Passivation of defects in inverted perovskite solar cells using an imidazolium-based ionic liquid†

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During perovskite film preparation, the defects in the film are almost impossible to avoid because of the migration of the halide ions, which is detrimental to achieving a high-quality film. In general, the introduction of an additive is an effective strategy to control the film morphology and to reduce the defect density. Here, the representative and simplest ionic liquid, 1-ethyl-3-methylimidazolium bromide (EMIB), is selected as an additive due to its high conductivity and lone-pair electrons in its cationic group. Remarkably, the addition of the EMIB additive into the perovskite film improves the power conversion efficiency (PCE) from 15.9% for the pristine device to 18.2%. With the help of characterization analysis by scanning electron microscopy, X-ray photoelectron spectroscopy, Fourier transform infrared spectroscopy, etc., two contributions of the EMIB additive are addressed: (1) the primary one is the passivation of the uncoordinated Pb2+ to reduce the defects in the perovskite film by the lone-pair electrons in its cationic group, and (2) the secondary one is beneficial to promote crystal growth to improve the film quality. Hence, this work provides an easy approach to achieve a high-performance perovskite solar cell via passivation of the uncoordinated Pb2+ in the perovskite film by the lone-pair electrons in the cationic group of the ionic liquid.

1. Introduction

Organometallic perovskite solar cells (PSCs) have been extensively investigated in the past few years due to their potential to promote high-efficiency, low-cost, solution-processable devices thanks to the inherent properties of perovskite materials, including high mobility, tunable bandgaps and long diffusion lengths. During the nucleation and crystal growth of perovskite films, vacancies and charged defects are always created because of the migration of the halide ions. Undoubtedly, these vacancies and defects are detrimental to the device performance due to undesirable charge recombination and then performance deterioration. To reduce the vacancies or defects in polycrystalline perovskite films, introducing additives in the active layer to is an effective strategy which controls the morphology and/or passivates the uncoordinated Pb2+ or passivates the uncoordinated Pb2+ and then to reduce the recombination of charge carriers and facilitate carrier transfer. However, the passivation agents based on small molecule Lewis bases may not sustain their interaction with the halide perovskite at high temperature due to their low thermal stability. To circumvent this, polymer additives with multiple Lewis base functional groups have been designed and synthesized to provide a durable passivation of defects in halide perovskite films. However, the low conductivity is another drawback of small molecules and polymers and may impede the carrier transport in perovskite films.

Within this context, ionic liquids (ILs) are considered alternative candidates to serve as additives for high-efficiency PSCs because of their low vapor pressure and high ionic conductivity. ILs have been widely employed as additives in PSCs via incorporating them into TiO2-modified layers, C60-modified layers, interface layers, and perovskite precursors. In general, the role of ILs as additives aims to promote the processes of crystal nucleation and growth to achieve better morphologies and high-quality perovskite films. Aside from this, IL additives could provide an opportunity to passivate the...
defects when added into perovskite precursors.\textsuperscript{28–30} Bai et al.\textsuperscript{31} incorporated 1-butyl-3-methylimidazolium tetrafluoroborate (BMIMBF$_4$) into a perovskite precursor to achieve long-term operational stability due to the passivation between the PbI$_2$ of the perovskite and the anion ([BF$_4$]$^-$) of the additive. In addition, Wang\textsuperscript{32} and co-workers designed and synthesized a new hydrophobic IL, 3-(3-aminopropyl)-1-methylimidazolium hexafluorophosphate (APMimPF$_6$), and then incorporated this IL into a perovskite precursor to improve the device stability due to the interaction between the IL anion ([PF$_6$]$^-$) and the perovskite precursor. To date, many research studies have concentrated on the interaction between the IL anions and perovskites. A question naturally arises about the possible utilization of cations of ILs to achieve high-performance PSCs.

1-Methyl-3-propylimidazolium bromide (MPIB, as shown in Fig. 1a) is one of the representative and simplest ILs with considerable thermodynamic properties\textsuperscript{33} and has never been used as an additive in perovskite precursors. In our study, a simple structure is a better choice as an additive. (1) Short-chain branching provides the opportunities to coordinate with the perovskite. It does not easily cause steric hindrance. (2) The simplified structure is necessary to promote the facile synthesis process and low-cost additive engineering. On the other hand, MPIB is a Lewis base with a structure having a nitrogen atom on the cationic group imidazole, which can provide lone-pair electrons in the electron-deficient system. Thus, MPIB could serve as an additive to passivate the uncoordinated Pb$^{2+}$ in perovskite films.

Herein, we demonstrate how the MPIB additive can be successfully exploited for controlling the film morphology and reducing the defects by passivation of the uncoordinated Pb$^{2+}$ in the perovskite film through the interaction between the cations of MPIB and Pb$^{2+}$. The p–i–n architecture was employed in this work, as shown in Fig. 1b. A dense and homogeneous film was achieved when 0.5 mg mL$^{-1}$ MPIB additive was added into the perovskite precursor due to its high wettability. In addition, the introduction of the MPIB additive into the perovskite precursor enhances the PCE from initial 15.9% to 18.2%. This enhancement of the electrical performance is mainly attributed to the reduced defects due to the passivation of the uncoordinated Pb$^{2+}$ through the interaction between the cations of MPIB and the uncoordinated Pb$^{2+}$ in the perovskite film, which was supported by the XPS and FTIR measurements. Benefiting from the passivation of uncoordinated Pb$^{2+}$, the PSC with 0.5 mg mL$^{-1}$ MPIB additive retains 78% of its original PCE after storing the device in an atmospheric environment at room temperature for 150 hours. This work provides a facile approach to obtain a high-quality perovskite film by incorporating a MPIB additive into the perovskite precursor.

2. Experimental section

2.1. Materials

Methylammonium iodide (CH$_3$NH$_3$I), lead chloride (PbCl$_2$, >99.99%), lead iodide (PbI$_2$, >99.99%), PEDOT:PSS (Heraeus-Clevios PVP AI 4083), [6,6]-phenyl-C$_6$1-butyric acid methyl ester (PC$_6$1BM, >99%) and bathocuproine (BCP, >99%) were purchased from Xi’an Polymer Light Technology Corp. (China). 1MPIB (98%) was bought from TCI (Shanghai) Development Co., Ltd. All the solvents, including N,N-dimethylformamide (DMF), dimethyl sulfoxide (DMSO), ethyl alcohol, isopropanol (IPA) and chlorobenzene (CB), were purchased from Sigma-Aldrich. All the chemicals were used without further purification.

Fig. 1 (a) Chemical structure of MPIB. (b) Structure of the planar heterojunction p–i–n perovskite solar cell. (c) Schematic representation of the preparation processes of the MPIB-perovskite film.
2.2. Device fabrication

To prepare the perovskite precursor, 0.14 M PbCl₂, 1.26 M PbI₂ and 1.4 M CH₃NH₃I were simultaneously dissolved in a 1 mL co-solvent of DMSO and DMF (volume ratio = 1 : 9). The solution mixture was prepared in a glove box and stirred overnight at room temperature. To prepare the perovskite precursor with different concentrations of the MPIB additive, different weights of the MPIB additive were directly added into 1 mL perovskite precursor solutions (Fig. 1c). PC₆₀BM (20 mg) and BCP (0.5 mg) were dissolved in 1 mL of CB and 1 mL of ethyl alcohol, respectively, and then stirred overnight at room temperature before using. PEDOT:PSS was diluted with deionized water (volume ratio = 1 : 9) and stirred for 3 hours at room temperature.

The indium tin oxide (ITO) glass substrates were sequentially cleaned by using the detergent Decon 90, deionized water and ethanol in an ultrasonic machine (KQ3200DV) for 15 min, respectively, followed by drying with a N₂ flow. Once cleaned, the PEDOT:PSS solution was spin coated on the ITO substrate at 6000 rpm for 40 s, followed by annealing at 130 °C for 25 min in air. After this, the PEDOT:PSS film was cooled down at room temperature and transferred to a glove box for the next step. The perovskite films were deposited by a one-step method (Fig. 1c), that is, the perovskite precursor and MPIB-perovskite solution were spin cast onto the PEDOT:PSS layer at 400 rpm for 3 s and 4000 rpm for 25 s. When the precursor was rotated for 12 s, the anti-solvent of CB (170 μL) was dropped onto the film. The wet perovskite film was placed on a hotplate for annealing at 50 °C for 120 s and 85 °C for 25 min in the glove box, respectively. Then, the PC₆₀BM solution (20 mg mL⁻¹) was spin cast on the perovskite layer at a speed of 5000 rpm for 30 s followed by exposing to the ambient environment (Room temperature, humidity ≈25%) for 30 min to oxidize the PC₆₀BM. Finally, the BCP solution was spin-coated on the pre-formed PC₆₀BM film at 2000 rpm for 30 s in the glove box followed by depositing a 100 nm Ag electrode in a vacuum chamber (5 × 10⁻⁵ pa) by using a shadow mask.

To prepare the sample for Fourier transform infrared (FTIR) spectroscopy measurements, PbI₂ and MPIB were mixed in an ultrasonic machine (KQ3200DV) for 15 min, respectively, followed by drying with a N₂ flow. Once cleaned, the PEDOT:PSS solution was spin coated on the ITO substrate at 6000 rpm for 40 s, followed by annealing at 130 °C for 25 min in air. After this, the PEDOT:PSS film was cooled down at room temperature and transferred to a glove box for the next step. The perovskite films were deposited by a one-step method (Fig. 1c), that is, the perovskite precursor and MPIB-perovskite solution were spin cast onto the PEDOT:PSS layer at 400 rpm for 3 s and 4000 rpm for 25 s. When the precursor was rotated for 12 s, the anti-solvent of CB (170 μL) was dropped onto the film. The wet perovskite film was placed on a hotplate for annealing at 50 °C for 120 s and 85 °C for 25 min in the glove box, respectively. Then, the PC₆₀BM solution (20 mg mL⁻¹) was spin cast on the perovskite layer at a speed of 5000 rpm for 30 s followed by exposing to the ambient environment (Room temperature, humidity ≈25%) for 30 min to oxidize the PC₆₀BM. Finally, the BCP solution was spin-coated on the pre-formed PC₆₀BM film at 2000 rpm for 30 s in the glove box followed by depositing a 100 nm Ag electrode in a vacuum chamber (5 × 10⁻⁵ pa) by using a shadow mask.

To prepare the sample for Fourier transform infrared (FTIR) spectroscopy measurements, PbI₂ and MPIB were mixed in a DMF solution and stirred overnight in the glove box at room temperature. Then the sample powder was obtained by placing a DMF solution and stirred overnight in the glove box at room temperature. When the precursor was rotated for 12 s, the anti-solvent of CB (170 μL) was dropped onto the film. The wet perovskite film was placed on a hotplate for annealing at 50 °C for 120 s and 85 °C for 25 min in the glove box, respectively. Then, the PC₆₀BM solution (20 mg mL⁻¹) was spin cast on the perovskite layer at a speed of 5000 rpm for 30 s followed by exposing to the ambient environment (Room temperature, humidity ≈25%) for 30 min to oxidize the PC₆₀BM. Finally, the BCP solution was spin-coated on the pre-formed PC₆₀BM film at 2000 rpm for 30 s in the glove box followed by depositing a 100 nm Ag electrode in a vacuum chamber (5 × 10⁻⁵ pa) by using a shadow mask.

To prepare the sample for scanning electron microscopy (SEM, JSM-6700F) and X-ray diffraction (Shimadzu XRD-7000), respectively. Contact angle measurement was performed with a contact angle meter (POWEREACH, Shanghai Zhongchen Co., Ltd.). The FTIR spectra were recorded using a Thermo Scientific Nicolet 6700 FTIR spectrometer. XPS was performed on a Thermo Fisher ESCALAB 250Xi using a monochromatic Al Kα source and a pass energy of 50 eV at a base pressure of 1 × 10⁻⁸ mbar. The current density–voltage (J–V) characteristics were measured in the reverse direction (from 1.2 to −0.2 V) with a voltage step of 10 mV and 0 ms delay time by using a Keithley 2400 source measurement unit, coupled with a standard xenon-lamp-based solar simulator (Newport 94043A) to provide AM 1.5G irradiation (100 mW cm⁻²). Before measurement, the intensity of simulated solar light was calibrated by using a monocrystalline silicon reference solar cell. The external quantum efficiency (EQE) of the device was recorded by calculating the photocurrent and the light intensity with a lock-in technique.

3. Results and discussion

Fig. 2a shows the top-view SEM images of the perovskite films without and with the MPIB additive (hereafter abbreviated as the pristine perovskite and the MPIB-perovskite (x) respectively, where x is the concentration of the MPIB additive in the perovskite precursor with a unit of mg mL⁻¹) on the PEDOT:PSS layer.

A small average grain size (~200 nm) with some pinholes is observed in the pristine perovskite film, while the MPIB-perovskite (0.5) film exhibits a uniform and dense surface without any pinholes. In addition, the grain size gradually decreases upon further increasing the concentration of the MPIB additive in the perovskite film (see the top-view SEM images in Fig. S1†). The uniform and pinhole-free morphology in the MPIB-perovskite (0.5) film is possibly attributed to the low solid–liquid interfacial energy induced by the MPIB additive.35 Hence, a comparison of the contact angle between the pristine perovskite and MPIB-perovskite precursor solution has been carried out on the PEDOT:PSS film. As shown in Fig. 2b, the contact angles of the pristine perovskite precursor and MPIB-perovskite (0.5) precursor are about 19° and 11°, respectively. The higher wettability of the MPIB-perovskite (0.5) achieves a PCE of 18.2% with a Voc of 1.114 V, a Jsc of 24.3 mA cm⁻², and a FF of 0.81. On the other hand, the champion device of the pristine perovskite case, which seems to suppress the disordered crystal growth and provide well-distributed nucleation sites.36,37

The photovoltaic performances of the pristine perovskite device and MPIB-perovskite device have been investigated by employing a device structure of ITO/PEDOT:PSS/perovskite and MPIB-perovskite(x)/PC₆₀BM/BCP/Ag. The current density–voltage (J–V) characteristics of the pristine perovskite device and MPIB-perovskite (0.5) device under the illumination of AM 1.5G are presented in Fig. 3a. The pristine perovskite device exhibits a PCE of 15.9% with a short-circuit current (Jsc) of 19.20 mA cm⁻², an open-circuit voltage (Voc) of 1.028 V, and a fill factor (FF) of 0.81. On the other hand, the champion device of the MPIB-perovskite (0.5) achieves a PCE of 18.2% with a Voc of 1.114 V, a Jsc of 19.83 mA cm⁻², and a FF of 0.82. In other terms, an obvious enhancement of the photovoltaic performance has been observed in the MPIB-perovskite (0.5) device. This improvement is consistent with the result obtained from the external quantum efficiency (EQE) and integrated Jsc curves. There is no obvious hysteresis in both devices based on the p–i–n configuration, which can be ascribed to PCBM due to its important role in suppressing hysteresis.38,39 The lower
The hysteresis of the MPIB modified device compared with the pristine device can be attributed to the passivation effect of MPIB.

As evidenced in Fig. 3b, the calculated integrated $J_{SC}$ values of the pristine perovskite and MPIB-perovskite (0.5) device are 18.63 and 19.45 mA cm$^{-2}$, respectively. Undoubtedly, the integrated $J_{SC}$ of the MPIB-perovskite (0.5) device is higher than that of the pristine perovskite device, which is mainly attributed to the high-quality perovskite film. In our case, we successfully exploited the MPIB additive for controlling the film morphology and reducing the defects by passivation the uncoordinated Pb$^{2+}$. We believed that the reduction of carrier recombination is the major reason for the increased current density. On the other hand, it’s worth mentioning that the carrier recombination$^{46}$ and the quality of the perovskite film$^{47}$ have impacts on the FF. Overall, we believe that the improvement of all the performance parameters is due to the defect passivation in the perovskite by MPIB.

In addition, the high PCE of the MPIB-perovskite (0.5) device has been further confirmed by comparing the statistical data...
from 20 devices of the pristine perovskite and MPIB-perovskite (0.5) cases, as shown in Fig. S2.†

Furthermore, a series of PSCs with different MPIB concentrations have also been fabricated and measured, and their corresponding performance values are listed in Table 1. Obviously, the $V_{oc}$, $J_{sc}$, and PCE simultaneously increase by increasing the MPIB concentration from 0 to 0.5 mg mL$^{-1}$. However, further increasing the MPIB concentration leads to a decrease in the device performance, which can be ascribed to the reduction of the grain size and the increased density of grain boundaries in the films (Fig. S1†). It should be highlighted that the maximum PCE is achieved in the MPIB-perovskite (0.5) device. Hence, our further investigations have been carried out on the pristine perovskite device and MPIB-perovskite (0.5) device.

To understand the influence of the MPIB additive on the crystallinity of the perovskite film, X-ray diffraction (XRD) has been first carried out by comparing the pristine perovskite and MPIB-perovskite (0.5) film. As shown in Fig. 4a and S3,† the pristine perovskite film shows a small peak at 12°, which is mainly attributed to the residual PbI$_2$. In general, the residual PbI$_2$ originates from the incomplete growth of the perovskite crystal because of the fast but unbalanced reaction between PbI$_2$ and MAI during the annealing process. In contrast, no obvious peak at the same position is observed for the MPIB-perovskite (0.5) film, which indicates that the MPIB additive may be incorporated into the perovskite crystal and then remove the excess PbI$_2$. Another key issue is to understand the influence of the MPIB additive on the absorption of the perovskite. Therefore, the UV-vis absorption measurement was performed for the above two films. As reported in Fig. 4b, no obvious discrepancies have been observed in the absorption spectra between the pristine perovskite film and MPIB-perovskite (0.5) film. Such a behavior indicates that 0.5 mg mL$^{-1}$ MPIB additive in the perovskite film would not affect the optical absorption.

As stated before, a possible explanation for the improvement of the electrical performance in the MPIB-perovskite device is the reduced defects in this film due to the passivation of the uncoordinated Pb$^{2+}$. Aiming at confirming the above mechanism, we have performed a series of cross-checks. First, X-ray photoelectron spectroscopy (XPS) has been employed to check the binding energy of the Pb atom at the surface of the perovskite film. As shown in Fig. 5a and S3,† the binding energy of Pb 4f shifts by 0.2 eV to lower energy in the MPIB-perovskite when compared to that of the pristine perovskite case. A similar behavior has been observed by Wang et al. and Li et al., who attribute this shift to the binding energy change of the Pb atom due to the chemical interaction between 1-alkyl-4-amino-1,2,4-triazolium and uncoordinated Pb$^{2+}$. Thus, this indicates that the surface binding energy of Pb has been changed due to the addition of the MPIB additive in our case.

To further confirm that the passivation of uncoordinated Pb$^{2+}$ is due to the MPIB additive, we have performed Fourier transform infrared (FTIR) spectroscopy aiming to understand the change of the N atom in the MPIB additive. Three kinds of powder samples, including PbI$_2$, MPIB, and MPIB-PbI$_2$, have been prepared (see the Experimental section) and tested. As displayed in Fig. 5b and S4,† the stretching vibration of C=N at 1629 cm$^{-1}$ is observed for the MPIB sample. However, two absorption bands at 1618 cm$^{-1}$ and 1650 cm$^{-1}$ are recorded for the MPIB-PbI$_2$ sample. Kanatzidis and co-workers already showed that passivation of Pb$^{2+}$ responds in a similar manner to a thiazole additive, which can be ascribed to the chemical interaction of Pb=N. Therefore, in our case, both the red shift and the blue shift for the MPIB-PbI$_2$ sample are mainly associated with the splitting of the C=N band into two C=N bonds in the MPIB structure. In addition, it is found that the skeleton

<table>
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<th>Concentration (mg mL$^{-1}$)</th>
<th>$V_{oc}$ (V)</th>
<th>$J_{sc}$ (mA cm$^{-2}$)</th>
<th>FF (%)</th>
<th>PCE (%)</th>
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<tr>
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<tr>
<td>0.5</td>
<td>1.114</td>
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<tr>
<td>1.0</td>
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<td>2.0</td>
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<td>19.16</td>
<td>80.7</td>
<td>16.28(15.89 ± 0.60)</td>
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Table 1 Summary of the device performance with different concentrations of the MPIB additive

Fig. 4 (a) X-ray diffraction (XRD) patterns and (b) UV-vis absorption spectra of the pristine perovskite and MPIB-perovskite (0.5) films.
vibration peak of the aromatic ring (1572 cm⁻¹) is also split into two peaks at 1568 and 1560 cm⁻¹, which indicates that the electron cloud density of the imidazole ring has been changed. Considering these results, it can be unambiguously affirmed that the passivation of Pb²⁺ is due to the formation of a Pb–N bond in our case.

A schematic representation of the passivation process that took place between the lone-pair electrons and uncoordinated Pb²⁺ in the MPIB-perovskite sample is illustrated in Fig. 5c. In general, the passivation of uncoordinated Pb²⁺ leads to reduction of the defects in the perovskite film. Within this context, the photoluminescence (PL) test has been carried out on the pristine perovskite film and MPIB-perovskite (0.5) film. As shown in Fig. 5d, a strong PL intensity is observed in the MPIB-perovskite (0.5) film when compared to the pristine perovskite film, which confirms the defect reduction due to the passivation of uncoordinated Pb²⁺. In addition, in Fig. 5e, we compared the time-resolved photoluminescence spectra of the two samples. For the pristine perovskite film, τave was determined to be 38.8 ns. Upon MPIB addition, τave was increased to 91.7 ns for the optimized film, indicating fewer defects and less charge recombination in the MPIB-modified perovskites. Thus, we conclude that the Voc improvement may derive from the low non-radiative recombination of the perovskite film. 39

As demonstrated above, the passivation of uncoordinated Pb²⁺ has been successfully achieved by adding the MPIB additive in the perovskite precursor. Such promising results prompted us to deepen our knowledge of the stability of these MPIB-perovskite device. To the best of our knowledge, the stability is still a big challenging issue in the research field of PSCs. 45,46 Therefore, the stability test has been carried out on the pristine perovskite and MPIB-perovskite (0.5) devices. The stability test was conducted by occasionally measuring the device performance during the shelf storage of the devices. It should be highlighted that all the devices were stored in the atmospheric environment (RH = 40–60%, room temperature). As displayed in Fig. 6a, a total PCE of 52% was maintained after 150 hours by the pristine perovskite device, while the MPIB-perovskite device retained 78% of its original PCE after 150 hours. Clearly, the PCE of the MPIB-perovskite device undergoes a slow degradation than that of pristine perovskite device, which is mainly attributed to the passivation of uncoordinated Pb²⁺ in the former case. These results have been further confirmed by comparing the XRD and film color between the fresh and aged films of the above two cases. As shown in Fig. 6b, a sharp increase of the peak at 12° (related to PbI₂) is observed for the pristine perovskite film after 150 hours of storage under ambient conditions. In contrast, a little increase of the peak at the same position is found for the MPIB-perovskite (0.5) film after storing for the same duration. Furthermore, no obvious color change after 150 hours is observed in the MPIB-perovskite film, while a half of the surface of the perovskite crystals breaks down into PbI₂ and turns yellow in the pristine perovskite film after storing for the same hours. In addition, a similar stability experiment has been performed by storing the device in a glove box. As displayed in Fig. S5,† the pristine perovskite device retains 80% of its original PCE, while the MPIB-perovskite device retains 95% of its original PCE. To further expand our understanding of perovskite stability, we measured the tolerance of the device at high temperature. As shown in Fig. S6,‡ for the pristine perovskite device, 91% of its initial PCE was achieved after 85° heating on
a hot plate for 30 min. Under the same conditions, the MPIB device maintained 97% of its initial PCE. Undoubtedly, all the above results confirm that the MPIB additive is beneficial in improving the stability of the device thanks to the passivation of uncoordinated Pb$^{2+}$ in the MPIB-perovskite film.

4. Conclusions

In conclusion, we have incorporated the representative and simplest ionic liquid additive, MPIB, into the perovskite precursor solution to fabricate an inverted perovskite solar cell. A dense and homogeneous perovskite film without any pinholes has been obtained thanks to the high wettability of the MPIB-perovskite precursor. Remarkably, the PCE increases from 15.9% for the pristine perovskite device to 18.2% for the MPIB-perovskite (0.5) device.

This performance enhancement is mainly attributed to the reduced defects in the perovskite film due to the passivation of the uncoordinated Pb$^{2+}$ and the lone-pair electrons in the imidazole of MPIB, which has been solidly confirmed by the XPS and FTIR results. As a result, a prolonged stability has been achieved in the MPIB-perovskite (0.5) device because of the passivation of uncoordinated Pb$^{2+}$. Thus, in this work, the incorporation of the MPIB additive into the perovskite precursor solution provides an easy approach to obtain high-performance devices through reducing the defects by passivating the uncoordinated Pb$^{2+}$ in the perovskite film.

Conflicts of interest

There are no conflicts to declare.

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Notes and references