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Structural, Optoelectronic and Thermoelectric Properties of Ternary CaBe$_2$X$_2$ (X = N, P, As, Sb, Bi) Compounds

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Abstract: The structural, electronic, optical and thermoelectric properties of ternary CaBe$_2$X$_2$ (X = N, P, As, Sb and Bi) have been investigated comprehensively for the first time using density functional theory. All the compounds are optimized to obtain their ground states. Computed structural parameters agree to the available experimental results. Electronic band structure calculations reveal the semiconducting nature of the compounds, while band gap decreases by changing the anion X from N to Bi the band gap decreases. In the valence band, major contribution is due to Ca-p state, while in conduction band (CB) the major contribution is mainly due to the Ca-d state. Furthermore, electron charge density plots reveal ionic bonding character with small covalent bonding. Optical properties are calculated in detail. Static value of refractive index shows inverse variation with band gap. The refractive indices of these compounds are high in the infrared region and gradually decreased in the visible and ultra-violet region. The thermoelectric properties are studied using Boltzmann statistics through BoltzTraP code. High optical conductivity peaks and figure of merits (ZT) for ternary compounds reveal that they are good candidates for the optoelectronics and thermo-electric devices.

Keywords: Band Structure; Optical Response; Thermoelectrics; Zintl Compounds.

1 Introduction

The Nitridoberyllate Li[BeN] was the first and only known reported compound in 1996 [1]. In this crystal structure Be and N alternate contains puckered 4.8$^2$ nets. Li cations are connected to neighboring 2$^\infty$[(Be$_3$/2N$_4$/3)$^-$] nets, and are tetrahedrally coordinated by nitrogen. Replacement of Li by the heavier and larger alkali metals like Na or K has not been fruitful, whereas a heavier homologue of beryllium is successfully achieved. A microcrystalline powder of Ae[Be$_2$N$_2$] (Ae = Mg, Ca, Sr and Ba) compounds were successfully prepared [2, 3]. These compounds crystalize as a substitutional alternative of the polymorphic modifications of cubic Be$_2$N$_2$ present in a low-temperature variation [4, 5] with tetrahedrally coordinated by nitrogen and Mn$_3$O$_7$-type structure, in addition beryllium at high-temperature variation [6, 7] is matched in a tetrahedral and trigonal-planar manner by nitrogen. The mixed alkaline earth metal nitride CaMg$_2$N$_2$ [8], Li$_2$CeN$_2$ [9] and Li$_2$ZrN$_2$ [10] also made in (anti-) La$_2$O$_3$-type structure. The compounds Ae[Be$_2$N$_2$] [11, 12] are characterized as Nitridoberyllates as well as it contain complex anion layers. Because beryllium and nitrogen contain covalent bonds whereas Mg[Be$_2$N$_2$] made in the preliminary La$_2$O$_3$-type structure [13]. Compounds containing Ca, Sr, and Ba are iso-structural to Ca[Be$_2$C$_2$] [14].

The compound Mg[Be$_2$N$_2$] contains puckered Be–N six-membered rings, which are reduced to single layers parallel (001) and which are pair-wise linked to form double layers along [001]. Magnesium is octahedrally bounded by nitrogen (d(Mg–N) = 220.9(2) pm) and is located between the complex anions 2$^\infty$[(Be$_2$N$_2$)$_2^-$] [15]. Lithium–nitrogen in Ca(Li$_2$[Mn$^3$N$_3$]) [16, 17] adopted the same congruent motif. With a full-potential calculations [18, 19] the series of Be and N along [001] in the crystal structure of Ca[Be$_2$N$_2$] were checked in space group P4/mmb. The corrected values for the $X_{corr}$ (300 K) amount to $-35.3$ (Ca[Be$_2$N$_2$]), $-28.5$ (Mg[Be$_2$N$_2$]), and $-60.3 \times 10^{-6}$ emu mol$^{-1}$ (Ba[Be$_2$N$_2$]). A value of $X_A$ (300 K) $= (-27 \pm 2) \times 10^{-6}$ emu mol$^{-1}$ can be intended.
for the \([\text{Be}_2\text{N}_2]\), with the diamagnetic increments \(X_{\text{dia}}\) for the alkaline-earth ions \(\text{Ae}^{2+}\) [20]. Therefore, nitridoberyllates are diamagnetic. The bonding condition in the compounds \(\text{Mg}[\text{Be}_2\text{N}_2], \text{Ca}[\text{Be}_2\text{N}_2]\), and \(\text{Sr}[\text{Be}_2\text{N}_2]\) were analyzed [21, 22]. Compounds \(\text{CaBe}_2\text{P}_2, \text{CaBe}_2\text{As}_2, \text{MgBe}_2\text{P}_2\) and \(\text{MgBe}_2\text{As}_2\) have been prepared [23], and crystallized in trigonal \(\text{CaAl}_2\text{Si}_2\)-type structure.

The \(\text{CaBe}_2\text{X}_2, \text{X} = (\text{N, P, As, Sb, Bi})\) have been investigated mainly through experimental techniques. However, experimental work is mostly on the structural properties of these compounds. No work is present on the energy band structure, optical and thermoelectric properties. Therefore, we have calculated the different properties of the compounds through first principles technique of density functional theory. Most of the results on these compounds are described for the first time.

\section{2 Computational Details}

First-principles density functional calculations carried out using the all electron full-potential linearized augmented plane wave (FP-LAPW) [24] method implemented in the Wien2k code [25]. The Perdew–Burke–Ernzerhof (PBE) [26] and Tran-Blaha modified Becke-Johnson (TB-mBJ) [27] functionals were employed for account of exchange-correlation effects. We relaxed both the atomic positions and lattice constants taking into account the plane wave cut-off was set to 500 eV. The atomic positions were relaxed until the forces and the energy converged to \(10^{-3}\) eV/Å and \(10^{-4}\) eV, respectively. Monkhorst–Pack of gamma-centered \(k\)-mesh of 1000 points was employed for integration of the Brillouin zone. Particularly, the converged PBE wave functions were used as the starting points for the TB-mBJ calculations.

\section{3 Results and Discussion}

\subsection{3.1 Structure Properties}

\(\text{CaBe}_2\text{X}_2\) exist in trigonal structure having space group \(\text{P}3\text{m}1\) (#164), with cell parameters \(a = b \neq c, \alpha = \beta = 90^\circ\) and \(\gamma = 120^\circ\). \(\text{Ca}\), usually occupied Wyckoff position 1b, while \(\text{Be}\) and \(\text{X}\) occupied 2d position in \(\text{CaBe}_2\text{X}_2 (\text{X} = \text{N, P, As, Sb and Bi})\). Compounds structural behavior is explained by calculating structure parameters. The lattice parameters \(a(\text{Å}), c(\text{Å}), c/a\) ratio, the bulk modulus \(\text{B(GPa)}\) and its pressure derivative \(\text{B'}\), ground state energy \(E_0\) (Ry.) and volume \(V_0\) (a.u.)\(^3\) are obtained by the volume optimization of the unit cell of \(\text{CaBe}_2\text{X}_2 (\text{X} = \text{N, P, As, Sb and Bi})\). Investigated compounds optimize structure and optimization curve is shown in Figures 1 and 2, respectively. Lowest energy of the unit cell is the ground state energy and volume corresponding to this optimum energy is the ground state volume. Calculated values of this parameter are presented in Table 1. There is increase in \(a(\text{Å})\) which is clearly seen in the table, as one move down the periodic table from \(\text{N}\) to \(\text{Bi}\). By changing the anion from \(\text{N}\) to \(\text{Bi}\) atomic size increases and \(\text{B(GPa)}\) value decreases, which show the material compressibility increases from top to bottom anion replacement.

\subsection{3.2 Electronic Properties}

Band structures of \(\text{CaBe}_2\text{X}_2\) are calculated using TB-mBJ. The conduction band minima (CBM) of \(\text{CaBe}_2\text{X}_2\) lies at the \(\Gamma\) symmetry point and valence band maxima (VBM) lies

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Crystal structure of \(\text{CaBe}_2\text{X}_2 (\text{X} = \text{N, P, As, Sb and Bi})\) compounds.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.png}
\caption{Volume optimization curves of \(\text{CaBe}_2\text{P}_2\) as a prototype for \(\text{CaBe}_2\text{X}_2 (\text{X} = \text{N, P, As, Sb, Bi})\) compounds.}
\end{figure}
Table 1: Structural parameter used in the present calculation as well as other study, lattice parameter $a(\AA)$, $c(\AA)$, $c/a$ ratio, Pressure derivative ($B'$), the Bulk Modulus $B$(GPa), Volume $V_0$, and Energy $E_0$ are obtained, respectively.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$a(\AA)$</th>
<th>$c(\AA)$</th>
<th>$c/a$</th>
<th>$V_0$</th>
<th>$B$(GPa)</th>
<th>$B'$</th>
<th>$E_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CaBe$_2$N$_2$</td>
<td>3.044</td>
<td>5.877</td>
<td>1.930</td>
<td>318.22</td>
<td>145.81</td>
<td>5.0</td>
<td>$-1639.24$</td>
</tr>
<tr>
<td>CaBe$_2$P$_2$</td>
<td>3.599, 3.760 [23]</td>
<td>8.126, 6.641 [23]</td>
<td>2.257, 1.77 [23]</td>
<td>615.48</td>
<td>71.07</td>
<td>5.0</td>
<td>$-2788.49$</td>
</tr>
<tr>
<td>CaBe$_2$As$_2$</td>
<td>3.908, 3.876 [23]</td>
<td>6.804, 6.814 [23]</td>
<td>1.741, 1.76 [23]</td>
<td>607.19</td>
<td>70.47</td>
<td>5.0</td>
<td>$-10464.46$</td>
</tr>
<tr>
<td>CaBe$_2$Sb$_2$</td>
<td>4.171</td>
<td>7.709</td>
<td>1.848</td>
<td>759.86</td>
<td>55.99</td>
<td>5.0</td>
<td>$-27354.54$</td>
</tr>
<tr>
<td>CaBe$_2$Bi$_2$</td>
<td>4.476</td>
<td>7.342</td>
<td>1.640</td>
<td>860.51</td>
<td>46.21</td>
<td>5.0</td>
<td>$-87746.11$</td>
</tr>
</tbody>
</table>

at $M$ symmetry point; hence all compounds show indirect band gap nature along $\Gamma \rightarrow M$ direction as shown in Figure 3. In all the cases, CaBe$_2$N$_2$ yielded the highest band gap (2.890 eV). The band gap decreases as the pnictogen anion replaced from N to Bi. The calculated band gaps and bond lengths between Be-X, Ca-X and Ca-Be are listed in Table 2; there is increase in the bond length value as anion replaced from N to Bi. So, there is inverse relation which is clearly observed between the bond length and band gap values of the compounds.

Total density of states (TDOS) and partial density of states (PDOS) plots of CaBe$_2$X$_2$ ($X = N, P, As, Sb and Bi$) compounds are shown in Figure 4. In the valence band, major contribution is due to $X-p$ state and a very little contribution is seen from Be-$p$ state and Ca-$d$ state. While in conduction band (CB) the major contribution is mainly due

Figure 3: Calculated band gap energy using TB-mBJ for (a) CaBe$_2$N$_2$, (b) CaBe$_2$P$_2$, (c) CaBe$_2$As$_2$, (d) CaBe$_2$Sb$_2$, and (e) CaBe$_2$Bi$_2$ compounds.
Table 2: Band gap energy and bond lengths of compounds.

<table>
<thead>
<tr>
<th>Compounds</th>
<th>Band gap energy (eV)</th>
<th>Other works</th>
<th>Bond lengths (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CaBe₂N₂</td>
<td>2.890</td>
<td>–</td>
<td>2.412 1.795 2.677</td>
</tr>
<tr>
<td>CaBe₂P₂</td>
<td>1.327</td>
<td>–</td>
<td>2.946 2.095 3.144</td>
</tr>
<tr>
<td>CaBe₂As₂</td>
<td>1.140</td>
<td>–</td>
<td>2.942 2.348 3.397</td>
</tr>
<tr>
<td>CaBe₂Sb₂</td>
<td>0.916</td>
<td>–</td>
<td>3.261 2.458 3.613</td>
</tr>
<tr>
<td>CaBe₂Bi₂</td>
<td>0.132</td>
<td>–</td>
<td>3.323 2.591 3.445</td>
</tr>
</tbody>
</table>

Figure 4: Calculated TDOS and PDOS for CaBe₂X₂ (X = N, P, As, Sb and Bi) compounds.

to the Ca-\(d\) state and a very small contribution from X-\(p\) states and Be-\(p\) states are appeared.

3.3 Chemical Bonding

Charge density distribution maps are plotted in (110) plane for investigating the chemical bonding nature in CaBe₂X₂ (X = N, P, As, Sb and Bi) compounds. The counter plots of charge density in (110) plane are shown in Figure 5. Following Figure 5, there is no obvious charge density at the Ca-Be bonding regions, the distribution of electronic charge around Ca is spherical which results in the bonding between Ca-Be showing prevailing ionic features because of electro negativity difference between Ca (1.0) and Be (1.57). Also in (110) plane, Ca forms ionic bonding with X atoms having electro negativity (X = N (3.04), P (2.19), As (2.18), Sb (2.05) and Bi (2.02)) and the charge distribution around Ca is remain spherical. While there exist charge densities between Be atom and its neighboring X atoms, the distribution of charge is not spherical around Be atoms, indicating some covalent bond. This is due to the strong hybridization of Be-\(p\) and X-\(p\) states (discussed in Dos). Therefore, from the above it is concluded that a mixture of covalent and ionic-like character, characterizes the bonding nature in CaBe₂X₂.

3.4 Optical Properties

The optical properties are calculated by random phase approximation; only interband transitions are included
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Figure 5: Charge density maps on [110] plane of CaBe$_2$X$_2$ (X = N, P, As, Sb, Bi) compounds.

[28–33]. Dispersion of an electromagnetic wave, when it enters in a medium can be explained by real part of dielectric function, $\varepsilon_1(\omega)$. Frequency-dependent $\varepsilon_1(\omega)$ spectra for CaBe$_2$X$_2$ (X = N, P, As, Sb, Bi) compounds are presented in Figure 6a. It is clearly seen from the figure, that band gap of the compounds strongly related with the static dielectric constant, $\varepsilon_1(0)$. The calculated values of $\varepsilon_1(0)$ for CaBe$_2$N$_2$, CaBe$_2$P$_2$, CaBe$_2$As$_2$, CaBe$_2$Sb$_2$ and CaBe$_2$Bi$_2$ are 4.92, 7.20, 9.18, 11.76 and 15.42, respectively. The calculated data show that the smaller band gap produced a larger $\varepsilon_1(0)$ value, when we move down in this pnictogen group from N to Bi. This inverse feature could be associated with Penn’s Model [34]. After zero frequency limit, $\varepsilon_1(\omega)$ start grow and reaches its peak value (7.15 at 4.04 eV for CaBe$_2$N$_2$ compound, 10.07 at 2.14 eV for CaBe$_2$P$_2$ compound, 15.93 at 2.68 eV for CaBe$_2$As$_2$ compound, 18.05 at 1.89 eV for CaBe$_2$Sb$_2$ compound and 22.46 at 1.24 eV for CaBe$_2$Bi$_2$, respectively) at higher energies followed by a decreasing trend of $\varepsilon_1(\omega)$. Except SrMgN$_2$, whose energy value is lying in ultraviolet regions, all the other four...

Figure 6: Real and imaginary part of the dielectric functions for CaBe$_2$X$_2$ (X = N, P, As, Sb and Bi) compounds, (a) $\varepsilon_1(\omega)$ and (b) $\varepsilon_2(\omega)$. 
compounds main characteristic peak located in the visible region of electromagnetic spectrum. The spectra decrease toward low energy by changing X anion from N to Bi. It falls below zero after certain energy ranges, shows complete attenuation of light in the optical medium. Materials become highly reflective in this energy range.

In Figure 6b imaginary part of dielectric function, \( \varepsilon_2(\omega) \), is presented. The spectra of the compounds started at a particular energy, which is the absorption edge of the compounds. The absorption edges for CaBe\(_2\)N\(_2\), CaBe\(_2\)P\(_2\), CaBe\(_2\)As\(_2\), CaBe\(_2\)Sb\(_2\) and CaBe\(_2\)Bi\(_2\) CaBe\(_2\)N\(_2\) are 0.026, 0.069, 0.091, 0.166 and 0.286 eV, respectively. Beyond the absorption edge characteristics absorptions peaks appeared. These peaks are due to the interband transitions from the valance band to the unoccupied CB states. High absorption obtained where the joint density of states is high. The main peaks of CaBe\(_2\)N\(_2\), CaBe\(_2\)P\(_2\), CaBe\(_2\)As\(_2\), CaBe\(_2\)Sb\(_2\) and CaBe\(_2\)Bi\(_2\) compounds have magnitude 7.99, 10.32, 14.01, 15.57 and 19.38 at energy 8.72, 6.33, 5.46, 4.39 and 2.49 eV, respectively.

Zero frequency reflectivity \( R(0) \), which is the static part of the reflectivity is at 14%, 20%, 25%, 29% and 35% for CaBe\(_2\)N\(_2\), CaBe\(_2\)P\(_2\), CaBe\(_2\)As\(_2\), CaBe\(_2\)Sb\(_2\) and CaBe\(_2\)Bi\(_2\) compounds as shown in Figure 7. After the limit of zero frequency, reflectivity coefficient \( R(\omega) \) increases with increasing incident photon frequency. Maximum reflectivity arises from the inter band transitions. The maximum reflectivity \( R(\omega) \) is 35% at 16.77 eV, 46% at 8.61 eV, 61% at 9.40 eV, 60% at 7.33 eV and 57% at 6.89 eV for CaBe\(_2\)N\(_2\), CaBe\(_2\)P\(_2\), CaBe\(_2\)As\(_2\), CaBe\(_2\)Sb\(_2\) and CaBe\(_2\)Bi\(_2\) compounds, respectively. All the compounds have roughly similar reflectivity spectra; it shows good response at energies 9.13–16.7 eV region for SrMg\(_2\)N\(_2\) while 5–12.5 eV region for the rest of compounds. In high reflectivity regions, compounds have high thermoelectric properties and potentially prevent it from solar heating.

Frequency dependent optical conductivities (\( \sigma(\omega) \)) for CaBe\(_2\)X\(_2\) (X = N, P, As, Sb, Bi) are shown in Figure 8. Optical conductivity \( \sigma(\omega) \) start at approximately 3.08, 1.89, 2.03, 1.32 and 0.99 eV for CaBe\(_2\)N\(_2\), CaBe\(_2\)P\(_2\), CaBe\(_2\)As\(_2\), CaBe\(_2\)Sb\(_2\) and CaBe\(_2\)Bi\(_2\), respectively. It increases slowly with smaller peaks for CaBe\(_2\)N\(_2\), CaBe\(_2\)P\(_2\), CaBe\(_2\)As\(_2\) and CaBe\(_2\)Bi\(_2\) and reaches to maximum value, whereas CaBe\(_2\)Sb\(_2\) increase sharply and reach to their maximum value and then decrease slowly. The maximum value of \( \sigma(\omega) \) are found to be 9412 \( \Omega^{-1}\cdot\text{cm}^{-1} \), 8832 \( \Omega^{-1}\cdot\text{cm}^{-1} \), 10389 \( \Omega^{-1}\cdot\text{cm}^{-1} \), 9332 \( \Omega^{-1}\cdot\text{cm}^{-1} \) and 8253 \( \Omega^{-1}\cdot\text{cm}^{-1} \) around 8.77 eV, 6.381 eV, 5.537 eV, 4.50 eV and 3.38 eV for CaBe\(_2\)N\(_2\), CaBe\(_2\)P\(_2\), CaBe\(_2\)As\(_2\), CaBe\(_2\)Sb\(_2\) and CaBe\(_2\)Bi\(_2\), respectively, where the magnitude of \( \sigma(\omega) \) is largest for CaBe\(_2\)As\(_2\). After achieving the maximum values of optical conductivity in the high energy range decreases.

The calculated refractive indices for CaBe\(_2\)X\(_2\) (X = N, P, As, Sb, Bi) compounds are shown in Figure 9a. The refractive index \( n(\omega) \) has an important role in consideration of the electronic properties of materials. \( n(\omega) \) has a similar character as that of \( \varepsilon_1(\omega) \). This similarity of spectra is supported with the established theory [34]. The values of static refractive index \( n(0) \) are noted as 2.22, 2.68, 3.03, 3.42 and 3.92 for CaBe\(_2\)N\(_2\), CaBe\(_2\)P\(_2\), CaBe\(_2\)As\(_2\), CaBe\(_2\)Sb\(_2\) and CaBe\(_2\)Bi\(_2\) compounds, respectively. These results show that \( n(0) \) increases as we move from CaBe\(_2\)N\(_2\) to CaBe\(_2\)Bi\(_2\). After this point, the spectra increase sharply to 2.65 at 7.52 eV, 3.26 at 2.84 eV, 4.04 at 2.71 eV, 4.32 at 1.94 eV and 4.75 at 1.26 eV, for CaBe\(_2\)N\(_2\), CaBe\(_2\)P\(_2\), CaBe\(_2\)As\(_2\), CaBe\(_2\)Sb\(_2\) and CaBe\(_2\)Bi\(_2\), respectively. It is obvious from the plots...
that the refractive indices of these compounds are high in the lower energy region and gradually decreased in the ultraviolet region.

The local maxima of $K(\omega)$ are found to be 1.80 for CaBe$_2$N$_2$ at 9.05 eV, 2.19 for CaBe$_2$P$_2$ at 6.57 eV, 2.80 for CaBe$_2$As$_2$ at 6.33 eV, 2.89 for CaBe$_2$Sb$_2$ at 4.72 eV and 2.91 for CaBe$_2$Bi$_2$, respectively as shown in Figure 9b. $K(\omega)$ has a same trend just like $\varepsilon_2(\omega)$, which shows absorption of the incident electromagnetic energy. This similarity of spectra is supported with the established theory [35].

Figure 10 shows the birefringence $\Delta n(\omega)$ for CaBe$_2$X$_2$ ($X = N, P, As, Sb$ and Bi) compounds, which is basically the difference between the extraordinary and ordinary refraction indices, $\Delta n = n_e - n_o$. The presence of birefringence is essentially in the non-absorbing region, which is below the energy gap. The $\Delta n(\omega)$ spectral dependence displays oscillations in the energy range from 1 to 10 eV.

### 3.5 Thermoelectric Properties

The calculated values of Seebeck coefficient for the compounds CaBe$_2$X$_2$ as a function of temperature is shown in Figure 11. It is clear from plots that for the compounds CaBe$_2$N$_2$, CaBe$_2$P$_2$, CaBe$_2$As$_2$, CaBe$_2$Sb$_2$ and CaBe$_2$Bi$_2$, the Seebeck coefficient is appreciably changing with the rise in temperature. At 300 K, the calculated Seebeck coefficient for compounds CaBe$_2$N$_2$, CaBe$_2$P$_2$, CaBe$_2$As$_2$, CaBe$_2$Sb$_2$ and CaBe$_2$Bi$_2$ are 267.394 µV/K, 257.9166 µV/K, 252.7845 µV/K, 257.105 µV/K and 201.175 µV/K, respectively. However, the values of Seebeck coefficients for the compounds CaBe$_2$N$_2$, CaBe$_2$P$_2$, CaBe$_2$As$_2$ and CaBe$_2$Sb$_2$, gradually increase while CaBe$_2$Bi$_2$ decreases when temperature increases up to 800 K. The calculated values of Seebeck coefficient for the compounds CaBe$_2$N$_2$, CaBe$_2$P$_2$, CaBe$_2$As$_2$, CaBe$_2$Sb$_2$ and CaBe$_2$Bi$_2$ are 297.8905 µV/K, 260.885 µV/K, 262.1325 µV/K, 267.229 µV/K and 106.4424 µV/K at temperature 800 K, respectively.
Figure 12 shows the variation of electrical conductivity of CaBe$_2$X$_2$ in per relaxation time with temperature. From the plot, it is obvious that the electrical conductivity of the compounds CaBe$_2$N$_2$, CaBe$_2$P$_2$, CaBe$_2$As$_2$, CaBe$_2$Sb$_2$ and CaBe$_2$Bi$_2$ vary nearly linear with the increase in temperature. However, the compound CaBe$_2$Bi$_2$ shows somewhat more pronounced increments in electrical conductivity, due to increase in temperature, as compared with others. This behavior can be attributed to small energy bandgap of the compound. The highest calculated values of electrical conductivity at 800 K are $0.05701 \times 10^{20}$ (Ω·m·s)$^{-1}$, $0.0443 \times 10^{20}$ (Ω·m·s)$^{-1}$, $0.0294 \times 10^{20}$ (Ω·m·s)$^{-1}$, $0.04025 \times 10^{20}$ (Ω·m·s)$^{-1}$ and $0.10376 \times 10^{20}$ (Ω·m·s)$^{-1}$ for the compounds CaBe$_2$N$_2$, CaBe$_2$P$_2$, CaBe$_2$As$_2$, CaBe$_2$Sb$_2$ and CaBe$_2$Bi$_2$, respectively.

Figure 13 shows the variation of thermal conductivity for the compounds CaBe$_2$X$_2$ with temperature. It is obvious from plot that the values of thermal conductivity for CaBe$_2$X$_2$ in per relaxation time increase with temperature. The maximum calculated values of thermal conductivity are $0.48878 \times 10^{15}$ (W/m·k$^2$·s)$^{-1}$, $0.25621 \times 10^{15}$ (W/m·k$^2$·s)$^{-1}$, $0.20983 \times 10^{15}$ (W/m·k$^2$·s)$^{-1}$, $0.29406 \times 10^{15}$ (W/m·k$^2$·s)$^{-1}$ and $0.58941 \times 10^{15}$ (W/m·k$^2$·s)$^{-1}$ for the compounds CaBe$_2$N$_2$, CaBe$_2$P$_2$, CaBe$_2$As$_2$, CaBe$_2$Sb$_2$ and CaBe$_2$Bi$_2$, respectively.

Figure 14 shows the variation of the figure of merit for the compounds CaBe$_2$X$_2$ with temperature and thermal conductivity. The figure of merit (ZT) for the compounds is optimized. The modified Becke Johnson exchange potential along with the GGA is used.

Figure 14: Figure of merits (ZT) obtained for CaBe$_2$X$_2$ (X = N, P, As, Sb and Bi).

4 Conclusions

The structural, electronic, optical and thermoelectric properties of ternary CaBe$_2$X$_2$ (X = N, P, As, Sb and Bi) compounds are investigated using all electrons full potential linearized augment plane wave method. By using generalized gradient approximation (GGA) the unit cell volume of the compounds is optimized. The modified Becke Johnson exchange potential along with the GGA is used.
for calculation of electronic and optical properties. All compounds show energy band gap and it is observed that by changing the anion X from N to Bi the band gap decreases. Furthermore, electron charge density plots concluded that ionic bonding is dominant in these compounds with small covalent character. Optical spectra of the compounds shifted towards lower energy by replacing the anion from N to Bi. Further high absorption peaks are observed in the visible and ultraviolet energy regions. The indirect and small bandgap nature of the compounds including ionic bonding in these materials characterizes these materials very suitable for the thermoelectric applications.

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