# Computer Simulation and Performance Optimization of Metal-Semiconductor-Metal Back-Contact Perovskite Solar Cells

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## Abstract

In this work, a computer simulation of the optical and electrical properties of metal-semiconductor-metal (MSM) back-contact (BC) perovskite solar cells (PSCs) is presented. An experimental MSM BC PSC reported in the literature is taken as a basis for the computer simulation experiments. The thickness of the perovskite layer and its charge carrier diffusion lengths in MSM BC PSCs are varied to obtain devices with the maximum power conversion efficiency (PCE).

(Keywords: Computer simulations, perovskite solar cells, back contact architecture, Schottky-junction)

## Introduction

Currently, hybrid organic-inorganic halide perovskites are the most promising low-cost materials for solar cell fabrication with decent optoelectronic properties compared to widely used crystalline silicon. Recently, devices with PCEs of around 25.7% were obtained with perovskite-based solar cells [1].

Conventionally, PSCs have a multi-layer structure, in which the perovskite layer is sandwiched between the two charge transporting layers (CTLs). This structure requires a high level of precision and accuracy in fabrication to achieve a reasonable level of performance in devices [2]. To overcome this challenge, a so-called back-contact architecture has been proposed to manufacture high-performance PSCs. One of the examples of BC PSCs, in which a MSM BC electrode system is implemented to construct PSCs, is reported by Line et al. in 2017 [2]. Here, unlike in the traditional PSCs, no CTLs are used to collect charges. The charge extraction process in these devices solely relies on a build-in field formed at the interface of the perovskite photo-active layer and two metallic BC electrodes with distinct work functions. Hence, the perovskite photo-active layer forms two different Schottky-junctions with the two metallic BC electrodes.

In the work by Lin et al., the experimental MSM BC PSCs showed a PCE of around 3.11%. However, this value for PCE is obtained for unoptimized devices. Hence, the aim of this work is to perform a theoretical analysis on MSM BC PSCs reported by Lin et al. and computationally determine the maximum attainable PCEs in these devices by optimizing the thickness of the perovskite active layer and its charge carrier diffusion lengths ($L_d$).

## Methodology

### *A. Optical and electrical simulations*

The MSM BC PSCs do not have a one-dimensional (1D) uniformity along the direction of the incident light as illustrated in Figure 1. Hence, a multidimensional optical approach is used to determine the exact electromagnetic (EM) responses of devices. The details of this approach can be found in the report by Li et al. and in our previous works [3-4]. We employed the thermionic emission for the simulation of the electrical currents in MSM BC PSCs [5-6].

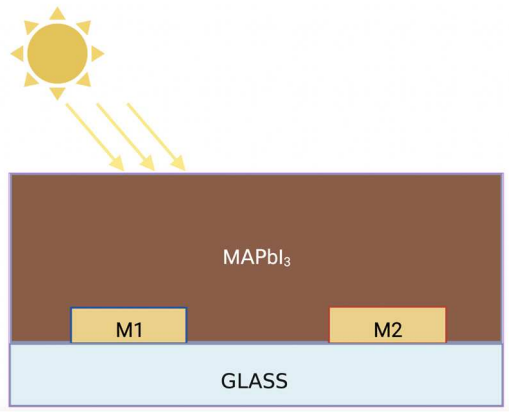



**Figure 1.** Device structure for MSM BC PSCs.

### *B. Device structure*

A general structure of MSM BC PSCs used in the computer simulation experiments follows the design reported by Lin et al. and is shown in Figure 1 [2]. Here, a 500 nm thick $MAPbI_3$ perovskite layer is placed over a pair of 60 nm thick and 2 μm wide metallic electrodes on a glass substrate. The distance between the metallic electrodes is 2 μm. The work function values of the first (M1) and the second (M2) BC electrodes are 4.5 and 5.1 eV, correspondingly.



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These parameters for the device geometrical dimensions and work functions of BC electrodes are taken from the work by Lin et al. [2].

## Results and discussion

Figure 2 shows a simulated current density vs. voltage (*J-V*) curve for MSM BC PSCs under 1 Sun condition (100 mW/cm$^2$ AM1.5G irradiation). The photovoltaic parameters extracted from the *J-V* curve are displayed in Table 1. The obtained value for the open circuit voltage ($V_{OC}$) is 0.6 V and it corresponds to the difference between the work functions of the M1 and M2 BC electrodes. The values for the short-circuit current ($J_{SC}$) and the fill factor (*FF)* are around 11.44 mA/cm$^2$ and 0.47, correspondingly. The resulting *PCE* is around 3.26%. These values are obtained when during the simulation experiments, the electron/hole mobility ($\mu_{e,h}$) and lifetime ($\tau_{e,h}$) are set 1 cm$^2$/V·s and 1 μs, correspondingly.

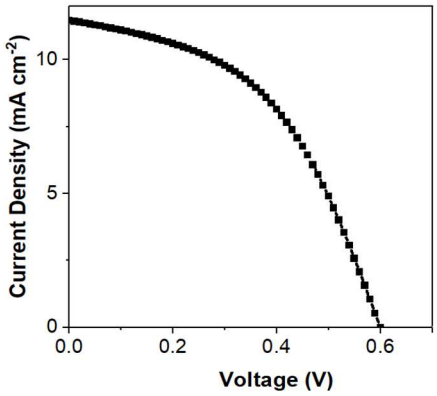



**Figure 2.** Simulated *J-V* curve of MSM BC PSCs.

**Table 1.** Photovoltaic parameters of MSM BC PSCs.

| | $J_{SC}$ (mA/cm$^2$) | $V_{OC}$ (V) | *FF* | *PCE* (%) |
|---|---|---|---|---|
| **Simulation** | 11.44 | 0.6 | 0.47 | 3.26 |
| **Experiment [2]** | 11.38 | 0.57 | 0.4 | 2.59 |

Comparing the photovoltaic parameters obtained from the computer simulation experiments with the experimental values obtained in the work by Lin et al. (also presented in Table 1), it is evident that there is a good correspondence between them. Such a close match between the simulated and experimentally obtained photovoltaic parameters suggests that the constructed computer model of MSM BC PSCs, the assumptions made and approaches employed in the simulation experiments are reasonable and valid. Hence, the developed computer model can be used to further investigate the optoelectronic properties of MSM BC PSCs with a certain confidence.

In the next step of the computer simulation experiments, the thickness of the perovskite layer of MSM BC PSCs is varied to analyze its effect on the photovoltaic parameters of devices. Figure 3 depicts the dependence of the photovoltaic parameter of devices on the thickness of the perovskite photo-active layer. Figure 3a shows that with the increase in the thickness of the perovskite layer, $J_{SC}$ of devices also increases. At a thickness value of around 1 μm, $J_{SC}$ of devices reach its saturation value and do not change much with further increase in the thickness of the perovskite layer. Figure 3b and 3c indicate that $V_{OC}$ and *FF* of devices do not change much with the thickness of the perovskite layer. Due to these trends in $J_{SC}$, $V_{OC}$, and *FF*, the *PCE* of devices also increases with the thickness of the perovskite layer and also reaches its saturation value at around 1 μm. The highest *PCE* (4.58%) in the simulation experiments is obtained when the thickness of the perovskite layer was 1.1 μm. Based on these findings, hence, it can be suggested that the thickness of the perovskite layer should be around 1 μm for given geometric dimensions and electronic parameters of MSM BC PSCs.

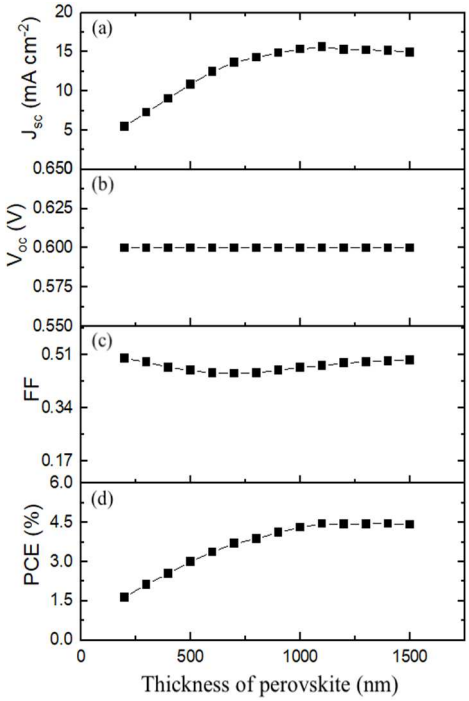



**Figure 3.** Dependence of the photovoltaic parameters of MSM BC PSCs on the thickness of the perovskite layer.



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Finally, the influence of the electronic properties of the perovskite layer on the performance of MSM BC PSCs is investigated in the quest for a maximum attainable PCE in these devices. One of the important electronic parameters that has a strong influence on the performance of solar cells is the charge carrier diffusion length ($L_d$). Hence, in the next step of device simulation experiments, the influence of this parameter on the photovoltaic properties of MSM BC PSCs is investigated.

Figure 4 shows the dependence of the photovoltaic parameter of devices on the magnitude of $L_d$. As in Figure 3b, it appears that $V_{OC}$ does not depend on $L_d$ (see Figure 4b). However, $J_{SC}$ and $FF$ vary significantly with $L_d$ (see Figure 4a and 4c). With the increase in $L_d$, $J_{SC}$ and $FF$ also increase and reach their saturation values around $L_d = 3$ µm. Due to these trends in $J_{SC}$, $V_{OC}$, and $FF$, PCE also increases and reaches its saturation value of ~ 5.05% at $L_d = 3$ µm. Further increase in $L_d$ does not seem to have any significant effect on these parameters. Based on these findings, it can be stated that the optimum $L_d$ value in MSM BC PSCs is around 3 µm for the given geometric design of the BC electrodes and 1.1 µm thickness of the $MAPbI_3$ perovskite layer.

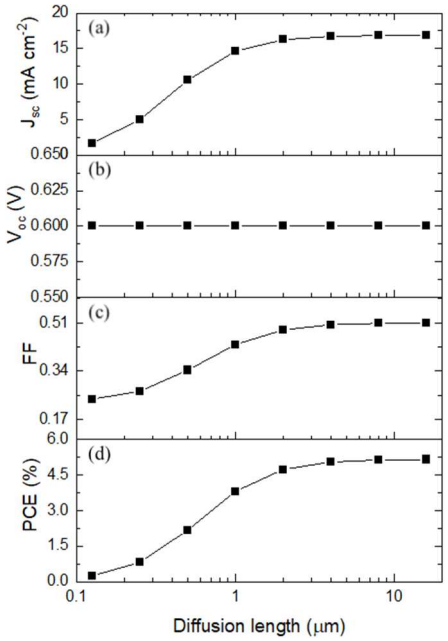



**Figure 4.** Dependence of the photovoltaic parameters of MSM BC PSCs on $L_d$ of the perovskite layer.

## Conclusion

In conclusion, computer modeling methods are employed to investigate the photovoltaic properties of MSM BC PSCs. The validity of the obtained modeling results are assessed by comparing them to the reported experimental findings. The influence of the thickness of the perovskite layer and its charge carrier diffusion lengths on the performance of devices is investigated and optimum values for these parameters are determined. The findings of this work can be used as a guideline for designing and fabrication of high-performance MSM BC PSCs.


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