Strain Induced Topological Insulator Phase in CsPbBr$_3x$I$_{3-x}$ ($x = 0, 1, 2, and 3$) Perovskite: A Theoretical Study

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Abstract: First-principles density functional theory was used to determine the surface band structures of CsPbBr$_3x$I$_{3-x}$ ($x = 0, 1, 2, and 3$) perovskites. The equilibrium lattice constants of CsPbBr$_3x$I$_{3-x}$ were obtained from the minimum of the total energy as a function of the iodine concentration. We discovered that the band gaps of CsPbBr$_3x$I$_{3-x}$ decreased monotonically under pressure. The phase change from a normal insulator to a topological insulator was found at approximately 2–4 GPa. The Pb$p$- and Br$s$-orbitals inverted at the R symmetric point with and without spin–orbit coupling. Nontrivial $Z_2$ topological numbers were obtained, and the surface conduction bands were demonstrated theoretically using a $1 \times 1 \times 10$ supercell. We ascertained that CsPbBr$_3x$I$_{3-x}$ has the largest electric polarization 0.025 C/m$^2$ under a compression strain of 10%. We also observed that in the normal insulator phase, the band gap increases with a small displacement of the central Pb atom in the $z$-direction, but in the topological insulator phase, the band gap decreases with the movement of the Pb atom in the $z$-direction. Additionally, in the supercell structure, CsPbBr$_3x$I$_{3-x}$ is a ferroelectric topological insulator because the Pb atom leaves its own equilibrium position.

Keywords: CsPbBr$_3x$; CsPbI$_3$; topological insulator; band structures; first-principles calculations

1. Introduction

Topological insulators (TIs) have an insulating gap in the bulk and gapless surface states at the same time, and these insulators have been extensively studied in past decades [1,2] due to their potential applications in spintronic devices [3,4]. Therefore, TIs have attracted much attention in both the fundamental physics and experimental research fields. Studies on BiSe$_2$ [5], half-Heusler alloys such as LnPtBi$_3$ [6,7], and binary compounds such as HgTe [8,9] have demonstrated that those materials are normal insulators, but they may also be transformed into TIs by applying spin-orbit coupling (SOC), axial or uniaxial strain, and impurities. Topologically trivial to nontrivial transitions of TIs are identified by observing the band inversion in the Brillouin zone. Fu and Kane [10] introduced a useful and practical Chern number or topological number $Z_2$, which is calculated by analyzing the bulk band structure and provides a physical meaning in the prediction of edge states at interfaces.

Perovskite crystals are of interest in the fields of high thermoelectric power, ferroelectricity, superconductivity, spin electronic devices, and colossal magnetoresistance [11–13]. Studies on perovskites have been aimed at, for example, energy-saving and cost efficiency as well as the manufacture of stable solar cells [14]. For example, the cesium lead halide perovskite (CsPbX$_3$; X = Cl, Br, and I) has received considerable attention for its potential...
application in high-performance solar cells [15,16] and light-emitting diodes [17,18]. Furthermore, organic lead halide (CH$_3$NH$_3$PbX$_3$) nanocrystals and bulk crystals are promising high-efficiency solar cells with power conversion efficiencies exceeding 20% [19]. The TI phase in perovskites and double perovskites has been studied theoretically [20–22]. The coexistence of the TI phase and other phases, such as those of superconductivity, magnetism, and ferroelectricity, are of particular interest. Liu et al. [23] reported that cesium lead halide perovskite (CsPbI$_3$) has a TI phase under strain together with a ferroelectric phase.

Previous theoretical studies on CsPbX$_3$ (X = Cl, Br, and I) have focused on its electronic [23–26] and optical [24,25] properties. For example, Afsari et al. [25] reported that CsPbI$_3$ becomes a TI under very high pressure [23,26]. However, the reported band gap for the CsPbI$_3$ in the fully relativistic scheme is significantly underestimated. The calculated band gap of CsPbI$_3$ is 1.48 eV without SOC in the generalized gradient approximation (GGA) and becomes 0.29 eV when the SOC is considered, revealing that the SOC effect is strong in these cesium lead halide perovskites. Nonetheless, the optical band gap for CsPbI$_3$ has been reported to be 1.73 eV experimentally [27,28].

In this study, we investigated the TI phase of CsPbBr$_3$I$_{3-x}$ (x = 0, 1, 2, and 3) under hydrostatic strain. The paper is organized into the following sections: Section 2 describes the crystal structures and computational methods, initially addressing the structural and electronic properties with and without consideration of SOC. Section 3 depicts the bulk and surface band structures and describes the calculation of the electric polarization produced by Pb atom distortion. We confirm theoretically that the slight distortion will not disrupt the TI phase of cesium lead halide perovskite. In the final section, we draw conclusions.

2. Structures and Computational Methods

The perovskite ABX$_3$ is a cubic structure with a space group of Pm3m. The B-site cations correspond to six anions to form cuboctahedra, which are chemically inert ions arranged in a cuboctahedron. The B-site and Z-site refer to the atomic arrangement in the unit cell of cations and anions, respectively. The Wyckoff position for the A-site cation is located at the corner (0, 0, 0), that of the B-site cation is located at the center (1/2, 1/2, 1/2), and those of the Z-site anions are located at face-center (1/2, 1/2, 0), (1/2, 0, 1/2), and (0, 1/2, 1/2). Studies have reported that, under experimental conditions, lead halide perovskites have a simple cubic phase at high temperatures. In this study, the structural and electronic properties of CsPbBr$_3$I$_{3-x}$ (x = 0, 1, 2, and 3) perovskites were calculated using density functional theory as implemented in the Vienna ab initio simulation package (VASP) [29,30] along with the Perdew-Burke-Ernzerhof (PBE) GGA [31] for the exchange-correlation functional. The Γ-centered Monkhorst-Pack scheme with a k-mesh of 12 × 12 × 12 was used for the first Brillouin zone integration. The self-consistent total energy criterion was set to 1.0 × 10$^{-6}$ eV. The plane wave cutoff energy was set to 350 eV. The equilibrium lattice constant of the cubic perovskite structure was obtained from the minimum of the total energy as a function of the lattice constant. The SOC effect was considered after the equilibrium lattice constant was found. To identify the surface conduction band of CsPbBr$_3$I$_{3-x}$ perovskites, we prepared a supercell containing 10 formula units with a vacuum spacing of approximately 20 Å, which is wide enough to decouple the interlayer interaction. The surface atoms were fixed (i.e., with no further structural optimization possible) to correspond with the one in the bulk form. The atomic structure of CsPbI$_3$ (X = Br and I) bulk is shown in Figure 1a, and schematics of two initial surface structure models—specifically with one PbX$_2$- and CsX- and two PbX$_2$-terminated slabs as shown in Figure 1b,c, respectively—were constructed from known bulk geometries to help clarify which plane contributes to the surface conduction bands. The nonpolar supercells contained 10 formula units with a vacuum of 20 Å, which is large enough to help obtain the surface conduction bands.

We studied the electric polarization caused by the movement of the Pb atom in the z-direction. Displacement of Pb atom in the z-direction breaks the inverse space symmetric of the CsPbBr$_3$I$_{3-x}$, resulting in a finite electric polarization. In addition to using the band inversion, the so-called Chern number or topological number Z$_2$ can be used to prove the
characteristics of TIs. We calculated $Z_2$ by considering the parity of the wave function at specific $k$ points reported by Fu and Kane [10].

![Figure 1](image_url)

**Figure 1.** Schematic of the CsPbX$_3$ ($X =$ Br or I) crystal structure (a), one PbX$_2$- and CsX- (b) and two PbX$_2$- (c) terminated slabs. The atoms are represented by spheres: Cs (green, large), Pb (dark blue, medium), and X (purple, small).

### 3. Results and Discussion

The calculated equilibrium lattice constants, scalar relativistic band gap $E_{SP}^S$, and fully relativistic band gap $E_{SP}^{SOC}$ (eV) of the CsPbBr$_{3-x}$ perovskites are listed in Table 1.

For the CsPbBr$_3$, we obtained a relaxed lattice constant of $a = 5.99$ Å in the equilibrium structure, which was consistent with the theoretical value of 5.99 Å [24]. The calculated lattice constant for the CsPbI$_3$ was 6.39 Å, in excellent agreement with its theoretical values of 6.40 [25], 6.39 [24], and 6.05 Å [32]. The equilibrium lattice constants increased monotonically with iodine concentration. The Wigner–Seitz radii for the Cs, Pb, Br, and I atoms are 1.323, 1.725, 1.164, and 1.487 Å, respectively. Therefore, the calculated lattice constants of the CsPbBr$_{3-x}$ perovskites were increased due to the larger Wigner–Seitz radius of iodine. The fully relativistic band gap was significantly lower than the scalar relativistic band gap of the CsPbBr$_{3-x}$ perovskites due to the strong SOC effect. When SOC is considered, the band gaps of the CsPbBr$_{3-x}$ perovskites lead to a substantial underestimation of calculated band gaps. The calculated band gaps of the CsPbBr$_{3-x}$ perovskites induced by SOC were 0.67, 0.49, 0.39, and 0.33 eV for the CsPbBr$_3$, CsPbBr$_2$I, CsPbBrI$_2$, and CsPbI$_3$, respectively. This underestimation of the band gap can be corrected by applying, for example, the $G^0W^0$ or PBE0 approximations, but the tendency of the band gap to decrease under strain will remain unchanged. The reduction in the band gap caused by the SOC effect commonly appears in not only bulk TIs but also two-dimensional transition metal dichalcogenides (TMDCs) [33]. A useful and practical empirical formula of TMDCs in terms of the PBE band gap and $G^0W^0$ band gap was introduced by Garcia et al. [34] who introduced the form $E_{SP}^{G^0W^0} = 1.358 \times E_{SP}^{PBE} + 0.904$, where the $G^0W^0$ is an approximation with Hartree-Fock (HF) Green function G and the screened interaction W without further iterations. Here we adopt the $G^0W^0$ approximation because it is the most physically grounded method to accurately predict the energy band gap, as presented in Table 1 and Figure 2. To compare our calculated band gaps, we also employed the PBE0 hybrid functional which combines the PBE exchange energy and HF exchange energy in a set 3:1 ratio, along with the full PBE correlation energy, as also summarized in brackets in Table 1. The CsPbBr$_{3-x}$ perovskite obtained from the $G^0W^0$ empirical approach has the largest band gap. The PBE0 band gaps with SOC are between the PBE and $G^0W^0$ band gaps. For the experimental results of CsPbBr$_3$ and CsPbI$_3$ perovskites, the $G^0W^0$ band gaps
with SOC are underestimated by approximately 23% and 22%, respectively. Analysis of the fully relativistic band gaps suggests that more external pressure may be required to produce a normal TI phase transition under the empirical correction with a constant of 0.904 eV.

Table 1. Calculated equilibrium lattice constant $a$, scalar relativistic band gap $E_{S}^{SP}$, and fully relativistic band gap $E_{S}^{SOC}$ of the CsPbBr$_3$, CsPbBr$_2$I, CsPbBr$_2$, and CsPbI$_3$ perovskites.

| Lattice Constant (Å) | Band Gap (eV) | Theory | Experiment |
|----------------------|---------------|--------|------------|
|                      |               | G$_0$W$_0$ [34] (PBE0) |           |
|                      | $E_{S}^{SP}$  | $E_{S}^{SOC}$ | $E_{S}^{SP}$ | $E_{S}^{SOC}$ |
| CsPbBr$_3$           | 5.99, 5.99$^{24}$ | 1.76, 2.41$^{24}$ | 0.67, 1.32$^{24}$ | 3.29, (2.95) | 1.81, (1.74) | 2.36 $^{[35]}$ |
| CsPbBr$_2$I          | 6.14          | 1.52   | 0.49       | 2.97         | 1.57         |
| CsPbBr$_2$           | 6.27          | 1.40   | 0.39       | 2.81         | 1.43         |
| CsPbI$_3$            | 6.39, 6.39$^{24}$ | 1.47, 2.00$^{24}$ | 0.33, 0.86$^{24}$ | 2.90, (1.47) | 1.35, (1.18) | 1.73 $^{[36]}$ |

Figure 2. Top and bottom panels illustrating external stress ($a/a_{theo}$) and calculated band gaps ($G_0W_0$), respectively, for CsPbBr$_3$, CsPbBr$_2$I, CsPbBr$_2$, and CsPbI$_3$ perovskites as a function of the lattice constant and its equilibrium lattice constant, $a/a_{theo}$, as a percentage.

3.1. Band Structures

To estimate the strain effect on the trivial topology feature, we illustrate in Figure 2 the stress-ratio $a/a_{theo}$ and band gap-ratio $a/a_{theo}$ relationships for hydrostatically strained...
CsPbBr\textsubscript{x}I\textsubscript{3-x} over the wide $a/a_{\text{theo}}$ range from −10% to 6%. At the hydrostatically compressed strain value of about 4% to 5%, our calculations indicate that the band gaps of CsPbBr\textsubscript{x}I\textsubscript{3-x} become zero, indicating that the CsPbBr\textsubscript{x}I\textsubscript{3-x} perovskites become TIs. In addition, the phase transition from normal insulators to TIs occurs at approximately 2–4 GPa. The critical external pressure of the CsPbBr\textsubscript{x}I\textsubscript{3-x} phase transition from the normal insulators to TIs decreases monotonically with iodine concentration. On the other hand, the TI regime of the CsPbBr\textsubscript{x}I\textsubscript{3-x} perovskite occurs at $a/a_{\text{theo}}$ from −3% to −5%. To observe how external pressure and SOC affect the band structure, the band structures of CsPbI\textsubscript{3} under different lattice constants and with and without SOC are represented in Figure 3. We discovered that the calculated band gaps of CsPbI\textsubscript{3} were direct without SOC and decreased monotonically as external pressure increased, as shown in Figure 3a–c. When SOC was considered, the calculated band gap of CsPbI\textsubscript{3} at the equilibrium lattice constant was only a quarter of the corresponding one without SOC, as illustrated in Figure 3a,d. Figure 3e indicates that the calculated band gap of CsPbI\textsubscript{3} is reduced to zero under an $a/a_{\text{theo}}$ ratio of −3.5%. To further clarify the TI behavior described in Figure 3f, we determined how the calculated band gap of CsPbI\textsubscript{3} increases under an $a/a_{\text{theo}}$ ratio of −8%, demonstrating that the Dirac corn appears at the high symmetric R point. The so-called band inversion also occurred at the point R where the Pb\textsubscript{p}- and I\textsubscript{s}- orbitals are inverted due to SOC. This energy band reversal illustrates a theory of material topology. We also noted that as stress increased, the energy of the highest occupied band at point M also increased.

![Figure 3](image.png)

**Figure 3.** CsPbI\textsubscript{3} band structures corresponding to (a) the equilibrium lattice constant, (b) the $a/a_{\text{theo}}$ ratio of −3.5% with spin–orbit coupling (SOC) and (c) the $a/a_{\text{theo}}$ ratio of −8% without SOC; (d) the equilibrium lattice constant, (e) the $a/a_{\text{theo}}$ ratio of −3.5% with SOC and (f) the $a/a_{\text{theo}}$ ratio of −8% without SOC, respectively. The dashed line is the Fermi level. The green line represents Pb\textsubscript{p}- and I\textsubscript{s}-orbitals. The red line depicts Pb\textsubscript{s}- and I\textsubscript{p}-orbitals.
A detailed comparison of the calculated band gaps of CsPbBrI2 perovskites, which are virtually identical to doping iodine atoms in CsPbBr3, is also warranted. The band structures of CsPbBrI2 perovskites under different lattice constants with and without SOC are shown in Figure 4. The calculated band gaps of CsPbBrI2 were also similar in behavior to those of CsPbI3, which show that the calculated band gaps of CsPbBrI2 are direct without SOC and decrease monotonically as external pressure increases, as illustrated in Figure 4a-c. Figure 4c clearly indicates that Pb-p- and Brs-orbitals are degenerate or close together in energy (0.2 eV), whereas Pb-p- and Is-orbitals are degenerate in energy, which was 0.6 eV above the Fermi level under the \( \frac{a}{a_{\text{theo}}} \) ratio of \(-8\% \) at the R point. When SOC was considered, the calculated band gap of CsPbBrI2 at the equilibrium lattice constant was approximately one-third of the corresponding one without SOC, as shown in Figure 4a,d. Figure 4e shows the calculated band gap of CsPbBrI2 approaching zero under the \( \frac{a}{a_{\text{theo}}} \) ratio of \(-3.8\% \). When SOC was considered, band reversal still occurred at the R point, as shown in Figure 4f. Notably, the energy of the highest occupied band at the M point became higher than the energy band at the R point at the \( \frac{a}{a_{\text{theo}}} \) ratio of \(-8\% \), showing that the transition may not be useful for optical applications.

![Figure 4. CsPbBrI2 band structures corresponding to (a) equilibrium lattice constant, as well as (b) the ratio \( \frac{a}{a_{\text{theo}}} \) of \(-3.8\% \) with and (c) \(-8\% \) without the spin–orbit coupling; (d) equilibrium lattice constant, (e) the ratio \( \frac{a}{a_{\text{theo}}} \) of \(-3.8\% \) with and (f) \(-8\% \) without the spin–orbit coupling. The dashed line is the Fermi level.](image-url)

A useful and practical topological number of \( Z_2 \) in terms of the Green function and corresponding to the charge density derived from VASP and the Wannier90 package [37] was used to determine the characteristics of TIs. As shown in Figure 5, the Wannier
functions of the CsPbI₃ perovskite were applied in the range of −6 to 3 eV, which closely matched the band structure of the CsPbI₃ perovskite derived from VASP. Here, we followed the work by Fu et al. [10] and calculated the Z₂ invariants from six time-reversal invariant planes in the Brillouin zone [38], which have four independent Z₂ indices, to obtain the four indices (v₀; v₁, v₂, v₃). Note that v₀ is called the strong insulator index and v₁, v₂, and v₃ are called weak TI indices. In addition, Z₂ = 1 and Z₂ = 0 correspond to topological and trivial insulators, respectively. Our calculations indicated that all indices of CsPbBrₓI₃−ₓ (x = 0, 1, 2, and 3) with hydrostatic strain were (1,0,0,0), demonstrating that CsPbBrₓI₃−ₓ are strong TIs.

Figure 5. CsPbI₃ band structures derived from VASP (dashed blue line) and Wannier function (red line).

3.2. Electric Polarization

The preference for inversion symmetry with respect to CsPbBrₓI₃−ₓ causes band structure changes. To clarify this, we applied a small displacement of the central Pb atom in the z-direction in CsPbBrₓI₃−ₓ to break the inversion symmetry. Figure 6 shows the calculated band gap and electric polarization as a function of the Pb displacement in the z-direction of the CsPbBrₓI₃−ₓ cell, indicating that the all band gaps of CsPbBrₓI₃−ₓ at the equilibrium lattice constants increased markedly with the Pb displacement in the z-direction as shown in Figure 6a–d. Notably, the band gaps of CsPbBrₓI₃−ₓ at the equilibrium lattice constants decreased with the iodine concentration, showing that the movement of Pb around the iodine atoms significantly narrows the energy band gap, as shown in Figure 6a–d. The largest electric polarizations Pₑₑₑ of CsPbBr₃, CsPbBr₂I, CsPbBrI₂, and CsPbI₃ at the equilibrium lattice constants were 0.003, 0.02, 0.015, and 0.013 C/m², respectively. The electric polarizations Pₑₑₑ increased monotonically with the Pb displacement in CsPbBr₂I, CsPbBrI₂, and CsPbI₃ at the equilibrium lattice constants, but the CsPbBr₃ was close to the highest Pₑₑₑ on the Pb displacement of 0.0275 Å in the z-direction. The aforementioned data indicate that the behavior of TIs is intimately related to their respective electronic band structures and can be enhanced by increasing the iodine concentration or the Pb displacement of CsPbBrₓI₃−ₓ. By contrast, all band gaps of CsPbBrₓI₃−ₓ compressed by 10% relative to their equilibrium bulk lattice parameters; the lattice constants used for
CsPbBr₃, CsPbBr₂I, CsPbBrI₂, and CsPbI₃ were 5.39, 5.53, 5.64, and 5.75 Å, respectively, which decreased substantially as shown in Figure 6e–h, suggesting that more external pressure may be required to approach TI behavior. With the displacement of Pb in the z-direction, the band gaps of the hydrostatically compressed CsPbBrₓI₃₋ₓ decreased significantly as the polarizations increase. The largest electric polarization of 0.025 C/m² was found in CsPbBr₂I under compression strain of 10% when Pb was moved along the I–Pb–I direction, as shown in Figure 6f. A theoretical study [23] reported that the electric polarization of CsPbI₃ induced by a Pb displacement of 0.04 Å was approximately 0.030 C/m², which was about two times greater than but still consistent with our result.

**Figure 6.** Plots on the left (a–d) and right (e–h) depict the calculated electric polarization $P_{ele} (\text{C/m}^2)$ (red solid lines) and band gaps (eV) (blue dashed lines), respectively, for the CsPbBr₃ (a,e), CsPbBr₂I (b,f), CsPbBrI₂ (c,g), and CsPbI₃ (d,h) perovskites as a function of Pb displacement in equilibrium (compressive strain of 10%).
3.3. Surface Band Structure

The topological surface band structures of CsPbBr$_3$ and CsPbI$_3$ from the supercell structure illustrated in Figure 1b, namely one PbBr$_2$ (PbI$_2$) and CsBr- (CsI-) terminated slabs, are depicted in Figure 7a,e, respectively, and they exhibited a Dirac cone near the Fermi level at the M points of the surface Brillouin zones with the respect to the natural behavior. The polar surface band structures of CsPbBr$_3$ and CsPbI$_3$ come from the center Pb atom moved out-of-plane at approximately 0.08 Å, as shown in Figure 7b,f, respectively. This indicates that the surface conduction band is separated into positive and negative surfaces in terms of energy or achieves a ferroelectric TI. The Dirac cone split because of the break in the time-reversal symmetry, suggesting the presence of a Rashba band-splitting mechanism caused by the electric polarization from the Pb displacement. The topological surface band structures of CsPbBr$_3$ and CsPbI$_3$ from the supercell structure are illustrated in Figure 1c and two PbBr$_2$- and PbI$_2$- terminated slabs are depicted in Figure 7c,g, respectively. The PbBr$_2$ (PbI$_2$) surface did not appear to contribute to Dirac cone-like energy dispersion, but the CsBr (CsI) surface did. Furthermore, the polar surface band structures of CsPbBr$_3$ and CsPbI$_3$ with PbBr$_2$- and PbI$_2$- terminated surfaces on both sides are depicted in Figure 7d,h, respectively, showing that PbBr$_2$ (PbI$_2$) surfaces change from not contributing topological surface conduction bands to contributing such bands under the effect of polarization.

![Figure 7](image_url)

**Figure 7.** Comparison of the topological surface band structures of CsPbBr$_3$ in (a–d) and CsPbI$_3$ in (e–h) with surface normal (a,e), polarization in the z-direction (b,f), and two PbBr$_2$- and PbI$_2$-surface normals (c,g), and polarization in the z-direction (d,h), respectively.

4. Conclusions

The electronic band structures of the CsPbBr$_{x}$I$_{3-x}$ perovskites were studied theoretically using density functional theory with the GGA. The CsPbBr$_{x}$I$_{3-x}$ perovskite was found to become a TI when the external pressure exceeded its critical stress. The band inversion of the CsPbBr$_{x}$I$_{3-x}$ perovskite occurred at the high symmetric R point with and without SOC. All indices of CsPbBr$_{x}$I$_{3-x}$ (x = 0, 1, 2, and 3) determined from a $Z_2$ topological invariant with hydrostatic strain were (1,0,0,0), further confirming that CsPbBr$_{x}$I$_{3-x}$ perovskites are strong TIs. The largest electric polarization of 0.025 C/m$^2$ was found in the electric polarization of CsPbBr$_2$I induced by Pb displacement along the I–Pb–I direction. The
Dirac-cone-like energy dispersion of CsPbBr$_3$I$_{3-x}$ at the M point was enhanced in regions where electric polarization was increased, leading to ferroelectric TIs.

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