this molecule were examined using the semi-classical Boltzmann theory and the BoltzTrap method [38]. Moreover, by employing the Vienna Ab initio Simulation Package (VASP) [39], we performed the phonon dispersion study in order to study the dynamic stability of the investigated RbNbCd and RbNbZn.

3. Results and Discussion

3.1. Structural Properties

The analysis of the structural characteristics of RbNbCd and RbNbZn is the focus of this section. This type of research holds great promise because it enables the gathering of data related to the microscopic structure that assists in the forecasting of other properties, such as the electronic, elastic, and thermodynamic. The HHs generally belong to the generic formula XYZ that exists on the non-centrosymmetric cubic structure (#216, F-43m) [40]. However, the HH structure is shown in Figure 1 by the three different cubic face-centered networks, or X, Y, and Z, that are coupled with one another. This kind of structure can exist in any one of the three non-equivalent atomic configurations listed in Table 1. Structural optimization has been carried out for the ferromagnetic (FM) and non-magnetic (NM) phases that were carried out on the three diverse configurations (α, β, γ), as represented in Figure 1.

![Crystal Structure of RbNbCd and RbNbZn](image)

**Figure 1.** A view of the crystal structure of the RbNbCd and RbNbZn.

<table>
<thead>
<tr>
<th>Compounds</th>
<th>Phase</th>
<th>a (Å)</th>
<th>B (GPa)</th>
<th>B’</th>
<th>Energy (eV)</th>
<th>E$_{\text{form}}$ (eV/atom)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RbNbCd Alpha</td>
<td>NM</td>
<td>7.27</td>
<td>18.07</td>
<td>5.59</td>
<td>−337,359.50342</td>
<td>0.06</td>
</tr>
<tr>
<td></td>
<td>FM</td>
<td>8.06</td>
<td>7.43</td>
<td>4.43</td>
<td>−337,360.48248</td>
<td>−0.03</td>
</tr>
<tr>
<td>Beta</td>
<td>NM</td>
<td>7.21</td>
<td>24.78</td>
<td>4.68</td>
<td>−337,361.02856</td>
<td>−0.02</td>
</tr>
<tr>
<td></td>
<td>FM</td>
<td>7.64</td>
<td>14.22</td>
<td>4.65</td>
<td>−337,361.59782</td>
<td>−0.30</td>
</tr>
<tr>
<td>Gamma</td>
<td>NM</td>
<td>7.42</td>
<td>24.57</td>
<td>4.68</td>
<td>−337,360.98197</td>
<td>−0.25</td>
</tr>
<tr>
<td></td>
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<td>7.68</td>
<td>17.47</td>
<td>4.81</td>
<td>−337,361.7835</td>
<td>−0.95</td>
</tr>
<tr>
<td>RbNbZn Alpha</td>
<td>NM</td>
<td>6.96</td>
<td>21.11</td>
<td>5.67</td>
<td>−233,958.79599</td>
<td>−1.03</td>
</tr>
<tr>
<td></td>
<td>FM</td>
<td>7.93</td>
<td>6.47</td>
<td>4.93</td>
<td>−233,959.5225</td>
<td>−1.03</td>
</tr>
<tr>
<td>Beta</td>
<td>NM</td>
<td>6.96</td>
<td>26.45</td>
<td>4.47</td>
<td>−233,960.27421</td>
<td>−1.03</td>
</tr>
<tr>
<td></td>
<td>FM</td>
<td>7.37</td>
<td>14.06</td>
<td>5.49</td>
<td>−233,960.6733</td>
<td>−1.03</td>
</tr>
<tr>
<td>Gamma</td>
<td>NM</td>
<td>7.09</td>
<td>27.40</td>
<td>4.42</td>
<td>−233,960.41307</td>
<td>−1.03</td>
</tr>
<tr>
<td></td>
<td>FM</td>
<td>7.39</td>
<td>19.13</td>
<td>4.46</td>
<td>−233,961.06317</td>
<td>−1.03</td>
</tr>
</tbody>
</table>
To determine the equilibrium lattice constant as well as the structural stability of RbNbCd and RbNbZn, Birch Murnaghan EOS [41] was considered, with the variation of total energy as a function of volume, as displayed in Figure 2. Because the energy-volume curve of $\gamma$ in the FM arrangement is smaller than that of the other two arrangements, this suggests its stability. Table 1 lists the equilibrium energy, bulk modulus, as well as its pressure derivative for RbNbCd and RbNbZn, along with the optimized lattice parameters. The formation energy was used to evaluate the thermodynamic stability that affects the possibility of synthesizing RbNbCd and RbNbZn. The computed formation energies for the RbNbCd and RbNbZn are represented in Table 1. The negative formation energy indicates their stability [42]. To confirm the stability of the RbNbCd and RbNbZn, we estimated the phonon dispersion (PD) against momentum, as shown in Figure 3. The transverse and longitudinal modes in the phonon dispersion diagram typically resemble spaghetti. With a range of 0 to 6 THz, we employed frequency (THz) along the $y$-axis and momentum along the $x$-axis. However, practically all of the modes in the RbNbCd and RbNbZn compounds are positive and have genuine phonon branches, reflecting their stability [43,44].

![Figure 2. Variation of the energy as a function of the volume for RbNbCd and RbNbZn.](image)

3.2. Elastic Properties

The elastic properties required for the study of diverse mechanical properties such as strength of material, ductile and brittle nature, influence on stress and strain, as well as interatomic bonding can be determined from the first principle method based on the density functional theory [45,46]. The mechanical behavior of the investigated substance is quantified from the elastic properties. These characteristics have a significant impact on the compounds selected for innovative photovoltaic applications [47]. Three distinct elastic constants exist for cubic compounds ($C_{ij}$). Table 2 provides an overview of the computed elastic constants for RbNbCd and RbNbZn. The Born-Huang stability condition [48,49] is used to determine the mechanical stability of both of these compounds, which is expressed as

$$C_{11} - C_{12} > 0, C_{11} > 0, C_{44} > 0 \text{ and } (C_{11} + 2C_{12}) > 0$$

(1)
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\[ C_{11} - 2C_{12} > 0, \quad C_{11} > 0, \quad C_{44} > 0, \quad (C_{11} + 2C_{12}) > 0 \]  

Satisfying the above condition, the mechanical stability of the RbNbCd and RbNbZn was established [50,51]. Using Voigt-Reuss-Hill (VRH) approximations [52], these compounds’ physical properties, including their bulk modulus (B) and shear modulus (G), were determined. The bulk modulus values derived by applying VRH approximations (Table 2) agree well with the EOS Bulk modulus (Table 1), illustrating the high internal consistency of the research. Other elastic constants such as the Young’s modulus (Y), Poisson’s ratio (v), and shear anisotropy factor (A) of these compounds are computed as follows:

\[ B = \frac{C_{11} + 2C_{12}}{3} \]  
\[ G = \frac{C_{11} - C_{12}}{2} \]  
\[ Y = \frac{9GB}{3B + G} \]  
\[ y = \frac{3B - 2G}{2(3B + G)} \]  
\[ A = \frac{2C_{44}}{C_{11} - C_{12}} \]

When a material is compressed, its bulk modulus (B) reveals how resistant it is to volume change. The high B value denotes good crystal strength, whereas the shear modulus (G) shows the crystal opposition offered for plastic deformation [53–55]. For

Table 2. Computed elastic constants (C$_{ij}$) (in GPa), elastic modulus (B, G and E) (in GPa), Poisson’s ratio (v), G/B, Cauchy pressure and shear anisotropic parameters.

<table>
<thead>
<tr>
<th>Compound</th>
<th>C$_{11}$</th>
<th>C$_{12}$</th>
<th>C$_{44}$</th>
<th>B</th>
<th>G</th>
<th>G/B</th>
<th>E</th>
<th>v</th>
<th>P$_X^{Cauchy}$</th>
<th>A</th>
</tr>
</thead>
<tbody>
<tr>
<td>RbNbCd</td>
<td>30.7941</td>
<td>11.7813</td>
<td>9.6574</td>
<td>18.118</td>
<td>9.596</td>
<td>0.52</td>
<td>24.468</td>
<td>0.274</td>
<td>2.12</td>
<td>1.01</td>
</tr>
<tr>
<td>RbNbZn</td>
<td>36.1129</td>
<td>6.9461</td>
<td>7.8413</td>
<td>16.668</td>
<td>10.078</td>
<td>0.61</td>
<td>25.162</td>
<td>0.248</td>
<td>−0.89</td>
<td>0.53</td>
</tr>
</tbody>
</table>
RbNbCd and RbNbZn compounds, the estimated magnitudes of B are 18.11 GPa and 16.66 GPa, respectively. RbNbZn is more robust to volume change than RbNbCd because it has a higher B value.

Additionally, RbNbZn has a higher G value (10.07) than RbNbCd (9.59). As a result, RbNbZn has higher resistance to the transverse bending. For the determination of brittleness or ductility, it is quantified by Pugh’s ratio (B/G) [56,57]. Having more than 1.75 B/G, the substance is ductile or brittle. Table 2 displays the estimated B/G for RbNbCd and RbNbZn compounds, demonstrating the ductility of the compounds in question. Frantsevich et al. [58] used Poisson’s ratio (ν) to distinguish between brittleness and ductility, with a threshold value 0.26. If ν is greater than 0.26 it is considered to be ductile or brittle. The RbNbCd and RbNbZn compounds have estimated values of 0.27 and 0.24, respectively, showing that RbNbCd is ductile by nature, whereas RbNbZn is brittle. This is further supported by Cauchy pressure $C_p = C_{12} - C_{44}$, as represented in Table 2 [59,60]. A positive (negative) magnitude identifies ionic (covalent) bonding. The positive $C_p$ for RbNbCd signifies ionic bonding, whereas a negative $C_p$ for RbNbZn signifies covalent bonding. The capacity for creating microcracks in materials has been strongly associated with elastic anisotropy. The anisotropy factor (A) has a value of unity for an entirely isotropic system; the divergence from unity represents the degree of elastic anisotropy [61–63]. RbNbZn is anisotropic and more prone to developing microcracks or structural faults during the growth process than RbNbCd according to the computed values of A, which are displayed in Table 2.

Two thermodynamic factors associated with elastic properties: the melting point $T_m$ and the Debye temperature ($\theta_D$), were also studied:

$$\theta_D = \frac{h}{k_B} \left[ \frac{3n}{4\pi} \left( \frac{N_A \rho}{M} \right) \right]^{-1/3} \nu_m$$  \hspace{1cm} (7)

where $n$ is the number of atoms in a single cell, $k$ is Boltzmann’s constant, $h$ is Planck’s constant, $N_A$ is Avogadro’s number, $\rho$ is the material’s density, and $M$ is its molecular weight. Table 3 contains the computed Debye temperature. The investigated materials’ mean sound speeds were determined using,

$$\nu_m = \left[ \frac{1}{3} \left( \frac{2}{\theta_l} + \frac{1}{\theta_t} \right) \right]^{(1/3)}$$  \hspace{1cm} (8)

where the shear modulus and bulk modulus, respectively, are used to determine the longitudinal and transverse components of sound velocity as,

$$\theta_l = \sqrt{\frac{G}{\rho}} \quad \text{and} \quad \theta = \sqrt{\frac{3B + 4G}{3\rho}}$$  \hspace{1cm} (9)

**Table 3.** The total and local magnetic moments of both compounds.

<table>
<thead>
<tr>
<th>Compounds</th>
<th>Total ($\mu_B$)</th>
<th>Rb ($\mu_B$)</th>
<th>Nb ($\mu_B$)</th>
<th>Cd/Zn ($\mu_B$)</th>
<th>Interstitial ($\mu_B$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RbNbCd</td>
<td>4.05</td>
<td>0.03</td>
<td>2.52</td>
<td>0.04</td>
<td>1.44</td>
</tr>
<tr>
<td>RbNbZn</td>
<td>4.01</td>
<td>0.05</td>
<td>2.49</td>
<td>0.07</td>
<td>1.39</td>
</tr>
</tbody>
</table>

Table 4 presents the computed magnitude of $\nu_l$, $\nu_t$, $V_m$, $\theta_D$, and $T_m$.

### 3.3. Magnetic Properties

When examining the material magnetic properties, the magnetic moment is a crucial consideration. It provides information on the material magnetic field components as well as the magnetic field frequency [23]. The magnetic moments of spins in RbNbCd and
RbNbZn compounds were investigated. Table 3 depicts the calculated total and partial magnetic moments with polarized spin in the interstitial sites and the muffin-tin spheres. The total magnetic moment ($\mu_B$) per cell unit for both materials approached an integer Bohr magneton of 4 $\mu_B$, confirming their half-metallic character. It is clear that although the magnetic moments of the Rb and Cd/Zn atoms are small and do not significantly contribute to the total moment, they are extremely important for the development of magnetism. Furthermore, the environment of these atoms has an impact on the width of the predominant band gap in the compound RbNbCd and RbNbZn. A significant magnetic moment can be discovered in the interstitial region, as demonstrated in Table 3. This outcome is the result of a large charge transfer from Rb and Nb to Cd/Zn, which can be used to explain the magnetic moment at the interstitial region. This is explained by the fact that the Cd/Zn anion has a higher electronegativity than the Rb and Nb, and is responsible for the magnetic moment in the interstitial region.

Table 4. Computed density, longitudinal, transverse, and average elastic wave velocity ($\rho$ (in g/cm$^3$), $v_l$, $v_t$, $v_m$ (in m/s)), the Debye temperatures ($\Theta_D$ in K), Melting temperature ($T_m$ in K), and minimum and lattice thermal conductivity at 300K ($k_{min}$, $k_{ph}$ in W/m-K).

<table>
<thead>
<tr>
<th>Compounds</th>
<th>$\rho$ (g/cm$^3$)</th>
<th>$v_l$</th>
<th>$v_t$</th>
<th>$v_m$</th>
<th>$\Theta_D$</th>
<th>$T_m$</th>
<th>$k_{min}$</th>
<th>$k_{ph}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>RbNbCd</td>
<td>4.2546</td>
<td>2695.51</td>
<td>1501.82</td>
<td>1672.28</td>
<td>148.309</td>
<td>734.309</td>
<td>0.161</td>
<td>0.701</td>
</tr>
<tr>
<td>RbNbZn</td>
<td>4.0022</td>
<td>2742.67</td>
<td>1586.86</td>
<td>1761.39</td>
<td>162.329</td>
<td>766.427</td>
<td>0.098</td>
<td>0.947</td>
</tr>
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</table>

3.4. Electronic Properties

The dispersion of electrons in the valence and conduction bands and the width of the gap are the primary determinants of the electronic characteristics, band structure, and state density [64,65]. These characteristics are determined for Half Heusler RbNbCd and RbNbZn equilibrium states using the most stable $\gamma$-structure optimized lattice parameter. Figure 4 shows the computed spin-up as well as the spin-down polarized electronic band structures for RbNbCd and RbNbZn. For both RbNbCd and RbNbZn compounds, the results of the band structure investigation demonstrate that both compounds are metallic and that there is no energy difference between the conduction and valence bands. Similar behavior is obtained for the spin down state.

We computed the density of states (Dos, both total and partial) for RbNbCd and RbNbZn, as, depicted in Figure 5, to better understand the interaction between different orbitals of the atoms. With the exception of the values of their densities of states with changing energies, the computed band structure and DoS for the compounds under consideration behave similarly. In all the materials taken into consideration, the electrons of the d-orbital of the ‘Nb’ atom make up the majority of the contribution in the lower valence band region from $-2.5$ eV to 0 eV, while the electrons of the p-orbital of the Y-atom (Y = Zn, Cd) make up the minor portion at the conduction band with small contribution of the Rb atom. The metallic behavior is again confirmed from the DoS plot, with the valance state crossing the Fermi energy [64].

3.5. Thermodynamic Properties

Using Gibbs2 [37], we estimated the thermodynamic properties of the investigated RbNbCd and RbNbZn materials. Within the temperature range of 0–800 K, the thermal characteristics of the compounds under consideration were calculated. The effects of pressure in the range of 0–15 GPa were taken into consideration by using the quasi-harmonic model. The essential physical characteristic that indicates whether a material is suitable for usage in high temperature situations is the lattice or phonon thermal conductivity ($k_{ph}$) [66]. Figure 6 shows the $k_{ph}$ values determined at room temperature (300 K). Its dependency on temperature between 0 to 1000 K is represented, which demonstrates with increase in temperature the $k_{ph}$ value decreases. At 300 K the $k_{ph}$ is found to be 1.1 W/mk and 0.98 W/mk for RbNbCd and RbNbZn, respectively. These values are significantly lower.
than the lattice thermal conductivity of other reported thermoelectric materials; however, experimental work on this will be more beneficial.

Figure 4. Calculated band structures for RbNbCd and RbNbZn along the high-symmetry axes of the first Brillouin zone.

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Figure 5. Calculated total and partial density of states (TDOS, PDOS) in spin up and spin-down for RbNbCd and RbNbZn.
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Figure 6. Temperature dependence of lattice thermal conductivity of RbNbCd and RbNbZn.

Variations in the volume of the unit cell versus temperature at a diverse pressure (0, 5, 10, 15 GPa) are shown in Figure 7. It is evident that when the pressure increases and temperature remains constant, the volume decreases. Contrarily, the volume increases with the temperature at a very slow rate at a given pressure for RbNbCd and RbNbZn. Examining the data in Figure 7 reveals that the volume absolute zero pressure and zero temperature is 680 bohr$^3$ and 775 bohr$^3$ for RbNbCd and RbNbZn, respectively.

Figure 7. The Volume (V) as a function of temperature at different pressures for RbNbCd and RbNbZn.
The variability in heat capacity ($C_V$) for various temperatures for the pressure range of 0 to 15 GPa is illustrated in Figure 8. We can infer from the figure that $C_V$ complies with the $T^3$ law. It is simpler to understand the vibrational properties of the material by taking into account heat capacity, which has multiple uses. At high temperatures, the value of $C_V$ is nearly constant due to the Dulong-Petit limit [67,68], which is the result of the suppression of an anharmonic. The variation of Debye temperature ($\theta_D$) [69] with diverse temperature and pressure are represented in Figure 9. With the rise in temperature at a given pressure, the pressure reduces almost linearly; however, it increases for increasing pressure at a certain temperature. Therefore, the Debye temperature is significantly affected by pressure as well as temperature in the opposite directions.

![Figure 8. The heat capacity ($C_v$) as a function of temperature at different pressures for RbNbCd and RbNbZn.](image)

These findings suggest that temperature and pressure have an impact on particle vibration frequency across all computed compounds. The fluctuation of the coefficient of thermal expansion ($\alpha$) with temperature and pressure is shown in Figure 10. It can be seen in the figure that $\alpha$ rises sharply between 0 and 200 K, then rises gradually, and above 300 K, particularly in high-pressure locations, it rises almost linearly, with a low slope. The thorough examination of the thermodynamic characteristics will shed light on the experimental efforts.

3.6. Thermoelectric Properties

The capacity of thermoelectric materials to transform thermal energy into usable energy and vice versa has increased interest in them significantly around the globe [70]. Because of their capacity for energy production, dielectric properties, and refrigeration, these the efficiency of these materials finds a significant demand in the thermoelectric realm. The BoltzTraP code [38] was employed to compute thermoelectric parameters using an approximation of charge carrier constant relaxation times. This section focuses on analyzing several transport coefficients of RbNbCd and RbNbZn in both up- and down-spin states, including electrical conductivity ($\sigma/\tau$), Seebeck coefficient ($S$), and the merit factor ($ZT$).

For
RbNbCd and RbNbZn, the variation in Seebeck coefficient (S) is represented in Figure 11. Over the whole temperature range, it can be seen that the Seebeck coefficient for RbNbCd is positive for the up-spin state, whereas S for RbNbZn is negative up to 250 K, which ends up being positive after a further increment in the temperature. In the spin-down condition, we also see that the Seebeck coefficient for the RbNbCd and RbNbZn increases linearly with temperature in the entire temperature range.

![Figure 9](image1.png)

**Figure 9.** Debye temperature ($\theta_D$) as a function of temperature at different pressures for RbNbCd and RbNbZn.

![Figure 10](image2.png)

**Figure 10.** Thermal expansion coefficient ($\alpha$) as a function of temperature at different pressures for RbNbCd and RbNbZn.
When the temperature is between 100 K–800 K, the computed for the spin-up state and that discovered for the spin-down state are different. For both Half Heuslers, the electrical conductivity temperature for RbNbCd and RbNbZn. For RbNbCd, the magnitude of ZT rises with temperature for the spin-up state, whereas an opposite trend is observed for the spin-down state. The computed results indicate that RbNbCd and RbNbZn are suitable for thermoelectric applications at low temperatures.

Figure 11. Temperature dependence of Seebeck coefficient (S) for RbNbCd and RbNbZn.

Furthermore, Figure 12 depicts the fluctuation of electrical conductivity (σ/τ) with temperature for RbNbCd and RbNbZn. For both Half Heuslers, the electrical conductivity computed for the spin-up state and that discovered for the spin-down state are different. When the temperature is between 100 K–800 K, the σ/τ is observed to increase with temperature for the RbNbY for spin-up. However, for spin-down, the σ/τ unexpectedly dropped between 200–800 K. Finally, to measure the thermoelectric efficiency of these compounds, we examined the fluctuation of the figure of merit throughout a temperature range from 0 to 800 K, as represented in Figure 13. For RbNbCd, the magnitude of ZT rises with temperature for the spin-up state, whereas an opposite trend is observed for the RbNbZn. For RbNbCd and RbNbZn, the ZT values at 300 K for the spin-up state are around 0.007 and 0.035, respectively. The magnitude of ZT rises as the temperature rises for the spin-down state. The computed results indicate that RbNbCd and RbNbZn are suitable for thermoelectric applications at low temperatures.

Figure 12. Temperature dependence of the conductivity integral (σ/τ) for RbNbCd and RbNbZn.
Figure 13. Temperature dependence of the figure of merit (ZT) for RbNbCd and RbNbZn.

4. Conclusions

We analyzed the structural, electronic, elastic, thermodynamic and thermoelectric features of RbNbCd and RbNbZn employing first-principle computations and Boltzmann transport theory. The elastic properties demonstrate that RbNbCd and RbNbZn are mechanically stable. Furthermore, the computed lattice thermal conductivity values for RbNbCd and RbNbZn at 300 K are 1.1 (0.98) Wm\(^{-1}\)K\(^{-1}\). The best thermoelectric properties are believed to be produced by the lattice thermal conductivity with the least magnitude. We also discovered that the Seebeck coefficient and electrical conductivity yield good results to match the performance requirements of thermoelectric devices with low thermal conductivity. According to the calculated results, RbNbCd and RbNbZn are suitable for thermoelectric applications at low temperatures. The aforementioned study will motivate researchers to pursue this avenue; however, rubidium is an element that is extremely sensitive to air and moisture, hence any experimental operation has to be performed with special precautions in place.


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References


27. Zerrouki, T.; Rached, H.; Rached, D.; Caid, M.; Cheref, O.; Rabah, M. First-principles calculations to investigate structural stabilities, mechanical and optoelectronic properties of NbCoSn and NbFeSb half-Heusler compounds. *Int. J. Quantum Chem.* **2021**, *121*, e26582. [CrossRef]


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