Effect of mixed halide contents on structural, electronic, optical and elastic properties of CsSnI$_{3-x}$Br$_x$ for solar cell applications: first-principles study

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Abstract

In this study, structural, electronic, optical and elastic properties of CsSnI$_{3-x}$Br$_x$ perovskites are investigated by full potential linearized augmented plane wave method (FP-LAPW) with exchange correlation functionals GGA-PBE and GGA-mBJ as implemented in Wien2k. The calculated structural parameters for all compositions are in good correlation with literature. The band structures and density of states (DOS) are calculated by GGA which indicated that all these alloys have direct band gap. Furthermore, the band gaps are also calculated by employing modified Beck-Johnson’s (mBJ) exchange potential. The obtained band gaps with this method are found to be improved as compared to GGA. The calculated optical parameters show that these materials have the competency for light absorption and to retain it. These characteristics make them promising materials for solar cell applications. The elastic constants have also been calculated which revealed that all these compounds have ductile nature. The mixed halide contents are pioneered in this study and therefore, no data is in hand for estimation.

1. Introduction

It has become a fact that energy is the most basic and primary need of society. Its demand is continuously increasing with the increase in population. The gap between demand and supply is growing large with the passage of time. The conventional energy production methods have been failed to meet the energy requirements. Therefore, the non-conventional methods such as photovoltaic devices and windmills have attained much interest. These methods are the most promising solution to fulfill the energy gap. In addition to other methods, the photovoltaic devices are considered as the best cheap approach to meet this requirement of energy. Halide based perovskites with general formula ABX$_3$ have gained great interest because of efficient light accumulation attribute and applications as next generation photovoltaics. In addition to it, these materials have also found applications such as memory devices, dielectrics, superconductors, LED’s and in LASER diodes [1]. These technological applications make them significant class of materials for both theoretical and experimental research point of view. In general, the perovskites have cubic structure with AB$_3$ stoichiometry. The cations A and B are of different sizes and X may belong to Halogen family (X = I, Br, Cl), where I (Iodine), Cl (Chlorine) and Br (Bromine). The larger cation A occupies the corner positions, the smaller cation B at body center and Halogen member occupies face centered making the octahedron cage with body centered cation. Perovskites mainly exists in three phases named as α (Cubic), β (tetragonal) and γ (orthorhombic) [2]. Furthermore, it is imperative to mention that, to have stable structure of a perovskite material, selection of A and B atoms is diametrically confined and have been defined by Goldsmith coefficient;
\[ t = \frac{(r_A + r_X)}{\sqrt{2}} \frac{1}{(r_B + r_X)} \] (1)

To obtain high symmetry, \( t \) should have the range \( 0.76 \leq t \leq 1.1 \). Perovskites based photovoltaics have the power conversion efficiency (PCE) limit to 22.1\% as reported by National Renewable Energy Laboratory (NREL) [1, 3]. In photovoltaic applications the band gap has pivotal role and in Halide based perovskites it can be tuned either by varying Halide contents or with cations size. Therefore, in order to obtain an optimal band gap for photovoltaic applications, several studies have been carried out by various researchers as reported in the literature and are discussed here. Firstly, Moller et al studied the pure inorganic perovskite material i.e. CsPbX₃, which have the same structure as CaTiO₃ (a perovskite materials reported by for the first time) but have lower conversion efficiency [4]. Later, Cs was replaced by Methyl-ammonium (MA) and Farmamidinium (FA) in CsPbX₃ which resulted in blue shift in band gap with 1.48 eV band gap. But these materials have stability issues [5]. The large size of FA cation leads to FA based perovskites with high tolerance factors \( t > 1 \) resulting a yellow-hexagonal non-perovskite \( \delta \)-phase at room temperature and found not suitable for solar cell applications [6]. FA based perovskites have very limited value of optical absorption coefficient [7]. The major drawback reported for MA based perovskites was its reversible phase transition between tetragonal and cubic for temperature range 54 °C–57 °C [8]. It has been highlighted in the literature that the perovskites with small band gap are suitable for solar cell practices. Since, the materials with small band gap can absorb maximum light from solar spectrum.

To obtain the desired result we must architect a useful computational model which meticulously describe the electronic properties of materials. GGA-PBE exchange potentials nicely illustrate the ground properties of a system but do not consider the excited-state properties [9]. A different exchange potential has been made known by Becke and Johnson [10]. For the computation of band gap mBJ improves over the PBE. The value of modified Becke and Johnson potential is given by the below equation,

\[
v_{s, 0}^{mBJ}(r) = \frac{1}{\pi} \sqrt{5} \frac{1}{6} \frac{t_s(r)}{\rho_e(r)}
\]

where \( t_s(r) \) is Kohn–Sham kinetic energy density and \( \rho_e(r) \) is electron density. Although, this potential can’t be used for the calculation of forces acting on nuclei as mandatory for geometry optimization rather, the sole function of mBJ is to overcome the underestimation of band gap and get the values to meet up with experimental results [11, 12].

Halide based perovskites i.e. APbX₃ (A = Cs, MA, FA) have attained much attention for photovoltaic application. However, the existence of Pb in these compounds make them toxic. Therefore, the Pb based perovskites are difficult to handle which further reduced their commercialization [13–17]. In keeping view these issues and limitations, the researchers are finding alternative and Pb free materials for photovoltaic devices. In addition to high efficiency of halide based photovoltaic device, these devices also have high carrier mobility, long diffusion lengths, and small effective masses of holes and electrons. Therefore, to obtain an alternative or Pb free material for photovoltaic application, a tin based mixed halide perovskites CsSnI₃₋ₓBrₓ (\( x = 0, 1, 2, 3 \)) have been investigated and reported for the first time. This study consists of 4 sections. In first section the literature has been discussed. Second section consists of computational detail employed in this study. Third section contains results with detailed discussion on structural, electronic, optical and elastic properties. In the last section we have concluded our results.

2. Computational details

In this strive the calculations were executed by using FP-LAPW with GGA + PBE and GGA + mBJ as implemented in Wien2k code. We have applied the full potential scheme on the unit cell of CsSnI₃₋ₓBrₓ halide based mixed perovskites. The crystal system is divided into two localities i.e. the atomic spheres and the zone outside the atomic spheres (interstitial regions) [18]. The plane wave function explicated into two distinct basis sets. Wave function can be defined in atomic-type functions in every atomic sphere whereas it is defined as plane wave basis at interstitial positions [19]. We set the value of RMT, so that the whole crystal system is in equilibrium, that no forces are being applied by the atomic spheres on each other [17]. Muffin tin radius (RMT) for Cs, Sn and Br were taken 2.5 Bohr while for I, it was 2.07 Bohr [19]. Cubic phase and \( m \bar{3} m \) space group with atomic positions (0, 0, 0), (0.5, 0.5, 0.5), (0.5, 0.5, 0) for Cs and (I, Br) were taken in this work. Calculations are performed using \( 10 \times 10 \times 10 \) \( k \)-mesh. The energy convergence criteria were taken 0.0001 eV to avoid any charge leakage. Band gap was calculated by both GGA and (mBJ)-GGA exchange potential. The band gap values can be made suitable by using the mBJ potential. Further, optical and elastic parameters for all compositions range were calculated within the framework of DFT.
3. Results and discussion

3.1. Structural properties

The determination of structural specification is unavoidable for the description of structural behavior of materials. The structural parameters i.e. lattice constant \(a_o\), bulk modulus \(B\) and the pressure derivative of the bulk modulus \(\frac{\partial B}{\partial P}\) are determined. The total energy (Ryd) of the unit cell for every compound was calculated by fluctuating the volume of the unit cell and plotted against the correlative energies for optimization. The Murnaghan’s equation of state is used to calculate bulk Modulii and the lattice constants. Murnaghan’s equation of state assumes that the bulk modulus varies inversely with pressure \[20\]. Mathematical form of Murnaghan’s equation of state is given by

\[
P (\nu) = \frac{B}{B'} \left[ \left( \frac{V_o}{V} \right)^{\frac{B'}{B}} - 1 \right]
\]

\[
(\nu) = \frac{B}{B'} \left[ \left( \frac{a_o}{a} \right)^{\frac{3B}{2}} - 1 \right]
\]

Where \(P (\nu)\) is the pressure, \(B\) is the bulk modulus, \(B'\) is the pressure derivative of bulk modulus, \(V_o\) and \(a_o\) are the equilibrium volume and lattice constant i.e. when the system is in relax state. The calculated structural parameters are compared with literature as listed in the table 1.

The calculated parameters of end compounds are in good correlation with other theoretical and experimental results \[25\]. However, the mixed halide contents are reported for the first time, therefore, no data is available in literature. From the obtained results as listed in the table 1, it can be observed that with the increase in Bromine concentration, the lattice constant ‘\(a\)’ found to be decreased \[9\] and bulk modulus is increased as shown in figure 1.

The graphical narration of geometry optimizations is shown in figures 2(a)–(d).

3.2. Electronic properties

The electronic properties of the CsSnI\(_{3-x}\)Br\(_x\) are calculated by using GGA and mBJ. Band structure diagram tells us whether the material has direct or indirect band gap in addition to band gap value. Furthermore, it also tells us about the \(p\)-type, \(n\)-type or intrinsic nature of the semiconducting materials based on the position of Fermi level \(E_F\). The calculated results revealed that the conduction band minima and valance band maxima are located at the R high symmetry points, hence evidenced for the direct band gap semiconductors. The calculated band gaps by both potentials (GGA and mBJ) are listed in the table 2, from where it can be seen that the band gaps calculated with mBJ have been improved as compared to other theoretical results reported in literature but lower than to experimental values which is due the limitations and under estimations of GGA \[26, 27\].

Direct band gap can also be detected at other symmetry points (M, \(\Gamma\) and X). It is clear from the band structure diagrams in figure 3 that band gap is increased when we replace the I atoms by Br atoms due to decrease in atomic size. This is due to fact that as the I has the more number of nucleons than Br atom, so the I, due to its large size have the less electrostatic force of attraction between nucleus and the outermost electrons (shielding
Figure 1. Variation of lattice constant and bulk modulus with composition for CsSnI$_{3-x}$Br$_x$ for ($x = 0, 1, 2, 3$) alloys.

Table 2. Comparison between calculated and other theoretical and experimental band gaps.

| Composition    | CsSnI$_3$ | CsSnI$_2$Br | CsSnBr$_2$ | CsSnBr$_3$ |
|----------------|-----------|-------------|------------|------------|
| This work $E_g$ (eV) GGA-mBJ | 0.59 | 0.60 | 0.63 | 0.95 |
| This work $E_g$ (eV) GGA | 0.30 | 0.31 | 0.40 | 0.58 |
| In literature (eV) | Theo. 0.34[28], 0.15[29] | Exp. 1.37[30] | Exp. 1.65[30] | Theo. 0.3[28], 0.35[29] | Exp. 1.75[29] |

* [28].
* [29].
* [30].
* [17].
effect) which results the shrinkage in the bonding energies and the separation between CB (conduction band) and the VB (valence band). The main reason behind this effect is to have large number of electrons in their corresponding bands and thus in the occupancy states close to the Fermi level.

The calculated band gap $E_g$ (eV) values at R-symmetry point in this work and other values available in literature are given in table 2.

In one way or other, the physical properties of a compound are based on the electronic band gap which lies in the DOS (density of states). Therefore, the understanding of its formation becomes vital for the development and fabrication of opto-electronic, magneto-optic and magneto-electronic devices [14]. The total and partial DOS for all compositions (CsSnI$_3$ – $x$Br$_x$) have been calculated and are presented in figures 4(a)–(d). The DOS graphs can be explained with two aspects, the orbitals which are contributing near the band edges and the overall contribution of the states. In composition CsSnI$_3$, I-$p$-states and Sn-$p$-states are contributing near the band edges in VB and CB respectively. The overall contributions in band gap are mainly of the Cs-$p$ and I-$s$-states in VB and Cs-$d$ in CB. In case of CsSnI$_2$Br, only I-$p$-states are contributing near the band edge in VB. While Cs-$p$ and Br-$s$ have the major contribution in band gap with slight contribution of I-$s$-states in VB and Cs-$d$ states in CB. In DOS graphs of CsSnBr$_2$, I-$p$, Br-$s$ and Sn-$p$-states are contributing near the band edges in VB and CB respectively. Firstly, Cs-$p$-states have maximum contribution followed by Br-$p$ and I-$s$-states in VB and Cs-$d$ have very small contribution in upper part of CB. If we talk about the states contributions of CsSnBr$_3$, our calculated results reveal that Br-$p$ and Sn-$p$-orbitals have the main impact in band gap formation (near the band edges) and the overall contribution of states in valance and conduction band are of Cs-$p$, Br-$s$ and Cs-$d$-orbitals respectively. In summary, $p$-states of I, Br, Ce and Sn have the main role in band gap formation in simple and mixed halides perovskites.

Figure 3. Band structures of CsSnI$_3$ – $x$Br$_x$ calculated by employing mBJ-GGA.
The band gap will enhance by the decrement in lattice constants \(^{31}\). In other words, we can say that by controlling the halide (Br) contents, the band gap can be tuned in order to approach optimal band gap. This variation of band gap can be understood easily that how band gap is changed with the inclusion of Br contents from figure 5(a). Secondly lattice parameter and the band gap value have the inverse relation between them according to results obtained. Band gap increased with the increase in lattice constant. This is shown in figure 5(b) below.

### 3.3. Optical properties

Cesium tin mixed halide perovskites are the efficient light absorbing materials amongst the family of photovoltaic family \(^{32–34}\). So, the researchers have huge concern in these materials for solar cell applications. The computed optical parameters such as absorption coefficient, and refractive indexes have explored that what type of response these materials will show when the photons will be incident upon them \(^{35}\). Optical properties of the compound which is being investigated (CsSnI\(^3-x\)Br\(_x\)) are explained with the help of their dielectric function \(\varepsilon_1\) and \(\varepsilon_2\), where \(\varepsilon_1\) and \(\varepsilon_2\) are the real and imaginary parts of the dielectric functions. The mathematical formulae for the calculation of different optical parameters are given by the following equations.

\[
\begin{align*}
    n &= \sqrt{\varepsilon_1} \\
    k &= \sqrt{\varepsilon_2} \\
    \alpha &= \frac{4\pi}{\lambda}k
\end{align*}
\]

Real part \(\varepsilon_1\) shows the stored energy of the material that available to be given out at zero energy or zero frequency limit and considered to be intrinsic characteristic of any material. These materials show high value of \(\varepsilon_1\) which means that at zero energy these materials have enough energy to be given out for useful purposes in opto-electronic devices. The values of \(\varepsilon_1\) for CsSnI\(_3\), CsSnI\(_2\)Br, CsSnIBr\(_2\) and CsSnBr\(_3\) are 8.4, 5.1, 4.4 and 6.8 respectively.
respectively. The $e_1$ and band gap have the inverse relation between them. The $e_1$ and band gap have the inverse relation between them. We can investigate the metallicity of the compound by real function $e_1$. The negative value of the $e_1$ shows the metallic nature of the compound [36]. From figure 6(a) we can see that at high enough value of energy $\sim 10$ eV these materials show metallic behavior.

On the other hand imaginary part $e_2$ represents the absorption ability and behavior of these materials show the energy gain for the photovoltaic devices [37]. Basically, it gives us information that how a material response when a disturbance is caused by electromagnetic radiation. The dielectric function having imaginary part represents the absorptive response of materials and directly varies with their band structure [38]. The critical points in the spectra of $e_2$ for CsSnI$_3$, CsSnI$_3$Br, CsSnIBr$_2$, CsSnBr$_3$, are found at 1.9, 2.8, 3.4, 2.3 eV and 6.65, 6.58, 5.26, 4.81 eV, respectively [Table 3]. The $e_2$ values show that these materials may absorb the maximum amount of the energy over the wide photon energy range and coincidentally may hold that energy.

Extinction coefficient ($k$) refers as how actively a substance absorbs light at a given wavelength. It is an optical property of the material related to index of refraction of the material. Positive value of $k$ shows that the absorption is going to be take place, while $k = 0$ shows that the light travels straight through the material [39].

| Composition | Real function $e_1$ | Imaginary function $e_2$ | Refractive index $n$ | Extinction coefficient $k$ | Absorption coefficient $\alpha$ |
|-------------|---------------------|--------------------------|----------------------|---------------------------|-------------------------------|
| CsSnI$_3$   | 8.4                 | 1.9                      | 2.9                  | 2.57                      | 157000                        |
| CsSnI$_3$Br | 5.1                 | 2.8                      | 2.1                  | 2.56                      | 154000                        |
| CsSnIBr$_2$ | 4.4                 | 3.4                      | 2.75                 | 2.30                      | 146000                        |
| CsSnBr$_3$  | 6.8                 | 2.3                      | 2.6                  | 2.21                      | 214000                        |

Figure 5. Variation of band gap w. r. t (a) lattice constants and (b) with compositions.

Figure 6. Dielectric function (a) real part and (b) imaginary part.

Table 3. Optical parameters of CsSnI$_3$-$_x$Br$_x$ ($x = 0, 1, 2, 3$).
The extinction coefficient graphs have similar features (critical points) to imaginary part $\varepsilon_1$. Absorption coefficient ($\alpha$) depends upon both the incoming light and the intrinsic property of the material [40, 41]. Absorption coefficient determines how far into a material of a particular wavelength can drill inside the material before it absorbed. The calculated value of absorption coefficients for different compositions are 214000 at 2.2 eV for CsSnBr$_3$, 157000 at 1.9 eV for CsSnI$_3$, 154000 at 2.8 eV for CsSnI$_3$Br and 146000 at 3.4 eV for CsSnIBr$_2$. CsSnBr$_3$ showed the maximum absorption in IR region and will cover the maximum solar spectrum range, hence suitable for devices like solar cells, LED’s and LASER’s. Figures 7(a)–(b) shows calculated values for extinction and absorption coefficients.

To use the materials in practical applications like solar cells, LED’s and waveguides the knowledge of refractive index is very important. The dimensionless number, refractive index shows that how light propagates through that material [42]. Figure 8 shows the variation of refractive index as a function of incident electromagnetic wave energy for all compounds. Refractive indexes show the increasing trend with the increase in frequency/energy of incident light and we have noted the following maximum values i.e. 2.9 for CsSnI$_3$, 2.1 for CsSnI$_3$Br, 2.75 for CsSnIBr$_2$ and 2.6 for CsSnBr$_3$. After certain energy limit the refractive indexes started decreasing and reach to minimum values less than unity. As the formula for refractive index is $n = c/v$, from this formula we conclude that value of refractive index is less than unity indicates that phase velocity of incident radiation is greater than $c$, so, the incident radiation can penetrate through depth. Hence, material will become transparent for incoming radiations. The refractive indices of these perovskites show that these materials are favorable for photovoltaic devices. Figure 8 shows the variation of refractive index as a function of incident photon energy.
3.4. Elastic properties

To study the crystal behavior under the influence of the applied macroscopic pressure can be interpreted with the help of three elastic constant tensor $C_{ij}$ ($C_{11}$, $C_{12}$, $C_{44}$) for the cubic perovskite crystal structures. These elastic constants show how a system undergoes a deformation under the applied pressure and how these materials return to their initial stage [43]. With the help of these three elastic constants one can extract the useful information about the crystal structure stability, type and quality of the bonds between the plains, anisotropic or isotropic type of the material and even the melting points of the materials. As there is no experimental data on these elastic properties is available for the cubic perovskites CsSnI$_3$, CsSnI$_2$Br, CsSnIBr$_2$, and CsSnBr$_3$. So, these results are being reported for the first time. A consistency analysis of the calculated values can be performed by implementing the criterion of mechanical stability of the perovskite crystal [43].

$$\begin{align*}
C_{11} + 2C_{12} &> 0 \\
C_{11} - C_{12} &> 0 \\
C_{11} &> 0, \ C_{44} > 0
\end{align*}$$

(8)

These three conditions will have to be fulfilled by all the four compositions (i.e. CsSnI$_3$, CsSnI$_2$Br, CsSnIBr$_2$, and CsSnBr$_3$) and have to execute the mechanical and structural stability according to the justified benchmark. Bulk modulus $B$ measures the strength or hardness of the crystal. Large $B$ of the crystal ensures the strength of the crystal against brittleness. We can calculate the $B$ using $C_{11}$, $C_{12}$

$$B = \frac{C_{11} + 2C_{12}}{3}$$

(9)

The calculated $B$ for all the four composition of cubic perovskite crystal structures are given in table 4. By analyzing and comparing the $B$ of these materials with other materials like diamond and glass, they are found to be soft materials. The shear modulus $G$ indicate the strength of the crystal against plastic deformation [44]. The elastic constants are used to calculate the value of $G$ and the following principle equations are used.

$$G = \frac{G_V + G_R}{2} \text{ where } \begin{align*}
G_V &= \frac{C_{11} - C_{12} + 3C_{44}}{5} \\
G_R &= \frac{(C_{11} - C_{12})5C_{44}}{4C_{44} + 3(C_{11} - C_{12})}
\end{align*}$$

(10)

We can use the ratio of $B$ to $G$ to take an estimate of softness or friability of materials [30].

$$\begin{align*}
\frac{B}{G} &> 1.75, \ \text{the material is ductile} \\
\frac{B}{G} &< 1.75, \ \text{the material is brittle}
\end{align*}$$

(11)

The results in table 4 show that these materials are ductile in nature. The young’s modulus $E$ is another important constant which can be used to analyze the stiffness of the materials. The equation for the $E$ is given by

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

(12)

In physics the term anisotropy is used to describe the direction dependent properties of the materials. It refers as the difference in physical or mechanical properties like refractive index, absorbance, conductivity and tensile strength etc when measured along different axis. Based on anisotropic coefficient, we can check whether the material is isotropic or anisotropic in nature. The anisotropic coefficient $A$ can also be evaluated with the help of elastic parameters formulated below

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \text{ with } \begin{align*}
A &= 1 \text{ material is isotropic} \\
A &\neq 1 \text{ material is anisotropic}
\end{align*}$$

(13)

All four materials CsSnI$_3$, CsSnI$_2$Br, CsSnIBr$_2$, and CsSnBr$_3$ which are under investigation have $A \neq 1$. So, these are anisotropic in nature. The dimensionless quantity, Poisson ratio $\sigma$ declares the fluctuation in the volume of crystal as a result of type of bond and interatomic forces. For ionic crystals $\sigma \geq 0.25$ and for covalent crystals $\sigma < 0.1$ [45].

$$\sigma = \frac{3B - E}{6B}$$

(14)

CsSnI$_3$, CsSnI$_2$Br, CsSnIBr$_2$, and CsSnBr$_3$ are predominately ionic in nature because they have $\sigma > 0.25$. The below stated formula can be used to find out the melting point of crystals and all
### Table 4: Elastic and physical parameters for CsSnI$_3$–xBr$_x$ ($x = 0, 1, 2, 3$)

| Composition | Bulk Modulus ($B$) | Shear Modulus ($G$) | Young’s Modulus ($E$) | Anisotropic coefficient ($A$) | Poisson ratio ($ν$) | Melting Point ($T_{\text{mel}}$) |
|-------------|-------------------|---------------------|-----------------------|------------------------------|-----------------|-----------------------------|
| CsSnI$_3$  | 16.56  | 9.03  | 22.92  | 1.83  | 0.25  | 0.26  | 806.53 ± 300 K |
| CsSnI$_2$Br | 18.52  | 4.63  | 12.82  | 4.00  | 0.77  | 0.38  | 792.94 ± 300 K |
| CsSnIBr$_2$ | 19.31  | 8.48  | 22.19  | 2.27  | 0.39  | 0.30  | 808.90 ± 300 K |
| CsSnBr$_3$ | 21.09  | 11.48 | 29.15  | 1.83  | 0.25  | 0.26  | 843.77 ± 300 K |
\[ T_{\text{nd}} = [553^\circ K + (5.91 \times C_{\text{A}})] \pm 300^\circ K \] (15)

the discussed parameters with their calculated values are given stated below in table 4.

4. Conclusions

FP-LAPW technique is used to measure the physical properties of CsSnI3, CsSnI2Br, CsSnIBr2, and CsSnBr3 revealed that they are ductile, anisotropic and ionic in nature. The high absorption power and direct band gaps in ultraviolet range predicts that these materials are suitable for solar cell applications. Elastic properties of these materials show that these materials are ductile because they have low 'B' values. Their ratio of bulk 'B' to 'G', anisotropic coefficient A and Poisson ratio of the materials CsSnI3, CsSnI2Br, CsSnIBr2, and CsSnBr3 revealed that they are ductile, anisotropic and ionic in nature. The findings of this study are predictive and can be used toward experimental work.

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References

[1] Afshari M, Boochani A and Hantezadeh M 2016 Electronic, optical and elastic properties of cubic perovskite CaPbI3: Using first principles study Optik-International Journal for Light and Electron Optics 127 11433–45
[2] Aharon S, Cohen B E and Elgar L 2014 Hybrid lead halide iodide and lead halide bromide in efficient hole conductor free perovskite solar cell The Journal of Physical Chemistry C 118 17160–5
[3] Arar R, Ouahraoui T, Varshney D, Khemata R, Murtaza G, Rached D and Reshak A 2015 Structural, mechanical and optical properties of sodium based fluoroperovskites NaXFe3 (X = Mg, Zn) from first-principle calculations Mater. Sci. Semicond. Process. 33 127–35
[4] Ayatullahah H, Murtaza G, Muhammad S, Naeem S, Khalid M and Manzar A 2013 Physical properties of CsSnM3 (M = Cl, Br, I): A first principle study, Acta Phys Polym 124 102–7
[5] Babu K E, Murali N, Babu B K and Veeraiah V 2015 Structural, elastic and electronic properties of KCaF3 and RbCaF3 for vacuum-ultraviolet-transparent lens materials AIP Conf. Proc.
[6] Borriello I, Cantele G and Ninno D 2008 Ab initio investigation of hybrid organic-inorganic perovskites based on tin halides Physical Review B 77 235214
[7] Bretschneider S A, Weikert J, Dorman J A and Schmidt-Mende L 2014 Research update: physical and electrical characteristics of lead halide perovskites for solar cell applications APL Mater. 2 155204
[8] Brik M 2011 Comparative first-principles calculations of electronic, optical and elastic anisotropy properties of CsXBr3 (X = Ca, Ge, Sn) crystals Solid State Commun. 151 1733–8
[9] Jishi R A 2016 Modified Becke–Johnson exchange potential: improved modeling of lead halides for solar cell applications Mater. Sci. 3 149–59
[10] Tran F, Blaha P and Schwarz K 2007 Band gap calculations with Becke–Johnson exchange potential J. Phys. Condens. Matter 19 196208
[11] Koller D, Tran F and Blaha P 2011 Merits and limits of the modified Becke–Johnson exchange potential Physical Review B 83 195134
[12] Raesaenen E, Pittalis S and Proetto C R 2010 universal correction for the Becke–Johnson exchange potential J. Chem. Phys. 132 044112
[13] Castelli I E, Thygesen K S and Jacobsen K 2015, Calculated optical properties of different perovskite phases Journal of Materials Chemistry A 3 12343–9
[14] Even J, Pedesseau L, Jancu J M and Katan C 2014 DFT and k·p modelling of the phase transitions of lead and tin halide perovskites for photovoltaic cells, physica status solidi (RRL)–Rapid Research Letters 8 31–5
[15] Filip M, Haber J and Neaton J 2019 First-principles studies of the electronic and optical properties of halide perovskites: from three to two dimensions Bull. Am. Phys. Soc. 64 2
[16] Filip M R and Giustino F 2015 Computational screening of homovalent lead substitution in organic–inorganic halide perovskites The Journal of Physical Chemistry C 120 166–73
[17] Heyd J, Peralta J E, Scuseria G E and Martin R L 2005 Energy band gaps and lattice parameters evaluated with the Heyd–Scuseria–Ernzerhof screened hybrid functional J. Chem. Phys. 123 174101
[18] Jacobsson T J, Correa-Baena J-P, Paozki M, Saliba M, Schenk K, Grätzl M and Hagfeldt A 2016 Exploration of the compositional space for mixed lead halogen perovskites for high efficiency solar cells Energy & Environmental Science 9 1706–24
