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Pressure induced mechanical, opto-electronics, and transport properties of ZnHfO3 oxide for solar cell and energy harvesting devices

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Abstract

Based on the density functional theory, we systematically investigate the effect of pressure on the mechanical, optoelectronic, and transport properties of ZnHfO3. The pressure has been employed up to 30 GPa in a step-size of 10 GPa. A slight variation in the lattice constant and Bulk modulus have been observed at the applied pressure steps. The electronic properties are significantly tuned by applying pressure. The calculated bandgap values slightly increase with increasing the pressure and its values start to decrease after the critical pressure of 20 GPa. More interestingly, a transition from indirect to direct band has been observed at the critical pressure. This transition of the bandgap is also justified by studying the optical properties like dielectric constant, refraction, and absorption at different pressure. Furthermore, we studied the electronic transport properties in terms of electrical conductivity, thermal conductivity, Seebeck coefficient, and power factor at temperature (300–800 K). The calculated lattice thermal conductivities are low while the electrical conductivities and Seebeck coefficients are high at all pressure. Thus, the properties of the ZnHfO3 show high potential for thermoelectric applications.

1. Introduction

Energy harvesting is a very important field due to the insufficiency of natural energy sources and global warming. The search for new material with both fundamental research and device applications is emerging in the field of optoelectronics, energy conversion, and storage. The perovskite oxides have attracted attention due to their fascinating properties such as optical and thermal efficiency [1, 2], low cost [3], and environment-friendliness [4]. The perovskite oxides have already shown their promising applications in the field of light-emitting diodes, solar cells, and photo-detector [5]. Additionally, the perovskite oxides with high thermal efficiency are quite suitable for use in thermoelectric generators, thermo-coolers, and thermocouples [6]. However, the lead (Pb) contents in the perovskite hindered its applications for real devices due to its toxic nature [7], though they have been promising the electronic devices.

Thus, Hf-based perovskites have been reported to be a more suitable substitute for lead-based perovskites. Currently, the lead-free perovskites AHiO3 (A = Zn, Cd) have attracted the attention of iso-structure such as PbZrO3 [8]. Generally, the perovskite oxides exist in the para-electric phase (cubic) and ferroelectric phase (tetragonal) [9, 10]. The nano-particles of AHiO3 (A = Mg, Ca, Sr and Ba) have been grown in the experiment [11–15]. Additionally, the bandgap of AHiO3 (A = Mg, Ca, Sr and Ba) has also been tuned via applying strain to optoelectronics devices [16]. The pressure and temperature play a vital role in determining the stabilities of the compounds. In such cases, the pressure becomes more important. Pressure-induced semiconductors are gaining interest for multifunctional applications [17].
This report explores the effect of high pressure on the optoelectronic and transport properties of ZnHfO₃. Furthermore, the dynamic and structural behavior of the perovskites has been identified. We study the structural properties of ZnHfO₃ under high pressure ranging from 0 to 30 GPa, and found a slight variation in the lattice constant and Bulk modulus. Additionally, an increase in the bandgap has been observed at 10 GPa, and then a decrease after the critical pressure of 20 GPa. Interestingly, an indirect to direct bandgap transition has been observed at the critical pressure. We find low lattice thermal conductivities and high electrical conductivities and high Seebeck coefficients for ZnHfO₃ at (300 K–800 K). Thus, the ZnHfO₃ shows high potential for thermoelectric applications. To our knowledge, there is no other study available on the effect of high pressure on ZnHfO₃. Therefore, we investigated the pressure-dependent mechanical, electronic, and thermoelectric properties of ZnHfO₃.

2. Method of calculations

All the density functional theory calculations are carried out using the Wien 2 k Package with the projector augmented wave method [18]. The PBEsol-GGA is used as an exchange-correlation functional [19]. The electron core has been kept for the muffin-tin region with its density in all the calculations. As the GGA is known to underestimate the band gap value, we performed the modified Becke and Johnson potential (mBJ) [20–22] for the analysis of electronic properties. The $R_{MT} \times K_{max} = 7$ are the fundamental measures instructed into the software. $R_{MT}$ represents the muffin-tin sphere radius and $K_{max}$ symbolizes the wave vector. We have used $G_{max} = 16$ and $l_{max} = 10$ for the Gaussian factor in our computations. A $k$-mesh with the sequence of $12 \times 12 \times 12$ has been employed for the exactness of union for the ground state energy, even after scrutinizing the repetitive measurements. The energy is kept fixed as $10^{-2}$ mRy throughout the iteration process. Further, the classical transport theory (CTT) based BoltzTraP code [23] is for the computation of the thermoelectric characteristics.

3. Results and discussion

3.1. Mechanical properties

Before going into the detail of mechanical, electronic, and thermal properties, first, we have to discuss the structure of ZnHfO₃. The A-site cation lies at the corners and the B-site cation is located at the center of the cube whereas the O atoms rest at the face center in the perovskite unit cell, as shown in figure 1. The space group of the perovskite ZnHfO₃ is Pm-3m, where all atoms are at the special Wyckoff positions, e.g., Zn at (0, 0, 0), Hf at (0.5, 0.5, 0.5) and O’s at (0.5, 0.5, 0). The mechanical properties of material play a vital role in defining practical applications. It is thus an essential prerequisite for the integration of material in many devices to acquire detailed knowledge on the mechanical properties of ZnHfO₃. The volume versus energy curves are plotted (figure 2) and
predict the phase stability of the ZnHfO$_3$. The equilibrium lattice parameters, bulk moduli, and ground-state energies have been obtained by fitting total energies with Murnaghan’s equation (Table 1) at 0 GPa. Our calculated parameters are in good agreement with [24]. To find the structural stability of ZnHfO$_3$, we have calculated the formation enthalpy ($\Delta H_f$) (see Table 1). Our calculated $\Delta H_f$ is negative and hence suggesting the favorable nature of ZnHfO$_3$. The $\Delta H_f$ is calculated using the relation,

$$
\Delta H_f = E_{\text{Total}}(\text{ZnHf}_m\text{O}_n) - nE_{\text{Zn}} - mE_{\text{Hf}} - nE_{\text{O}}
$$

(1)

The pressure-induced volume variations are computed with the help of the following expression:

$$
V(P) = V_0 \left(1 + P \left(\frac{d\ln B_0}{d\ln P}\right)\right)
$$

(2)

The variation of cubic lattice parameters depending on pressure has been optimized using $a_0 = (V(P))^{1/3}$. The optimized lattice constant has been considered for further investigation of electronics and the thermal properties of ZnHfO$_3$. The calculated bulk modulus and lattice constant of ZnHfO$_3$ at different pressure, 0 to 30 GPa has been tabulated in Table 2. The increasing external pressure produced compression in the electrons states and reduced the lattice constant resulting in an enhancement of the mechanical behavior of ZnHfO$_3$. Additionally, the pressure-mediated hybridization between anions and cations may cause ferroelectricity in perovskites [25].

To assure the mechanical stability at different pressure, the elastic constants (C$_{11}$–C$_{12}$–C$_{44}$) has been calculated from the tensor matrix. Table 2 shows an increasing trend of the lattice constant, which is in line with the Born mechanical stability criteria $C_{12} < B < C_{11}$, $C_{44} > 0$, $C_{11} - C_{12} > 0$, and $C_{11} + 2C_{12} > 0$ [26], suggesting that the ZnHfO$_3$ is mechanically stable. The elastic moduli have been determined through Voigt-

### Table 1. Calculated lattice constant ($a$\,(Å)), bulk moduli ($B$\,(GPa)), enthalpy of formation ($\Delta H$\,(eV/unit cell)), and elastic parameters of ZnHfO$_3$ at 0 GPa.

| Parameter | ZnHfO$_3$ |
|-----------|-----------|
| $a_0$ (Å) | 4.04 |
| Existing data $a_0$ | 4.07$^*$ |
| $B_0$ (GPa) | 147.32 |
| $\Delta H$ | $-2.62$ |
| $B$ (GPa) | 181.54 |
| $G$ (GPa) | 55.75 |
| $Y$ (GPa) | 151.79 |
| $B/G$ | 3.25 |
| $\nu$ | 0.36 |
| $v_{\text{tot}}$ | 1546.79 |
| $\theta_0$ | 333.57 |

$^*$ [24]

**Figure 2.** Calculated volume versus energy plot at 0 GPa.
Table 2. Calculated elastic and 0 eV energy optical parameter of ZnHfO3 by employing different pressure 0–30 GPa.

| Pressure (in GPa) | a0(Å) | B(GPa) | C_{11} | C_{12} | C_{44} | ε_1(0) | m(0) | R(0) |
|------------------|-------|--------|--------|--------|--------|--------|------|------|
| 0                | 4.04  | 181.54 | 335.35 | 104.64 | 32.68  | 2.63   | 1.62 | 0.056|
| 10               | 3.98  | 216.19 | 533.10 | 106.74 | 34.28  | 2.67   | 1.63 | 0.058|
| 20               | 3.91  | 276.44 | 607.01 | 108.76 | 38.44  | 2.70   | 1.64 | 0.059|
| 30               | 3.86  | 318.07 | 715.07 | 111.42 | 42.50  | 2.74   | 1.65 | 0.061|

Reuss-Hill [27–29], using the elastic constants table 1 indicates the observed values of Shear modulus (G), Young modulus (Y), and Bulk modulus (B). The Poisson ratio (ν) with its critical limit ν > 0.26 and Pugh’s ratio (B/G) with its critical limit B/G > 1.75 have been used for the evaluation of the ductility and brittleness of the material [30]. Table 2 expresses the Pugh’s ratio (B/G) and Poisson ratio (ν) computed values that show the perovskite is ductile. Table 2 further implies that the ductility of the perovskite enhances with external pressure. The specific heat capacity (withstanding limit of the compound against the Debye temperature (θ_D) dependent heat) confirmed the stability of the material.

The value of θ_D is obtained from the tensor matrix of Charpin as under [31, 32]:

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

where molar mass is symbolized by M, Avogadro number is represented by N_A, density is shown by ρ, and v_m stands for average sound velocity.

From the longitudinal v_p, and the transverse parts of the Saviour equations v_s, the average sound velocity is achievable as under:

\[ v_m = \left[ \frac{1}{3} \left( \frac{2}{v_p^2} + \frac{1}{v_s^2} \right) \right]^{\frac{1}{2}} \]  (4)

Here, v_p and v_s are transverse and longitudinal velocities that have independently been put as follows:

\[ v_p = \left( \frac{G}{\rho} \right)^{\frac{1}{2}} \] and \[ v_s = \left( \frac{3B + 4G}{3\rho} \right)^{\frac{1}{2}} \]  (5)

Table 2 displays the obtained value v_m. It discloses that when the pressure-induced (0 GPa to 30 GPa) caused an increase in the elasticity of the medium, their values also started to increase. In addition, v_m and θ_D are directly proportional to each other, because of which value θ_D also increased with the pressure-induced 0–30 GPa [33].

3.2. Opto-electronic properties

From the analysis of the band structure of the perovskite, the electronic features have been determined at various pressure levels from 0 to 30 GPa in step size of 10 GPa (see figure 3). The conduction band minima (CBM) and the valence band maxima (VBM) lie at Γ -symmetry point and M -symmetry point respectively at 0 GPa. This indicates that the band structure has an indirect bandgap response the computed value of which has been put in table 1. The direct bandgap lies at Γ -symmetry point has been shown in figure 3 at 20 GPa, from which it becomes clear that the method of calculation has accuracy in providing electronic characteristics of the oxide without applying pressure. In indirect bandgap compounds, phonons have a dominant role in optical transitions, therefore, are not appreciated because they cause energy loss. Hence, the compounds must have a direct bandgap for being used in solar cell device applications to avoid energy losses.

Interestingly, a band shift from Γ-M (indirect) bandgap to Γ-Γ (direct) on increasing external pressure up to 20 GPa, where both CBM and VBM became alike at the same k-value. The direct gap nature of ZnHfO3 retain even at a higher pressure of 30 GPa. Thus, the ZnHfO3 can be utilized in device applications particularly at high external pressure. The partial and complete shift of electronic density of states (Zn, Hf, and O atoms) to external pressure has been indicated in figure 4(b). It shows that the conduction band bottom was made of Zn-4 s and O-2p states whereas the top of the valence band was made of O-2p states. Therefore, electronic transitions between the above-narrated states are very attractive for the exposure of thermoelectric and optoelectronic applications. Figure 4(a) shows the shifting of the symmetry point from Γ-M (indirect) to Γ-Γ (direct).

The transition energy is reduced by the symmetry point shift due to which the reliability of the compound for being used in device fabrication reasonably enhances. Additionally, the electronic states spectra indicate that the increasing pressure makes these states flatter that demonstrated the transformation of the covalent nature of the oxide into an ionic one. However, the flat states existing at the boundaries of the conduction and valence bands specify the enhancement in dispersion, which is according to the real dielectric constant. If the
compounds particularly Hf containing are of direct band structure become of the higher potential for being used solar cells and optoelectronic applications. Figures 5(a), (b) and (a)–(c) show various optical parameters of ZnHfO₃. The mathematical expressions requisite for the calculation of these parameters have been provided elsewhere [34, 35]. As it has already been elaborated that the contribution of phonons is suppressed when the external pressure is increased it happens when the indirect bandgap transforms into a direct bandgap. The interaction of external energy with oxide has been investigated in terms of complex dielectric constant i.e. 

\[ \varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \]

where \( \varepsilon_1(\omega) \) and \( \varepsilon_2(\omega) \) are the imaginary and elements of it respectively.

Both parameters are associated with the Kramer–Kronig relation [36, 37]. Different further parameters have also been extracted from these two parameters with changing pressure in the energy ranges 0–16 eV. Figure 5(a) displays the energy-dependent \( \varepsilon_1(\omega) \) and \( \varepsilon_2(\omega) \) with varying pressure levels. The graphs present that their shapes were not significantly changed with external pressure. With the energy up to 6 eV, there is a slight increase in the value of \( \varepsilon_1(\omega) \), where the plasmonic resonance is indicated by a small valley. Then it started to decrease up to 7 eV and it again increasing up to 9 eV. Beyond 16 eV, it exhibited its negative values. The metallic nature of ZnHfO₃ has become obvious due to the negative values of \( \varepsilon_1(\omega) \) in comparatively high energy ranges. The pressure caused a reduction in the static value of \( \varepsilon_1(\omega) \) for zero energy with the development in band structure to which Penn’s model confirmed [38]. Due to the up-gradation of band gaps, the minor shifting of the \( \varepsilon_1(\omega) \) spectrum towards ultraviolet from visible region advocates the potential candidature of ZnHfO₃ for being utilized in optoelectronic device applications. Figure 5(a) also displays the fraction of absorbed energy that has been determined regarding the imaginary part of dielectric constant \( \varepsilon_2(\omega) \). The border values after and before which absorption and transmission take place are defined by the computation of \( \varepsilon_2(\omega) \) [39].

![Figure 3. The calculated band structures of ZnHfO₃ plotted as a function of applied pressures (0–30 GPa).](image-url)
between the obtained boundary values for energy and electronic bandgap verification at various levels of induced pressure \([40]\). \(\varepsilon_{2}(\omega)\) obtained its peak value at energy ranges from 8 eV to 10 eV and its least value at energy ranges from 12 eV to 14 eV.

The extinction coefficient and refractive index have been computed while employing \(2nk = \varepsilon_{2}\) and \(n^{2} = \varepsilon_{1}(\omega)\) respectively (see figure 5(b)). The dispersion and transparency properties of oxide are determined by the value of \(n(\omega)\) for being employed in optoelectronic device fabrication, and its value must be almost 2. However, it gained its peak value of 2.2 at 8.4 eV that was dropped down to 1 at 11.40 eV. Another maximum value of it emerged above 9 eV indicating the group velocity \((V_g)\) exceeded the speed of light that describes the

**Figure 4.** (a) Bandgap crossover at 20 GPa of ZnHfO\(_3\) along with \(\Gamma\)-M and \(\Gamma\)-\(\Gamma\) symmetry directions, and (b) total DOS along with partial DOS at different pressure.
Figure 5. Real part $\varepsilon_1(\omega)$, imaginary part $\varepsilon_2(\omega)$ of dielectric constant and refractive index $n(\omega)$, extension coefficient $k(\omega)$ of ZnHfO$_3$ at pressure 0–30 GPa.

Figure 6. Computed (a) electrical conductivity and (b) Seebeck coefficients of ZnHfO$_3$ against temperature (300–800 K).
polarization of the compound started to oppose the energy of the photon \[41\]. Figure 5(b) shows the variations in the extinction coefficient that proves the behavior alike as that of \(\varepsilon_2(\omega)\).

### 3.3. Transport properties

The pressure-dependent electronic transport parameters have been computed for ZnHfO\(_3\), as shown in figures 6–8. The variations of electrical conductivity \((\sigma/\tau)\) of the perovskite in the temperature range 300–800 K have been displayed in figure 6(a). The external temperature motivates the conduction electrons that cause this conductivity \([42, 43]\). There is a continuous and linear increase in \(\sigma\) from \(2 \times 10^{19} \text{(\(\omega\) ms)}^{-1}\) to \(3 \times 10^{19} \text{(\(\omega\) ms)}^{-1}\) (see figure 6(a)). Further, its value is directly connected to the bandgap of the perovskite. The considerably various values of bandgap have been noted 30 GPa. The transformation of indirect towards direct bandgap transitions might be the major cause of this variation \([44]\). The lattice vibration produces thermal conductivity \((k/\tau)\) in crystalline compounds. We have plotted the electronic division of thermal conductivity here. The increasing temperature causes an increase in the thermal conductivity that approaches \(10^{14} \text{W/(m K s)}\) at 800 K. On the other hand, the electronic component of thermal conductivity is enhanced due to the shift of the bandgap. The power factor and Seebeck coefficient \((S)\) help to understand the thermoelectric efficiency of ZnHfO\(_3\) (see figures 7(a), (b)). The potential gradient \((\Delta V)\) that itself is developed through temperature difference \((\Delta T)\) helps in computing the Seebeck coefficient \((S)\). Seebeck coefficient \((S)\) varies significantly in the temperature range 300–800 K at various pressure (figure 7(a)). From figure 7(a), it can be seen that \(S\) slightly increased up to 600 K, and remain constant (164 \(\mu\)V/K) till 800 K. We found that increase in pressure (30 GPa) can enhance the Seebeck coefficient \((S)\). Additionally, a further increase led the \(S\) value to its minimum value, which is not considered in this report. Moreover, the power factor \((PF)\) that is equal to \(\sigma S^2\) has also been calculated. The PF value increases in the temperature with raise in temperature (200–800 K) (see

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**Figure 7.** Computed (a) thermal conductivity and (b) power factor of ZnHfO\(_3\) against (c), (d) temperature (300–800 K).

**Figure 8.** The ZT values of ZnHfO\(_3\) against temperature (300–800 K).
Table 3. Room temperature thermoelectric coefficients of ZnHfO₃ at different pressure.

| Pressure (in GPa) | σ/τ (× 10¹⁴/Ω ms) | κ/σ (× 10⁴ W mK⁻¹) | Seebeck coefficient (μV/K) | PF (× 10⁻⁵ W mK⁻²) | ZT |
|------------------|-------------------|-------------------|----------------|-------------------|-----|
| 0                | 2.00              | 2.17              | 139.71        | 3.90              | 0.53|
| 10               | 2.36              | 2.51              | 132.62        | 4.15              | 0.49|
| 20               | 12.54             | 7.47              | 28.30         | 1.01              | 0.04|
| 30               | 16.76             | 17.79             | 7.83          | 0.10              | 0.01|

In summary, we used first-principles calculations to explore the effects of high pressure on the mechanical, optoelectronic, and transport properties of ZnHfO₃. We found that the ZnHfO₃ is energetically stable due to high enthalpy formation energy. The mechanical property is suggested to be ductile due to the higher Pugh’s ratio. Furthermore, the ZnHfO₃ is a semiconductor with an indirect bandgap of 1.5 eV. We found that a transition from indirect to direct bandgap (1.9 eV) occurs at a critical pressure of 20 GPa. The polarizability and absorption ability of the compound increases with the increase in pressure. ZnHfO₃ absorbs highly in the ultraviolet (UV) region of the energy spectrum. The obtained value of the figure of merit (ZT = 0.53) at room temperature expressed a similar behavior as that of S that decreased with increasing pressure. Moreover, the high ZT and the direct bandgap nature of ZnHfO₃ at a critical pressure of 20 GPa could furnish a way for the promising application of ZnHfO₃ in energy harvesting devices.

4. Conclusion

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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