A comprehensive DFT study to evaluate the modulation in the band gap, elastic, and optical behaviour of CsPbBr₃ under the effect of stress

S M Junaid Zaidi, M Ijaz Khan, S A Gillani, M Sana Ullah Sahar, Sana Ullah and Muhammad Tanveer

1 Department of Physics and Mathematics, Faculty of Sciences, Superior University, Lahore 54000, Pakistan
2 Institute of Mechanical and Manufacturing Engineering, Khwaja Fareed University of Engineering and Information Technology, Rahim Yar Khan 64200, Pakistan
3 Department of Physics, GC University, Lahore 54000, Pakistan
4 Department of Physics, Khwaja Fareed University of Engineering and Information Technology, Rahim Yar Khan 64200, Pakistan

Abstract

The computational Generalized Gradient Approximations (GGA) are applied on cubic Cesium Lead Bromide (CsPbBr₃) with different stress values of 0, 5, 10, and 15 GPa for a supercell with PBE exchange relationship parameters to study the structural, mechanical, and optoelectronic characteristics. This study aims to determine how stress affects structural and electronic properties, how optical behaviour changes in reaction to electronic change, and how mechanical properties change as a result. The structure remains cubic, and there is no phase shift, but a reduction in the lattice parameters is seen. The reduction in band gap (1.900 eV) is found from 0–15 GPa and zero at 17 GPa. The partial densities of states (PDOS) of bulk CsPbBr₃, Cs, Pb, and Br are also calculated. The partial density states PDOS of bulk CsPbBr₃ show that in the valence band range, the sharpest observed peak is for d-states, while in the conduction region, the sharpest peak is for p-states and then for s-states. The significant variation in values of absorption, conductivity (imaginary and real), dielectric function (imaginary and real), loss function, reflectivity, and refractive index (imaginary and real) are found by applying stresses of 0, 5, 10, 15 GPa. Using the energy deformation relationship, the elastic constants are computed. From these constants, various mechanical characteristics such as the bulk modulus, shear modulus, Young modulus, and Poisson ratio are derived and discussed. Additionally, it is a good component in optoelectronic devices due to its high refractive index, absorption, reflectivity, and conductivity.

1. Introduction

Inorganic perovskite material Cesium Lead Bromide (CsPbBr₃) has gained considerable attention due to its high stability and improved carrier mobility [1]. The Electrical and optical properties of this perovskite are dependent on compositions, morphologies, and crystallographic phases [1–3]. These properties make it appropriate for applications in numerous optoelectronic devices such as photovoltaic cells, light-emitting diodes, and lasers [4–7]. The general chemical formula of single inorganic perovskite is AMX₃, where A is a cation (Cs, Na, K, Li, etc), M is the second cation (Pb/Sn normally), and X is a halide (Br, Cl, I, F) [8–10]. The structural properties of the Cubic CsPbBr₃ reveal that it belongs to the Pm3m phase group, Cs is at the position (0, 0, 0.5), Pb holds (0, 0, 0), while Br possesses (0, 0, 0.5) position. Bromide atom incorporation into the halide anion generates a black phase at room temperature and gives a lower phase transition and increased tolerance factor. The Larger band gap and shorter bond length exist in CsPbBr₃ due to the larger difference in electronegativity of lead and
halogen. This factor has excessive potential for semitransparent photovoltaic applications [11]. Stability plays a vital role in the applied application perspective as well as in various methods used in adapting the desired characteristic of the material. In perovskites, the band gap changes due to three factors (a) phase transition due to temperature ($E_{g\text{cubic}} < E_{g\text{tetragonal}} < E_{g\text{orthorhombic}}$) (b) change in chemical composition and (c) hydrostatic pressure. The pressure change is a facile method to alter the band gaps [12, 13]. It is well-identified that the greater band gap value of halides is not suitable for optoelectronic devices.

The cubic inorganic perovskites phase represents the highest structural symmetry as compared to the tetragonal and orthorhombic phases. Xiao et al found that increasing the applied stress on the nanocrystal CsPbBr$_3$ can successively elevate bandgap narrowing [14]. Kong et al delivered experimental proof that by applying hydrostatic pressure to MAPbBr$_3$, band gaps are narrowed down and then widened up with increasing stress [15]. The recent works on the applications of CsPbBr$_3$ in laser-driven projection display, white light emission and visible light communication, thin films decorated by nanoparticles, and light-emitting diodes, can be seen in [16–21]. Y. Huang et al studied the effect of stress up to 12 GPa on cubic and orthorhombic perovskite halide CsPbBr$_3$ [22]. A decrease in the band gap is found, and it is equal to zero when stress increased from 12 GPa. The work on Room Temperature Synthesis of Stable Single Silica-coated CsPbBr$_3$ Quantum Dots can be found in [23].

In the current research, the structural, elastic, mechanical, electrical, and optical aspects of various material characteristics are studied with external stress (0–15 GPa). This study is set up so that the computational details are given in the next section; the results for the electronic properties, the densities of states, the optical properties, and the elastic and mechanical properties are presented and discussed in the third section. Finally, the results are concluded in section 6.

2. **Computational details**

In this study, the structural, elastic, mechanical, electronic, and optical characteristics of CsPbBr$_3$ are computed using the Material Studio setup. The Cambridge Serial Total Energy Package (CASTEP) code is taken into account by utilizing the principles of density functional theory (DFT) [24–26] and the plane wave pseudopotential technique.

To explore the relationship between electron transfers, Perdew–Burke–Ernzerhof (PBE) established a generalized gradient approximation (GGA) approach [27, 28]. The computational Generalized Gradient Approximations (GGA) are applied on cubic CsPbBr$_3$ having space group Pm3m with different stress values of 0, 5, 10, 15 GPa for a $2 \times 2 \times 2$ supercell as shown in figure 1(a). The plane wave functions apply as a set of bases. For Brillouin zone integration, MPG (Monkhorst-Pack grid) of $8 \times 8 \times 8$ k-points are used. The cutoff energy for this computation is 260 eV for the depiction of electron-ion interaction by the ultrasoft pseudopotential. The band energy tolerance in the whole process is $1 \times 10^{-5}$ eV. The variation of lattice parameter with stress values and concerning volume can be seen in figure 1(b), which indicate the decrease of both parameters with the increase of external stress. One can readily see the values of lattice parameters are decreasing from 6.13764 Å to 5.38028 Å with increasing stress up to 15 GPa. The computations are performed using the Kohn–Sham equations [29–31]. The results for the lattice parameter and the band gap are in good agreement with previous work as shown in table 1.

3. **Result and discussion**

3.1. **Electronic properties**

Figure 2(a–d) represents the electronic band structure of cubic CsPbBr$_3$ with perfect symmetry lines of the Brillouin zone with a stress of 0.0 GPa. After applying crystallographic geometrical conditions of CsPbBr$_3$, the electronic and optical properties of the material are analyzed. The parameters of the Perdew–Burke–Ernzerhof PBE exchange relationship are used for band gap calculations in CsPbBr$_3$. The energy band gap has two types one is called direct band gap and the other is indirect band gap. If the minima of the conduction band and maxima of the valence band lies on the same line then the band gap is called a direct band gap, if they exist on different lines then the band gap will be indirect. In our calculated results the minima of the conduction band lie at point ‘G’ while the maxima of the valence band lie also on ‘G’, which shows the direct band nature shown in figure 2(a). The energy band gap for the 0 GPa crystal structure is found at 1.90 eV. The value of the band gap is found to decrease up to 0.165 eV with the increase in stress. The decrease in band gap is found at about 91.3% from its value at 0 GPa with the increase in stress up to 15 GPa shown in figure 1(c), and finally, the band gap is zero at 17 GPa. The inverse relation between stress and band gap is found, as shown in figure 1(c). The stress calculations are estimated up to that value where the material is able to maintain its cubical crystallographic structure.
3.2. Density of states

The electron distribution in the energy spectrum is explained by the density of states (DOS) shown in figures (3–7). The partial density of states PDOS of bulk CsPbBr3 is shown in figure 4. It is clear that in the valence band range, the sharpest peak is for $d$-states, while in the conduction region, the sharpest peak is for $p$-states and then for $s$-states. By increasing stress from 0 GPa to 15 GPa, the collective response of states or sum curves decreases.

Table 1. Comparison of Lattice parameters and band gaps.

| Lattice parameter (Å) | Band gap (eV) |
|-----------------------|---------------|
| CsPbBr3 (Present work)| 6.13764 1.900 |
| 6.0061 | 1.61 |
| 6.009 | 1.764 |
| 5.9905 | 1.663 |
| 5.874 | 2.3 |

$^a$ Reference [32] Theo.
$^b$ Reference [33] Theo.
$^c$ Reference [34] Theo.
$^d$ Reference [35] Exp.
$^e$ Reference [36] Exp.

Figure 1. (a) Supercell of CsPbBr3, (b) the lattice parameters and volume of the cell as a function of stress. (c) The effect of stress on the band gap.
Figure 2. Band structure of CsPbBr$_3$ (a) at 0 GPa, (b) at 5 GPa, (c) at 10 GPa, (d) at 15 GPa.

Figure 3. The total density of state (TDOS) of CsPbBr$_3$.

Figure 4. Partial density of state (PDOS) of CsPbBr$_3$. 
The effect of stress from 0 to 15 GPa on elemental partial densities of states (PDOS) can be seen in figures 5–7. PDOS of Cesium (Cs) shown in figure 5 show the contribution of p-states for both valence and conduction bands. The sharpest peak of the p-state at 0 GPa is detected at $-7.085$ eV with an intensity of $94.64$ electrons/eV. With the increase in stress (0–15 GPa), the intensities of p-states are decreasing. The PDOS of Lead (Pb) is shown in figure 6. It can be seen clearly that the major shown contributing peaks are for d-states. The sharpest peak is observed at $-15.95$ eV with an intensity of $156.5$ electrons/eV for 0 GPa. By increasing the value of stress from (0–15 GPa), the intensity of the sharpest peaks is decreasing.

In the case of Bromine (Br), shown in figure 7, the sharp peaks of p-states are observed. At 0 GPa, the sharpest peak is observed at $-0.63$ eV with a peak intensity of $113.2$ electrons/eV. The total density of states (TDOS) of bulk CsPbBr$_3$ is shown in figure 3. The sharpest peaks of 0, 5, 10, and 15 GPa are observed at $-15.95$, $-16.09$, $-16.30$, and $-16.48$ eV respectively. A gradual decrease in peak intensities is observed from (0–15 GPa). In our results, we determined that there is a decrease in the band gap as the stress is increased and the Fermi level is shifted downward.

### 4. Optical properties

The optical properties of CsPbBr$_3$ like absorption, conductivity (real and imaginary), dielectric function (real and imaginary), loss function, reflectivity, and refractive index (real and imaginary) are measured to explain how...
light interacts with matter. All the optical properties are measured at (0, 5, 10, 15 GPa) as shown in figure 8(a)–(f). All the properties are frequency-dependent. The absorption spectrum for CsPbBr₃ at different values of stress is given in figure 8(a). This compound exhibits significant UV absorption. The threshold energy is a specific amount of electromagnetic radiation that the substance quickly absorbs. The properties are interlinked with each other with the following equations [37, 38].

\[ I(\omega) = \sqrt{2} \omega (\sqrt{\epsilon_1(\omega)^2 + \epsilon_2(\omega)^2} - \epsilon_1(\omega))^{1/2} \]  
\[ K(\omega) = \frac{I(\omega)}{2\omega} \]  
\[ L(\omega) = \frac{\epsilon}{(\epsilon_1(\omega)^2 + \epsilon_2(\omega)^2)} \]  
\[ n(\omega) = \left(\frac{1}{\sqrt{2}}\right) (\sqrt{\epsilon_1(\omega)^2 + \epsilon_2(\omega)^2} - \epsilon_1(\omega))^{1/2} \]  
\[ r(\omega) = \frac{n + iK - 1}{n + iK + 1} \]  
\[ \sqrt{\epsilon'(\omega)} = n(\omega) + iK(\omega) \]  
\[ \epsilon_1(\omega) = n^2 - K^2 \]  
\[ \epsilon_2(\omega) = 2nK \]
Where $I(\omega)$ is absorption coefficient, $K(\omega)$ is extinction coefficient, $L(\omega)$ is the energy loss function, $r(\omega)$ reflectivity coefficient, $n(\omega)$ is the refractive index, $\epsilon(\omega)$ is the dielectric function with $\epsilon_1(\omega)$ as real part and $\epsilon_2(\omega)$ is the imaginary part.

The level of absorption increases with the increase in energy. At 0.0 GPa, the absorption edge occurs at 0.0 eV. With the increase in stress from 0 to 15 GPa, the absorption edge lifts towards the higher energies, and the peaks become sharper and shift towards the right. In the absorption spectrum, the blue shift can be seen.

The highest intensity peak observed in the absorption graph is for 15 GPa stress at 14.07 eV. The dielectric function (real) and dielectric function (imaginary) versus frequency graphs are plotted as shown in figures 8(d)–(e). In figure 8(d), the dielectric function varies with the increase in energy; one can readily see four curves at 0, 5, 10, and 15 GPa. The lowest value of the dielectric constant is found at 14.58 eV for 10 GPa. The real part of the dielectric function explains the polarization of material, and the imaginary part gives information about the wasted energy of the system or absorption. The computed results for the imaginary part of the dielectric function of cubic CsPbBr$_3$, in figure 8(e) showed the two major peaks at 3.05 and 7.51 eV and the other two major peaks at 29.01 and 34.21 eV. The transition of electrons from the valence band to the conduction band is due to these points.

The electron energy loss function $L(\omega)$ is drawn in figure 8(f), and it is the function that explains the typical plasmonic oscillations. The rapid electrons crossing the compound characterize the macroscopic and microscopic characteristics of the substance. In this process, energy loss is initialized, and the entire process is directly linked with the electron energy loss function $L(\omega)$. The plasmon peak is the most notable peak found in the energy loss function spectrum. The volume plasmon $(\hbar \omega_{V_{p}})$ is taken by the energy of the major maximum which is equal to 35.13 eV for 15 GPa.

The optical reflectivity of the materials is plotted as a function of energy for different values of stress, as shown in figure 8(g). A major peak of reflectivity is observed at 14.79 eV for 10 GPa. It means that the highest reflectivity is observed in the case of 10 GPa. The results computed for this compound show that it is particularly transparent in low-energy regions, for example, in the infrared, ultraviolet, and visible regions. From 6 to 17 eV, the reflectivity of compounds at 5, 10, 15 GPa is relatively higher than 0 GPa. It can be seen clearly from figure 8(g) that at 0 eV, there is some value of reflectivity in each compound from 0 to 15 GPa.

One can readily see in figures 8(h) and (i) that the refractive index $n$ (real and imaginary) are plotted as a function of energy at different stress ranges from 0 to 15 GPa. Both real and imaginary parts depend upon the frequency in eV. The certain value of the refractive index at zero photon energy is related to the smaller absorption of energy in compounds. The value of the refractive index is 1.98 at zero energy, shown in figure 4(h). The maximum value of the refractive index (real) is found at 2.95 eV for 0 GPa. The values of the highest peak intensities of other compounds are gradually increasing with increasing stress from 0–15 GPa. A drastic increase in refractive index is found at 34.5 eV for a 15 GPa.

5. Elastic and mechanical properties

Understanding the mechanical properties of solids, such as hardness, stiffness, and stability depends heavily on the material’s elastic constants [39]. Elastic constants named $C_{11}$, $C_{12}$, and $C_{44}$ are necessary for defining the stability of the cubic structured compound, as shown in figure 9. Shear stresses are explained by coefficient $C_{12}$, and material transverse growth is explained by coefficient $C_{44}$. Due to the cubic structure of the substance (RbPbF$_3$), it satisfies the Born stability requirements [41]. Following inequality relations are the necessary conditions for a compound to be stable cubically, $(C_{11}−C_{12})>0$, $C_{11}>0$, $C_{44}>0$, $C_{12}<B<C_{11}$, $(C_{11}+2C_{12})>0$.

The elastic characteristics that are obtained from our computed results are Bulk modulus ($B$), Young’s modulus (E), Shear modulus (G), Pugh’s Ratio (B/G), Frantsevish Ratio (G/B), Poisson’s ratio ($\nu$) and Cauchy Pressure ($C_P$) represented in (table 2). Young’s modulus is an important parameter to state the rigidity of a substance [42]. All these parameters are derived through the collected results of elastic constants $C_{11}$, $C_{12}$, and $C_{44}$ from the following equations,

$$E = \frac{9GB}{3B + G} \quad (9)$$

$$\nu = \frac{3B - G}{2(3B + G)} \quad (10)$$

The terms B and G are extracted from Reuss and Voigt limits of Shear ($G_R$ and $G_V$) andBulk ($B_R$ and $B_V$) moduli,

$$G_V = \frac{1}{5}(3C_{44} + C_{11} - C_{12}) \quad (11)$$
For representing the inflexibility and stiffness of a compound, the assessment of bulk modulus \((B)\) is mandatory. The compound shows higher rigidity and tightness when the value of \(B\) is noticeable. In our computed results, the maximum rigidity is found in 10 GPa because the value of Bulk modulus is maximum (57.373). From 0 to 15 GPa, the rigidity or stiffness of the material increases as shown in figure 10(a). A large estimate of the Bulk modulus \((B)\) and Shear modulus \((G)\) values of a compound suggests its greater dynamics to resist certain changes. The Young’s modulus \((E)\) value also describes the inflexibility of a compound, which increases with the increase of stress as shown in figure 10(a).

An important parameter to demonstrate material stiffness is Young’s modulus \([42]\). The values of Young’s modulus is increasing with the increase in stress as shown in table 2.

Furthermore, we measured the yielding or fragile nature of the material by using the Pugh ratio \((B/G)\) \([43]\). Pugh’s principle suggests that if \(B/G > 1.75\) the compound is ductile otherwise brittle \([44]\). In our computed estimations of CsPbBr\(_3\), the Pugh’s ratio for 0 to 15 GPa is greater than 1.75, representing the ductile nature of the material as shown in figure 10(b). The ductile and brittle behaviour of the material can also be explained by Cauchy pressure \((C_P)\) obtained through elastic constants \((C_{12}-C_{44})\) \([45]\). The positive value of \((C_{12}-C_{44})\) specifies ductile while the negative value brittle behaviour \([40, 46]\). In our case, the values of Cauchy pressure are positive from 0 to 15 GPa representing the ductile behaviour of CsPbBr\(_3\). Extreme ductile behaviour is found at 15 GPa, as shown in figure 10(d).

Furthermore, the bond between the atoms of hard compounds consists of covalent nature reinforced by a large shear modulus. Frantsevich rule also suggests a ductile nature when \(G/B < 0.57\) and brittle when \(G/B > 0.57\) \([47]\). All values of \(G/B\) are less than 0.57, so it also confirms the ductile behaviour of this compound as shown in figure 10(c). Poisson’s ratio \((\nu)\) is one more imperative mechanical factor; it also verifies the ductility or brittleness of any material. One can readily see from figure 10(e) that the values of Poisson’s ratio \(\nu > 0.26\) also confirm the ductile nature of CsPbBr\(_3\) \([39]\).

### Table 2. Elastic and Mechanical properties of cubic CsPbBr\(_3\).

| Stress | Bulk modulus (B) | Shear modulus (G) | Young’s modulus (E) | Cauchy pressure \((C_P)\) | Pugh ratio \((B/G)\) | Frantsevich ratio \((G/B)\) | Anisotropic factor \((A)\) | Poisson’s ratio \((\nu)\) |
|--------|-----------------|------------------|---------------------|--------------------------|---------------------|--------------------------|--------------------------|--------------------------|
| 0      | 17.341          | 6.6705           | 17.7602             | 3.8619                   | 2.6296              | 0.3803                   | 0.2347                   | 0.3313                   |
| 5      | 37.015          | 9.3229           | 26.3123             | 11.8901                  | 3.8869              | 0.2573                   | 0.0737                   | 0.3815                   |
| 10     | 57.3732         | 12.4081          | 34.7211             | 20.3786                  | 4.6239              | 0.2163                   | 0.0302                   | 0.3991                   |
| 15     | 72.511          | 14.318           | 40.301              | 26.364                   | 5.0643              | 0.19746                  | 0.0083                   | 0.40737                  |

\[
G_{R} = \frac{5(C_{44} - C_{12})C_{44}}{3(C_{11} - C_{12}) + 4C_{44}} \quad (12)
\]

\[
B_{V} = B_{R} = \frac{C_{11} + 2C_{12}}{3} \quad (13)
\]
Elastic anisotropy of compounds is also calculated by the anisotropic factor (A). If the computed value is larger or less than unity, the compound will be anisotropic, and when A is unity, it will be isotropic [48]. The following mathematical expression is used to calculate anisotropy:

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

For this compound (CsPbBr₃), the results of anisotropic factor A are found to be less than 1, representing anisotropic elastic behavior for 0 to 15 GPa, as shown in figure 10(f).

6. Conclusion

The optical and electronic characteristics of CsPbBr₃ are calculated by applying PBE generalized gradient approximation. The computed lattice parameter and cell volume are found in decreasing factors from 6.138 to 5.426 (Å) and 231.21 to 159.74 (Å³), respectively. The results predicted from band gap calculations show that the computed values of the band gap are in inverse relation with respect to stress. The decrease in band gap (1.900–0.077 eV) is found under the stress of 0 to 15 GPa. On further increase in stress value up to 17 GPa, the band gap vanishes, and the material lacks its semiconductor properties. The partial densities of states (PDOS) of bulk CsPbBr₃, Cs, Pb, and Br are also calculated. The partial density states PDOS of bulk CsPbBr₃ showed that in the valence band range, the sharpest observed peak is for \( d \)-states, while in the conduction region, the sharpest peak is for \( p \)-states and then for \( s \)-states. The maximum value of absorption is found 288020 cm\(^{-1}\) for 15 GPa. The absorption capability is found in increasing order with respect to stress. The dielectric loss function is found maximum for 0 GPa, energy loss for 15 GPa, and refractive index for 0 GPa stress. According to the Pugh ratio (B/G) value, the material is ductile. The values of the Frantsevish ratio (G/B), Poisson’s ratio (\( \nu \)), and Cauchy pressure (\( C_P \)) show also the ductile behavior of this compound. This compound is anisotropic according to...
anisotropic factor (A), which is less than 1 for all ranges of stress. It is also a great choice for usage in optoelectronic devices due to its high refractive index, high absorption, high reflectivity, and high conductivity.

Data availability statement

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

ORCID iDs

M Ijaz Khan @ https://orcid.org/0000-0001-7679-4319
S S A Gillani @ https://orcid.org/0000-0002-4678-4758

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