First-principle calculations of the electronic, structural, optical, thermoelectric and elastic properties of CeXO3 (X = Ti, V and Cr) perovskites

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ABSTRACT
The electronic, structural, optical, thermoelectric and elastic properties of cubic CeXO3 perovskites (X = Ti, V and Cr) were studied within the density functional theory via full-potential linearized augmented plane wave (FP-LAPW) process. It found that CeXO3 are stable in ferromagnetic phase with less energy than in the nonmagnetic phase. The band structures and density of states show that CeTiO3 exhibits a metallic nature whereas CeVO3 and CeCrO3 have a half-metallic (HM) property. The dielectric function was used to calculate the optical parameters like the absorption spectra, energy-loss spectra, refractive index, reflectivity and conductivity. Moreover, the thermoelectric properties include the electrical conductivity, Seebeck coefficient and power factor, were evaluated using BoltzTrap code, which infer that CeXO3 have p-type doping characteristics. The results of elastic parameters indicate that CeXO3 compounds have anisotropic and ductile nature. The obtained results suggest that the CeXO3 have promise for potential in thermoelectric and optoelectronic applications.

1. Introduction
Perovskites have a broad variety of crystal structures, fascinating spintronic and multiferroic properties as well as other interesting physical properties [1,2]. Perovskites based on oxides and their derivatives are contained in a small range of compounds. In the perfect ABO3 cubic structure, the cation A is the base element located at the unit cell corner, the cation B is a metal located in the middle and oxygen is found at the unit cell’s face-centered locations [14,15]. The perovskite oxides RE–TM–O3 have recently attracted a lot of attention in experimental and theoretical studies (RE indicates rare earth while TM refers to transition metal elements). This type of oxides crystallizes as an ABO3 cubic perovskite with the space group Pm-3m (No.221) [16].

Several experimental studies have been performed on cerium based CeXO3 (X = Co, Ni, Cu) perovskites. From these studies, it was found that these compounds can be used in supercapacitor electrode materials [17]. Hasni et al. used the ab initio APW + lo technique to examine the effect of the Ga and In cations on the magnetic and electronic properties of CeBO3 (B = Ga, In). These calculations showed that there was favourable energy stability for CeInO3 with the hexagonal structure (P63/mmc) and for CeGaO3 with the orthorhombic structure (Pnma) [18]. The cubic CeCrO3 compound was studied for the first time by Rashid et al. via density functional theory [19]. They examined only the magnetic and electronic properties of CeCrO3 in the FM phase by using mBJ approximation. They found that this compound shows ferromagnetic half-metallic properties with a total magnetic moment equal to 4.0 μB. No
detailed reports are available on the optical and thermoelectric properties resulting from substitution of the B site in CeBO₃ with Ti, V, and Cr ions.

The lack of data regarding some physical properties of Ce-based perovskites CeBO₃ motivated us to carry out a comprehensive DFT study on this type of compounds. Therefore, the main goal of this work is to study the structural, electronic, optical, and thermoelectric and elastic properties of CeXO₃ (X = Ti, V, and Cr) perovskite compounds. These successive 3d transition-metals, which show a similar electronic configuration, Ti (Z = 22): [Ar]¹⁸ 4s² 3d², V (Z = 23): [Ar]¹⁸ 4s² 3d³, and Cr (Z = 24): [Ar]¹⁸ 4s¹ 3d⁵ in perovskite oxides, have been carefully chosen to study their deep effect on the physical properties of the parent perovskite CeXO₃. To this end, the FP-LAPW process was utilized with the generalized gradient approximation (GGA) functional.

2. Calculation methods

In frame of the density functional theory (DFT), the structural calculations and optimizations of CeXO₃ (X = Ti, V and Cr) compounds were carried out utilizing the FP-LAPW process implemented in the WIEN2k software [20]. The optimizations of the structure were achieved by GGA within the Perdew, Burke and Ernzerh (PBE) method [21]. The utilized electronic configurations were [Xe] 4f¹5d¹6s² for Ce, [Ar] 3d²4s² for Ti, [Ar] 3d³4s² for V, [Ar] 3d⁵4s¹ for Cr, and [He] 2s²2p⁴ for O. The crystal structure of CeXO₃ (X = Ti, V and Cr) perovskites is cubic with a Pm-3m space group (#221), where Ce atoms are positioned at 1a (0,0,0), X atoms are located at 1b (0.5,0.5,0.5), and the three O atoms are located at 3c (0.5,0.5,0), as presented in Figure 1.

The electronic and structural properties of CeXO₃ perovskites were measured at 1728 k-points (12 × 12 × 12) k-mesh, while the thermoelectric properties, in the first Brillouin zone, were examined using 64,000 k-points. The cut-off energy, the separation energy between valence and core states in atoms, is selected as of −6.0 Ry. The convergence test is used to predict the value Kmax × RMT. This test assumes the calculation is converged under (Kmax × RMT = 7.0), where RMT is the radius of the muffin tin and Kmax is the plane wave cut-off for the reciprocal lattice vector. Here, to avoid leakage of the charges from their atomic core, the RMT values are set as: 2.50, 1.84 and 1.67 for CeTiO₃; 2.50, 1.85 and 1.68 for CeVO₃; 2.50, 1.79 and 1.62 for CeCrO₃. The maximum value of angular momentum (Lmax = 10.0) and Fourier expanding (Gmax = 12.0 1/a.u.) are set for the partial waves inside atomic MTs and the charge density, respectively. Iterations up to the accuracy of 1 × 10⁻⁴ Ry were carried out for maximum total energy convergence.

The thermoelectric properties were calculated utilizing the BoltzTrap code as a function of carrier concentration and temperature [22]. The code is utilizing the semi-classical Boltzmann theorem. In BoltzTrap code, the Seebeck coefficient (S) is independent of the relaxation time (τ), but the electrical conductivity (σ) and thermal conductivity (κ) can only be determined with respect to τ [23]. The elastic constants were evaluated utilizing the Charpin method [24], which was employed in the WIEN2k.

3. Results and discussion

3.1. Structural properties

The elastic constants at the ground-state of CeXO₃ perovskites (X = Ti, V and Cr) are determined via the total energy fitting as a function of the unit cell volume with the Murnaghan equation of state (EOS) [25]. The structural optimized plots for these compounds in ferromagnetic (FM) and nonmagnetic (NM) configurations are presented in Figure 2. The evaluated bulk modulus (B), lattice constant (a), and pressure derivative of the bulk modulus (B0) of CeXO₃ at T = 0 K are listed in Table 1. The main remark here, that the FM state has the minimum energy than that for NM, where the total energy differences are ΔE = E_FM − E_NM ≈ −0.0034, −0.00468 and −0.05134 Ry per unit cell of CeTiO₃, CeVO₃, and CeCrO₃, respectively. Therefore, FM will be adopted as a stable state to calculate and analysis the proposed properties of all CeXO₃ perovskites. Also, it is observed from Table 1 that the lattice constants increase with the atomic radii of the transition metals R(Ti) = 1.47 Å > R(V) = 1.34 Å > R(Cr) = 1.28 Å [26]. Correspondingly, the variation in bulk modulus values based on FM state has the dissimilar behaviour to
Figure 2. Energy-volume optimization curves of CeXO₃ (X = Ti, V and Cr) perovskite structure calculated in ferromagnetic (FM) and nonmagnetic (NM) phases.

Table 1. Lattice constant (a in Å), bond lengths (in Å), pressure derivative of the bulk modulus (B₀), bulk modulus (B in GPa) and tolerance factor for CeXO₃ (X = Ti, V and Cr) perovskites.

| Compound | a     | V₀     | B (GPa) | B₀   | E (Ry) | ΔHᵣ | Ce-O | X-O | Ce-X | t   |
|----------|-------|--------|---------|------|--------|------|------|-----|------|-----|
| CeTiO₃   | NM    | 3.9367 | 411.6996| 183.5822| 4.4182 | −19890.61346| −5.99 | 2.8686 | 2.0284 | 3.5133 | 1.00 |
|          | FM    | 3.9457 | 414.5291| 182.3771| 3.5508 | −19890.61963|        |        |        |      |     |
| CeVO₃    | NM    | 3.8646 | 389.4990| 195.4508| 4.2362 | −20081.507010| −5.76 | 2.8613 | 2.0233 | 3.5044 | 0.999|
|          | FM    | 3.8853 | 395.8334| 164.4263| 3.7148 | −20081.511691|        |        |        |      |     |
| CeCrO₃   | NM    | 3.8227 | 376.9590| 206.6250| 4.3547 | −20284.523444| −5.64 | 2.8394 | 2.0078 | 3.4776 | 0.999|
|          | FM    | 3.8759 | 392.9314| 171.6025| 2.4070 | −20284.574786|        |        |        |      |     |

|       |       |       |        | 0.997 | a = 3.8770 Å, t = 0.999, [19]. |

that verified for the lattice constants, B of CeTiO₃ is greater than that of CeCrO₃ and CeVO₃. To the best of our knowledge, the experimental or theoretical values of the bulk modulus, the pressure derivative of the bulk modulus and the lattice parameters have not been stated except for the cubic CeCrO₃ [19]. The lattice parameter calculated for CeCrO₃ agrees with the previously reported theoretical value.

The length of the bond among atoms is significant for determining the symmetry of the structure of the perovskite compound. Goldschmidt’s tolerance factor (t) [27] is used to determine the crystal structure stability based on the length of the bond and is calculated using:

\[ t = \frac{0.707 \left( \langle A - O \rangle \right)}{\langle B - O \rangle} \] (1)

Here \( \langle A - O \rangle \) and \( \langle B - O \rangle \) represent the bond lengths of Ce-O and X-O (X = Ti, V and Cr), respectively. In general, the t-value for cubic compounds is in the range of 0.93–1.04 [28,29], and the determined tolerance factor values for CeTiO₃ (t = 1.00) and for both CeVO₃ and CeCrO₃ (t = 0.999) confirm the stability of the cubic structure of these perovskite compounds. The formation energy is also a good parameter to predict the stability of compounds. This energy value is calculated through the following equation:

\[ \Delta Hᵣ = E(CeXO₃) - (E_{Ce} + E_{X} + 3E_O) \] (2)

where \( E(CeXO₃) \) is the total energy of the compound, \( E_{Ce}, E_{X} \), and \( E_O \) represent the bulk energy of content atoms. The calculated values of formation energy...
appear with negative sign, as shown in Table 1, which confirm the structural stability of these compounds.

3.2. Electronic properties

The electronic properties of CeXO₃ (X = Ti, V and Cr) perovskites were studied by investigating their total and partial density of states (DOS) and band structure in both spin-up and spin-down channels. The calculated band structures are presented for the three studied compounds at 0 K and 0 GPa alongside the Brillouin zone symmetry lines. The lattice constants are in the energy range −8.0 eV to 8.0 eV at the equilibrium.

From Figure 3, one can see that the band structures tend to be quite similar, and all three perovskites CeTiO₃, CeVO₃, and CeCrO₃ exhibit a metallic behavior in spin-up direction, which is characterized by an overlap between the top of the valence band and the bottom of the conduction band. Figure 3(a) shows that the electronic band structure of the CeTiO₃ compound has a metallic character as a result of a Fermi-level (EF) crossing one of the permitted bands in both the minority and majority electronic spins with zero band gap. Whereas the electronic band structures demonstrate that the two CeVO₃ and CeCrO₃ compounds to be half-metallic (HM) nature, consistent with those detected in similar V- and Cr-based perovskites using the GGA method [19,29]. In CeVO₃ and CeCrO₃ compounds as shown in Figure 3(b and c), respectively, all approved bands cross the EF in the spin-up direction, but all spin-down bands show an energy gap through the EF. The predicted energy gap in the spin-down channel is 3.057 eV along the Γ−X symmetry point for CeVO₃ and 2.720 eV along the Γ−X symmetry path for CeCrO₃.

To investigate the role of different ion states in electronic band structures, we computed the total density of states (TDOS) and partial density of states (PDOS) of the studied CeXO₃ (X = Ti, V and Cr) cubic perovskites, as shown in Figures 4–6, respectively. In the case of CeTiO₃ (Figure 4), the participation of each state, such as s, p, d, and f states of Ce, Ti, and O atoms, is displayed in majority-spin (spin-up) and minority-spin (spin down). In the spin-up case, the Ce-4f states have the highest participation in the conduction band, expand between −1.0 eV and +1.0 eV, the Ce-5d states have a participation only in the conduction band from +2.0 eV to +4.0 eV, while the Ce-4f, Ti-3d and O-2p states in spin-up channel, and a little Ti-3d states in spin-down channel, cross the EF to yield the metallic character of this material.

Whereas, in the case of CeVO₃ and CeCrO₃, the TDOS exhibits metallic behavior in the majority spin and semiconductor behavior in the minority spin. Thus, CeVO₃ and CeCrO₃ compounds have a half-metallic (HM) nature, making them potential candidates for spintronics applications. As shown in Figures 5 and 6, the bottom of the conduction bands and the top of the valence bands are at the same place in the Brillouin zone, confirming that CeVO₃ possesses a direct band gap in the minority spin electrons with a large value of 3.057 eV. The valance band in CeVO₃ (Figure 5) and CeCrO₃ (Figure 6) comes from the O-2p and V-3d/Cr-3d states. The Ce-4f states are responsible for the bands in the conduction region, (−1.8 to +1.0 eV) and (−1.0 to +1.0 eV) in these two compounds, respectively, with a small contribution from the 3d and 2p states of V, Cr and O atoms.

The distributions of TDOS and PDOS for CeXO₃ (X = Ti, V and Cr) in Figures 4–6 are categorized into two regions. The first is from −7.0 eV to −3.0 eV which is in the valence band with the maximum influence to the DOS drawing from X-3d, O-2p, and few of X-3p states. The second region started in the valance band from −0.6 eV for CeTiO₃, −1.0 eV for CeVO₃, and −1.4 eV for CeCrO₃ to 8.0 eV in the conduction band. At this region, the maximum contribution is from Ce-4f states together with few contributions from O-2p and X-3d states at the EF, as well as bands that are present above the EF in the conduction band occupied by Ce-5d, X-3d, and O-2p states.

Comparing the TDOSs of CeXO₃ and local density of states (PDOSs) for Ce, O, and X (X = Ti, V Cr), it can be inferred that the Ce electrons have the highest contribution to the CeXO₃ conduction band. It is also noticed that the studied compounds do not have a band gap in spin-up panel because their TDOS values at the EF are not zero, and this indicates a metallic feature in spin-up of the studied compounds. While the spin-down TDOS shows a metallic nature for CeTiO₃ (Figure 4) and a band gap with half-metallic nature for the compounds CeVO₃ (Figure 5) and CeCrO₃ (Figure 6). The total states in spin-up direction, at the EF, are 12.2, 8.90, and 17.5 states/eV/unit cell for CeTiO₃, CeVO₃, and CeCrO₃, respectively. It can be concluded that the difference in these values and the above results give clear evidence of the effect of X-site type due to the variance in electronic nature between the Ti, V, and Cr elements, which governed by their configurations Ti: 4s² 3d², V: 4s² 3d⁵ and Cr: 4s¹ 3d⁵, in their corresponding CeXO₃ compounds. This effect is evident in the HM property that was detected in both compounds of CeVO₃, and CeCrO₃, in contrast to that in the first one, CeTiO₃.

3.3. Magnetic properties

One of the most interesting aspect is the investigation on the magnetic properties of perovskites CeXO₃ (X = Ti, V and Cr) that containing rare-earth and transition-metal atoms because apart from the major contribution of transition-metal atom X, rare-earth atom Ce also contributes a large portion to total
magnetic moment of the unit cell CeXO$_3$. As summarized in Table 2, the spin-polarized magnetic properties of CeXO$_3$ are evaluated by calculating the three partial magnetic moments $M_{\text{Ce}}$, $M_X$ and $M_O$ per atoms for Ce, $X$ ($X = \text{Ti}$, V and Cr) and O, respectively, besides the partial magnetic moment contributed by the interstitial...
Figure 4. TDOS and PDOS of Ce, Ti and O for the perovskite CeTiO₃.

sites ($M_{\text{int}}$). Also, the values of total magnetic moment per unit cell ($M_{\text{tot}}$) for the investigated perovskites are displayed in a separate column. It can be seen from these results the main contribution of total magnetic moment is due to X and Ce atoms, whereas the atoms O and interstitials have minor effect on the total magnetic moment of their unit cell. The main observation here is that the type of transition-metal atom enhances the value of the partial magnetic moment on the X-site, which increases their total magnetic moment per unit cell. The partial and total magnetic moments reveal the FM behaviour in CeXO₃, which confirm the obtained result via the optimization calculations in Section 3.1. Besides, due to the number of unpaired electron in 3d-orbitals, Ti$^{3+}$: $3d^1$: $t_{2g}^{1}; S = 0.5$, V$^{3+}$: $3d^2$: $t_{2g}^{2}; S = 1.0$, and Cr$^{3+}$: $3d^3$: $t_{2g}^{3}; S = 1.5$, the calculated
values for the total magnetic moment increase in this sequence. Moreover, the obtained values of $M_{\text{Tot}}$ close to the theoretical, 2.0, 3.0 and 4.0 $\mu_B$, which verifies the presence of HM-FM properties in CeVO$_3$ and CeCrO$_3$, and in good agreement with those reported by Rashid et al. for the Cr-based perovskite using mBJ method [19].

### 3.4. Optical properties

Optical materials have become increasingly important due to their broad applications in various fields such as optical coatings, optical communication windows, mirrors, reflectors, lasers, and solar collectors [30,31]. Perovskites are good candidates as optical materials for the
Figure 6. TDOS and PDOSs of Ce, Cr and O for the perovskite CeCrO$_3$.

generation of high-performance optoelectronic devices [1]. The optical properties of perovskites compounds can be defined by the complex dielectric function ($\varepsilon$), which is used to characterize a specific material’s reaction to an applied field of electromagnetic radiation. $\varepsilon$ is represented as [32]:

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

where $\varepsilon_1(\omega)$ is the real part and $\varepsilon_2(\omega)$ is the imaginary part of the complex dielectric function ($\varepsilon$).

Figure 7(a) and (b) presents $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ of CeXO$_3$ (X = Ti, V, and Cr) in the energy spectrum up to 25.0 eV. $\varepsilon_1$ was calculated via the Kramers–Kronig dispersion relationship [19] is presented in Figure 7(a). It represents the ability of the material to store energy. For $\varepsilon_1(\omega) > 0$ the photons propagate in the material, for $\varepsilon_1(\omega) < 0$ the waves of electromagnetic radiations are
damped, and for $\varepsilon_1(\omega) = 0$ only longitudinally polarized waves is likely propagating [33]. The limit $\varepsilon_1(0)$ gives the static real part of the optical dielectric constant and is an essential characteristic of $\varepsilon_1(\omega)$. Table 3 summarizes the static values of $\varepsilon_1(0)$ locate at ($E = 0.0$ eV), which indicate that the value of $\varepsilon_1(0)$ increases from CeTiO$_3$ to CeVO$_3$ then decreases to CeCrO$_3$. After $\varepsilon_1(0)$, the $\varepsilon_1(\omega)$ starts to decrease sharply and attains negative value for CeTiO$_3$, CeVO$_3$ and CeCrO$_3$ compounds, then $\varepsilon_1(\omega)$ approaches zero at the high energy region. The imaginary component $\varepsilon_2(\omega)$ in Figure 7(b) demonstrates the material’s ability to absorb light at various energy levels. The spectrum is measured using the total transfer from the occupied valence band states to the unoccupied states in the band of conduction. The imaginar part shows that all of the CeXO$_3$ compounds are metallic. This behaviour is attributed to the high value of $\varepsilon_2(\omega)$, which is a characteristic of metallic compounds at zero frequency. Therefore, both $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ indicate metallic, and of course HM, nature of the studied compounds.

Furthermore, the real and imaginary parts of the dielectric function are used to determine the optical parameters of CeXO$_3$ along the xx-direction which include the reflectivity $R(\omega)$, loss function $L(\omega)$, absorption coefficient $I(\omega)$, extinction coefficient $k(\omega)$, refractive index $n(\omega)$, and optical conductivity $\sigma(\omega)$. The estimated $n(\omega)$ and $k(\omega)$ values are presented in Figure 8(a) and (b), respectively. The refractive index determines how much light is refracted when entering the material and has identical characteristics to the $\varepsilon_1(\omega)$ spectrum. The static refractive index at zero-frequency $n(0)$ is a significant parameter that is used to characterize the optical character of a material. The estimated values $n(0)$ for CeTiO$_3$, CeVO$_3$ and CeCrO$_3$ respectively. Figure 8(a) shows that the $n(\omega)$ values sharply decrease in the low energy region until around 1.9 eV above which and they fluctuate between decreasing and increasing. Figure 8(b) presents the $k(\omega)$ values as a function of photon energy. $k(\omega)$ values show a maximum peak in the near-infrared region (NIR) above which the $k(\omega)$ values continue to decrease up to 3.0 eV. The maximum values of $k(\omega)$ appear at the energy range 0.0–2.5 eV for CeXO$_3$ ($X = Ti$, V and Cr), see Table 3. Above 3.0 eV the $k(\omega)$ values start oscillating where two humps around 8.0 and 22.5 eV are observed.

The absorption coefficient, $I(\omega)$, shows the amount of energy needed for any interband transfer. The absorption spectrum shows some peaks that can be elucidated by the interband transition via the results of the band structure. It is obvious from Figure 9(a) that all studied perovskites have strong absorption at two different energies: 8.0 and 23.0 eV. The absorption of CeTiO$_3$, CeVO$_3$ and CeCrO$_3$ starts at 0.0 eV. Figure 9(b) displays the optical conductivity spectrum for CeXO$_3$ compounds in the photon energy range of 0.0–25.0 eV. The conductivity of CeXO$_3$ compounds exhibits a metallic nature because photoconductivity begins at zero photon energy. The optical conductivity range has many peaks associated with bulk plasmon excitations.

Table 2. Calculated interstitial, partial and total magnetic moments (in $\mu_B$) for perovskites CeXO$_3$ ($X = Ti$, V and Cr).

| Compound   | $M_{\text{int}}$ | $M_{Ce}$ | $M_{\text{Ti,VO, Cr}}$ | $M_{O}$ | $M_{\text{Tot}}$ |
|------------|------------------|----------|-------------------------|---------|-----------------|
| CeTiO$_3$  | 0.33436          | 1.25570  | -0.02105                | 1.97381 |                 |
| CeVO$_3$   | 0.49460          | 1.13577  | 1.37549                 | -0.00993| 2.97607         |
| CeCrO$_3$  | 0.55303          | 1.06122  | 2.37205                 | 0.00949 | 4.01478         |

*Note: mBJ method; MCe = 2.52830, M_{Ce} = 0.98310$\mu_B$, $M_{\text{Tot}}$ = 4.0040, and $M_{O}$ = 0.06420 [19].

Table 3. The static values of the real part of dielectric function $\varepsilon_1(0)$ and refractive index $n(0)$, and the maximum values of extinction coefficient $k(0)$ and optical conductivity $\sigma(0)$ (in $\Omega^{-1}\text{cm}^{-1}$).

| Compound   | $\varepsilon_1(0)$ | $n(0)$ | $\sigma_{\text{max}}(0)$ | $k_{\text{max}}(0)$ |
|------------|---------------------|--------|------------------------|---------------------|
| CeTiO$_3$  | 69.9090             | 8.54255| 13669.9                | 3.20000             |
| CeVO$_3$   | 147.489             | 12.4678| 13640.2                | 5.52000             |
| CeCrO$_3$  | 113.730             | 6.46305| 13496.9                | 7.36000             |

*Note: $\varepsilon_1(0)$ and $n(0)$ locate at ($E = 0.0$ eV), and $k(0)$ and $\sigma(0)$ values are present in Figure 8(a) and (b), respectively.

Figure 7. Variations of the real (a) and imaginary (b) parts of the dielectric function for CeXO$_3$ ($X = Ti$, V and Cr) cubic perovskites with photon energy.
induced by electron transfers from the occupied states in the valence band to the unoccupied states in the band of conduction. As shown in Table 3, the maximum values of $\sigma(\omega)$ are observed at 21.24, 21.40 and 21.51 eV for CeTiO$_3$, CeVO$_3$ and CeCrO$_3$, respectively.

Figure 9(c) displays the reflectivity spectrum of CeXO$_3$ compounds. These spectra are attributed to the contribution of O-2p states in the valence band and X-3d states in the band of conduction. The reflectivity at zero-frequency $R(0)$ is estimated to be 63.70%, 73.66% and 77.65% for CeTiO$_3$, CeVO$_3$ and CeCrO$_3$ respectively. The loss function, $L(\omega)$, denotes the fast electrons crossing through a material. The maximum peak observed in the energy loss spectrum occurs because of bulk
plasmonic excitation at specific photon energy and the related frequency called the bulk plasma frequency. The plasma frequency, in the loss spectrum, is situated at 12.585, 11.823, and 11.497 eV for CeTiO₃, CeVO₃ and CeCrO₃, respectively, at an energy that corresponds with a rapid decrease in reflectivity \( R(\omega) \). The peak location in the loss spectrum presented in Figure 9(d) shows the transfer point from the metal behaviour to the dielectric behaviour. At this point, the compound displays dielectric behaviour, whereas, beneath it, the compound acts as a metal [5].

3.5. Thermoelectric properties

It is well known that materials with good thermoelectric properties transform thermal energy directly to electrical energy and reversibly into thermal energy. The material with good thermoelectric properties must have low thermal conductivity, high electrical conductivity, high Seebeck coefficient and reasonable physical and chemical stability at high temperatures [34].

Thus, the thermoelectric properties such as the ratio of electrical conductivity to relaxation time \( \sigma/\tau \), the Seebeck coefficient \( S \) and the ratio of power factor to the relaxation time \( S^2\sigma/\tau \) of CeXO₃ (X = Ti, V, and Cr) perovskites were determined based on Boltzmann transport theory.

Figure 10(a) shows the variations of Seebeck coefficient of CeXO₃ (X = Ti, V and Cr) with temperature up to 1800 K. It is observed that the maximum evaluated absolute Seebeck coefficient associated with electron doping is greater than that evaluated for hole doping, which indicates that the majority charge carriers, for conduction, are electrons rather than holes. Table 4 presents the maximum Seebeck coefficient values with their congruent temperature \( T \) and the concentration of charge carriers \( n \) for hole and electron doping. It is seen from Table 4 that the estimated values of the charge carriers concentration are positive for the \( S_{max} \) values of the electron doping. This infers that these perovskites have p-type doping characteristics.

Figure 10(b) shows the variation of charge carrier concentration with temperature. The variation is mostly linear and proportional with temperature. As the temperature increases the thermal excitations get high, which raises the concentration of the carriers. The increase in concentration increases the electrons that cross from the valence band, over the \( E_F \), to the conduction band and produces hole–electron pairs.

Figure 11(a) shows the variation of the electrical conductivity relative to the relaxation time \( \sigma/\tau \) of the electron charge carriers with temperature. The total electrical conductivity demonstrates a similar pattern for all studied compounds. The calculated values of \( \sigma/\tau \) are increasing directly with temperature whereas they inversely change with \( S \), which is consistent with the Mott Equation [35]. This behaviour is in agreement with the high values of the charge carrier concentrations and indicates the transition of electrons to the band of conduction. The \( \sigma/\tau \) plot at 1800 K reaches high value of \( 1.12 \times 10^{17} \), \( 7.22 \times 10^{17} \), and \( 1.92 \times 10^{18} \) (1/\( \text{Ω}\) ms) for CeTiO₃, CeVO₃, and CeCrO₃, respectively.

Figure 11(b) indicates that the power factor \( S^2\sigma/\tau \) for the electron charge carriers is also directly proportional

![Figure 10](image1.png)

**Figure 10.** Variations of the calculated Seebeck coefficient (a), charge carrier concentration (b) with temperature for electrons (solid line) and holes (dashed line) charge carriers of CeXO₃ (X = Ti, V and Cr) perovskites.

| Compound  | Hole-doping  | Electron-doping |
|-----------|--------------|-----------------|
|           | \( S_{max} \) (μV/K) | \( T \) (K) | \( n \) (e/au) | \( ZT \) | \( S_{max} \) (μV/K) | \( T \) (K) | \( n \) (e/au) | \( ZT \) |
| CeTiO₃    | 5.46 × 10¹⁷ | 540            | -3.96142 | 0.1108557 | -2.75 × 10³ | 380           | 1.769329 | 0.99830 |
| CeVO₃     | 7.25 × 10¹⁷ | 1020           | -1.63874 | 0.175138  | -2.72 × 10³ | 280           | 2.92339  | 0.99843 |
| CeCrO₃    | 8.05 × 10¹⁷ | 920            | -0.52959 | 0.2119481 | -2.78 × 10³ | 220           | 4.26139  | 0.9980  |

**Table 4.** The maximum value of the Seebeck coefficient \( (S_{max}) \) corresponding to the temperature \( (T) \), the carrier concentration \( (n) \) and \( ZT \) values.
to temperature and rises rapidly above 700 K, which is accompanied by semi-linear rise up to 1800 K. At 1800 K, the values of $S^2\sigma/\tau$ are $5.147 \times 10^{10}$, $2.13 \times 10^{11}$ and $3.494 \times 10^{11}$ (W/K²ms) for CeTiO$_3$, CeVO$_3$ and CeCrO$_3$, respectively. The values of $S^2\sigma/\tau$ show that these compounds have good thermoelectric behaviour at higher temperatures. The $S^2\sigma/\tau$ values also demonstrate strong thermoelectrical efficiency at high temperatures.

The efficiency of CeXO$_3$ perovskite compounds is judged by the dimensionless thermoelectric figure of merit (ZT):

$$ZT = \frac{\sigma S^2 T}{\kappa}$$

where $\sigma$, $S$, $T$ and $\kappa$ denote to the electrical conductivity, Seebeck coefficient, the absolute temperature, and the total thermal conductivity, respectively. The calculated values of $ZT$ which correspond to the electrons, charge carriers, for the current compounds are listed in Table 4 and plotted in Figure 12(a). For CeTiO$_3$, CeVO$_3$ and CeCrO$_3$, the ZT value at the maximal $S$ value are equal

Figure 11. Variations of electrical conductivity (a) and power factor (b) with temperature for CeXO$_3$ (X = Ti, V and Cr) perovskites.

Figure 12. Variations of figure of merit (a) and thermal conductivity(b), specific heat capacity (c) with temperature for CeXO$_3$ (X = Ti, V and Cr) perovskite.
to 0.998 at 380, 280, and 220 K, respectively. Therefore, it can be concluded that the CeXO₃ compounds with a high thermoelectric ZT are suitable for thermoelectric applications and cooling systems.

The total thermal conductivity (κ) is the sum of the lattice and electronic contributions: \( \kappa = \kappa_L + \kappa_E \) [36–38]. Since this work is devoted to the study of the electronic properties, based on the all electrons FP-LAPW method, that control the rest of the other physical properties. Besides, because it is exceedingly expensive to include the lattice vibrations by all electrons using the WIEN2k code, we only included the electronic component (\( \kappa_E \)) and excluded the phonons contribution (\( \kappa_L \)) in our analysis. Figure 12(b) shows the change of electronic part of the thermal conductivity relative to relaxation time (\( \kappa_E / \tau \)) as a function of temperature (\( T \)) for the CeXO₃ compounds. It can be seen that the values of \( \kappa_E / \tau \) increase with increasing temperature, where this trend is the same for all three metallic and half-metallic compounds.

The specific heat capacity (\( C_v \)) is a measure of the heat amount required to increase the temperature of one mole of a material by one temperature degree. Figure 12(c) presents the variation of \( C_v \) for the studied compounds with temperature. It is observed that \( C_v \) remains close to zero up to 700 K and above which it rises rapidly with increasing temperature.

### 3.6. Elastic properties

The elastic constants (\( C_{ij} \)) are essential for characterizing the mechanical properties of solids [39]. The material’s elastic constants give details on the influences that happen to the material upon applying forces [40]. By evaluating these constants, the mechanical characteristics such as the hardness, the rigidity, the brittleness/ductility and the stability of the material can be determined. Three independent elastic constants (\( C_{11}, C_{12}, \) and \( C_{44} \)) are identified for the cubic structure [29,41,42]. In the present study, the elastic constants were determined using the Charpin method [24] as applied in WIEN2k software.

The elastic constants \( C_{11}, C_{12}, \) and \( C_{44} \) were evaluated via the application of isotropic strain and volume-preserving rhombohedral and tetragonal strains to the primitive cells of the optimized cubic structure. The computed elastic constants for CeXO₃ perovskite compounds are summarized in Table 5.

The stability of the CeXO₃ compounds was tested using the well-known three Born stability criteria of the cubic system [38,42]:

\[
C_{11} - C_{12} > 0; \quad C_{11} + 2C_{12} > 0; \quad C_{44} > 0; \quad C_{12} < B < C_{11}
\]

(5)

It is observed from Table 5 that the elastic constants of the compounds fulfil the Born mechanical stability.

### Table 5. Elastic constants (\( C_{ij} \)), bulk (\( B \)), shear (\( G \)), and Young (\( E \)) moduli, Pugh’s index ratio (\( B/G \)), Poisson’s ratio (\( \nu \)), anisotropic factor (\( A \)), Cauchy’s pressure (\( C^c \)), average (\( \nu_m \)), transverse (\( \nu_t \)) and longitudinal (\( \nu_l \)), Velocities, Debye temperature (\( \Theta_D \)), melting temperature (\( T_m \)) and Vicker’s hardness factor at equilibrium volume for CeTiO₃, CeVO₃ and CeCrO₃ perovskites.

| Elastic parameters | CeTiO₃ | CeVO₃ | CeCrO₃ |
|--------------------|--------|-------|--------|
| \( C_{11} \) (GPa) | 272.798248 | 307.155 | 249.3673 |
| \( C_{12} \) (GPa) | 139.361635 | 142.6604 | 183.1797 |
| \( C_{44} \) (GPa) | 34.078151 | 34.3741 | 40.685651 |
| \( B \) (GPa) | 183.841 | 197.492 | 205.242 |
| \( \Theta_D \) (K) | 124.179 | 136.192 | 105.928 |
| \( \nu_m \) | 0.387421 | 0.385065 | 0.413981 |
| \( \nu_t \) | 4.108 | 4.01695 | 5.47934 |
| \( \nu_l \) | 0.510777 | 0.417937 | 1.22941 |
| \( \Theta_D \) (K) | 105.28348 | 108.2863 | 142.9490 |
| \( \left( \frac{C_{44}}{C_{11}} \right) \) | 102.8348 | 108.2863 | 142.9490 |
| \( \nu \) (m/s) | 1319.9 | 1337.78 | 1146.31 |
| \( \nu \) (m/s) | 3078.89 | 3094.37 | 2990 |
| \( \nu \) (m/s) | 1419.58 | 1511.29 | 1299.26 |
| \( \nu \) (m/s) | 258.331 | 266.722 | 231.906 |
| \( \nu \) (m/s) | 2165.24 | 2368.28 | 2026.76 |
| \( \nu \) (m/s) | 52.0168 | 58.6992 | 31.1324 |

This means that the compounds are mechanically stable. Furthermore, the values of \( C_{11} \) are greater than the values of \( C_{44} \) by more than 60% for the compounds. This means that the perovskite compounds are probably to experience pure shear deformation in response to the uniaxial compression [43–45]. Also, the value of \( C_{44} \) indicates the pure shear deformation along the (100) plane in the crystal. From the results of \( C_{44} \) in Table 5, it is clear that the value of \( C_{44} \) increases in a small amount from CeTiO₃ to CeVO₃ and CeCrO₃, which allow us to predict that CeCrO₃ has strong resistance against the pure shear deformation making it more stiffness material than the other two compounds, and similar La-based perovskites [44].

Other mechanical constants such as anisotropy factor (\( A \)), shear modulus (\( G \)), Young’s modulus (\( E \)), bulk modulus (\( B \)) and the Poisson ratio can be calculated using elastic constants \( C_{ij} \). The various mechanical properties of these compounds are presented in Table 5.

The bulk modulus of the cubic crystal structure is given by:

\[
B = \frac{1}{3} \left( C_{11} + 2C_{12} \right)
\]

(6)

which is a linear combination of \( C_{12} \) and \( C_{11} \). The bulk moduli values for the studied perovskites are determined and listed in Table 5. The strong agreement between the bulk moduli of Murnaghan’s state equation (Table 1) with the bulk moduli of the elastic constant measurements is a measure of the accuracy of the evaluated elastic constants of CeXO₃. The bulk modulus increases with the decrease in atomic size of atoms from Ti to V to Cr for CeXO₃ and is inversely proportional to the lattice constant.

Determining of Young’s modulus value is an essential aspect for applications in technological engineering. It is known as the stress to strain ratio and is utilized to evaluate the stiffness of a material [11]. As the Young’s
modulus becomes higher, the material becomes stiffer. Young’s Modulus \( (E) \) is calculated from the following equation:

\[
E = \frac{9BG}{3B + G}
\]

(7)

where \( G \) is the value of Hill shear [46], which is the average of the Reuss Shear and Voigt shear. \( G \) designates the response of the material to shearing strain [47]. It is found that the value of \( E \) is greater for CeVO\(_3\) than for CeTiO\(_3\) and CeCrO\(_3\), which confirms that CeVO\(_3\) is stiffer than the other studied compounds.

Another important factor is the elastic anisotropic factor \((A)\) that is typically utilized to explain the structure stability of a material. This aspect is of pronounced significance in engineering sciences [48] and is closely connected to the risk of micro-cracks in the material [49]. It is given by the following formula:

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

(8)

The value of \( A \) is equal to one \((A = 1.0)\) for an isotropic material, however, any deviation from this value refers to a certain degree of anisotropy. It is clearly seen from Table 5 that the perovskite compounds are fully anisotropic with higher anisotropy for CeCrO\(_3\) relative to the other perovskites.

Pugh’s index \((B/G)\), Cauchy’s pressure and Poisson’s ratio \((\vartheta)\) are used to determine whether a material is brittle or ductile [23]. Positive Cauchy values reflect ductile compounds, and negative values indicate brittle compounds. The estimation values of Cauchy’s pressure

\[
C'' = C_{12} - C_{44}
\]

(9)

are listed in Table 5, which show that all CeTiO\(_3\), CeVO\(_3\), and CeCrO\(_3\) compounds are ductile materials in nature.

The Pugh’s index has a critical value of 1.75. A material will be ductile when the calculated value is more than the critical value and brittle if the value is lower. Based on data in Table 5, \( B/G > 1.75 \), meaning that the CeXO\(_3\) compounds are ductile.

Poisson’s ratio \((\vartheta)\) is a significant predictor about the bonding forces and is given by the following formula:

\[
\vartheta = \frac{3B - 2G}{2(3B - G)}
\]

(10)

Usually, the lower and upper limits of the Poisson ratio for the central forces in materials are 0.25 and 0.50, respectively [50]. The Poisson ratio for metals is between 0.25 and 0.45, with very few exceptions [51]. The calculated values of \( \vartheta \) are 0.387, 0.385, and 0.414 for CeTiO\(_3\), CeVO\(_3\), and CeCrO\(_3\), respectively. These indicate that the three examined perovskites own metallic bonding, and the interatomic forces between atoms are central. The Poisson ratio is less than 0.26 for brittle materials; otherwise, the materials are considered ductile [46].

Thus, the values of \( \vartheta \) ensure that the CeXO\(_3\) compounds are ductile.

The Vickers hardness of the compounds was calculated under ambient conditions using the following relation:

\[
H_v = \frac{(1 - 2\vartheta)E}{C(1 + \vartheta)}
\]

(11)

Here, \( E \) is the Young modulus and \( \vartheta \) is the Poisson ratio. This property shows the ability of compounds to resist denting. The largest value of \( H_v \) is 58.70 GPa for CeVO\(_3\), indicating high hardness of this compound.

The thermodynamic parameters, which are connected to the elastic properties, such as melting point \((T_m)\) and Debye temperature \((\theta_D)\) were also examined. The \( \theta_D \) was determined from the mean speed velocity \((V_m)\) using the relation [52,53]:

\[
\theta_D = \frac{h}{k_B} \left[ \frac{3n}{4\pi} \left( \frac{N_A \rho}{M} \right) \right]^{\frac{1}{3}} V_m
\]

(12)

where \( h \) Plank’s constant, \( k \) is Boltzmann’s constant, \( N_A \) is Avogadro’s number, \( M \) is the molecular weight, \( \rho \) is the density of the material, and \( n \) is the number of atoms in a single cell. The evaluated Debye temperature values are given in Table 5. For the studied compounds, the mean sound speed was determined by:

\[
V_m = \left[ \frac{1}{3} \left( \frac{2}{\nu_l^3} + \frac{1}{\nu_t^3} \right) \right]^{-\frac{1}{3}}
\]

(13)

where \( \nu_l \) and \( \nu_t \) are longitudinal and the transverse components of the velocity of sound, respectively, measured using the shear modulus and bulk modulus, and are given by:

\[
\nu_l = \sqrt{\frac{G}{\rho}} \quad \text{(14)}
\]

\[
\nu_t = \sqrt{\frac{3B + 4G}{3\rho}} \quad \text{(15)}
\]

The melting temperature \((T_m)\) is derived from the elastic constant \(C_{11}\) using the following equation:

\[
T_m = 553 + \frac{(5.91 \times C_{11})}{\text{GPa}}
\]

(16)

The measured values of \( \nu_l, \nu_t, V_m, \theta_D, \) and \( T_m \) are shown in Table 5. A high-frequency mode for phonon oscillations is observed for the temperature range of \( \theta_D < T > T_m \). Phonon oscillations are supposed to be frozen at \( T < \theta_D \) [53]. Based on our calculations of Debye temperature and melting-point values, we expect these compounds to be a possible candidate for high-temperature electronic applications.

4. Conclusions

In this work, the electronic, structural, optical, thermoelectric and elastic properties of CeXO\(_3\) perovskites
(X = Ti, V and Cr) were investigated using the LP-FAPW method implemented in the WIEN2k software. The obtained results of structural optimization, tolerance factor and formation energy confirmed the chemical stability and cubic structure of these three compounds with Pm-3m space-group in FM phase. The band structures and density of states in spin-up and spin-down diagrams revealed that CeTiO$_3$ is a metallic compound, whereas CeVO$_3$ and CeCrO$_3$ are half-metallic (HM) compounds with an energy-gap in spin-down direction of 3.057 and 2.720 eV, respectively. Besides, the calculated partial and total magnetic moments revealed the FM behaviour in CeXO$_3$, in good agreement with the previous publications. Various optical parameters of CeXO$_3$ such as the static dielectric constants, absorption coefficient, extinction coefficient, refractive index, reflectivity, electron loss function and optical conductivity were estimated and evaluated in atmospheric conditions. The high absorption and reflectivity values raise the likelihood that CeXO$_3$ compounds could be used for heat shields and in optoelectronics. The thermoelastic properties of CeXO$_3$ compounds were analysed through measuring their thermoelastic characteristics such as thermal conductivity, electrical conductivity and coefficient Seebeck using the BoltzTrap code implemented in WIEN2k. Furthermore, the elastic constants calculations showed that the constants $C_{11}$, $C_{12}$, and $C_{44}$ verified the Born’s criteria of the mechanical stability for cubic structure of CeXO$_3$. The three compounds were found to be characterized as elastically stable and anisotropic, and all CeTiO$_3$, CeVO$_3$ and CeCrO$_3$ compounds were determined to be ductile materials.

**Disclosure statement**

No potential conflict of interest was reported by the author(s).

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