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Research Article

Ab initio analysis of the optoelectronic properties of single perovskites CsPbX3 with (X=Br, I)

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Abstract-In this comparative study between two simple perovskites, we focus on the study of the optoelectronic characteristics of CsPbX3(X=Br, I) which allows a view in their applications in Led, Solar cell and for Imagery applications too.

Using the FPLAPW method implemented in the wien2k code give us the electronic and optical characteristics of the simples perovskites CsPbI3 and CsPbBr3, this by calculating the states of bands struct and density of state. Comparison between results of characteristics for this two simple perovskites will allow, through their gap, to show the development of the yield of singljonction solar cell. Allowing to observe the valence, conduction bands and to note the gap of CsPbI3, CsPbBr3 essential factor for thin films of solar cell.

Also using a FP-LAPW method implemented in the wien2k code give us optical characteristics of the simple perovskites CsPbI3 and CsPbBr3. the study of optical properties and indices together with the results of electronic properties, in particular gap, permits through absorption, reflectivity and conduction characteristics to determine the different applications of these two materials whether in imagery or the solar cell fields.

Key Words: Perovskites, Wien2k, Semiconductor, Structband, Optoelectronics, Solar Cell, Imagery.

I. INTRODUCTION

The primordial needs of the world and humanity for solar energy have aroused the interest in scientific research for simple or tandem or hybrid materials which form the thin films of solar panels. the element silicon, abundant on earth and inexpensive, was the essential element of these panels before the emergence of other materials such as perovskites essentially CaTiO3 discovered in Russia by Germanic scientist, which gives in solar cell panel ,greater yields ranging 15 to 20 alone and up to 28 percent in tandem silicon perovskites.[1] In this study we compare simple perovskites essentially in their gap which directly influences the performance of single junction solar panels developed with these simple materials. The study

of the electronic and optical characteristics of the simple perovskites CsPbI3 and CsPbBr3 will allow, through their gap, to show the development of the yield of single junction solar panels following the transition from simple perovskites to another with different Gap.

II. COMPUTATIONAL METHODE

The present calculations were done in the framework of the density function al theory (DFT) based on the solutions of the Kohn–Shame quations [2]. The well-founded full potential-linearized augmented plane wave FP-LAPW [3,4] methodology as implemented in the WIEN2K computer package [5] allows us to predict properly the structural, electronic and optic properties of $CsPbI_3$ and $CsPbBr_3$ Perovskites. The density functional theory (DFT) intends to solve the problems inherent from many body quantum mechanics is the basis on which FP LAPW method is heavily based. using the lapw and apw dft implemented in the wien2k code Although ab-initio calculations have successively predicted the electronic and structural properties of various perovskites, these calculations are very often restricted to the 0 K temperature [5], this method give us the electronic and optical characteristics of the simple perovskite CsPbI3 and CsPbBr3 materials through the study of its structure respecting the order of simple perovskites ABX3 which crystallizes in a cubic phase system 221pm3m, For structural optimization of CsPBI3 and CsPbBr3, we Chosen for dft-based calculation through fp-lapw implemented in the wien2k code: GGA 13 approximation and RMTKmax=8 Gmax=14 and separation energy =-6Ry for kpoint=2500 and (13 13 13) mech. Where atoms Cs occupies (0.0.0) position and atom Pb occupies (0.5.0.5.0.5) position and atoms I, Br occupies (0.5.0.5.0) ;(0.5.0.5.0) respectively. And lattice parameter for CsPbI3 $a_{0=}11.26$ A^0 and for CsPbBr3 a_0`$= 10.58$ A^0 see Fig 1 and Fig 2.

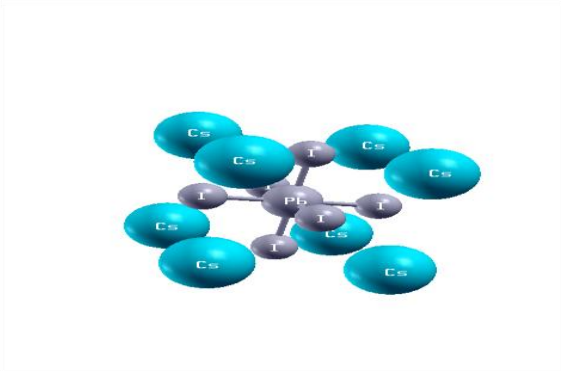


Fig. 1 The cubic -Perovskite CsPbI3. prototype

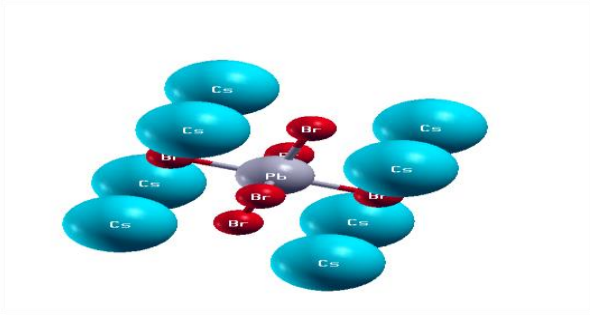


Fig. 2 The cubic -Perovskite CsPbBr3. prototype

Having a Goldschmidt factor respectively:

$$t=0.707 \times \frac{(rCs+ + rI-)}{(rPb2+ + rI-)}$$

$$t=0.707 \times \frac{(rCs+ + rBr-)}{(rPb2+ + rBr-)}$$

Which give Satifesaint stability in cubic phase for CsPbI3 and CsPbBr3

Table 1

Ionic radii Coordinance 12 Cs+ (A^0)	Ionic radii Coordinance 6 Pb2+(A^0)	Ionic radii Coordinance 6 I-(A^0)	Ionic radii Coordinance 6 Br-(A^0)	Factor of Goldschmidt of CsPbI3	Factor of Goldschmidt Of CsPbBr3
1.88	1.19	1.12	1.96	0.91	0.86

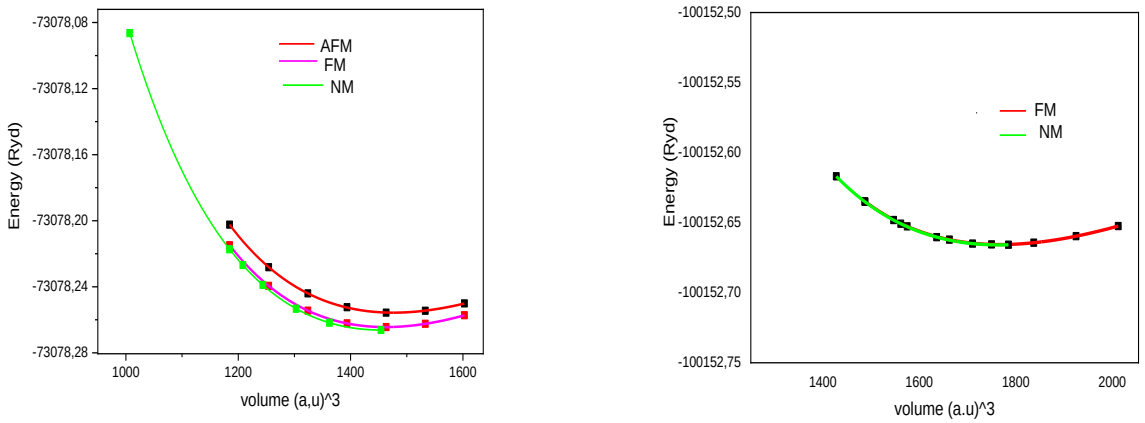
we carried out the optimization study allowing us to have the best lattice parameter and the best minimum energy state guaranteeing the stability of the materials also we calculated band structure and density of state the back allowing to note the valence and conduction bands and to note the gap of CsPbI3 and CsPbBr3 essential invoice for thin films made from these materials.

For structural optimization and to define the energy-volume variation and the most stable state at minimum energy, which turned out to be nonmagnetic, we opted for the GGA approximation **[6].**After the study with the wien2k code that we carried out for the simple perovskites CsPbI3, CsPbBr3 we have compared these results essentially making it possible to draw the values of the gap and the optical absorption of CsPbI3 with the same electronic and optical characteristics essentially in the GAP, absorption of these materials.

III. RESULT AND DISCUSSION

3-1 Structural Properties:

In terme of structural properties, our study has shown the stability of structure of CsPbI3 and CsPbBr3 in Non-Magnetic states.



CsPbBr3 CsPbI3

Fig. 3 Stability of the crystalline structure in the non-magnetic state for CsPbX3 with X= (I, Br)

The study of the structural properties is a prerequisite to predict other physical properties using first principal methods by means of the variation of the unit cell volume of the studied compounds and its adjustment with the well-known Murnaghan equation [7]. This allows us to determine the different structural parameters such as lattice parameter, the bulk modulus and its pressure derivative , For structural optimization of CsPBI3 and CsPbBr3, we Chosen for dft-based calculation through fp-lapw implemented in the wien2k code: GGA 13 approximation , Fig.3 and Fig.4 show the variation of the unit cell volume as function of energy for studied compounds (CsPbI3, CsPbBr3) where the continuous line presents the Murnaghan fit of our calculated points. Minimum energy state guaranteeing the stability of the material also.

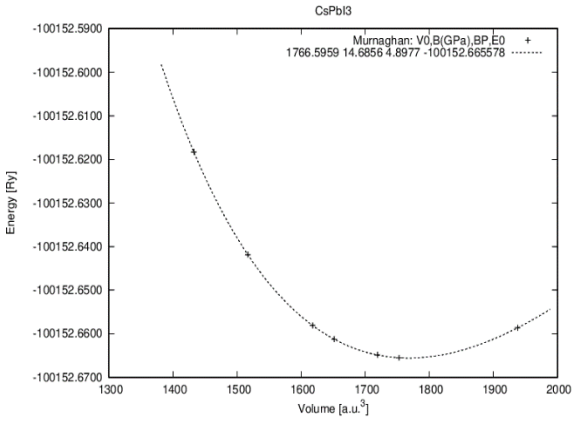


Fig. 4

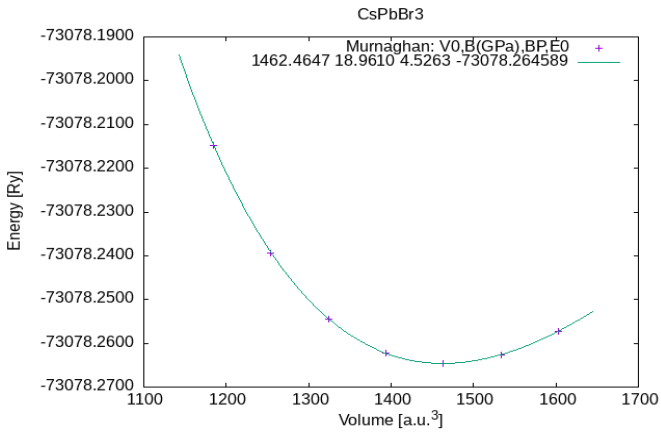


Fig. 5

3-2 Electronic Properties: The electronic properties of lithium oxide protactinium perovskite $LiPaO_3$ are described by the calculation of band structure energy and total and partial density states using the GGA approximation We calculated band structure and density of states the back allowing to note the valence and conduction bands and to note the gap of CsPbI3, CsPbBr3 [8]These figures (Figure 5 and Figure 6) reveal the existence of a direct gap along R -R for the GGA approximation ,with Gap (CsPbI3) is 1.445 eV and Gap (CsPbBr3) is 1.156 eV.

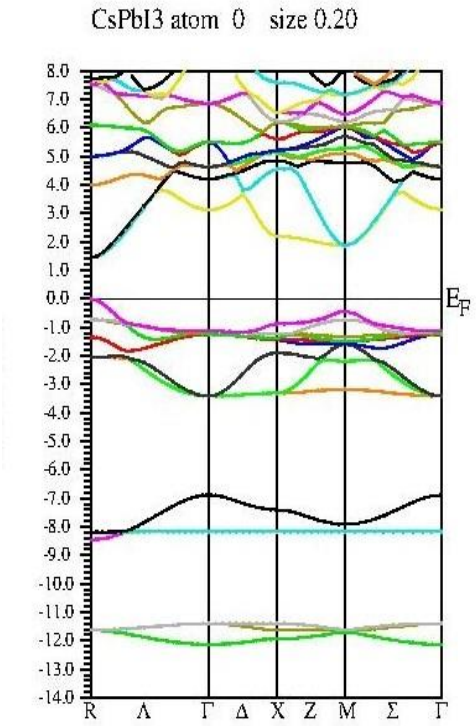


Fig. 6 Band struct CsPbI3

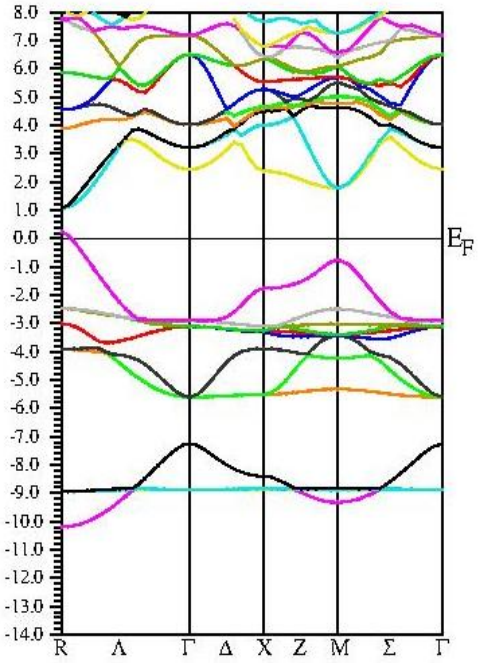


Fig. 7 Band struct CsPbBr3

Schema of tdos and pdos (figure 7 and figure 8) shows the number of states available (to occupy) at each energy level, observed in terms of total and partial density of states (TDOS & PDOS). and also shows atomic participation in energy states.

Finally, we confirmed gap values by comparison between the result of density of state and band structure.

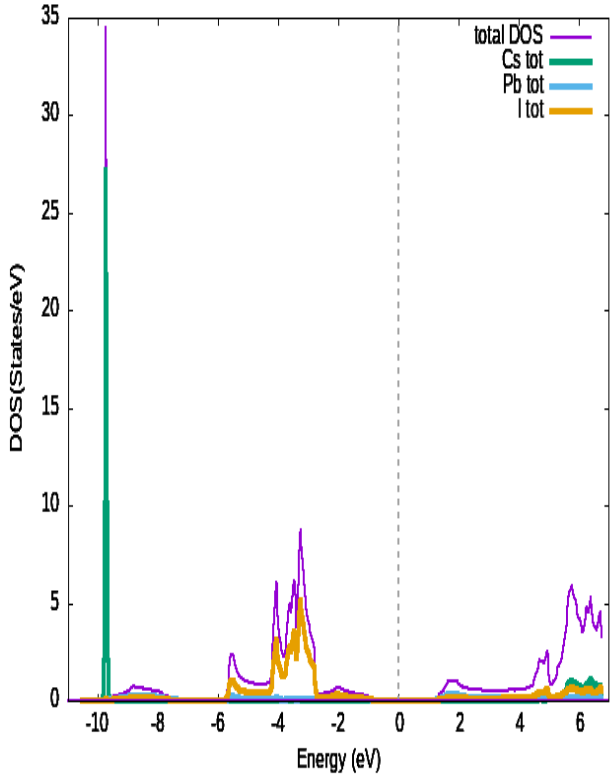


Fig. 8 DOS STATES CsPbI3

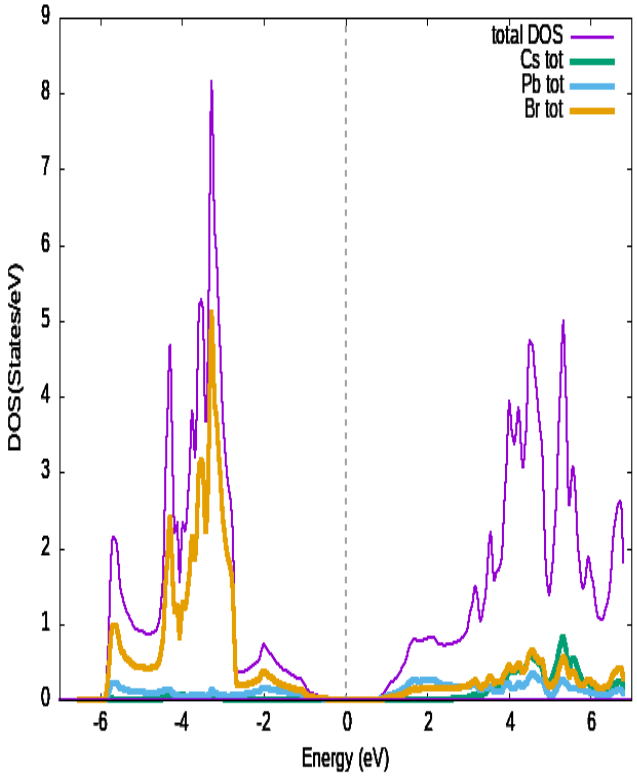


Fig. 9 DOS STATES CsPbBr3

3-3 Optical Properties

We have through wien2k calculated the optical characteristics of CsPbI3 and CsPbBr3, analyzed the absorption values through the calculations made by FP- LAPW we compar CsPbI3 and the other simple PEROVSKITES, we also noted the optical graphs such as reflectivity , refraction ,conductivity especially absorption (Figure 9 to Figure 16)in relation with the energy of simple perovskites CsPbI3 [10] which has an important absorption and two peaks in 10 EV and 22.5ev equivalent to landa wavelength from 124.8 nanometer to 55.46 nanometer which makes it possible to cover a large part of UV and we note that the CsPbBr3 materials have a high absorption and can cover part of the visible range and a wide range of the UV range. With a wide energy range from 3ev to 17.5ev equivalent to landa wavelength from 416 nanometer to 71.31 nanometer [9].

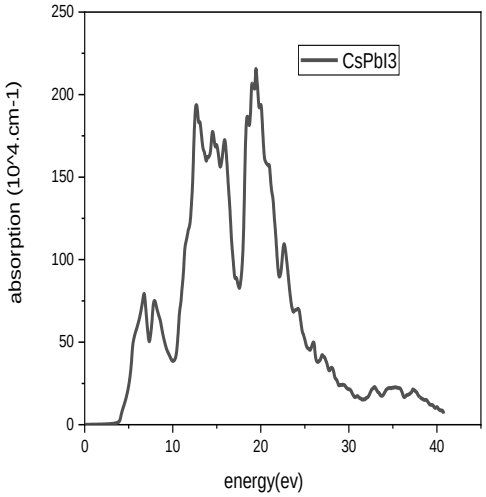


Fig. 10

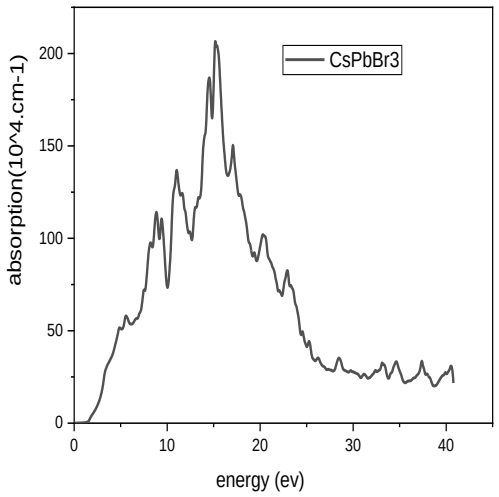


Fig. 11

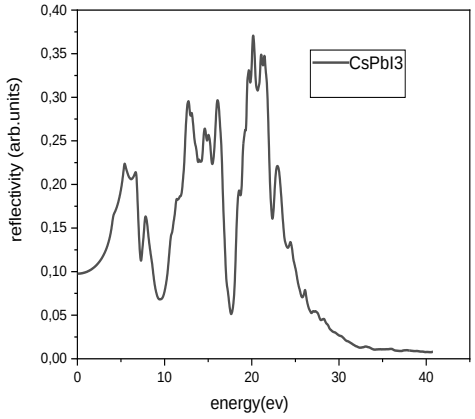


Fig. 12

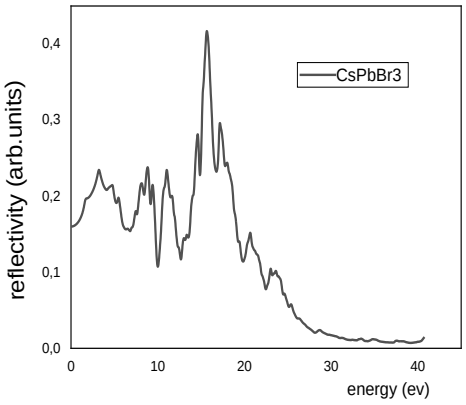


Fig. 13

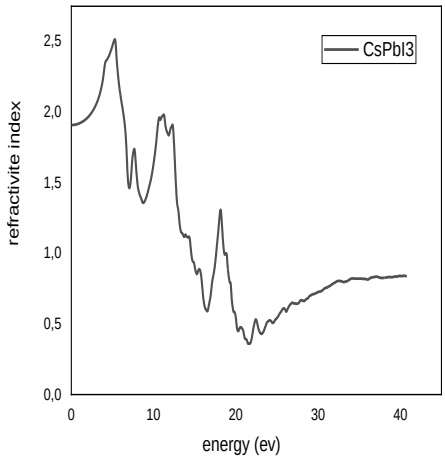


Fig. 14

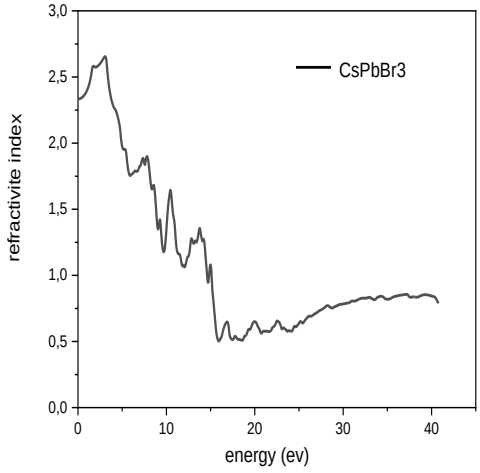


Fig. 15

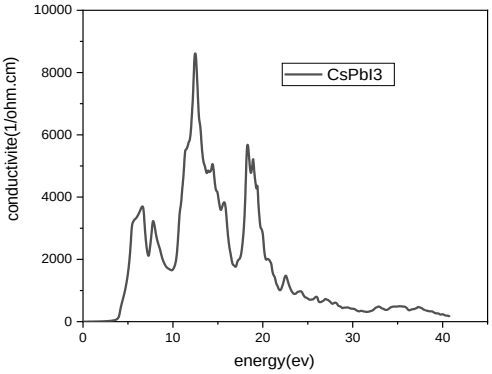


Fig. 16

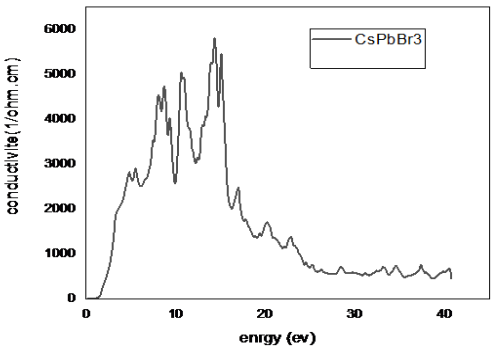


Fig. 17

IV. CONCLUSION

After the study of structural and optoelectronic characteristics of the simple perovskites CsPbI3 and CsPbBr3 result from our studies with wien2k code. Through the calculations made by FP- LAPW and with comparing the properties of CsPbI3 and CsPbBr3 derived from calculations and optoelectronic states, we conclude that they are close to the gap range for the material forming the thin films of the single junction solar panels with range between 1.1to1.4ev ,but we note the optical graphs and especially the absorption in relation to the energy of simple pervskites CsPbI3 which has a good absorption but in UV game only which makes it impossible to cover a large part of the solar rays essentially in visible range to reconvert them into energy and we note that the CsPbBr3 materials have a high absorption and can cover part of the visible range and a wide range of the UV. With band gaps in the range of 1.1ev to 1.4ev only CsPbBr3 perovskites have usage in solar cells and leds and other applications .high absorption $1.07 \times 105\ cm^{-}1$ for 4.02ev, low reflectivity and high conductivity of this material, represent a great advance in the field of solar panels, especially single junction, thanks to their adequate gap for uni-junction solar panels, which can be improved by doping or with Si in tandem, to achieve the ideal gap=1.3ev. Also for theres good characteristics optics CsPbBr3 is used in imagery and microscopieand give low-saturation-intensity, high-photostability, and high-resolution. $CsPbBr_3$-assisted STED nanoscopy has great potential to investigate microstructures that require super-resolution and long-term imaging. [11] To make CsPbI3 perovskites efficient as solare cells, we need to make various changes, such as doping with an Ionic defect such as Cl, use tandem or, multi-Junction solar cell panel [12].

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