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A tin-based perovskite solar cell with an inverted hole-free transport layer to achieve high energy conversion efficiency by SCAPS device simulation

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Abstract:

Recently, organic-inorganic halide perovskite solar cells (PSCs) have received extensive research in the field of optoelectronic materials due to their unique optical and electrical properties, especially lead-based PSCs. However, the toxicity and stability of these devices, as well as the expensive hole transport layer (HTL) and other factors inhibit their commercial production. In this work, the non-toxic tin was applied as the battery material, the perovskite solar cell adopts an inverted HTL-free structure, and the one-dimensional solar cell capacitor simulator SCAPS-1D (Solar Cell Capacitance Simulator) was adopted for numerical simulation and found that FTO/CH₃NH₃SnI₃/C₆₀/Au structure PSCs also showed excellent photovoltaic performance. We studied the influence of the thickness of the absorber layer, the defect density, the doping concentration of different layers, and the thickness of the electron transport layer (ETL) under different directions of illumination on the battery performance. The simulation results show that the optimized inverted HTL-free tin-based PSCs based on C₆₀ are with inspiring performance: a short-circuit current density (J_{sc}) of 30.1646 mA/cm², open-circuit voltage (V_{oc}) of 1.0465V, fill factor (FF) of 59.49% and power conversion efficiency (PCE) of 18.78%. We also introduced light from different directions to irradiate PSCs, and the results show that the HTL-free perovskite adopting an inverted structure can retain the light intensity of the irradiated perovskite layer to the greatest extent and exhibit superior performance. Based on the inverted HTL-free tin-based PSCs, we also investigated the performance parameters of ETL batteries with different materials. This work provides new ideas for PSCs development in the future.

Keywords: Tin-based perovskite; Inverted structure; HTL-free; SCAPS-1D

1. Introduction

In recent years, PSCs have attracted great attention due to their simple structure [1,2], low preparation cost [3], suitable and adjustable band gap [4,5], high extinction coefficient [6,7], bipolar carrier transmission characteristics [8,9] and flexible devices [10]. The energy conversion efficiency has been improved from 3.8% [11] to 25.2% [12]. Such a speed of development is unprecedented in the photovoltaic field. Although the current research on PSCs has achieved remarkable results, these perovskite materials used to absorb sunlight contain the toxic heavy metal lead, which is not friendly to the environment. This will undoubtedly limit the large-scale application of PSCs in the future, so there is an urgent need for development of new green and environmentally friendly lead-free PSCs.

Tin-based perovskite has even better photoelectric properties than lead-based perovskite, such as high absorption coefficient, small exciton binding energy and high carrier mobility, etc., which is currently the strongest candidate [13-16]. According to the Shockley-Queisser limit theory [17], the highest efficiency of a single solar cell is 33% corresponding to an absorption band gap of 1.34 eV. The absorption band gap of lead halide perovskite is generally larger in the range of 1.5-1.8 eV, while that of tin-based perovskite is narrower in the range of 1.3 eV, which is very close to the ideal value of 1.34 eV. Therefore, tin-based PSCs are expected to obtain higher short-circuit current density and reach the theoretical limiting conversion efficiency.

In contrast to the rapid development of lead-based PSCs, the PCE of tin-based PSCs has not seen a major breakthrough since 2014. Only in recent years has it been raised to nearly 10%. There are several possible reasons for this: (1) Sn^{2+} is unstable and very easy to be oxidized into Sn^{4+} or become vacancies, which causes the concentration of holes in the perovskite to increase sharply and lose its original semiconductor characteristics; (2) The crystallization rate of tin-based perovskite is fast at room temperature, and it is difficult to synthesize uniform and be completely coated tin-based films without additives; (3) Most lead-free tin-based PSCs usually adopt a regular battery structure, in which HTL is deposited on the tin perovskite layer, and HTL with high performance usually contains lithium (Li) or cobalt (Co) salts, which destroy the thin film of tin-based perovskite and in turn leads poor device performance.

With a special design, PSCs inverted structure (p-i-n) has some the advantages: the reverse structure has good stability and the J-V hysteresis effect is weak. HTL takes up nearly half of the cost of PSCs, so it is important to develop HTL-free PSCs to address the issue of manufacturing

cost [2]. The inverted HTL-free PSCs are expected to ensure the light intensity of the irradiated perovskite layer to the greatest extent to get better performance. In this work, we design and develop a simple inverted HTL-free tin-based PSCs structure, FTO/CH₃NH₃SnI₃/C₆₀/Au, which is non-toxic, no HTL to destroy the perovskite absorption layer film, and can reduce manufacturing costs and guarantee the light intensity irradiated on the perovskite layer, so that higher battery power conversion efficiency has been achieved.

2. Methodology

PSCs model is established in this work through theoretical methods to analyze the influencing factors of PSCs so as to optimize its performance, which is conducive to avoiding experiment duplication and reducing resource waste. In the process of simulating and optimizing solar cells, SCAPS-1D software developed by M. Burgelman of the University of Gent in Belgium is applied, which is suitable for simulating cells with various homojunction and heterojunction structures. Its basic principle is to solve the Poisson equation and current continuity equation under these constraints based on the established battery structure model and the input material parameters [18,19].

$$\begin{aligned} \nabla \cdot \epsilon \nabla \phi &= -q(p - n + N_D - N_A) \\ -\nabla \cdot J_p &= q(R - G) + q \frac{\partial p}{\partial t} \\ \nabla \cdot J_n &= q(R - G) + q \frac{\partial n}{\partial t} \end{aligned} \quad (1)$$

By setting the material parameters and corresponding boundary conditions, the above equations are solved with SCAPS-1D software through numerical calculations to obtain the relevant characteristics of the solar cells. Where, ϕ is the electric potential, p and n are the concentration of free carrier holes and electrons, J_n and J_p are electron current density and hole current density, R and G are the recombination rate and generation rate of electron hole pairs, N_A and N_D represent the acceptor and donor doping concentration.

2.1 Device structure and simulation parameters

The device structure diagram and energy band structure diagram of inverted HTL-free tin-based PSCs are shown in Fig. 1 (a) and (b). The cell is composed of glass substrate/transparent conductive oxide (FTO)/ absorption layer (CH₃NH₃SnI₃) / electron transport layer (C₆₀) / metal back contact (Au). As well known, exact values of the parameters are generally difficult to obtain,

so we carefully selected relatively reasonable parameters of FTO, ETL and perovskite absorption layer based on the available simulation literatures and reported experimental results of tin-based PSCs. Table 1 includes the basic physical and device parameter settings of each layer [20-25]. ϵ_r is the relative permittivity, χ is the electron affinity, E_g is the band gap energy, μ_n and μ_p are the electron mobility and hole mobility, and N_t is the defect density. The thermal velocities of the electrons and holes are set to 10^7 cm/s. The defect state in the absorption layer is set to a neutral Gaussian distribution, and the characteristic energy is 0.1 eV, and the defect energy level is in the middle of the band gap. The trapping cross-section of electrons and holes in the absorption layer is 2×10^{-14} cm², and the trapping cross-section of electrons and holes in other layers is 1×10^{-15} cm². Taking into account the carrier recombination at the interface, an interface defect layer is added between the FTO/absorption layer and the absorption layer/electron transport layer. The energy distribution of the interface defect layer is set as a single neutral defect, and the trapping cross section of the defect is 1×10^{-15} cm², and the total defect density is 1×10^{18} cm⁻³, which is located 0.6 eV above the top of the valence band. Table 2 lists the defect density inside and at the interface of the light-absorbing layer. In this simulation, the surface of each layer and the optical reflection of the interface between the layers are not considered.

Fig. 1. (a) Device configuration of simulated PSC, (b) Energy band diagram of the device

Table 1. Basic parameters of each layer of the device

Parameters	FTO	FASnI ₃	C ₆₀
Thickness (nm)	500	500	30
Band gap (eV)	3.5	1.3	1.7
Electron affinity (eV)	4.0	4.17	3.9
Dielectric Permittivity	9	8.2	4.2
CB effective density of states (cm ⁻³)	2.20×10^{18}	1.0×10^{18}	8×10^{19}

VB effective density of states (cm⁻³)	1.80×10^{19}	1.0×10^{18}	8×10^{19}
Electron mobility (cm²/Vs)	20	1.6	0.08
Hole mobility (cm²/Vs)	10	1.6	0.0035
Shallow donor density N_D (cm⁻³)	1.00×10^{19}	0	0
Shallow Acceptor density N_A (cm⁻³)	0	1.0×10^{17}	1.0×10^{18}
Defect density N_t (cm⁻³)	1.00×10^{15}	1.0×10^{16}	1.0×10^{15}
Electron Thermal Velocity cm/s	10^7	10^7	10^7
Hole Thermal Velocity cm/s	10^7	10^7	10^7

Table 2. Defect density values inside the absorber layer and at interface of the device

Parameters	FTO/ CH₃NH₃SnI₃	CH₃NH₃SnI₃/C₆₀	CH₃NH₃SnI₃
Defect type	Neutral	Neutral	Neutral
Capture cross section for electron and holes (cm⁻²)	1.00×10^{-15}	1.00×10^{-15}	2.00×10^{-14}
Energetic distribution	Single	Single	Gaussian
Energy level with respect to E_v	0.6	0.6	0.65
Characteristic energy (eV)	0	0	0.1
Total density (cm⁻³)	10^{18}	10^{18}	1.0×10^{15}

2.2 Simulation analysis of the proposed device

According to the initial parameters given in Table 1 and Table 2, Fig 2 shows the calculated energy band diagram (a), current density-voltage (J-V) curve (b) and quantum efficiency (QE) curve (c). The reflection of each functional layer and interface and the additional series resistance caused by FTO or back contact are not considered. The energy band diagram in Fig 2 (a), E_v (eV), F_p (eV), F_n (eV), E_c (eV) represent the highest energy level of the valence band, the hole Fermi level, and the electron Fermi level and the lowest energy level of the conduction band, respectively. LUMO level of C₆₀ matches with the conduction band minimum of absorber layer, so efficient electron transport can happen from FASnI₃ to Au electrode. HOMO level of C₆₀ is also lesser than that of valance band maximum of perovskite, so there is no hole transportation from FASnI₃, i.e., holes are blocked effectively. In this way, charge recombination at interface is prevented and photovoltaic performance is in turn improved. Fig 2(b) is based on the initial parameters of the above table1,2, and it demonstares that the simulated V_{oc} =0.8291 V, J_{sc} =19.5411 mA/cm², FF=64.33%, and PCE=10.42%, which are close to the experimental data in the literatures as shown in Table 3, proving the effectiveness of the simulation. The quantum efficiency (QE) curve

shown in Fig 2(c) is also the simulated result under the same parameters. Based on the analysis of the data shown in Fig.2, the band gap of $\text{CH}_3\text{NH}_3\text{SnI}_3$ is 1.3eV, which is narrower than the 1.55eV of $\text{CH}_3\text{NH}_3\text{PbI}_3$, so that the absorption wavelength of tin-based perovskite is shifted to 950nm. The range of the external quantum efficiency curve covers the entire visible spectrum, and the absorption from 360nm to 750nm is the strongest, exceeding 50%, which is consistent with the PCE spectrum measured in the literature [31]. The red-shifted external quantum efficiency curve is more conducive to light absorption in the infrared wavelength range.

Fig 2. (a) Energy band diagram (b) Current density-voltage (J-V) (c) Quantum efficiency (QE)

Table 3. Experimental data in the literature

Voc (eV)	Jsc (mA/cm2)	FF (%)	PCE (%)	Reference
0.8291	19.5411	64.33	10.42	This work
0.4700	22.4500	67.80	7.09	[26]
0.4650	22.0700	60.67	6.22	[27]
0.4700	20.0700	74.00	6.98	[28]

0.5200	20.0000	71.60	7.40	[29]
0.4500	24.8700	63.00	7.05	[30]

3. Results and discussion

The following results and discusses are based on the simulation results.

3.1 Effect of changing absorption layer parameters

For PSC, the spectral response of the device is highly dependent on the thickness of the absorption layer, which has a great influence on the overall performance of the device. The absorption layer thickness varies from 50nm to 700nm, and other input parameters are shown in [Table 1](#) and [Table 2](#). First, J-V curves of devices with different absorption layer thickness are obtained, as shown in [Fig 3 \(a\)](#). When the absorption layer is 550nm and 700nm, their J-V curves almost coincide. As shown in the inset of [Fig 3\(c\)](#), V_{OC} increases as the thickness of the absorbing layer increases, and increases significantly before the thickness of the absorbing layer reaches 400nm, after which the V_{OC} curve tends to be flat and even has a downward trend as the thickness of the absorbing layer continues to increase (More absorption layer thicknesses are not listed here), indicating that a thicker absorption layer thickness can increase charge recombination. The carrier number of the perovskite absorption layer increases with the increase in thickness, and the PCE and short-circuit current density J_{sc} also increase. When the thickness reaches 550nm, the curve tends to be flat. As the thickness of the perovskite absorption layer increases, the thicker perovskite absorption layer can absorb more photons and thus produce more excitons. However, excessive absorption layer thickness may lead to the increase of harmful recombination and diffusion length, and finally the PCE curve tends to flatten or even decline. If the thickness of the absorption layer is greater than diffusion length of the carrier, the carriers may recombine before reaching the metal electrode. Based on the above analysis, the optimal value of the absorption layer thickness is 550nm. [Fig 3\(b\)](#) depicts the influence of the thickness change of the absorption layer on the QE (%) changing with wavelength. As the thickness increases, more long-wave external quantum efficiency increases and the absorption becomes stronger, so the carrier extraction increases.

Fig 3. Change the thickness of the absorption layer: (a) J-V, (b) quantum efficiency (QE), (c) PCE (the illustration shows the V_{oc}, J_{sc} and FF)

Tin-based PSCs are in an unfavorable self-doping process, and their unstable oxidation state Sn²⁺ is easily oxidized to a stable Sn⁴⁺ oxidation state at room temperature. In this work, the doping concentration of CH₃NH₃SnI₃ absorption layer varies from 10¹⁴cm⁻³ to 10¹⁸cm⁻³, and the optimized V_{oc}, J_{sc}, FF and PCE are 0.7690V, 24.8115 mA/cm², 62.61% and 11.95% respectively when N_A is 10¹⁶cm⁻³, as shown in Fig. 4 (a) and (b). With the increase of doping concentration in the absorption layer, the electric field inside the perovskite layer also increases. The enhancement of electric field promotes the separation of charge carriers, which leads to the improvement of photovoltaic performance and PCE curve shows an upward trend. However, the main interference

factor is that with the increase of doping concentration, unnecessary recombination process may be increased. When the doping concentration of the absorption layer is increased, that is, more than 10^{16}cm^{-3} , it is easy to increase the photon recombination, and the PCE curve shows a downward trend. Only proper doping concentration can improve J_{SC} and V_{OC} well, and then improve the energy conversion efficiency. Therefore, it is necessary to adjust the N_A at a reasonable doping concentration.

(a)

(b)

Fig 4. Changing the doping concentration N_A : (a) J-V, (b) PCE, V_{OC} , J_{SC} and FF

In order to further improve the performance of the battery, another important influencing factor, the defect density of the perovskite layer, is investigated. The morphology and quality of $CH_3NH_3SnI_3$ thin films have recently been considered to be an important factor in determining the performance of PSCs. The photogenerated electrons and charge recombination behavior play a leading role in the V_{OC} , J_{SC} , FF and PCE of the device. The tin-based perovskite film covering the electron transport layer was observed to have poor film quality, the recombination of carriers in the perovskite light absorption layer will dominate. The poor quality film means that the perovskite absorption layer has a greater defect density (N_t). The effect of perovskite defects density on battery performance is studied based on Shockley-read-Hall composite model (SRH). The simulated defect is set to a neutral Gaussian distribution with a characteristic energy of 0.1 eV, which is located in the middle of the band gap. The SRH composite model is as follows:

$$R = \frac{np - n_i^2}{\tau_p (n + N_c e^{(E_g - E_t)/kT}) + \tau_n (p + N_v e^{E_t/kT})} \quad (2)$$

where n and p are electron and hole concentration respectively, which can be obtained by solving Poisson's equation and continuity equation. In order to obtain sufficient forward bias, $qV > 3kT$, we can ignore n_i^2 . E_t and N_t are the energy level and density of defects, respectively. τ_n and τ_p are the lifetimes of electrons and holes respectively. The parameters are modified by changing the defect density from 10^{12}cm^{-3} to 10^{16}cm^{-3} . As shown in Fig 5, when the defect density is below 10^{13}cm^{-3} , the defect density does not have a great influence on PCE and other parameters. Beyond this value, all parameters begin to be seriously affected. Obviously, the existence of defects in the perovskite film does lead to a significant decrease in all photovoltaic parameters. The higher the defect density, the higher the recombination rate and the less the number of conductive carriers.

Fig 5. Changing the defect density N_t : (a) J-V, (b) quantum efficiency (QE), (c) PCE (the illustration shows the V_{oc} , J_{sc} and FF)

3.2 Research on PSCs under different light conditions

In order to verify that the inverted structure is more conducive to improving the photovoltaic performance of HTL-free tin-based PSCs, it was studied under different lighting conditions and the results are shown as Fig. 6 (the input parameters are shown in Table 1 and Table 2). The light irradiated from both sides of FTO and Au was simulated, being with other parameters unchanged. It is worthy being noted that it is difficult to achieve in a practical device due to the visible reflectivity of the gold electrode, whereas it is very easy to achieve in the simulation of the SCAPS program. With the SCAPS program, the basic parameter of the gold electrode is its work

function, which is not absolute and essentially contains other parameters such as band gap, light absorption coefficient, and etc. As an electrode, gold can be regarded as a transparent material in the ultraviolet-visible wavelength range, and its work function is 5.1 eV. Therefore, we can theoretically discuss and simulate the light irradiated from the Au side.

The J-V curves and V_{oc} , J_{sc} , FF and PCE curves of light irradiated from the Au side corresponding to different C_{60} thickness are shown in Fig. 6 (a) and (c). The thickness of electron transport layer C_{60} is between 10nm and 100nm. The graphs of light irradiated from the FTO side corresponding to different C_{60} thicknesses are shown as Fig 6 (b) and (d). From Fig (b) and (d), it is obvious that J-V curves corresponding to different C_{60} thicknesses almost coincide when light is irradiated from the FTO side, and V_{oc} , J_{sc} , FF and PCE curves tend to be horizontal, with slight fluctuations at about 3.4V, 19.85mA/cm², 21.7% and 14.65%, respectively. When light is irradiated from the Au side, J-V curves corresponding to different C_{60} thickness are different. With the increase of C_{60} thickness, V_{oc} , J_{sc} and PCE all show a downward trend, and the maximum PCE is 2.34%. In conclusion, when the light irradiated from the FTO side, C_{60} thickness has little effect on the photovoltaic performance of inverted HTL-free tin-based PSCs, and the PCE is higher. When the opposite light is irradiated from the Au side, C_{60} thickness has a great influence on the photovoltaic performance of inverted HTL-free tin-based PSCs, and the PCE is low. The results show that when the light reaches the absorption layer through ETL, there is a partial loss of light intensity. On the basis of HTL-free, PSCs with the inverted structure achieve to keep the light intensity of the irradiated perovskite layer to the greatest extent, possessing showing better photovoltaic performance.

(a)

(b)

Fig 6. When light is irradiated from the Au side (FTO side), change the thickness of C_{60} to get the J-V and V_{OC} , J_{SC} , FF, PCE ((a), (c) is the light irradiated from the Au side. (b), (d) is the light irradiated from the FTO side)

3.3 Effect of changing the doping concentration of FTO N_D

For an inverted HTL-free tin-based PSC, the FTO directly contacts the perovskite layer. Therefore, it is of great significance to study the effect of FTO properties (such as doping concentration) on the performance of the device. Such detection helps to further control the physical parameters of FTO to improve the efficiency of the device. Fig 7 (a) and (b) show the curves of J-V and V_{OC} , J_{SC} , FF, PCE under different FTO doping concentration N_D . It can be obtained from Fig 7(a) that when the doping concentration is lower than 10^{18} cm^{-3} , the simulated J-V curve is strange and the device performance is poor. It may be because FTO is not suitable for electrodes due to its low conductivity. When N_D reaches 10^{18} cm^{-3} , the simulated J-V curve becomes better. When N_D is greater than 10^{19} cm^{-3} , the J-V curve becomes overlapping and fuzzy, and the V_{OC} , J_{SC} and PCE values tend to stabilize. It is worthy being noted that as the doping concentration increases, the conductivity of FTO may inevitably increase due to the increase in carrier concentration, and the strong absorption of these additional carriers reduce the visible light transmittance of FTO. The final optimized value N_D is determined as 10^{19} cm^{-3} .

Fig 7. Different doping concentration N_D : (a) J-V; V_{oc} , J_{sc} , FF, PCE

Based on the optimization analysis of the above-mentioned various layer parameters, the optimized values determined finally are shown in Table 4: the thickness of the absorption layer is 550nm, the doping concentration is $1.00 \times 10^{16} \text{ cm}^{-3}$, and the defect density is $1.00 \times 10^{15} \text{ cm}^{-3}$. The FTO doping concentration is $1.00 \times 10^{19} \text{ cm}^{-3}$. The thickness of the ETL is 30 nm. Fig 8 shows the J-V curve and quantum efficiency (QE) curve obtained from the final optimized values (refer to Tables 1 and Tables 2 for other parameters), where $V_{oc}=1.0465\text{V}$, $J_{sc}=30.1646\text{mA/cm}^2$, $FF=59.49\%$, and $PCE=18.78\%$.

Table 4 Final parameter optimization values

Optimized Parameters	Thickness (nm)	Doping Density (cm ⁻³)	Defect Density (Nt) (cm ⁻³)
Absorber	550	1.00×10^{16}	1.00×10^{15}
FTO	—	1.00×10^{19}	—
ETL	30	—	—

Fig 8. J-V curve and quantum efficiency (QE) curve obtained from the final optimized value

3.4 Other ETL candidates

In addition to C_{60} as the electron transport layer, there are other materials that can be used as the ETL of the inverted hole-free tin-based PSC. Fig 9 shows the energy band structure diagram of the different ETL and the optimized J-V curve diagram. Table 5 summarizes the performance comparison of different ETL devices, including important parameters of V_{OC} , J_{SC} , FF and PCE. When C_{60} is used as ETL, PCE reaches 18.78%, PCBM also shows excellent photovoltaic performance, while other materials CdS, IGZO and ZnO show relatively weak photovoltaic performance. Fig 10 is a bar graph comparing the performance of different ETL devices.

Fig 9. Different ETL energy band structure diagram and optimized J-V curve diagram

Table 5 Performance comparison of different ETL devices

	Voc (eV)	Jsc (mA/cm2)	FF (%)	PCE (%)
C_{60}	0.8755	30.1646	71.11	18.78
PCBM	0.8759	29.4917	55.83	14.42
CdS	0.3411	31.3062	70.85	7.57
IGZO	0.2625	30.8498	65.25	5.28
ZnO	0.2640	31.0850	66.58	5.46

Fig 10. Histogram of the performance of different ETL devices

4.0 Conclusion

In this work, SCAPS-1D software was used to simulate the proposed inverted HTL-free tin-based PSC structure design, and the V_{oc} was 1.0465 V, J_{sc} was 30.1646 mA/cm², FF was 59.49%, and PCE was 18.78%. In order to optimize the structure, we individually changed the parameters of the device to observe and analyze its impact on the PSC performance.

The simulation results show that the photovoltaic performance can be improved by changing the thickness of the absorber layer, the doping concentration and reducing the density of defect states. When the thickness of the absorption layer is 550nm, the PCE growth tends to be stable, and the thickness of 550nm is the optimal value. As the doping concentration of the absorption layer increases, the PCE curve increases first and then decreases. This is because the continuous increase of the doping concentration easily leads to the recombination of photons. The maximum PCE is obtained when the N_A is 10¹⁶cm⁻³. The larger the defect density of the absorption layer is, the greater the impact on PSC and the worse the performance is. Therefore, the defect density should be reduced as much as possible. The defect density of this work was selected as 10¹⁵cm⁻³. By inverting the HTL-free tin-based PSC, the FTO will be in direct contact with the perovskite layer. It is valuable to study the influence of FTO parameters on the device. Changing the FTO doping concentration N_A , it is found that the smaller N_A devices have poor performance and abnormal J-V curve, which may be unsuitable for electrodes due to the low conductivity of FTO. PCE is the optimal value when N_A is 10¹⁹ cm⁻³.

Through the study of PSCs under different illumination conditions, the thickness of C_{60} is changed, and when light is irradiated from the Au (or FTO) side, it is found that the impact on the battery performance from the Au side is greater than that from the FTO side, and the PCE is lower. The results show that the inverted PSCs can ensure the light intensity of the incident perovskite layer to the maximum extent on the basis of HTL-free, and show better photovoltaic performance.

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Figures

Figure 1

(a) Device configuration of simulated PSC, (b) Energy band diagram of the device

(a)

(b)

(c)

Figure 2

(a) Energy band diagram (b) Current density-voltage (J-V) (c) Quantum efficiency (QE)

Figure 3

Change the thickness of the absorption layer: (a) J-V, (b) quantum efficiency (QE), (c) PCE (the illustration shows the VOC, JSC and FF)

Figure 4

Changing the doping concentration NA : (a) J-V, (b) PCE, VOC, JSC and FF

Figure 5

Changing the defect density N_t : (a) J-V, (b) quantum efficiency (QE), (c) PCE (the illustration shows the VOC, JSC and FF)

Figure 6

When light is irradiated from the Au side (FTO side), change the thickness of C₆₀ to get the J-V and VOC, JSC, FF, PCE ((a), (c) is the light irradiated from the Au side. (b), (d) is the light irradiated from the FTO side)

(a)

(b)

Figure 7

Different doping concentration ND: (a) J-V; VOC, JSC, FF, PCE

Figure 8

J-V curve and quantum efficiency (QE) curve obtained from the final optimized value

Figure 9

Different ETL energy band structure diagram and optimized J-V curve diagram

Figure 10

Histogram of the performance of different ETL devices