Electronic structure transition of cubic CsSnCl3 under pressure: effect of rPBE and PBEsol functionals and GW method

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1. Introduction

In the cutting-edge world, the synthesis of air and moisture-stable compounds are playing a significant role in the fabrication of high-performance devices. Importantly, a diversity of compounds and alloys is accessible, but the stability and physical properties impose restrictions on their use in technological devices. To resolve the problem, however, researchers are searching for air and moisture stable materials with useful properties in the required surrounding conditions. Some perovskites are air and moisture stable with useful physical properties for solar cell applications [1, 2]. Besides, these compounds show insulator, conductor, semiconductor, and superconductor properties as well [1, 2]. They have noteworthy physical properties including optical, charge ordering, magnetic, useful spin-dependent electronic transport, good thermoelectric performance, high magnetoresistance, and ferroelectric properties [3, 4, 5, 6, 7]. Recently, the physical properties of metal halide perovskite (AMX3, where A, M, and X represent a cation, metal (ion), and halogen (anion)) respectively materials have been investigated extensively as it has possessed several salient optoelectronic properties such as tunable optical bandgap, absorption spectrum in a wide range, narrow emission width, large numbers of mobile carriers with light effective mass, and high absorption and charge diffusion [8, 9]. Most importantly, it is abundant with low-cost precursor solutions on everywhere place in the world. To date, ABX3 has been applied to different electronic devices including light-emitting diodes (LEDs), photovoltaics (PVs), and fuel cells [8].

The application of hydrostatic pressure or strain engineering has arisen as an effective means of tuning the physical properties of ABX3 materials such as structural phases and electronic band structure, which provides a better understanding of the change in the rigid bonding [10, 11, 12]. In the conduction band maximum (CBM) of ABX3 perovskites, the X-p and B-p orbitals have dominant contributions, while valence band maximum (VBM) contributions come from X-p, B-s, and B-p orbitals [13]. On the other hand, the cation ‘A’ does not have a significant effect on the bandgap, but it mediates the metal halide interactions [14]. Besides, the bandgap is associated with the lattice parameters of the ABX3 perovskite structure which signifies the significance of octahedral tilting upon the optical properties of ABX3 perovskites [15]. As a result, the optimized band gaps of ABX3 perovskites are obtained, rises charge carrier life-times, diminishes trap state densities, and tunes carrier
conductivities. So, it is increasingly being used in p-n junctions, photovoltaic, and electronic devices [16].

Recently, the effects of hydrostatic pressure on the physical properties of metal halide ABX₃ perovskites were studied meticulously, for example, CsGeBr₃ and CsGeI₃ [17, 18, 19]. CsGeCl₃ has been also examined but not precisely. Internal and external pressure in cubic ABX₃ perovskite have been examined using HSE + SOC function by Metin et al. and reported that there is no phase transition, and the bandgap shrinkage with increasing internal pressure while bandgap increases by external pressure [13]. Conversely, Jakiul et al. reported that they have found semi-conductor to metallic transition at 20 GPa using GGA + PBE function, and an identical scissor value (1.857 eV) is taken from the experimental value for each pressure, which is completely wrong [19]. Besides, Ying et al. reported that the optical band gap reveals red-shifts and blue shifts with 3D topological non-trivial phase and band inversion by tuning the hydrostatic pressure [20]. But they did not much explain the bond length. Thus, there is still needed a convincible investigation of CsSnCl₃ materials under pressure and to find out the correlation between bond length and phase transition.

Therefore, the aim of our present study further investigates the physical properties of CsSnCl₃ materials accurately and detects association with the bond length and phase transition through GGA + PBEsol, GGA + rPBE functionals, and GW method. For the first time, we have calculated the electronic structure, absorption coefficient of CsSnCl₃ under different pressures by using the GW method.

2. Computational methods

The structural relaxations were performed by using density functional theory (DFT) within the plane-wave pseudopotential technique implemented in CASTEP (Cambridge Serial Total Energy Package) code [21, 22] by minimizing energy and interatomic forces simultaneously. For this, we initially used the experimental lattice parameters and atomic coordinates. We set strict convergence criteria, energy 10⁻⁶ eV and force 10⁻³ eV/Au. We treated the exchange-correlation energy term by using the generalized gradient approximation (GGA) with Perdew-Berke-Ernzerhof for solids (PBEsol) and revised Perdew-Berke-Ernzerhof (rPBE) settings. We used Vanderbilt ultrasoft pseudopotentials [23] and the BFGS (Broyden–Fletcher–Goldfarb–Shanno) technique [24] with the cutoff energy 550 eV with 12 × 12 × 12 Monkhorst–Pack [25] after extensive trials. The calculations of elastic constants were accomplished by using finite-strain theory [26] as implemented in CASTEP. For GW calculations, we used the plane-wave pseudopotential (PW) method, like that of CASTEP, in Quantum Espresso (QE) code [27]. We set the same convergence criteria as mentioned above and used Optimized norm-conserving Vanderbilt pseudopotentials [28, 29] and 2 × 2 × 2 k-point, as the calculations are very expensive. For the self-consistent calculations, we used PBEsol functional by using the above settings and calculated self-consistent potentials. By using this potential, we calculated Quasi-Particle energy implemented in BerkeleyGW code [30]. Then, the G0W₀ electronic structure calculations were performed by using the above outputs. In all calculations, we did not consider spin-orbit interactions, as these calculations with spin-orbit interactions are much expensive.

3. Results and discussion

The ground state cubic structure of CsSnCl₃ is depicted in Figure 1. The Cesium tin chlorides (CsSnCl₃) have an ideal cubic structure having space group Pm₃m (no. 221) [31]. Where, Cs atoms lie at the corner of the unit cell with 1a (0, 0, 0) Wyckoff position, Sn atom occupies the body-centered 1b (1/2, 1/2, 1/2), Wyckoff position, and Cl atom at the face-centered (0, 1/2, 1/2) Wyckoff positions [31].

Figure 1. A ground-state crystal structure of CsSnCl₃ compound.

The different functionals treat the exchange-correlation term differently and the calculated lattice parameters vary slightly depending on the type of function. That’s why the geometric optimization of the CsSnCl₃ structure has been performed by using different functionals, namely PBEsol and rPBE. The PBEsol and rPBE functionals give the lattice parameters, of CsSnCl₃, 5.51, and 5.75 Å, respectively, while the experimental value is 5.56 Å. Like PBE functional, rPBE also overestimates the experimental value, while as usual, the PBEsol underestimates the experimental lattice parameters slightly.

It, however, can be seen (also Figure 2) that the effects of hydrostatic pressures have great influences on the lattice parameters, volumes, and bond lengths (Cs–Cl, and Cl–Sn) in both PBEsol and rPBE method as demonstrated in Figure 2, which did not manifest by Zakiul et al [19]. The hydrostatic pressure gradually declines the lattice parameters by reducing the interatomic distance. Interestingly, both functionals calculate a longer bond length of Cs–Cl than Cl–Sn. These three types of bond lengths are deteriorated moderately by employing hydrostatic pressure due to the production of compressive strain within the CsSnCl₃ lattice network. This suggests that the change in bond lengths would profoundly inspire the electronic structures of the CsSnCl₃ compound. The detailed changes of these bond lengths are shown in Figure 2 (c, d).

3.1. Electronic properties

The accuracy of the calculation of electronic bandgap strongly depends on the type of functionals. Generally, GGA with different settings underestimates the experimental bandgap. To demonstrate this, we have calculated the electronic structure of CsSnCl₃ by using PBEsol and rPBE functionals. The computed band structures, by using PBEsol and rPBE, of CsSnCl₃ at ambient conditions and different pressures are shown in Figures 3 and 4, respectively.

The gross features of the electronic dispersions of CsSnCl₃ are almost the same for both functionals. The PBEsol functional is less effective to compensate for self-interaction energy. Thus, shifted the minima of the conduction band downward and underestimates the bandgap severely. On the other hand, the rPBE functional improves the bandgap but it still underestimates the experimental bandgap largely. At ambient conditions, the computed bandgap of CsSnCl₃ is 0.55 and 1.4 eV by using PBEsol and rPBE functional, while the experimentally measured bandgap is 2.9 eV [32].

The pressure excites the valence electrons upward. It pushes the conduction band minima downward and Fermi levels upward. Thus, the bandgap is reduced with the pressure linearly. The gap is disappeared above 4 GPa and 8 GPa for PBEsol and rPBE functional, respectively. However, the bandgap can be correlated with the change of bond length while applying various hydrostatic pressures (see Figure 2 c, d). The CsSnCl₃ shows a metallic band structure when the bond length reaches a certain limit. In PBEsol functional, the CsSnCl₃ shows a metallic band structure when the bond lengths of Cs–Cl and Cl–Sn are at or below 3.74
and 2.64 Å, respectively. Likewise, in rPBE functional, CsSnCl₃ also develops a metallic band structure when Cs–Cl and Cl–Sn bond lengths reach the same limit (see Figure 2d). This information may be useful for experimentalists to perform the Rietveld refinement analysis. The fact demonstrates how these functionals treat self-interaction energy and PBEsol is less effective than rPBE to compensate for self-interaction energy.

The electronic phase transition nature of the CsSnCl₃ perovskite under pressure can be further understood from the total electronic density of states (DOS) as shown in Figure 5 (a, b). The compound possesses an intrinsically high absorption coefficient of CsSnCl₃ and presented it graphically in Figure 7 (b). When the GW bandgap correction is applied to the experimentally measured values of the bandgap of CsSnCl₃ under pressure are not available, to date. Thus, we have calculated the absorption coefficient by using the GW method. However, the experimentally measured values of the bandgap of CsSnCl₃ under pressure may contain large uncertainties. Therefore, we need to calculate the absorption coefficient by using the GW method. The absorption coefficient is extremely vital to achieving deep information concerning the compatibility of materials for better performance device applications. For this reason, we have calculated the absorption coefficient of CsSnCl₃ and presented it graphically in Figure 7 (a, b). The compound possesses an intrinsically high absorption coefficient and pressure can only improve it slightly but shifts the peak to lower photon energy. As both functionals underestimate the values of the experimental bandgap severely, the calculated absorption coefficient might contain large uncertainties. Therefore, we need to calculate the absorption coefficient by using the GW method. However, the experimentally measured values of the bandgap of CsSnCl₃ under pressure are not available, to date. Thus, we have calculated the absorption coefficient by using the GW method. The absorption coefficient is extremely vital to achieving deep information concerning the compatibility of materials for better performance device applications. For this reason, we have calculated the absorption coefficient of CsSnCl₃ and presented it graphically in Figure 7 (a, b). The compound possesses an intrinsically high absorption coefficient and pressure can only improve it slightly but shifts the peak to lower photon energy. As both functionals underestimate the values of the experimental bandgap severely, the calculated absorption coefficient might contain large uncertainties. Therefore, we need to calculate the absorption coefficient by using the GW method. However, the experimentally measured values of the bandgap of CsSnCl₃ under pressure are not available, to date. Thus, we have calculated the absorption coefficient by using the GW method.
absorption coefficient, the absorption changes significantly, and the peak shifts to the higher photon energy. The absorption of photons with energy ~6 eV is significant for the GW method. However, the value of the absorption coefficient does not rise significantly. This fact demonstrates the importance of accurate electronic structure calculations to describe the optical properties of material accurately.

3.3. Mechanical properties

Material suitability to external force is determined by elastic constant, enormously significant in potential implementation. So, we have explored the elastic stability of the perovskite compound CsSnCl3 by pivotal parameter, elastic constants. Generalized Hook’s law is used for determining the elastic constants of CsSnCl3 [36]. According to Born–Huang’s mechanical stability criterion, the strain energy should be positive. This stability criteria for the cubic system can be expressed as

\[ C_{11} > 0, \quad C_{44} > 0, \quad C_{11} + 2C_{12} > 0 \quad \text{and} \quad C_{11} - C_{12} > 0 \]

Our calculated elastic constants by using PBEsol functional at different pressures are listed in Table 1. The computed values satisfy the stability criteria and hence, the compound is stable up to 30 GPa by using PBEsol functional within our computational accuracy. The mechanical instability appeared at 40 GPa with the PBEsol functional. The elastic constants \( C_{11}, C_{12}, \) and \( C_{44} \) are related to elasticity in length and shape, indicating how much it has deformed by applying various hydrostatic pressure. The \( C_{12} \) rises with pressure while \( C_{44} \) lowers with pressure. The Cauchy pressure also rises, suggesting that the ductility of the compound is improved by the applied pressure as listed in Table 1. The mechanical parameters such as a bulk modulus, \( B \), shear modulus, \( G \), Pugh’s ratio, \( B/G \) ratio, and Poisson, \( \nu \), are assessed based on prominent expressions as indicated in literature [38, 39] and listed in Tables 1, 2.

As the interatomic distance is reduced with pressure, the value bulk and shear moduli are increased with it. This indicates that the mechanical resistance of the CsSnCl3 is substantially improved under high pressure. In our exploration, the soft to hard transition occurred when the CsSnCl3 material was subjected to different hydrostatic pressures. On the other hand, Pugh’s ratio is another pivotal parameter for determining whether the CsSnCl3 perovskite material is ductile or brittle. The critical value considers as 1.75 [40], and if the value \( B/G \) exceeds the critical value, then the compound will be ductile, otherwise brittle [41]. From Tables 1, 2 we see that the perovskite compound of CsSnCl3 has no brittle nature. The pressure, therefore, has enhanced the ductile behavior of CsSnCl3.

Another important parameter in deciding the brittle and ductile condition of CsSnCl3 is the Poisson’s ratio \( \nu \), which has a critical value of 0.26, over which the material becomes ductile [41]. The computed value of \( \nu \) of CsSnCl3 at ambient conditions is 0.278 as listed in Table 1, which suggests the ductile nature of the CsSnCl3. The pressure reduces the interatomic distance and increases the value of Poisson’s ratio. As a consequence, the ductility of the perovskite compound CsSnCl3 increases.

Figure 3. The computed band structure, by PBEsol functional, of CsSnCl3 under different pressures: (a) 0 GPa, (b) 2 GPa, (c) 4 GPa, (d) 6 GPa, (e) 8 GPa, (f) 10 GPa, (g) 20 GPa, (h) 30 GPa, and (i) 40. The dashed line at the zero-energy represents the Fermi level.
with hydrostatic pressure. Generally, the mechanical hardness of a compound is directly related to Poisson’s ratio [42], so it is expected that the hardness might also be increased with the pressure. The computed elastic constants and elastic moduli by using rPBE functional are listed in Table 2. The C_{11} and C_{44} strongly depend on the functional type, while C_{22} shows almost independent of functional. Interestingly, the compound is mechanically stable up to 40 GPa for rPBE functional, as the functional overestimates the experimental lattice parameters by 3.4%. 

![Graph](image-url)
4. Conclusions

In summary, we have studied the structural, electronic, absorption coefficient, and mechanical properties of cubic CsSnCl$_3$ compound at different pressures by using the first-principles method based on the density functional theory (DFT). We used PBEsol, rPBE functionals, and the accurate GW method and found that the PBEsol gives the lattice parameters close to the experimental value compared to that of rPBE.

Figure 6. The computed band structure, by GW method, of CsSnCl$_3$ under pressure: (a) 0 GPa, (b) 20 GPa, (c) 30 GPa, and (d) 40 GPa. The dashed line at the zero-energy represents the Fermi level.

Figure 7. Calculated optical absorption of perovskite CsSnCl$_3$ as a (a) PBEsol and (b) rPBE functionals and with GW bandgap correction.

| Pressure (GPa) | C$_{11}$ (GPa) | C$_{12}$ (GPa) | C$_{44}$ (GPa) | C$_{12}$–C$_{44}$ (GPa) | B (GPa) | G (GPa) | B/G | $\nu$ |
|---------------|----------------|---------------|----------------|------------------------|--------|--------|-----|------|
| 0             | 58.98          | 9.18          | 5.59           | 3.59                   | 25.78  | 13.21  | 1.94 | 0.28 |
| 2             | 77.94          | 12.31         | 5.40           | 6.91                   | 34.19  | 16.37  | 2.09 | 0.29 |
| 4             | 95.65          | 15.61         | 5.16           | 10.45                  | 42.29  | 19.10  | 2.21 | 0.30 |
| 6             | 112.71         | 19.15         | 4.88           | 14.27                  | 50.34  | 21.64  | 2.33 | 0.31 |
| 8             | 128.34         | 22.58         | 4.58           | 18.00                  | 57.83  | 23.9   | 2.42 | 0.32 |
| 10            | 143.58         | 26.03         | 4.24           | 21.79                  | 65.21  | 26.05  | 2.50 | 0.32 |
| 20            | 213.83         | 44.96         | 2.38           | 42.58                  | 101.25 | 35.20  | 2.88 | 0.34 |
| 30            | 275.41         | 63.99         | 0.19           | 63.8                   | 134.46 | 42.40  | 3.17 | 0.36 |
| 40            | 334.83         | 86.69         | -2.2           | 88.9                   | 169.40 | 48.30  | 3.51 | 0.37 |

Table 1. Computed values of elastic constants C$_{ij}$ (GPa), Cauchy pressure C$_{12}$–C$_{44}$ (GPa), bulk modulus B (GPa), shear modulus G (GPa), and Poisson ration $\nu$, of the cubic perovskite CsSnCl$_3$ under variant pressures by using PBEsol functional.
functional. However, the underestimation of the bandgap is more severe in the case of PBEsol functional than rPBE. The GW method gives the most accurate bandgap of 2.91 eV at ambient conditions, which is in excellent agreement with the experimentally measured bandgap of 2.9 eV. Our calculations reveal that the predictions of semiconducting to metallic transitions strongly depend on the exchange-correlation term used in the calculations and the GW method can predict the most accurate bandgap of 2.91 eV at ambient conditions, which is in excellent agreement with the experimentally measured bandgap of 2.9 eV.

Table 2. Calculated values of $C_{ij}$ (GPa), Cauchy pressure $C_{12-C_{44}}$ (GPa), bulk modulus B (GPa), shear modulus G (GPa), and Poisson ratio $\nu$ of cubic CsSnCl$_3$ perovskite under variant pressures by using rPBE functional.

| Pressure (GPa) | $C_{11}$ | $C_{12}$ | $C_{44}$ | $C_{12-C_{44}}$ | B (GPa) | G (GPa) | B/G | $\nu$ |
|---------------|----------|----------|----------|-----------------|--------|--------|-----|------|
| 0             | 39.47    | 9.04     | 6.51     | 2.53            | 19.19  | 10.00  | 1.92 | 0.278 |
| 2             | 58.15    | 12.48    | 6.58     | 5.90            | 27.70  | 13.08  | 2.12 | 0.296 |
| 4             | 74.15    | 15.57    | 6.53     | 9.04            | 35.10  | 15.63  | 2.25 | 0.306 |
| 6             | 90.37    | 18.77    | 6.42     | 12.35           | 42.64  | 18.17  | 2.35 | 0.313 |
| 8             | 105.95   | 21.75    | 6.25     | 15.50           | 49.82  | 20.59  | 2.42 | 0.318 |
| 10            | 121.68   | 24.84    | 6.05     | 18.79           | 57.12  | 23.00  | 2.48 | 0.322 |
| 20            | 188.98   | 41.14    | 4.68     | 36.46           | 90.42  | 32.38  | 2.79 | 0.340 |
| 30            | 250.21   | 58.71    | 2.93     | 55.78           | 122.54 | 40.06  | 3.06 | 0.352 |
| 40            | 306.15   | 76.64    | 0.88     | 75.76           | 153.14 | 46.43  | 3.30 | 0.362 |

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