A facile surface passivation method for efficient inorganic CsPbI₂Br perovskite solar cells with efficiencies over 15%

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ABSTRACT Recently, perovskite solar cells (PVSCs) based on CsPbI₂Br have attracted increasing attention owing to their good balance between efficiency and stability. Solution-processed CsPbI₂Br perovskites usually contain various defects which need passivation for PVSCs with high-performance as well as good stability. Since the degradation of perovskite films usually begins at the grain boundaries, here we report a facile defect passivation strategy by spin-coating a KF solution on the CsPbI₂Br perovskite surface. The deposited KF salt mostly locates at the grain boundaries of the perovskite surface, resulting in PVSCs with improved stability. Both steady-state and time-resolved photoluminescence results suggest that the defects of perovskite were significantly passivated by KF treatment. Consequently, the best-performance PVSC based on CsPbI₂Br with KF treatment shows an enhanced power conversion efficiency (PCE) of 15.01% with a larger open circuit voltage (V_{OC}) of 1.26 V in comparison with the pristine CsPbI₂Br-based counterpart which exhibits an inferior PCE of 14.14% with a V_{OC} of 1.18 V.

Keywords: fluorides, energy conversion, perovskites, defect passivation, grain boundary

INTRODUCTION

In the past five years, organic-inorganic halide perovskite solar cells (PVSCs) have been widely investigated and they have become one of the most promising technologies to convert sunlight to electricity with low-cost solution processing [1,2]. Although the best power conversion efficiency (PCE) of organic-inorganic PVSCs has now exceeded 23% [1], the volatility and thermal instability of organic cations (e.g., $[(NH_2)_2CH]^+$, $CH_3NH_3^+$) can lead to the stability problems of PVSCs which limit their further

commercialization [3]. To solve this issue, an emerging approach is to develop all-inorganic perovskites which can be prepared by replacing the organic cations with inorganic cations (such as Cs⁺). Such all-inorganic cesium lead halide perovskites CsPbX₃ (X = Cl, Br, and I) do not readily decompose under heat and moisture conditions due to the absence of organic components. For example, the inorganic CsPbBr₃ perovskite is stable at temperatures up to 580 °C, while the organic CH₃NH₃PbI₃ decomposes at a temperature of around 200 °C [4]. Among all kinds of CsPbX₃ perovskites, CsPbI₃ and CsPbBr₃ were studied at the early stage of all-inorganic PVSC research [5,6]. The PVSCs based on CsPbBr₃ with PCEs up to 5.95% were firstly reported by Kulbak *et al.* [6] in 2015. However, its relatively large bandgap (E_g) of ~2.30 eV limits its sunlight-harvesting ability. In contrast, with a more suitable E_g of ~1.73 eV [7], CsPbI₃ perovskite has been used for the most efficient all-inorganic PVSC [8]. Unfortunately, black phase α -CsPbI₃ perovskite is unstable and will rapidly convert into a non-perovskite phase (δ -CsPbI₃) upon exposure to ambient atmosphere [7]. In 2016, both McGehee [9] and Snaith [10] groups reported that the optical absorption and the structural stability of CsPbX₃ can be adjusted by regulating the halogen composition. Meanwhile, they found that the phase stability and phase transition temperature can be adjusted by partial incorporation of Br into the CsPbI₃ perovskite. Starting with a surprising PCE of 9.8% for the CsPbI₂Br-based PVSCs reported by Sutton *et al.* [10] in 2016, more and more PVSCs based on bromide-containing mixed-halogen perovskites (CsPbI_{3-x}Br_x) have been reported [11–16]. Previously, our group reported a best PCE of 7.3% for all-inorganic PVSCs based on polyethylene glycol (PEG)-

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passivated CsPbI₂Br₂ with an E_g of 2.07 eV [17]. To enhance the light-harvesting ability of PVSCs, we further developed a Zn-doped CsPbI₂Br perovskite with an E_g of 1.88 eV. The resulting best-performance PVSC showed an impressive PCE of 12.16% [18]. Unlike CsPbI₂Br and CsPbI₃, CsPbI₂Br is able to achieve both good light-harvesting ability and good phase stability, suggesting that CsPbI₂Br is a promising active-layer material for PVSCs with its good balance between the efficiency and stability. In recent two years, many strategies have been reported for the fabrication of high-performance CsPbI₂Br-based PVSCs [11,12,19–23].

High-quality thin films are essential to achieve high-performance PVSCs. However, many defects and traps are inevitably formed in most perovskite films obtained from solution-processing techniques. Prior studies have demonstrated that the defects at the crystal surface and grain boundaries (GBs) will generate trap states and have a detrimental effect on the performance of PVSCs [24,25]. More importantly, it was found that the degradation of perovskite films usually begins at the GBs [26]. To improve the PCE and stability of CsPbI₂Br PVSCs, many defect passivation approaches have been proposed for the perovskite films [27–34]. Chemical doping is an effective way to control the crystallization speed and to passivate the defects of perovskite films. For example, by incorporating a small amount of Sr into CsPbI₂Br, the surface of CsPbI₂Br film was enriched with Sr, which provides a passivating effect on the defects of the films. The PCE was increased from 7.7% for the CsPbI₂Br-based device to 11.3% for the CsPb_{0.98}Sr_{0.02}I₂Br-based device [27]. Recently, Bai *et al.* [28] demonstrated that interstitial Mn²⁺ ions doped in the CsPbI₂Br film could lead to suppressed nucleation and a decreased growth rate, thus resulting in films with better crystallinity and larger grains. Moreover, the excess Mn²⁺ cations would aggregate in the grain boundary and passivate the surface defects. An improved PCE of 13.47% was eventually achieved for the PVSCs based on the 2% Mn-doped perovskite film [28]. More recently, Europium (Eu) and Indium (In) cations were also used to stabilize the black phase CsPbI₂Br perovskite [29,30]. Besides, smaller alkali metal cations (such as K⁺) [31] and some other anions (such as SCN[−], Ac[−]) [32–34] were also incorporated into the CsPbI₂Br film to increase the grain size, passivate the grain boundary, and improve the performance of the corresponding PVSCs. In addition to the interior defects, perovskite films also have a lot of surface defects which are harmful to the performance and stability of PVSCs. Thus, surface passivation is of high importance in order

to achieve high-efficiency PVSCs. As mentioned previously, some doping ions (such as Sr²⁺ [27], Mn²⁺ [28], and Zn²⁺ [18]) can be enriched on the surface of the CsPbI₂Br film and passivate the traps at the surface and GBs. Unlike other types of perovskites, new passivation materials for surface modification of CsPbI₂Br perovskites are relatively less explored. As far as we know, there are only a few reports about solution-processed surface passivation of CsPbI₂Br perovskite, in which bulky organic amines, Pb(NO₃)₂, and poly(3-hexyl-thiophene) (P3HT) were used to modify the perovskite surface [35–38]. For example, Yuan *et al.* [35] introduced a post-processing strategy with Pb(NO₃)₂ solution to passivate the CsPbI₂Br surface defects, resulting in reduced traps and decreased nonradiative recombination rate, thus leading to an improved PCE of 12.34%. Moreover, P3HT was shown to have a passivating effect on the surface defects, resulting in an improved PCE of 12.02% [36].

In this work, for the first time, potassium fluoride (KF) is used as a surface passivation agent for the CsPbI₂Br perovskite with suppressed surface defects. The surface modification can be achieved by a simple solution process which will not destroy the original morphology or cause new phase formation in the perovskite films. We found that the KF salt was preferentially deposited at the GBs of the perovskite surface. Thus, the defects of the perovskite were significantly reduced and the recombination was significantly suppressed. As a result, PVSCs based on the KF-treated CsPbI₂Br film achieved a PCE as high as 15.01% with a large open circuit voltage (V_{OC}) of 1.26 V. In contrast, the control device based on the pristine CsPbI₂Br film only showed an inferior PCE of 14.14% with a lower V_{OC} of 1.18 V. Additionally, the devices with the KF-treatment showed improved stability and reduced hysteresis in comparison with the control devices. The solution passivation strategy demonstrated in this work is promising for PVSCs considering the low-cost of KF as well as the simple solution processes.

EXPERIMENTAL SECTION

Materials

The SnO₂ colloid precursor was purchased from Alfa Aesar (Tin(IV) oxide, 15% in H₂O colloidal dispersion). Dimethyl sulfoxide (DMSO, anhydrous, 99.8%), chlorobenzene (anhydrous, 99%), acetonitrile (anhydrous, 99.8%) and isopropanol (anhydrous, 99.8%) were purchased from Acros. PbBr₂ (99%) and PbI₂ (99%) were purchased from Tokyo Chemical Industry (TCI). KF

(99.999%) was purchased from Aladdin. CsI (99.9%), 4-*tert*-butylpyridine (4-TBP), tris(2-(1*H*-pyrazol-1-yl)-4-*tert*-butylpyridine)cobalt(III) bis(trifluoromethylsulfonyl)imide (FK 209), and bis(trifluoromethane)sulfonimide lithium salt (Li-TFSI) were purchased from Xi'an Polymer Light Technology Corp. 2,2',7,7'-Tetrakis[*N,N*-di(4-methoxyphenyl)amino]-9,9'-spiro-bifluorene (Spiro-OMeTAD) was purchased from Shenzhen Feiming Science and Technology Co., Ltd.

Characterizations

Perovskite solar cells were measured in air (with relative humidity of ~60%) after a simple encapsulation by epoxy kits (general purpose, Sigma Aldrich) in the glove-box. The PVSCs were illuminated through their indium tin oxide (ITO) sides, and the active areas were fixed at 4 mm². The current density *versus* voltage (*J*-*V*) curves were recorded using a Keithley 2400 source measurement unit under AM 1.5 G irradiation (100 mW cm⁻²) from an Oriel Sol3A simulator (Newport) with an NREL certified silicon reference cell. The *J*-*V* curves were measured along the reverse scan direction from 1.3 to -0.2 V or the forward scan direction from -0.2 to 1.3 V. The step voltage and scan rate were fixed at 20 mV and 150 mV s⁻¹. For device stability testing, all the PVSCs were stored and periodically tested in air under ambient conditions. The ambient conditions for the device storage in air were the darkness, temperature of 25°C, and relative humidity of ~60%. External quantum efficiency (EQE) measurements were conducted by using a Newport EQE measuring system. UV-vis absorption spectroscopy was performed using a Lambda35 spectrophotometer. X-ray photoelectron spectroscopy (XPS) measurements were performed on an ESCALAB 250Xi X-ray photoelectron spectrometer (Thermo Fisher) using an Al K α source (15 kV, 10 mA). X-ray diffraction (XRD) spectra were measured by a Rigaku MiniFlex 600 diffractometer equipped with a Cu K α radiation. Top-view and cross-sectional scanning electron microscopy (SEM) images were recorded on a Hitachi SU-8010 scanning electron microscope. Atomic force microscopy (AFM) was conducted with a Bruker Nanoscope V station. The thickness of the film was measured by a Bruker Dektak XT surface profilometer. Photoluminescence (PL) and time-resolved PL (TRPL) were measured with an Edinburgh Instruments FLS 980 spectrometer equipped with a 450 W xenon lamp and a 60 W μ F flash lamp as the excitation sources. The impedance spectroscopy was measured with a CHI 660D electrochemical workstation in the dark at an applied voltage of 1.1 V with the frequency ranging between

1 MHz and 100 Hz.

Fabrication of perovskite solar cells

ITO/glass substrate was cleaned in sequence with detergent, deionized water, acetone and isopropanol under sonication for 20 min each and then dried in an oven. The SnO₂ colloid precursor diluted with H₂O (1:2) was spin-coated at 3000 rpm for 30 s onto the ITO substrates which were pretreated by UV-O₃ for 15 min. Then the substrate was annealed at 150°C for 30 min. After cooling, the substrates were transferred into a glove box for the preparation of the perovskite layer. To form the CsPbI₂Br precursor solution, CsI, PbBr₂ and PbI₂ with an appropriate molar ratio were dissolved in DMSO with a concentration of 1.2 mol L⁻¹. The precursor solution was then spin-coated onto the SnO₂/ITO/glass substrate. Next, the perovskite film was annealed at 42°C for 1 min and 160°C for 10 min. For the KF-treated film, KF/isopropanol solution (1.0 mg mL⁻¹) was dropped on the perovskite film and then spin coated at 5000 rpm for 20 s in a N₂-filled glovebox. The resulting film was annealed at 80°C for 10 min to remove the residual solvent. Subsequently, a Spiro-OMeTAD solution was spin-coated at 4000 rpm for 20 s as the hole transport layer. The Spiro-OMeTAD (72.3 mg) was mixed with 28.8 μ L of 4-TBP, and 29 μ L of FK 209 (300 mg mL⁻¹ in acetonitrile) in 1 mL of chlorobenzene to form the Spiro-OMeTAD solution. Finally, MoO₃ (10 nm) and Ag (100 nm) were deposited by thermal evaporation.

Fabrication and measurement of electron-only devices

Electron-only devices were fabricated with a device configuration of ITO glass/SnO₂/perovskite/phenyl-C61-butyric acid methyl ester (PCBM)/Ag. The resulting devices were tested by current-voltage measurements in the dark. The trap densities of the films were calculated by the formula of $n_{\text{trap}} = 2\epsilon\epsilon_0 V_{\text{TFL}}/eL^2$, where ϵ is the relative dielectric constant of perovskite, ϵ_0 is the vacuum permittivity, V_{TFL} is the onset voltage of the trap-filling limited (TFL) region, e is the electronic charge, and L is the thickness of the films.

RESULTS AND DISCUSSION

A schematic diagram of the preparation and surface modification process for the CsPbI₂Br film is presented in Fig. 1. The CsPbI₂Br films were deposited *via* a simple one-step spin-coating method. The as-prepared perovskite films were annealed at 160°C, and then the films were treated by spin-coating with a KF isopropanol solution. To confirm the existence of KF on the film of

Figure 1 Schematic diagram for the preparation and surface modification of CsPbI₂Br film.

perovskite, the surface compositions of the CsPbI₂Br films with and without post-treatment were studied by using XPS. As shown in Fig. 2a, b, for the KF-treated films, typical F 1s peak (located at 683 eV) and K 2p peaks (295 and 292 eV, respectively) are observed. Notably, the binding energy of Pb 4f shifts towards a higher binding energy (Fig. 2c), suggesting a possible interaction

between the F atoms and the Pb atoms. XRD measurements were carried out to evaluate the influence of the KF-treatment on the crystallinity and phase purity of the perovskite. The XRD patterns of the CsPbI₂Br films with and without post-treatment are shown in Fig. 2d. It can be found that the XRD patterns for both films are almost identical, both of which show three main peaks at 14.7° (100), 20.9° (110), and 29.7° (200), indicating the good crystallinity of the films and no new phase formed during the solution post-treatment. Likewise, the post-treatment has a negligible effect on the absorption spectra of the CsPbI₂Br films. The absorption edges for both films are ~650 nm (Fig. 2e), corresponding to the same E_g of ~1.90 eV.

Steady-state PL and TRPL spectra of the CsPbI₂Br films with and without post-treatment on the glass substrates are presented in Fig. 2f, g, respectively. The PL intensity for the perovskite with KF treatment is much higher than the counterpart without any treatment, indicating that the incorporation of KF could passivate the GBs and/or surface defects. Moreover, from the TRPL spectra (Fig. 2g), one can observe that the film with KF-treatment reveals a longer PL lifetime compared with the one without any post-treatment. Both the TRPL curves show a biexponential decay behavior, and the detailed TRPL parameters are listed in Table S1. The average lifetimes

Figure 2 (a) XPS spectra, (b) specific XPS spectra showing F 1s and K 2p peaks, (c) specific XPS spectra of Pb 4f, (d) XRD patterns, (e) absorption spectra, (f) steady-state PL, and (g) TRPL spectra of the perovskites without and with KF-treatment.

τ_{ave} increases from 92.9 to 564 ns when the CsPbI₂Br perovskites are treated with KF, suggesting a reduction in nonradiative recombination due to the passivation of defect density at the surface and/or GBs, which is favorable for obtaining an improved V_{OC} of the corresponding PVSCs.

To check the effect of KF-treatment on the morphologies of the CsPbI₂Br perovskite films, top-view SEM and AFM were carried out. As shown in Fig. 3a, c, fully covered pinhole-free films with large crystallized grains (200–800 nm) were observed for the CsPbI₂Br perovskites with and without KF treatment. After the post-treatment with KF, many small platelets with bright contrast could be observed at the GBs preferentially (Fig. 3c). To identify these bright platelets in SEM images are KF or not, we conducted energy-dispersive X-ray spectroscopy (EDS) of two regions on the perovskite film treated with KF (Fig. S1). The results show that the K and F signals are much stronger in the areas with more bright platelets than where the bright platelets are sparse. It can be speculated that the KF salt was preferentially deposited at the GBs and filled the valley between grains, thereby reducing the height difference between the grain surface and the grain boundary. This effect was further verified by the AFM results. As shown in Fig. 3b, d, the roughness of the perovskite layer was reduced from 22.3 to 13.4 nm after the KF-treatment. Water contact angles of two films were also measured (Fig. 3e, f). A larger contact angle of 67° was observed for the film treated with KF, in comparison with a contact angle of 47° for the control film without the KF treatment, which can be attributed to the hydrophobic nature of the fluorine atoms. It should be noted that the hydrophobic surface can protect the hydrophilic perovskite from the moisture which is harmful to the device stability.

To confirm the effectiveness of the KF-treatment, we fabricated planar n-i-p type PVSCs with a configuration of ITO/SnO₂/CsPbI₂Br/Spiro-OMeTAD/MoO₃/Ag. The device structure and the corresponding cross-sectional SEM image are shown in Fig. S2. Firstly, we searched for the optimal post-treatment condition by varying the concentration of KF from 0.5 to 2 mg mL⁻¹. The best-performance device was achieved for the KF treatment with a concentration of 1 mg mL⁻¹ (Table S2). The devices with the KF-treatment exhibited enhanced performance. Particularly, the V_{OC} increased from 1.18 to 1.26 V (1 mg mL⁻¹ KF). The enhanced V_{OC} after the KF-treatment can be attributed to the reduced nonradiative recombination induced by the passivation effect of KF on the surface defects. In order to eliminate the interference

Figure 3 Top-view SEM images of the perovskite films without (a) and with (c) KF-treatment. AFM images of the perovskite films without (b) and with (d) KF-treatment (RMS: root-mean-squared roughness). Contact angles of water drops on the surface of the perovskite films without (e) and with (f) KF-treatment.

of solvent, the control devices with pure isopropanol treatment were also fabricated. The results show that the treatment of isopropanol has a neglectable effect on the performance of PVSCs (Table S2). With the treatment by KF solution with a concentration of 1 mg mL⁻¹, an average PCE of 14.71% was obtained for the PVSCs, while the control devices only showed a lower average PCE of 13.95%. This improvement is due to the increased short circuit current density (J_{SC}) and V_{OC} values, both of which are related to the reduced defects on the surface and GBs of the perovskite active layer. The J - V curves of the best-performance PVSCs based on CsPbI₂Br with and without KF-treatment are shown in Fig. 4a, and the detailed photovoltaic parameters of the corresponding PVSCs are summarized in Table 1. After the KF treatment, the best-performance device showed a PCE of 15.01% with a V_{OC} of 1.26 V, a J_{SC} of 15.89 mA cm⁻², and a fill factor (FF) of 75.18%, under the reverse scan. In comparison, the best-performance PVSC without the post-treatment only showed a PCE of 14.14% with a J_{SC} of 15.11 mA cm⁻², a V_{OC} of 1.18 V, and an FF of 79.17%. Both the reverse and forward scans of the PVSCs are shown in Fig. S3. A reduced hysteresis effect was observed for the device with the KF-treatment which may be related to the fewer traps

Figure 4 (a) J - V curves, (b) EQE spectra and the corresponding integrated J_{sc} curves of the champion PVSCs. (c) PCE statistical distribution histograms of PVSCs. (d) Normalized PCEs as a function of the storage time in dark.

Table 1 Detailed photovoltaic properties of the PVSCs based on CsPbI_2Br without and with KF-treatment

	Sweep	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF	PCE (%)	Average PCE (%)
Without KF	Reverse	1.18	15.11	79.17	14.14	13.95 $\pm$ 0.12
	Forward	1.08	15.07	54.63	8.92	
With KF	Reverse	1.26	15.89	75.18	15.01	14.71 $\pm$ 0.16
	Forward	1.21	15.88	55.23	10.59	

on the perovskite surface after the KF passivation. The steady-state output characteristics of devices without and with KF-treatment at maximum power point are shown in Fig. S4. The stabilized PCEs of the CsPbI_2Br and KF-treated CsPbI_2Br PVSCs are approximately 12.41% and 13.52%, respectively. The low stable power output (SPO) value indicated that there was hysteresis behavior of the device. EQEs of the best-performance PVSCs with and without KF-treatment were measured to verify the accuracy of the J_{sc} measurements. The obtained EQE spectra and the corresponding integrated J_{sc} curves are shown in Fig. 4b. The CsPbI_2Br -based PVSC with KF-treatment exhibits improved EQEs in the range from 380 to 640 nm compared with the one without post-treatment. The integrated J_{sc} values for the devices with and without KF

treatment are 15.10 and 14.38 mA cm^{-2} , respectively, which are in agreement with the measured values (J - V curves) within 5% errors. The PCE distributions of 20 devices with and without KF treatment are shown in Fig. 4c. No matter with the KF treatment or not, PVSCs show a narrow PCE distribution, indicating a good reproducibility of the CsPbI_2Br -based devices. In the meantime, the shelf-life stability of the best-performance PVSCs was investigated, and the result is shown in Fig. 4d. It is shown that the PCE for the device based on CsPbI_2Br with the KF treatment maintained 70% of its initial value after a storage for 11 days, while the PCE for the PVSC based on the pristine CsPbI_2Br decreases dramatically to 13% of its initial PCE during the same period's storage. This shelf-stability improvement is related

Figure 5 (a) Current-voltage characteristics of the electron-only devices with and without KF-treatment. (b) Nyquist plots of the PVSCs with and without KF-treatment.

to the more hydrophobic nature of the perovskite film after the introduction of fluoride ions, which is evidenced by the enlarged contact angle after the KF treatment (Fig. 3e, f).

To further assess the trap density of the PVSC films with and without KF-treatment, electron-only devices with a structure of glass/ITO/SnO₂/CsPbI₂Br/PCBM/Ag were fabricated. The trap densities were estimated by the space charge-limited-current (SCLC) method [39]. Typical dark current-voltage curves of electron-only devices with and without the KF-treatment are illustrated in Fig. 5a. It is clear that the current increases linearly at low bias voltages and then increases quickly when the bias voltage exceeds a certain value. This value at the kink point is known as the trap-filled limit voltage V_{TFL} . It can be seen that the V_{TFL} decreases from 0.42 V for the control device to 0.26 V for the KF-treated device. It means that the device with surface modification has a lower trap density ($3.85 \times 10^{15} \text{ cm}^{-3}$) compared with the trap density of $6.22 \times 10^{15} \text{ cm}^{-3}$ for the device without the KF modification. The decrease in trap density reconfirms the passivation effect of KF, which is in accord with the PL and TRPL results. Fig. 5b shows the Nyquist plots from the impedance spectroscopy measured in the dark with an applied voltage of 1.1 V. Generally, the low frequency region in the Nyquist plot is related to the recombination resistance (R_{rec}) [40–42]. The series resistance (R_s), transport resistances (R_{tr}) and R_{rec} were extracted by fitting the Nyquist plots with simplified equivalent circuit model (Fig. S5). As can be observed in Fig. 5b, the low-frequency region clearly suggested that recombination resistance was improved notably for the KF-treated device, indicating that the charge recombination was effectively suppressed by the passivation effect of KF. The result is consistent with the change in the performance of

corresponding devices.

CONCLUSIONS

In summary, we have demonstrated the use of KF as a surface modifier for all-inorganic CsPbI₂Br perovskite to enhance the performance and stability of the corresponding PVSCs. We have shown that the deposited KF gathered at the GBs of the perovskite surface can reduce the nonradiative recombination and trap density of the perovskite film. As a result, an improved PCE of 15.01% with a high V_{OC} of 1.26 V was achieved for the PVSCs based on the CsPbI₂Br with the simple solution post-treatment processing. In contrast, the control device without the treatment only showed a PCE of 14.14% with a V_{OC} of 1.18 V. Furthermore, improved storage stability and reduced hysteresis index were also achieved for the best-performance PVSC based on CsPbI₂Br with the KF treatment compared with the control device. This simple low-cost passivation strategy would be quite useful for high-performance and stable CsPbI₂Br-based PVSCs, and it could be applied for other all-inorganic PVSCs as well.

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Supplementary information Supporting data are available in the online version of the paper.

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高效无机CsPbI₂Br钙钛矿太阳能电池表面钝化的简便方法

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摘要 近年来, 基于CsPbI₂Br的钙钛矿太阳能电池(PVSC)由于能在效率和稳定性之间获得良好平衡而受到越来越多的关注. 通过溶液法制备的CsPbI₂Br钙钛矿薄膜通常包含各种缺陷, 为了获得具有高性能和良好稳定性的钙钛矿太阳能电池, 这些缺陷需要被钝化. 针对此问题, 本文报道了一种简便的缺陷钝化策略, 即通过在CsPbI₂Br钙钛矿表面旋涂KF溶液来对其进行缺陷钝化. 结果表明, 沉积的KF大部分位于钙钛矿表面的晶界处, 而钙钛矿膜的降解通常始于晶界, 因此钝化后的PVSC具有更高的稳定性. 稳态和时间分辨光致发光光谱均表明钙钛矿的缺陷被KF显著钝化了. 最终, 基于KF处理的CsPbI₂Br的电池器件能量转换效率(PCE)提高到了15.01%, 同时具有较大的开路电压(V_{OC} , 1.26 V). 与之相比, 基于CsPbI₂Br的对照器件的PCE仅为14.14%, V_{OC} 只有1.18 V.