Comparative study of distinct halide composites for highly efficient perovskite solar cells using a SCAPS-1D simulator

Sagar Bhattarai, Rahul Pandey, Jaya Madan, Soney Tayeng, P. K. Kalita, Mohd Zahid Ansari, Lamia Ben Farhat, Mongi Amami and M. Khalid Hossain

This research investigates the influence of halide-based methylammonium-based perovskites as the active absorber layer (PAL) in perovskite solar cells (PSCs). Using SCAPS-1D simulation software, the study optimizes PSC performance by analyzing PAL thickness, temperature, and defect density impact on output parameters. PAL thickness analysis reveals that increasing thickness enhances $J_{SC}$ for MAPbI$_2$ and MAPbI$_2$Br, while that of MAPbBr$_3$ remains steady. $V_{OC}$ remains constant, and FF and PCE vary with thickness. MAPbI$_2$Br exhibits the highest efficiency of 22.05% at 1.2 µm thickness. Temperature impact analysis shows $J_{SC}$, $V_{OC}$, FF, and PCE decrease with rising temperature. MAPbI$_2$Br-based PSC achieves the highest efficiency of 22.05% at 300 K. Contour plots demonstrate that optimal PAL thickness for the MAPbI$_2$Br-based PSC is 1.2 µm with a defect density of $1 \times 10^{15}$ cm$^{-3}$, resulting in a PCE of approximately 22.05%. Impedance analysis shows the MAPbBr$_3$-based PSC has the highest impedance, followed by Cl$_2$Br-based and I$_2$-based perovskite materials. A comparison of QE and J–V characteristics indicates MAPbI$_2$Br offers the best combination of $V_{OC}$ and $J_{SC}$ resulting in superior efficiency. Overall, this study enhances PSC performance with MAPbI$_2$Br-based devices, achieving an improved power conversion efficiency of 22.05%. These findings contribute to developing more efficient perovskite solar cells using distinct halide-based perovskite materials.

1. Introduction

After decades of research to improve the power consumption efficiency (PCE) of renewable solar cells, which can effectively substitute the depleting fossil fuels, perovskite solar cells (PSCs) have seen a significant increase in efficiency in the last decade, as evidently studied by many researchers. Their remarkable properties, which include a very high absorption coefficient, a tunable band gap, an extended diffusion length of the carriers, greater mobility of charge, a lower trap state density, a smaller binding energy of the excitons, and a low processing cost, have enabled them to achieve this feat. The chemical formula for perovskite is $\text{PbX}_3$, where $\text{P}$ stands for an organic/inorganic cation (Cs or MA or FA), $\text{Q}$ stands for heavy metals (Sn, Ge, Pb), and $\text{X}$ shows the halide anions (Br, Cl, and I). More specifically, the organic–inorganic perovskites have blazed a trail toward a highly efficient light-harvesting material and the PSC efficiency has now increased from 3% to 25.6%. Because of the tunable frequency, the PSCs can absorb different light frequencies effectively in different layers, improving PCE.

Many previous studies have been conducted on perovskite materials consisting of Pb$_2$, which are the most efficient and reliable. These PSCs have their own set of advantages and disadvantages, such as high efficiency and stability but poor performance, high stability but not eco-friendly, and so on. These issues can be addressed through improved engineered devices, encapsulation, and the use of 2D perovskites. Milot et al. verified that FASn$_3$ had higher carrier mobility, lower auger recombination rate constants, and a more substantial radiative rate of recombination constant that is comparable to GaAs. While Lee et al. combined FASnI$_3$ with the SnF$_2$–pyrazine complex to slow the crystallization and also attain a PCE up to 4.8%. Ban et al. fabricated an 8.03% efficient CsSnI$_3$ absorber layer-based PSCs with $V_{OC}$ of 520 mV and $J_{SC}$ of 23.4%. The work by Abdelaziz et al., where they used SCAPS software to investigate how the thickness, the defect density, and the doping affect the device output of [HC(NH$_2$)$_2$]$_2$SnI$_3$-.
FASnI$_3$ based PSCs that achieves a PCE up to 14.03%, $V_{OC}$ of 0.92 V, and $J_{SC}$ of 22.65 mA cm$^{-2}$ and a FF of 67.74%.

Certain studies have been reported to discover the characteristics of the PSCs. Such research is required to better understand perovskites and capitalize on their advantages. The results of these studies will provide valuable insights that will allow us to make informed decisions about how to use perovskite solar cells at best. The methylammonium-based PSC offered the most predominant efficiency, starting from 16% to 20% by Cao et al. and Bhattarai et al. The efficiency reached up to 22.16% in the recent numerical simulation study. It is crucial to investigate perovskites with exceptional optical and

![Figure 1](image)

**Figure 1.** (a) The proposed architecture of MA-based PSC, (b) absorption coefficient of perovskite materials under the illuminance of AM1.5G, and band energy diagram of PSCs.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Terms</th>
<th>ETL (WO$_3$)</th>
<th>PAL$_1$ (MAPbI$_3$)</th>
<th>PAL$_2$ (MAPbBr$_3$)</th>
<th>PAL$_3$ (MAPbI$_2$Br)</th>
<th>HTL (Mg-CuCrO$_2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d$ ($\mu$m)</td>
<td>Thicknesses</td>
<td>0.1–0.15</td>
<td>0.2–1.2</td>
<td>0.2–1.2</td>
<td>0.2–1.2</td>
<td>0.1–0.15</td>
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<td>$E_g$ (eV)</td>
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<td>2.3</td>
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<td>Relative permittivity</td>
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<td>6.3</td>
<td>15</td>
<td>9.5</td>
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<td>$\chi$ (eV)</td>
<td>Electron affinity</td>
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<td>3.9</td>
<td>3.6</td>
<td>3.7</td>
<td>2.1</td>
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<td>$N_e$ (cm$^{-3}$)</td>
<td>Eff. DoS at CB.</td>
<td>$1 \times 10^{20}$</td>
<td>$2.2 \times 10^{18}$</td>
<td>$2.2 \times 10^{18}$</td>
<td>$3 \times 10^{17}$</td>
<td>$1 \times 10^{19}$</td>
</tr>
<tr>
<td>$N_v$ (cm$^{-3}$)</td>
<td>Eff. DoS at VB.</td>
<td>$2 \times 10^{21}$</td>
<td>$1.8 \times 10^{18}$</td>
<td>$1.8 \times 10^{19}$</td>
<td>$4 \times 10^{18}$</td>
<td>$1 \times 10^{19}$</td>
</tr>
<tr>
<td>$\mu_0$ (cm$^2$ V$^{-1}$ s$^{-1}$)</td>
<td>Mobility of $\varepsilon$</td>
<td>100</td>
<td>2</td>
<td>20</td>
<td>15</td>
<td>0.1</td>
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<tr>
<td>$\mu_p$ (cm$^2$ V$^{-1}$ s$^{-1}$)</td>
<td>Mobility of $\mu$</td>
<td>25</td>
<td>2</td>
<td>20</td>
<td>15</td>
<td>2.53</td>
</tr>
<tr>
<td>$D_a$ (cm$^{-3}$)</td>
<td>Dop. den. of the acceptor</td>
<td>5.21 x $10^9$</td>
<td>0</td>
<td>0</td>
<td>6.4 x $10^{15}$</td>
<td></td>
</tr>
<tr>
<td>$D_d$ (cm$^{-3}$)</td>
<td>Dop. den. of donor</td>
<td>$1 \times 10^{21}$</td>
<td>5.21 x $10^9$</td>
<td>0</td>
<td>$1 \times 10^{16}$</td>
<td>0</td>
</tr>
<tr>
<td>$N_t$ (cm$^{-3}$)</td>
<td>Def. density</td>
<td>$1 \times 10^{14}$</td>
<td>$1 \times 10^{13}$</td>
<td>$1 \times 10^{13}$</td>
<td>$1 \times 10^{14}$</td>
<td>$1 \times 10^{14}$</td>
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</tbody>
</table>
electrical properties in order to achieve a balance between stability and performance. So, there is still a huge scope to study with the help of simulation to fully understand these materials’ distinct properties and associated performance parameters. Further, among the various types of perovskite materials, MAPbI$_3$–xBr$_x$, a hybrid organic–inorganic lead halide perovskite, has garnered significant attention as an absorber layer in PSCs. This compound offers a versatile platform for developing efficient and stable solar cells, holding great potential for revolutionizing the renewable energy landscape. MAPbI$_3$–xBr$_x$ is a solid solution of methylammonium lead iodide (MAPbI$_3$) and methylammonium lead bromide (MAPbBr$_3$). The incorporation of bromine (Br) atoms into the MAPbI$_3$ lattice allows for the controlled modification of its composition and bandgap. By fine-tuning the ratio of iodine (I) to bromine (Br) atoms, the bandgap of MAPbI$_{3-x}$Br$_x$ can be engineered to match specific solar spectra, optimizing light absorption and enhancing device efficiency. One of the key advantages of utilizing MAPbI$_{3-x}$Br$_x$ in PSCs is its high absorption coefficient, enabling efficient utilization of a broad range of solar wavelengths. This exceptional light-harvesting capability results in higher photocurrents and improved overall energy conversion efficiency. Furthermore, the energy levels of MAPbI$_{3-x}$Br$_x$ align favourably with the other functional layers within the PSC device, facilitating efficient charge transport and minimizing recombination losses.

Therefore, extensive PV study related to MAPbI$_{3-x}$Br$_x$ at varying halide compositions is much needed to comprehend the influence of different halide compositions on the outputs of the PSC. Therefore, in this work, the primary intent is to investigate and compare the properties of various Perovskite materials concerning their different halide materials in relation to their performance parameters. A comparative study of various perovskites, such as MAPbI$_3$, MAPbI$_2$Br, and MAPbBr$_3$, is carried out to help us to apprehend the distinct performances and the influence on the output parameters and to additional work for highly efficient and more suitable stable perovskite.

### Table 2  Parameter of interface defects used in simulations

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Mg–CuCrO$_2$/PALs</th>
<th>PALs/WO$_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Defect types</td>
<td>Neutral</td>
<td>Neutral</td>
</tr>
<tr>
<td>e cap. cross-section (cm$^2$)</td>
<td>$1 \times 10^{-19}$</td>
<td>$1 \times 10^{-19}$</td>
</tr>
<tr>
<td>h cap. cross-section (cm$^2$)</td>
<td>$1 \times 10^{-19}$</td>
<td>$1 \times 10^{-19}$</td>
</tr>
<tr>
<td>Energy distributions</td>
<td>Single</td>
<td>Single</td>
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<tr>
<td>Ref. for def. energy levels</td>
<td>Above the highest EV</td>
<td>Above the highest EV</td>
</tr>
<tr>
<td>Energy with respect to ref. (eV)</td>
<td>0.6</td>
<td>0.6</td>
</tr>
<tr>
<td>Total density (integrated over all energies) (cm$^{-2}$)</td>
<td>$1 \times 10^9$</td>
<td>$1 \times 10^9$</td>
</tr>
</tbody>
</table>

Fig. 2  The impact of the perovskite thicknesses on the outputs of the PSC devices.
2. Device configurations

In Fig. 1a, the heterojunction PSCs with the ITO/ETL/perovskite/HTL/Ag device configuration are used to simulate PSC devices. More specifically, a 0.1 \( \mu \)m top anode of ITO is placed after a 0.1 \( \mu \)m \( \text{WO}_3 \) layer in the simulated PSC devices, which serves as the ETL and effectively channels the produced electrons from the absorber layers in the PSC device. The HTL of \( \text{Mg-CuCrO}_2 \) is placed having a thickness of 0.1 \( \mu \)m. The material is used due to its appropriate band alignment with the perovskite absorber. During device fabrication, \( \text{Mg-CuCrO}_2 \)-based HTL can be fabricated using different deposition techniques such as spin-coating, doctor-blading, spray-coating, or inkjet printing. The perovskite absorber layer (PAL) for the devices is 0.4 \( \mu \)m thick and is sandwiched between an HTL and an ETL. The holes generated in the PSC are successfully collected and transferred to the cathode by the hooping mechanism. The cathode is made of 0.1 \( \mu \)m thicker Ag material, which is cheaper than other cathode materials such as Gold (Au). Table 1 and 2 list all of the input parameters used by the PSC device and interface defectivity details, respectively.

In Fig. 1b, the perovskites, namely MAPbI\(_3\), MAPbI\(_2\)Br, and MAPbBr\(_3\), are shown with their respective coefficients over the wavelengths. The absorption coefficients are obtained from the simulating software of SCAPS-1D. On the other hand, the band energy diagram for all the possible constituent layers in the three designs of the perovskites is also depicted in Fig. 1c, respectively.

3. Results and discussion

The discussion in this part is only focused on the findings and analysis of the current study. The results and discussion segment comprise five smaller portions, numbered 3.1 to 3.5. First, if appropriate, a bandgap analysis is performed, followed by impacts on absorber thickness, temperature, and overall defect density. In this part, the contour analysis for the MA-based solar cell has also been studied simultaneously.

The work is simulated at 300 K temperature to check the band alignment of the PSC device and obtain the desired results. The following is a detailed investigation of the current work.

3.1 The influence of PAL-thickness in outputs of the PSC

Thickness tuning of the PSC constituent layer is one of the most promising and successful methods for increasing the effectiveness of the PSC device. The PSC was thickened from 0.2–1.2
μm, and the compatible thicknesses for the optimal efficiency of the simulated device were determined. As shown in Fig. 2a, for MAPbI₃, the short-circuit current density (J_{SC}) rises from 16 mA cm⁻² and reaches the maximum point at 22 mA cm⁻² as the PAL thickness increases from 0.2 μm to 1.2 μm. This is due to the absorption rate’s proportional dependence on current density. J_{SC} remains constant, i.e., ~21 mA cm⁻² and 8 mA cm⁻² for MAPbI₂Br and MAPbBr₃ throughout the active layer thickness of 1.2 μm, respectively. Fig. 2b depicts the variation in V_{OC} of all three Perovskite materials and the active layer thickness, which ranges from 0.2 μm to 1.2 μm. The device’s V_{OC} is at a steady state with increasing thickness inside the PSC. In terms of numbers, the 1.2 μm thick MAPbBr₃-Pb has a higher V_{OC} value of 1.52 Volt. The devices in Fig. 2c demonstrate the Fill Factor (FF) property. The Fill factor indicates the squareness of the J-V curve and indicates the resistive losses in the device, and higher FF ensures higher output power and conversion efficiency as both the parameters are proportional to each other. The FF of MAPbI₃ decreases from 87.2% to 86.9%, while the PAL thickness increases from 0.2 μm to 1.2 μm. Among the three Perovskite materials used, the material MAPbI₂Br shows the maximum value. For MAPbI₂Br, the FF appears to remain constant, at around 86.2%, and the FF of MAPbBr₃ decreases from 87.89% to 86.89% for the PAL thicknesses varying from 0.2 μm to 1.2 μm, respectively. While Fig. 2d depicts PCE, the most crucial feature of the PSC. The PCE of MAPbI₃ remains at approximately 17.62% under the said variation of PAL and the PCE of MAPbBr₃ eventually reached 9.85% after steadily rising from 5.2% for the thickness values varying from 0.2 μm to 1.2 μm. The PCE of the material MAPbI₂Br rises from 14.8% to 22.05% at the maximum thickness level of the perovskite material. It can be noted from the data in Fig. 2d that the increase in PCE is significant during the initial rise in the thickness of the PAL. This is due to an improvement in photon absorption at higher thicknesses which results in an improvement in J_{SC} and PCE. The same can be validated through J_{SC}.

However, further increasing the thickness from 1.0 to 1.2 μm the improvement is not that prominent, and the FF trend showed degradation at higher thicknesses. So eventually a saturated J_{SC} and reduced FF will reduce the PCE if PAL thickness is increased beyond a certain limit. The current work offers a better outcome than the previous work by Dipta et al.⁴⁴

### 3.2 The influence of the temperature on the PSC outputs

Fig. 3a and b depicts a comprehensive examination of the PSC properties as temperature changes. As depicted in Fig. 3(a–d), the four parameters J_{SC}, V_{OC}, FF, and PCE decrease as the temperature rises from 300 K–400 K for the Perovskite material MAPbI₂Br. The maximum values for the Perovskite MAPbI₂Br parameters are 21.91 mA cm⁻², 1.16 V, 86.89%, and 22.05% at 300 K.
For the MAPbBr₃, the values of parameters $V_{OC}$ and FF both decrease as the temperature rises from 300 K – 400 K, with the maximum values at 300 K being 0.90 V and 81%, respectively. While the value of the parameter $J_{SC}$ rises from 16.6 mA cm$^{-2}$ to 17.4 mA cm$^{-2}$ as the temperature increases from 300 K to 400 K, in contrast, PCE remains nearly constant at approximately 9.8% as the temperature increases to the maximum value. Since the increase in temperature reduces the $V_{OC}$ of the PSC devices. As we know, due to the decrease in $V_{OC}$, the $J-V$ curve becomes steeper, as a result, the FF value is increased as compared to other PSC devices. This is the reason for a nonlinear increase in FF for MAPbBr₃-based PSC. And for the material MAPbI₃, values of the three parameters $J_{SC}$, FF, and PCE decrease with increasing temperature from 300 K to 400 K with values of 20.7 mA cm$^{-2}$, 62%, and 20.8% at peak for the respective parameters at 300 K, but the value of the parameter $V_{OC}$ for the MAPbI₃ appears to remain unchanged with a value of 0.982 V while the temperature increases. The current simulation offers an improvement in overall output parameters as compared to the previous work by Bhattacharai et al.²⁶

3.3 The combined influence of thickness and total defect density using contour plotting

There are three perovskites devices: firstly, the MAPbI₃-based PSC. As Fig. 4 shows the contour plot over the perovskite material’s thickness and total defect density. The following outcomes can be deduced. Firstly, the PCE is maximum at 1.2 μm thickness and defectivity of $1 \times 10^{13}$ cm$^{-3}$, which offers a high value of PCE, i.e., nearly 17.5%. The $V_{OC}$, on the other hand, is at its maximum, with a value of 1.144 V at 0.2 μm thickness and $1 \times 10^{13}$ cm$^{-3}$ defectivity. While the $J_{SC}$ keeps on increasing with the increase in thickness and reduces when the defectivity is higher. The maximum $J_{SC}$ value is 21.03 mA cm$^{-2}$ at a thickness of 1.2 μm and with a defectivity of $1 \times 10^{18}$ cm$^{-3}$. Lastly, the maximum FF is found to be 83% at thickness 0.2 μm thickness and defectivity $1 \times 10^{18}$ cm$^{-3}$, respectively.

The second PSC device with the perovskite material of MAPbI₂Br offers outstanding device outputs as depicted in Fig. 5. Firstly, the PCE is maximum at 1.2 μm thickness and $1 \times 10^{13}$ cm$^{-3}$, which offers a high value of PCE, i.e., nearly a value of 22.05%. On the other hand, the $V_{OC}$ is at maximum with the value of 1.156 V at the higher thickness regions and low defect density region, i.e., $1 \times 10^{13}$ cm$^{-3}$ defectivity. At the same time, the $J_{SC}$ keeps on increasing with higher thickness levels and smaller defectivity of the PAL. The maximum $J_{SC}$ value is 21.93 mA cm$^{-2}$ at a thickness of 1.2 μm and with a defectivity of $1 \times 10^{13}$ cm$^{-3}$. Lastly, the maximum FF is found to be 87.80% at a thickness of 1.2 μm and defectivity $1 \times 10^{18}$ cm$^{-3}$, respectively.

Fig. 5 The contour plotting of the perovskite material, i.e., MAPbI₂Br, for high output parameters at the optimized temperature and doping conditions.
Fig. 6 The contour plotting of the perovskite material i.e., MAPbBr₃, for high output parameters at the optimized temperature and doping conditions.

The PCE value continues to increase with the thickness and defectivity for MAPbBr₃-based PSC. The maximum value of PCE is 8.935% found at 1.2 μm thickness and 1 × 10¹³ cm⁻³ defectivity. While the maximum value of V_{OC} is 1.500 V found at a thickness of 0.2 micrometer and defectivity of 1 × 10¹³ cm⁻³, whereas J_{SC} increases with increasing thickness and defectivity, reaching a maximum of 6.971 mA cm⁻² at 1.2 μm thickness, and 1 × 10¹⁸ cm⁻³ defectivity. Lastly, the peak value of FF is 82.15%, which is found at 1.2 μm thickness and defectivity 1 × 10¹⁸ cm⁻³. Similar outcomes can be obtained from the previous SCAPS simulated work of Bhattarai et al.⁶⁶

3.4 Comparison of impedances of the PSCs

The impedance analysis is one of the better ways to understand the behavior of the perovskite materials having distinct halides. From Fig. 7, it is evident that the highest value of impedance is reached for the MAPbBr₃ perovskite, i.e., almost more than 100 000 ohm cm². While the Cl₂Br-based offers almost nearly 100 000 ohm cm², I-based Perovskite offers 95 000 ohm cm². The previous study also offers a similar impedance value, as depicted in Fig. 8. The report by Bhattarai et al. provides a high value nearly identical to the value obtained in this analysis.⁶⁷ The impedance plot or Nyquist plot of a solar cell provides a detailed qualitative understanding of resistive losses, capacitance, and recombination rate defects in the device. The impedance curve reported in Fig. 7 shows a similar trend in all three devices with minor changes.

3.5 Comparison of QE and J–V of the PSCs

The following points are attained from the J–V curve shown in Fig. 8. The MAPbBr₃ perovskite attains the highest V_{OC}, nearly
is almost 1.5 eV (MAPbI₃). The result can be matched with the

based PSC o

and 23 mA cm

highest point of wavelength,

necessary. The MAPbI₂Br attains the highest

perovskites show high QE values. Comparatively, the highest

two materials for better e

can be reached, as the steep curve of

MAPbI₃-based PSC 23.24 0.898 83.95 17.53

MAPbBr₃-based PSC 7.34 1.52 86.23 9.62

MAPbI₂Br-based PSC 21.91 1.16 86.89 22.05

Jayan PSC

with the previous works is reported in Table 3.

V

very low to contribute PCE as the

previous work by Jayan

et al.

MAPbI₂Br-based PSC devices. It is also worth to note that the

WO₃/PAL/Mg-CuCrO₂/Ag have been utilized using SCAPS-1D

simulating software. The WO₃ has been used as ETL, keeping in

view of maximizing the suitable band alignment and higher

mobility of the carrier with the perovskite material in the solar

devices, whereas, for the collection of the holes, Mg-CuCrO₂ as

the HTL for the numerical simulation of the PSC device.

Distinctive halide-based methylammonium-based perovskites

are used as active PAL that shows a greater influence on the

output parameter than the e–h transport layers of the PSC
device. So, the optimization of the absorber’s thicknesses for

the PSC is carried out for better outputs. The work attained an

optimal absorber thickness of 1.2 μm for the MAPbI₃Br-based

PSC device. The defectivity of the PSC shows that at the level of

1 × 10¹³ cm⁻³, which obtains higher outputs. Moreover, the

study also includes the impact of the resistances for enhancing

the higher efficiency of the PSC device. The simulation clearly

exhibits that the MAPbI₃Br can provide excellent outputs, as in

the present case, nearly 22.05%, which may be a fascinating and

suitable option in developing the PSC device. The overall

conclusion of the present study thus may offer valuable

contribution regarding the manufacturing of more efficient

MAPbI₃Br-based PSC devices. It is also worth to note that the

SCAPS-1D simulator used in this work is applicable to one-
dimensional devices and cannot support complex device

geometry. Therefore, advanced device simulators can also be

considered in future work.

Data availability

The raw/processed data required to reproduce these findings
cannot be shared at this time as the data also forms part of an
ongoing study.

Conflicts of interest

The authors declare that they have no known competing
financial interests or personal relationships that could have
appeared to influence the work reported in this paper.

Table 3 The overall assessment of the present work with the prior

<table>
<thead>
<tr>
<th>Device structures</th>
<th>Jₛᶜ (mA cm⁻²)</th>
<th>Vₒ𝑐 (V)</th>
<th>FF (%)</th>
<th>PCE (%)</th>
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<tr>
<td>MAPbI₃-based PSC</td>
<td>23.24</td>
<td>0.898</td>
<td>83.95</td>
<td>17.53</td>
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<tr>
<td>MAPbBr₃-based PSC</td>
<td>7.34</td>
<td>1.52</td>
<td>86.23</td>
<td>9.62</td>
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<tr>
<td>MAPbI₂Br-based PSC</td>
<td>21.91</td>
<td>1.16</td>
<td>86.89</td>
<td>22.05</td>
</tr>
<tr>
<td>Jayan et al.</td>
<td>21.83</td>
<td>1.00</td>
<td>71.19</td>
<td>15.55</td>
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<tr>
<td>Dipta et al.</td>
<td>16.27</td>
<td>1.06</td>
<td>76.22</td>
<td>13.03</td>
</tr>
</tbody>
</table>

1.5 V, and Jₛᶜ of 12.5 mA cm⁻². Though the Vₒ𝑐 is high, the Jₛᶜ is
very low to contribute PCE as the Vₒ𝑐 and Jₛᶜ are directly
proportional to the efficiency. On the contrary, the MAPbI₃-
based PSC offers the smallest value of Vₒ𝑐, which is unsuitable
for better efficiency. The MAPbI₃ attains the highest Vₒ𝑐 of 0.9 V
and 23 mA cm⁻² value of Jₛᶜ as shown in Fig. 8a. Since the need
of obtaining the best combination of Vₒ𝑐 and Jₛᶜ is mainly
necessary. The MAPbI₂Br attains the highest Vₒ𝑐 of 1.1 V and 22
mA cm⁻² of Jₛᶜ, which offers an excellent efficiency value. The
result can be compared with previous work by Adhikari et al.⁴⁸
The J–V curve of MAPbI₂Br also shows that a higher value of FF
can be reached, as the steep curve of J–V is higher than the other
two materials for better efficiency.

As from the QE curve in Fig. 8b, it is found that all three
perovskites show high QE values. Comparatively, the highest
bandgap perovskite of MAPbBr₃ drops at a very small wave-
length of nearly 540 nm as the dependency of QE is reciprocal to
each other. The lowest bandgap material of MAPbI₃ drops at the
highest point of wavelength, i.e., nearly 800 nm, as the bandgap
is almost 1.5 eV (MAPbI₃). The result can be matched with the
previous work by Jayan et al.⁴⁸ The overall comparison of the
present work with the previous works is reported in Table 3.

4. Conclusions

The simulation and investigation of the PSC structure with
different perovskite materials having a configuration of ITO/
Acknowledgements

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References