Simulation of carriers spatial distribution and transportation in co-mixing composition perovskite for solar cell

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Abstract

A planar device structure FTO/TiO2/SnO2/Cs0.1FA0.74MA0.13PbI2.48Br0.39/Cs0.1FA0.74MA0.13PbI2.48Br0.39/Cs0.1FA0.74MA0.13PbI2.48Br0.39/CuSCN/Au with cation and anion co-mixed Cs0.1FA0.74MA0.13PbI2.48Br0.39 as light harvester was modeled and investigated by using modeling program wxAMPS. The energy band structure, carrier concentration, carrier generation rate, recombination rate, and other data were obtained through simulation to analyze the specific influence on the performance of perovskite solar cells (PSCs). In order to better optimize device performance, we investigated the effects of perovskite and the interface between each functional layer defect density, film thickness, and test temperature environment on the performance of PSCs. The simulation results show that the device performance has higher dependence on the effect of perovskite and interface defect density. By further optimizing the parameters of defect density (1015 cm−3), film thickness (400 nm), and test temperature (300 K), the power conversion efficiency (PCE) of the finally obtained PSCs was enhanced from the initial 11.65% to 21.95%. This investigation will enable us to better understand the internal working mechanism of PSCs and provide theoretical guidance for the fabrication of high-performance PSCs in experiments.

1. Introduction

Solar cells have drawn tremendous attention of researchers due to their high absorption coefficient, low fabrication cost, and high PCE [1–5]. Among them, organic–inorganic halides PSCs have received many investigations in recent years [6], and the performance of device has also been continuously improved. Generally, conventional planar PSCs structure mainly include working electrode (cathode)/electron transport layer/perovskite light absorption layer/hole transport layer/counter electrode (anode). The perovskite light absorption layer plays a key role in energy absorption, conversion and exciton transport in PSCs [7, 8]. The quality of the perovskite film mainly affects the performance of the entire device. Among them, pure ABX3 structure compounds, such as CH3NH3PbX3, HCNH2PbX3, and CsPbX3 (X = Br, Cl or I) are mostly used as light absorption layer materials to fabricate PSCs [9].

In previous reported literature on PSCs, most of which are favored by experiments to discuss and investigate the effect of different fabrication processes on the photophysical properties and the performance of device, but if we can first understand the internal intrinsic multiphysical mechanisms of PSCs which also provide theoretical guidance for the fabrication of high-efficiency PSCs [10]. For example, one-dimension analytic method was used researchers to show how to enhance the device performance by adjusting the parameters of the device.

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Therefore, the wxAMPS software was used to simulate PSCs [15, 16]. But most of the previous reported literatures on device simulation, researchers have only investigated the effects of different functional layers materials or different parameters of the material itself on performance of the device [17, 18]. Different from these theoretical investigations, we simulated and analyzed the spatial distribution of carriers inside the PSCs under the conditions of dark and illumination, as well as the transport mechanism of charge, and finally the performance of PSCs was optimized on this basis.

In the design of PSCs structure, TiO2 is usually used as the material of the electron transport layer in planar heterojunction solar cells. But due to the thin single-layer TiO2 film cannot cover the rough FTO conductive substrate completely and uniformly; therefore, holes and cracks are prone to appear on the surface of the TiO2 film [19, 20]. According to the previous investigations of our research group, TiO2/SnO2 is used as an inorganic composite electron transport layer material, which can effectively compensate for the incomplete coverage of the single-layer TiO2 electron transport layer on the FTO substrate, and meanwhile reduce interface defects and device hysteresis [19]. As the pure ABX3 structure perovskite material mentioned above, due to the poor stability of this kind of materials under high temperature and light for a long time [21, 22]; chemical stability is also low in the atmosphere environment [23]. However, due to the high efficiency and better stability of the co-mixed perovskite materials composed of cations and anions, the devices fabricated in recent years have also obtained the best performance [9]. Therefore, the co-mixed Cs0.1FA0.74MA0.13PbI2.48Br0.39 was selected by us as the perovskite light absorption layer material. For commercial purposes, we choose CuSCN with low cost and simple synthesis process as the inorganic hole transport layer material [24, 25]. FTO and Au are used as electrodes because of their suitable work functions [26, 27].

In this simulation work, the planar PSCs with the structure of FTO/TiO2/SnO2/Cs0.1FA0.74MA0.13PbI2.48Br0.39/CuSCN/Au have been investigated. Through simulation, it was found that the carrier concentration, generation rate, recombination rate, life time, and electric field will change drastically at the interface of the functional layers, and the different spatial distribution of carriers in different functional layers was observed. At the same time, we also analyzed the effect of defect density and light absorption layer thickness, as well as the test temperature environment on the performance of PSCs. Finally, the high-efficiency and low-cost PSCs were obtained by optimizing design.

2. Device architecture and simulation parameters

In this work, the PSCs we designed were simulated and theoretically analyzed by using the wxAMPS simulation software. Figure 1 shows the structure of organic-inorganic planar heterojunction PSCs, in which p-type perovskite light absorption layer (Cs0.1FA0.74MA0.13PbI2.48Br0.39) is sandwiched between p-type hole transport layer (CuSCN) and the n-type electron transport layer (TiO2/SnO2). FTO and Au were used as photocathode and photoanode, respectively. In addition, the defect density at the interface between the perovskite light absorption layer and the electron transport layer/hole transport layer was also considered by us.
Table 1. Material parameters of the simulated perovskite solar cell [28–31].

| Parameters                     | FTO  | TiO$_2$ | SnO$_2$ | 1L1  | Cs$_{0.1}$FA$_{0.74}$MA$_{0.13}$Pb$_{1.46}$Br$_{0.39}$ | 1L2  | CuSCN |
|-------------------------------|------|---------|---------|------|-----------------------------------------------------|------|-------|
| Thickness/nm                  | 600  | 20      | 50      | 5    | 600                                                 | 5    | 90    |
| Relative permittivity $\varepsilon_r$ | 9    | 9       | 9       | 6.5  | 6.5                                                 | 6    | 10    |
| Electron affinity $\chi/eV$   | 4    | 4       | 4       | 3.95 | 3.8                                                 | 3.8  | 1.9   |
| Band gap $E_g/eV$             | 3.5  | 3.2     | 3.5     | 1.73 | 1.73                                                | 1.73 | 3.4   |
| Effective conduction band density $N_c/cm^3$ | $2.02 \times 10^{18}$ | $1 \times 10^{21}$ | $4.36 \times 10^{18}$ | $1.1 \times 10^{20}$ | $2.1 \times 10^{17}$ | $1.1 \times 10^{10}$ | $1.7 \times 10^{19}$ |
| Effective valence band density $N_v/cm^3$ | $1.8 \times 10^{19}$ | $1 \times 10^{21}$ | $2.52 \times 10^{19}$ | $8 \times 10^{19}$ | $1.7 \times 10^{18}$ | $8 \times 10^{19}$ | $2.5 \times 10^{11}$ |
| Electron mobility $\mu_n/(cm^2 V^{-1} s^{-1})$ | 20   | 0.006   | 20      | 16   | 11                                                  | 16   | 0.0002 |
| Hole mobility $\mu_p/(cm^2 V^{-1} s^{-1})$ | 10   | 0.006   | 10      | 16   | 4                                                   | 16   | 0.2   |
| Acceptor density $N_A/cm^3$   | 0    | 0       | 0       | $1 \times 10^{15}$ | $1 \times 10^{15}$ | $1 \times 10^{15}$ | $1 \times 10^{18}$ | $1 \times 10^{18}$ |
| Donor density $N_D/cm^3$      | $2 \times 10^{19}$ | $5 \times 10^{19}$ | $1 \times 10^{18}$ | —    | 0                                                   | —    | 0     |
| Defect density $N_t/cm^3$     | $1 \times 10^{15}$ | $1 \times 10^{15}$ | $1 \times 10^{15}$ | $1 \times 10^{15}$ | $1 \times 10^{15}$ | $1 \times 10^{15}$ | $1 \times 10^{15}$ |
The material parameters of the different functional layers in the PSCs are shown in Table 1. These material parameters are all taken from the previously reported literature \[28–31\]. We set the FTO conductive substrate, composite electron transport layer, perovskite light absorption layer, and the hole transport layer with initial thickness of 600 nm, 70 nm, 600 nm and 90 nm, respectively. The initial defect density of each functional layer was set to $10^{15}$ cm$^{-3}$. To consider the effect of interface recombination, two thin virtual layer (IL1 and IL2, not indicated in the figure 1) were inserted us between electron transport layer /Cs$0.1$FA$0.74$MA$0.13$PbI$2.48$Br$0.39$ and Cs$0.1$FA$0.74$MA$0.13$PbI$2.48$Br$0.39$ /hole transport layer to simulate realistic situation. Finally, the standard AM1.5G spectrum was used as the incident light source, and the simulation of the device was completed at the test temperature of 300 K.

3. Results and discussion

3.1. Simulation and internal working mechanism of perovskite solar cells

The energy band diagram of the PSCs simulated according to material parameters is shown in Figure 2, where the energy band is only related to the characteristics of the material itself. The photogenerated electrons generated in the perovskite are transmitted from the perovskite layer conduction band to the electron transport layer conduction band, and the photogenerated holes are transmitted from the valence band of the perovskite layer to the hole transport layer.
the valence band of the hole transport layer. The barrier of 2 eV in the conduction band at the interface of C$_{0.1}$FA$_{0.74}$MA$_{0.13}$Pb$_{1.248}$Br$_{0.39}$/CuSCN can prevent photogenerated electrons from being transferred from the perovskite to the CuSCN layer. The 2.0 eV energy barriers between C$_{0.1}$FA$_{0.74}$MA$_{0.13}$Pb$_{1.248}$Br$_{0.39}$ and SnO$_2$ valence band can also effectively block the transfer of holes generated in the perovskite layer to the SnO$_2$/TiO$_2$ composite layer, while the barrier between their conduction bands blocks the diffusion of electrons from the electron transport layer to the perovskite layer. Therefore, these barriers play an important role in forming appropriate heterojunctions and improving the photovoltaic performance of devices $^{28}$. In addition, we can observe that the position of SnO$_2$ conduction band bottom is slightly lower than that of TiO$_2$ in the enlarged image. There may be a concentration difference at the interface between TiO$_2$ and SnO$_2$, in this way, electrons transferred from the perovskite layer can also diffuse from SnO$_2$ layer to TiO$_2$ layer.

The carriers are transported under the action of internal electric field. Therefore, figure 3 shows the distribution of the built-in electric field of the sample at the different thickness position. The variation trend of the electric field is also related to the characteristics of the material itself. The positive electric field was generated at the interface of 0.07 µm and 0.67 µm, and the electric field at 0.07 µm was much higher than that at other interfaces, we speculated that it was due to the existence of the built-in electric field at the P-N junction at the interface of SnO$_2$/C$_{0.1}$FA$_{0.74}$MA$_{0.13}$Pb$_{1.248}$Br$_{0.39}$. But at 0.67 µm position, it is the C$_{0.1}$FA$_{0.74}$MA$_{0.13}$Pb$_{1.248}$Br$_{0.39}$/CuSCN interface, where the electric field may also be caused by the difference in concentration. In addition, we observe that the electric field intensity at these interfaces is much higher than that inside each functional layer, and the electric fields have a strong surge and fall. Therefore, the electric field at the interface plays an important role in driving the separation and transport of carriers $^{32}$.

In order to better understand the spatial distribution and transport mechanism of carriers in the device, we first simulated the variation curves of the electron and hole concentration values of the sample in the one-dimensional direction of the thickness, as shown in figure 4. Figures (a) and (b) are the carrier concentration...
Figure 5. Carrier generation and recombination rate curves inside perovskite solar cells simulated under illumination.

Figure 6. Carrier life time curves inside perovskite solar cells simulated under dark (a) and illumination (b).
diagrams obtained by simulation in the state of dark and illumination, respectively. In the state of dark, the device is equivalent to a diode at this time. When a bias voltage is added to the Schottky barrier, the applied voltage widens the depletion layer, the built-in electric field becomes larger, and the electric potential energy of the electrons was increased. The majority carrier holes of the perovskite layer P region and the majority carrier electrons of the electron transport layer N region are difficult to cross the potential barrier. Therefore, the concentration of electrons is high in the electron transport layer, and the concentration of holes is also high in the hole transport layer. It can also be seen that the hole concentration in the electron transport layer and the electron concentration in the hole transport layer are very low, which may be caused by few intrinsic minority carriers in the P region and N region. Since there are no electrons and holes generated inside the perovskite layer, which results in relatively low carrier concentration.

Under the illumination, it is observed from figure 4(b) that the electron concentration curve in the electron transport layer and the hole concentration curve in the hole transport layer are basically the same as those under dark, but the hole concentration in the electron transport layer and the electron concentration in the hole transport layer is relatively increased, which may be caused by the generation of more electrons and holes in the P-N junction under illumination. The electron concentration is increased when passing through the perovskite layer, and the hole concentration is gradually increased to the order of the 18th power when reaching the CuSCN layer. The concentration of electron in the FTO layer and the electron transport layer is very high, reaching the order of the 19th power. While the initial electron concentration is higher than the hole concentration when passing through the perovskite layer, and with the increases of thickness, the electron concentration starts to be lower than the hole concentration. In addition, it can be seen that at positions 0.6 μm, 0.62 μm, 0.67 μm, and 1.27 μm, the electron and hole concentrations are all surge and drop sharply with a large concentration
difference, indicating that these four position are the interface, which also confirms the reason for the existence of the electric field in figure 3.

Figure 5 shows the variation curves of carrier generation rate and recombination rate in the state of illumination. In the state of dark, since the carrier generation rate is almost zero, the carrier generation rate and recombination rate curves were not be simulated by us. In the state of illumination, when electron-hole carriers begin to be generated, the recombination of electron-hole starts almost at the same time. The magnitude of the recombination rate averages around the 18th power, and the magnitude of the generation rate averages around the 21th power. We found that the surge and sudden drop of the generation rate and recombination rate also occurred at the interface, which was also corresponding to the carrier concentration diagram in figure 4. It is worth noting that the recombination rate of the TiO2 layer is higher than the generation rate, which may be related to the position of the bottom of the conduction band of TiO2 being slightly higher than the bottom of the conduction band of SnO2 in the energy band diagram of figure 2.

Figures 6(a) and (b) respectively show the variation of carrier life time under simulation in the state of dark and illumination, which is closely related to the carriers recombination rate. In solar cells, the carrier life time is only meaningful for minority carriers. It can be observed from figure 6(a) that in the state of dark, there is no generation of electrons and holes. The hole concentration and electron concentration are low in the electron transport layer and the hole transport layer, respectively, so the life time of holes in the electron transport layer and the life time of electrons in the hole transport layer are very low. While due to the large recombination of carriers in the perovskite layer, leading to lower carriers life time gradually. From the carrier life time diagram under illumination in figure 6(b), it can be observed that in the electron transport layer and perovskite layer, the life time of the electron is higher than that of the hole, but at the position of 0.60 μm~0.62 μm, the life time of the electron is very low and lower than that of the hole life time, which may be caused by the high recombination rate of TiO2 layer. The overall life time of carriers under illumination is also lower than life time of carriers under dark; this may be due to the larger recombination of carriers under illumination.

Figure 7(a) shows the variation curve of electron current density and hole current density under dark. Since the current density is mainly formed by the drifting movement of the minority carriers in the P region and N region respectively under the action of the built-in electric field [33], but it can be seen from the carrier
concentration diagram that the carrier concentration is very low under dark, so the overall current density is very small. Figure 7(b) shows the variation curve of electron current density and hole current density inside the device under illumination, the sum of which is the value of current density in the J-V curve. It can be clearly seen from the figure that the electron in the SnO2/TiO2 layer are the majority carriers, and the holes in the CuSCN layer are the majority carriers. In addition, it can be seen that the current density of carriers has been greatly increased; this is because when light irradiates the P-N junction, electron-hole pairs can be generated in the P-N junction, which increases the concentration of minority carriers. These high-concentration carriers drift under the action of the built-in electric field, and finally increase the current density.

The J-V curves of the PSCs finally designed by us are shown in figure 8. The dark current curve under dark is shown in the red line in the figure 8(a). It is observed that there is no significant change in the dark current when the voltage is lower than 0.8 V, which may be the reason for the higher recombination of holes and electrons in the perovskite, so a higher dark current needs to be generated by adding higher bias voltage. The photo-generated current under lighting conditions is shown by the black curve in figure 8(a), where the open circuit voltage ($V_{OC}$) is 1.24 V, the short-circuit current density ($J_{SC}$) is 17.31 mA cm$^{-2}$ and the fill factor (FF) is 0.54. The final PCE obtained is 11.65% which is close to the experimentally reported with same electron transport layer and similar co-mixing absorber [19]. In an ideal state, the photogenerated current density ($J_0$) is as follows:

$$J_0 = J_{ph} - J_{dark},$$

Where $J_{ph}$ is total current density and $J_{dark}$ is dark current density, but given the solar cells with parallel resistance ($R_{sh}$), there is also the existence of leakage current ($J_{sh}$), as shown in figure 8(b) is the equivalent circuit diagram of solar cells considering the parallel resistance. From the figure 8(b), it can be seen that the actual photogenerated current density ($J$) can be expressed as

![Figure 9. J-V curves (a) and quantum efficiency curves (b) of perovskite solar cells with different defect densities of the perovskite layer.](image-url)
3.2. Effect of the defect density of the perovskite layer on the device performance

However, it is observed from the above simulation results of the device that the carrier concentration in the perovskite layer is lower than that of other functional layers, and there is a high carrier recombination rate, resulting in lower carrier life time and current density, as well as poor performance of the final device. So it is also necessary to optimize the performance of the PSCs with this structure. Since the perovskite layer and the interface between each functional layer play a major role in the device performance, the following mainly optimizes the parameters of perovskite layer and interface to improve the device performance.

The defect density of the perovskite layer is the key to the quality of the perovskite film. Here, five gradient defect densities were set for simulation, which are $10^{13}$ cm$^{-3}$, $10^{14}$ cm$^{-3}$, $10^{15}$ cm$^{-3}$, $10^{16}$ cm$^{-3}$, and $10^{17}$ cm$^{-3}$. Figure 9 shows the J-V curves (a) and the corresponding QE curves (b) of the device under various defect densities. From the J-V curve, it can be seen that with the increase of defect density, $V_{oc}$ is gradually decreased, while $J_{sc}$ is obviously reduced when the defect density is greater than $10^{15}$ cm$^{-3}$, which leads to the decrease of device performance. It can be seen from figure 9(b) that when the defect density is also greater than $10^{15}$ cm$^{-3}$, the absorption intensity of visible light decreases. Especially when the defect density reaches

$$J = J_{ph} + J_{dark} + J_{sh},$$

(2)

### Table 2. Comparison of the performance between the initial parameters and the optimum parameters.

| Samples          | Defect density (cm$^{-3}$) | Thickness (nm) | Test temperature (K) | $V_{oc}$ (V) | $J_{sc}$ (mA/cm$^2$) | FF   | PCE (%) |
|------------------|-----------------------------|----------------|----------------------|--------------|----------------------|------|---------|
| Initial PSCs     | $10^{15}$                   | 600            | 300                  | 1.24         | 17.31                | 0.54 | 11.65   |
| Optimization of PSCs | $10^{13}$               | 400            | 300                  | 1.44         | 17.16                | 0.89 | 21.95   |

![Figure 10. Performance parameters of perovskite solar cells with different defect densities of the perovskite layer: power conversion efficiency and fill factor curves (a), open circuit voltage and short circuit current density curves (b).](image-url)
10^{17} \text{cm}^{-3}$, the QE is very low. Therefore, when there are too large defects in the perovskite layer, the absorption intensity of visible light will be decreased for PSCs. Figures 10(a) and (b) show the performance parameters variation curves of PSCs. On the whole, these performance parameters are reduced as the increases of the defect density of the device, so the defect density has a great impact on device performance. The high defect density mainly affects the internal charge transport and collection process of the PSCs [6]. To sum up, low absorber defect density leads to longer diffusion length which reduces the carrier loss due to recombination and be more conducive to the improvement of device performance [18].

### 3.3. Effect of the thickness of the perovskite layer on the device performance

According to the above analysis, we set defect density of the perovskite to $10^{13} \text{cm}^{-3}$, and other parameters remain unchanged. The thickness of the perovskite absorber layer also plays a very important role in the performance of the perovskite solar cell. When the film thickness is too thin, it is not conducive to the absorption of light; and when the film thickness is too thick, which resulting in more defects distribution due to carrier recombination [29]. Figure 11 shows the simulated JV curves and QE curves of the PSCs under different thicknesses of the perovskite absorber layer. The setting gradient of thickness is from 200 nm to 800 nm. Figure 12 shows the changes in the four key performance parameters of PSCs. From the comparative analysis in the figure, it can be concluded that both $J_{sc}$ and QE are increased with the increase of the thickness of the perovskite layer, the $V_{oc}$ and FF initially have large value at smaller absorber thickness, while $V_{oc}$ and FF are decreased with the increase of the thickness of the perovskite layer, this is because when the thickness of the light absorption layer is thinner, there is lower series resistance at both ends of the solar cell, less recombination of internal carriers and higher charge extraction [34]. The PCE of the final device is first increased and then

![Figure 11. J-V curves (a) and quantum efficiency curves (b) of perovskite solar cells with different thicknesses of the perovskite layer.](image-url)
decreased. When the thickness of the perovskite layer is 400 nm, the PCE reaches the highest. As the thickness of the light absorption layer increases, more photons will be absorbed, thus generating more charge carriers, so the $J_{sc}$ and PCE of the device will also be enhanced. However, when the thickness of the light absorption layer is too thick, if the thickness of the absorption layer is greater than the diffusion length of the carriers, the carriers may recombine before they reach the metal electrode, which ultimately leads to the decrease of PCE of the device [18].

3.4. Effect of the test temperature on the device performance
In addition to the effect of light absorption layer parameters on the performance of perovskite devices, the test temperature of solar cells has also an important influence on the performance of devices [35, 36]. Here, the 400 nm perovskite film optimized above is used as the basic condition, and only the test temperature is changed, namely seven test temperature of 280 K, 300 K, 320 K, 340 K, 360 K respectively. From figures 13(a) and 14, it is observed that as the increases of test temperature, $J_{sc}$ is not changed obviously, while $V_{oc}$ and FF are slightly decreased, so the PCE of PSCs is reduced. Parameters such as carrier concentration and their mobility would be affected at a higher temperature, so the performance of the device is reduced [37]. Too high temperature would allow the electrons in the PSCs to gain additional energy. Therefore, they are more possible to recombine with holes before reaching the depletion zone and become unstable at higher temperatures [37]. In addition, it can be seen from figure 13(b) that QE hardly changes with the increase of test temperature. In conclusion, the test temperature environment has relatively a little effect on the performance of device in the atmosphere. We know that the room temperature is 25 ℃ (298.15 K), because most of the lab environment for room temperature, or is 25 ℃ constant temperature and humidity environment, considering the cost and easy access to the
environment. Therefore, our simulation test temperature is set to 300 K, and finally the optimized PCE of the device is 20.47%.

3.5. Effect of the defect density at the interface on the device performance

In addition to the perovskite light absorption layer defect density being considered, the defect density at the interface between the perovskite light absorption layer and electron transport layer/hole transport layer has also a great importance on the device performance. So we simulated adding interface layer parameters. Figure 15(a) shows the J-V curves of PSCs by changing the defect density at 1L1 at the interface between the perovskite light absorption layer and the electron transport layer. Other parameters are consistent with the above parameters. The defect density at the interface varies from $10^{13}$ cm$^{-3}$ to $10^{17}$ cm$^{-3}$. According to the simulation results, with the increase of defect density at interface layer 1L1, $J_{sc}$ hardly changed, $V_{oc}$ gradually decreased, and PCE also decreased from 20.74% to 15.21%. Figure 15(b) shows the effect of different defect densities at the interface 1L2 between the perovskite light absorption layer and the hole transport layer on device performance. The variation trend of J-V curve is consistent with figure 15(a). The final PCE dropped from 21.95% to 18.39%, a relatively small change. This is because with the increase of defect density, more carriers are trapped by defects at the interface, which is not conducive to carrier transmission, leading to the decline of $V_{oc}$ and FF, and directly affecting the performance of the device. In addition, since the interface layer 1L1 is closer to the light incident side than 1L2, more carriers are generated near the interface layer 1L1, so the excess carriers near the interface layer 1L1 are trapped by defects, resulting in a large amount of carrier loss. Therefore, compared with the interface layer 1L2, the defects in the interface layer 1L1 have a greater impact on the device performance, which is also consistent with the results obtained in the simulation [18].

Figure 13. J-V curves (a) and quantum efficiency curves (b) of perovskite solar cells with different test temperature.
Table 2 shows the performance parameters of the original structure of the PSCs and the optimized PSCs. Before optimization, the PCE of the PSCs with the structure of FTO/TiO\textsubscript{2}/SnO\textsubscript{2}/Cs\textsubscript{0.1}FA\textsubscript{0.74}MA\textsubscript{0.13}PbI\textsubscript{2.48}Br\textsubscript{0.39}/CuSCN/Au is 11.65%. After optimizing the parameters of defect density and thickness of the perovskite layer, and the test temperature of the PSCs, the Voc was increased to 1.44 V, the FF was increased to 0.89, and the Jsc reaches 17.16 mA cm\textsuperscript{-2}, and finally the optimized PCE of the PSCs was improved to 21.95%. The simulated optimum device performance is similar to the reported experimental result [38].

4. Conclusion

In summary, TiO\textsubscript{2}/SnO\textsubscript{2} was designed as composite electron transport layer, cation and anion co-mixed Cs\textsubscript{0.1}FA\textsubscript{0.74}MA\textsubscript{0.13}PbI\textsubscript{2.48}Br\textsubscript{0.39}/CuSCN/Au was used as the light absorption layer, and the inexpensive CuSCN was used as the inorganic hole transport materials. By using the wxAMPS device simulator, the new structure of the PSCs was respectively simulated in the state of dark and illumination, which allowed us to better understand the spatial distribution of internal carriers and charge transport mechanism. The simulated results have PCE of 11.65%, VOC of 1.24 V, JSC of 17.31 mA cm\textsuperscript{-2}, and FF of 0.54. However, it is observed from the figure obtained from the simulation that the internal recombination rate of the PSCs is relatively large, and there may be larger defects. Therefore, we simulated and analyzed the effects of defect density, perovskite layer thickness and test temperature environment on the performance of PSCs. The results show that the performance of PSCs was optimized when the defect density of the perovskite layer and the interface between each functional layer was 10\textsuperscript{13} cm\textsuperscript{-3}, and the perovskite film thickness was 400 nm. We chose 300 K as the appropriate test temperature due to the availability of the test temperature environment. Finally the PCE of the optimized PSCs was significantly enhanced from 11.65% to 21.95%. This investigation will be conducive to understanding of the operation mechanism of the functional layer for PSCs and favorable for its further efficiency improvement.
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The authors declare no conflict of interest.

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Figure 15. J-V curves of PSCs for various defect densities at interface layer IL1 (a) and interface layer IL2 (b), respectively.
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