Pressure induced band gap shifting from ultra-violet to visible region of RbSrCl₃ perovskite

Md Borhanul Asfia, Sahadat Jaman and Mohammad Abdur Rashid

Department of Physics, Jashore University of Science and Technology, Jashore 7408, Bangladesh

*Author to whom any correspondence should be addressed.

E-mail: rashid@just.edu.bd

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Abstract

Metal halide perovskites that do not contain lead are non-toxic and offer a wide range of uses in low-cost photovoltaic and optoelectronic systems. In this report, density functional theory is used to explore the influence of pressure (0–150 GPa) on the structural, electronic and optical characteristics of RbSrCl₃ perovskite metal halide. At 0 GPa, RbSrCl₃ was found to be an indirect wide-bandgap semiconductor. Under pressure, the electronic band gap transforms to visible range direct band gap which is suitable for optoelectronic devices. Higher absorption for RbSrCl₃ was found in the ultraviolet region under the influence of different pressures. As the pressure on the halide perovskite increased, absorption peak is shifted to higher energy range. The optical conductivity, reflectivity and extinction coefficient were significantly changed due to induced pressures. The results suggest that under uniform pressure RbSrCl₃ can be used in optoelectronic applications.

1. Introduction

Perovskite materials have recently piqued the interest of scientific community because of their outstanding characteristics such as tunable bandgap, superior charge-carrier mobility, high visible light absorption, low reflectivity, low recombination rate, high ductility, and low excitation binding energy [1, 2]. Because of their unusual characteristics and possibilities, inorganic metal halide perovskite materials have sparked a lot of attention in recent years. Metal halides have demonstrated excellent performance in optoelectronics and have significant potential as a solar cell materials. Furthermore, these metal halide perovskites are inexpensive and abundant on the planet. These semiconductors have a variety of uses outside of photovoltaics and optoelectronics, including photodetectors, LEDs (Light Emitting Diodes) and solar-to-fuel energy conversion systems [3–9]. Solar energy is now widely employed to generate electricity since it is more convenient and suited for usage, as well as useful in a variety of device applications [10]. The hybrid perovskite has been shown to have significant advantages over photoconductor-based x-ray detectors [11–13], spectroscopy [14], acoustic wave signal processing, and picture storage devices [15]. To foresee the specific device applications of this class of fascinating materials, a thorough grasp of their properties is necessary. As a result, it is critical to investigate the structural, mechanical, and optoelectronic capabilities, as well as the overall characteristics of various perovskites.

Metal halide perovskites have the formula ABX₃, where A is a monovalent cation, B is a divalent metal ion, and X is a halogen anion. Many Pb-based halide perovskites such as CsPbX₃ (X = Cl, Br) have been extensively studied [16, 17] and shown to have a good potential to be used in photovoltaic and optoelectronic device design. However, Roknuzzaman et al recently compared the structural, optical, electrical and mechanical characteristics of CsBX₃ (B = Ge, Sn and X = Cl, Br, I) semiconductors to the lead-containing semiconductors CsPbX₃ (X = Cl, Br, I) in a simulation study [18]. They indicate that the Ge-based CsGeI₃ metal halide is the best lead-free inorganic metal halide perovskite semiconductor for optoelectronic and solar cell applications based on a combinational study. Because of their hazardous impact on the environment, Pb-based hybrid halides will become obsolete in the future [19]. At ambient settings, lead-based metal halide perovskite materials disintegrate...
to PbI₃ in the presence of oxygen in the atmosphere, which is ecologically harmful [20–22]. As a result, one of the key disadvantages of lead halide cubic perovskites is device instability and J–V hysteresis [23]. Making lead-free, non-toxic halide perovskite is a key difficulty in commercializing perovskite solar cells. Hassan et al noticed, in the visible energy range, the indirect band gap widens and becomes direct at 75GPa for RbTaO₃, indicating potential optoelectronic applications [24]. They observed that the thermoelectric properties of RbTaO₃ at 0GPa and 75GPa may also be used in thermoelectric devices. Kholil et al reported that Fe-doped CsSnCl₃ is more promising for photovoltaic cells and other photoelectric technologies [25]. At 12 GPa, Saeed et al observed that CsYbBr₃ has a semi-metallic character, but when pressure increases, it becomes metallic. They also found that when pressure increased, the Debye temperature decrease, but the lattice thermal conductivity increased [26]. The radioactive element Fr-containing perovskite FrGeI₃ may have uses in nuclear medicine and diagnosis, such as x-ray imaging technologies, according to Hasan et al [27]. Zhang et al investigated the defect characteristics of CsSnCl₃, and proposed the necessary instructions for CsSnCl₃ synthesis and modulation [28]. Wu et al investigated metal (Mn, In) doping in CsSnCl₃ experimentally and calculated structural and electrical parameters to improve light emission [29]. RbSnCl₃ is a possible contender for solar energy conversion and photocatalytic water splitting, according to Yunsheng et al [30]. RbSnCl₃, RbSnBr₃, KSnCl₃, and KSnBr₃ perovskite compounds have promising electrical and optical characteristics, according to Khan et al, indicating their potential use in photovoltaic and other optoelectronic applications [31].

We report theoretically calculated electronic and optical characteristics of lead-free cubic RbSrCl₃ for different uniformly applied hydrostatic pressure. At zero pressure perovskite RbSrCl₃ is a wide indirect band gap semiconductor. With the application of uniform pressure the band gap becomes direct and after a small increase band gap decreases significantly to visible range with the increase of pressure. External pressure has also been shown to greatly increase theoretically measured optical characteristics, which is important for novel photovoltaic and optoelectronic device applications [32]. We use density functional theory (DFT) [33] simulations to show structural, electronic and optical characteristics of cubic RbSrCl₃ perovskite under pressure.

2. Computational method

Structures, electronic and optical properties of RbSrCl₃ at various applied pressures were estimated using DFT as implemented in the WIEN2k code [34, 35]. In solving the Kohn–Sham equations the exchange–correlation functional is constructed using the Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation [36]. In this method the space is divided into non-overlapping muffin–tin spheres separated by an interstitial region. The convergence of the basis set was controlled by a cutoff parameter \( R_{\text{mt}} \times k_{\text{max}} = 8.0 \), where \( R_{\text{mt}} \) is the smallest of the muffin–tin sphere radii and \( k_{\text{max}} \) is the largest reciprocal lattice vector used in the plane wave expansion. Total energy and charge convergence were set as 0.000 01 Ry and 0.0001 e respectively, during the self-consistency cycle. The number of \( k \)-points in Brillouin zone is selected to 2000, corresponding to \( 12 \times 12 \times 12 \) \( k \)-mesh, during the calculation. Furthermore, to get more accurate results in estimating density of states (DOS) and optical properties a denser \( k \)-point mesh of \( 21 \times 21 \times 21 \) \( k \)-point mesh corresponding to 10 000 \( k \)-points was considered.

3. Result and discussion

3.1. Structural properties

The cubic crystal structure of the inorganic lead-free metal halide perovskite semiconductor RbSrCl₃ corresponds to the space group \( Pm\bar{3}m \) (no. 221). Figure 1(a) depicts the structures of RbSrCl₃ containing five atoms in each unit cell (1 Rb, 1 Sr and 3 Cl atoms). The Rb, Sr and Cl atoms are located at 1a(0 0 0), 1b(0.5, 0.5, 0.5) and 3c(0.5, 0.5, 0) respectively, in Wyckoff coordinates. Minimum energy structure for zero induced pressure was obtained by fitting total energy versus volume (figure 1(b)) with the Murnaghan equation of state [37]. The estimated lattice parameter \( a \) for RbSrCl₃ is 5.698 Å at 0 GPa. The value of \( a \) can not be compared because of unavailability of any previous experiment or calculation. With the applied pressure the lattice parameter decreases so as the volume of the unit cell. The estimated lattice parameters with applied pressure as computed using Murnaghan equation of state [37] are presented in table 1. During the calculation of \( a \) with applied uniform hydrostatic pressure any possibility of phase change is ignored and the structure of RbSrCl₃ remain cubic throughout the process.

3.2. Electronic properties

Electronic band structure is an important factor for understanding the chemical bonding nature and physical characteristics of materials. The band structure of RbSrCl₃ is computed at different hydrostatic pressure at 0 GPa
to 150 GPa to investigate pressure-induced changes in band structure which shown in figure 2. The minimum value of conduction band (CB) located at the symmetry point Γ where the maximum value of valence band (VB) located at M symmetry point at 0 GPa. This indicates that indirect band gap is developed in lead-free RbSrCl3 with 4.629 eV at absence of pressure (figure 2(a)). Interestingly, when pressure is increased to 30 GPa, minimum value of CB shifted to higher energies and maximum value of VB shifted to Γ point from M point. As a result, indirect band gap is transformed to direct band gap which located at Γ point and calculated bandgap value is 5.166 eV. Beyond 30 GPa, the band gap started to decrease with the increase of pressure.

The calculated values of bandgap for different induced pressure are listed in table 1. The conduction band moves towards lower energies above 60GPa and direct bandgap is noticed. Finally at pressure 150 GPa the band gap is reduced at 2.090 eV. The transition nature from indirect bandgap to direct bandgap of RbSrCl3 is suitable for optoelectronic device applications.

To understand electronic structure of RbSrCl3 in details, density of state (DOS) is an important parameter. In figures 3(a)–(f) partial density of states (PDOS) and in figure 4 total density of states (TDOS) under different induced pressures for cubic perovskite RbSrCl3 are illustrated. In the absence of pressure the major contribution of Cl-3p is to form VB between the energy range from −2 to 0 eV and Sr-3d contributed to form CB in the energy range of 6–8 eV. Interestingly when pressures are applied from 60–150 GPa band gap continuously decreases due to strong hybridization between Cl-3p and Sr-4p or Cl-3p and Rb-4p orbitals. Conduction band minima may be created due to the interaction of Rb-3d and Cl-3p or Sr-3d and Cl-3p orbitals. As can be seen in the entire DOS plot, the minimum value of the conduction band displays an overall shift to the lower energy with progressively decreasing height as pressure increases.

### 3.3. Optical properties

The complex dielectric function, \( \varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \), which is connected to the interaction of photons with electrons, is used to quantify the linear response to an external electromagnetic field with a tiny wave vector [38]. The complex dielectric function must be used to determine the quantity of electromagnetic radiation response in a sample [39]. The momentum matrix components between the occupied and unoccupied wave functions might be used to generate the imaginary portion \( \varepsilon_2(\omega) \) of the dielectric function, which is given by [40]

\[
\varepsilon_2(\omega) = \frac{4\pi^2e^2}{m^2\omega^2} \sum \langle j|M|i\rangle^2 f_j(1 - f_i) \times \delta [E_j - E_i - \omega] d^3k. \tag{1}
\]
Using the Kramer–Kronig relations, the real portion $\varepsilon_1$ may be calculated from and is given by [41]

$$
\varepsilon_1(\omega) = 1 + \frac{2}{\pi} \int_0^\infty \frac{\omega' \varepsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega'.
$$

(2)
In the above equation \( P \) represents the integral’s principal value. All other optical characteristics may be computed simply from \( \varepsilon_1 \) and \( \varepsilon_2 \), including the absorption coefficient \( \alpha(\omega) \), the refractive index \( n(\omega) \), the extinction coefficient \( k(\omega) \), and the energy-loss factor \( [38, 41] \).

The imaginary component \( \varepsilon_2 \) of the dielectric function is related to electron excitation and the real part \( \varepsilon_1 \) contains information about the compound’s electronic polarization. The static peak of the dielectric function is a valuable measure for determining the charge carrier recombination rate and hence the overall potency of optoelectronic devices [42]. Materials with a higher dielectric constant have a lower charge carrier recombination rate, which implies they are more efficient in optoelectronic devices. Figures 5(a) and (b) show the imaginary and real parts of the dielectric constant of the pressure-induced RbSrCl\(_3\) at light energies up to 14 eV individually. It is observed that first peak of imaginary and real part of dielectric constant at 0 GPa is located at energy 7.28 eV and 6.52 eV respectively. As pressure is increased from 0 to 150 GPa, peaks are shifted towards higher energy values. A increase in the peak height is also observed with the increase of pressure for both \( \varepsilon_1 \) and \( \varepsilon_2 \). The material band structure is intimately related with the imaginary component of the dielectric function, which explains its absorption nature [39]. So maximum absorption occurs in ultraviolet region as seen from imaginary part of dielectric constant. After 9.3 eV, the real part of the dielectric function becomes negative, which indicates that in response to the high energy photon the behavior of the material is metallic.

The absorption coefficient is a measure of a material’s capacity to absorb light. Figure 5(c) shows the frequency dependent absorption coefficient for RbSrCl\(_3\) at various pressures. For 0, 30, 60, 90, 120 and 150 GPa, the largest absorption coefficient peaks are at 9.8, 10, 10.4, 11.4 and 11.8 eV, respectively. The absorption peaks at different pressures are in the UV region. Highest absorption peak transformed to higher energy in the UV range.

The variation of refractive index \( n(\omega) \) under various pressures is shown in figure 5(d). The fluctuations in refractive index \( n(\omega) \) and the real part of the dielectric function \( \varepsilon_1 \) are linked by the relationship \( n^2 - k^2 = \varepsilon_1 \), where \( k(\omega) \) is the extinction coefficient [43]. The interaction of photons with electrons slows them down when they penetrate a substance, therefore the refractive index is larger than one. The greater the refractive index of a substance, the more photons are retarded while passing through it. With the applied pressure the values of static refractive index \( n(0) \) increases as the pressure increases. Estimated values of \( n(0) \) are 1.49, 1.68, 1.77, 1.84, 1.90 and 1.96 for RbSrCl\(_3\), perovskite when the induced pressure is 0, 30, 60, 90, 120, and 150 GPa respectively. At different pressures initially the value of refractive index increases linearly in the energy range of 0–6 eV. In the energy range of 6–7.5 eV, a sharp peak is observed of refractive index \( n(\omega) \) and energy above 7.5 eV, refractive index is decreased at various pressures. Figure 5(e) shows the reflectivity spectra of RbSrCl\(_3\) under various pressures. The reflectivity increases gradually with the increase of photon energy up to 7 eV. Beyond that reflectivity increases rapidly for all induced pressure except for 0 GPa. Figure 5(f) shows graphs of optical conductivity \( \sigma(\omega) \) for RbSrCl\(_3\) perovskite materials under different induced pressure. It can be seen that the optical conductivity phenomena is not started 0 eV photon energy confirming the semiconducting nature of RbSrCl\(_3\). Optical conductivity at zero pressure starts with higher photon energy and as the induced pressure is increased the starting point moves toward the lower photon energies. Overall optical conductivity increase with the increase of induced pressure. The extinction coefficient for cubic halide perovskite RbSrCl\(_3\) under enhanced pressures are shown in figure 5(g). Overall the extinction coefficient is increased with increasing pressures.
4. Conclusions

In this paper, we reported our investigation on the variation of band structures of RbSrCl₃ lead-free metal halide perovskite material under different induced pressures up to 150 GPa. The wide indirect band gap value is transformed to visible range direct band gap with increasing pressures. At 150 GPa induced pressure the band gap value of RbSrCl₃ is decreased at 2.09 eV which is efficient to use in optoelectronic devices. We have also

Figure 5. Optical properties of RbSrCl₃ under different pressures at 0–150 GPa, (a) imaginary and (b) real part of the dielectric constant, (c) absorption coefficient, (d) refractive index, (e) optical reflectivity, (f) optical conductivity, (g) extinction coefficient.
investigated pressure induced structural and optical properties of RbSrCl₃. The optical absorption and conductivity of cubic perovskite RbSrCl₃ significantly increases with the increase of pressure.

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Data availability statement

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

Declaration of competing interest

There is no conflict of interest to declare.

ORCID iDs

Md. Borhanul Asif (https://orcid.org/0000-0001-7775-1644)
Sahadat Jaman (https://orcid.org/0000-0003-3737-0139)
Mohammad Abdur Rashid (https://orcid.org/0000-0001-9101-0869)

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