

Performance evaluation of different designs of back-contact perovskite solar cells

Erik O. Shalenov^{a,b}, Yeldos S. Seitkozhanov^a, Constantin Valagiannopoulos^b, Annie Ng^c, Karlygash N. Dzhumagulova^{a,b}, Askhat N. Jumabekov^{b,*}

^a Institute of Experimental and Theoretical Physics, Al-Farabi Kazakh National University, Almaty, 050040, Kazakhstan

^b Department of Physics, Nazarbayev University, Nur-Sultan, 010000, Kazakhstan

^c Department of Electrical and Computer Engineering, Nazarbayev University, Nur-Sultan, 010000, Kazakhstan

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ABSTRACT

Back-contact design for the architecture of devices is a promising approach to develop high-performance perovskite solar cells. Here, numerical simulation methods are used to investigate device properties of back-contact perovskite solar cells (BC-PSCs) with the quasi-interdigitated, flat-interdigitated, and interdigitated electrode designs. The results highlight the principal differences in the designs of the electrodes and provide an investigation and analysis of the impact of these electrodes on the photovoltaic properties of their BC-PSCs. The effect of the perovskite photoactive layer electronic properties on the performance of BC-PSCs is also investigated. It is revealed that while BC-PSCs with the quasi-interdigitated electrode design can potentially produce power conversion efficiencies (*PCEs*) well above 25 %, BC-PSCs with the flat-interdigitated and interdigitated electrode designs are more tolerant to electronic imperfections in the perovskite layer and can produce *PCEs* higher than those in devices with the quasi-interdigitated electrode design. Manufacturing and prospective use of electrodes with the quasi-interdigitated, flat-interdigitated, and interdigitated designs in developing BC-PSCs are discussed from the experimental standpoint.

1. Introduction

Perovskite solar cells (PSCs), due to their ability to produce high (>25 %) power conversion efficiencies (*PCEs*), have been recognized as one of the most promising technologies in contemporary photovoltaic (PV) research. The standard PSC devices have a sandwich-like architecture, in which the perovskite layer is placed between two thin layers referred to as electron and hole transporting layers (ETL and HTL) [1–3]. In recent years, an alternative architecture known as back-contact design has been proposed to further increase the light harvesting ability of PSCs and, thus, enhance the device efficiency [4–8]. In PSC devices with the back-contact architecture, both the ETL and HTL layers with their electrical contacts are placed on the rear side of the perovskite layer. The PSCs with such a design are named as back-contact perovskite solar cells (BC-PSCs) [4–8]. The peculiarity of this new architecture is that it allows an exposed perovskite layer on the front side of devices so that the incident light can directly enter the perovskite layer when devices are illuminated from the front side. This is in contrast to PSCs with

the conventional sandwich architecture, in which the incident light has to pass through various device functional layers before reaching the perovskite photo-absorber layer. This results in some light transmission losses due to absorption and reflection of a certain fraction of the incident light in these layers [9,10]. Hence, by using the back-contact architecture, the photon loss can be minimized, resulting in a higher number of photogenerated charge carriers in the absorbing layer of BC-PSCs, which gives an opportunity to manufacture PSCs with *PCEs* higher than in those with the standard sandwich architecture. The detailed investigation of this phenomenon has been reported by Ma et al. [11], Yang et al. [12,13] as well as in our previous reports [14,15]. The additional advantages of the back-contact architecture include: 1) pre-fabrication of back-contact electrodes before deposition of the final perovskite layer, which allows the use of a wider range of fabrication methods that might be challenging or unfeasible in the standard sandwich architecture; 2) less impact of shunt pathways in the active layer of devices, since the existence of pinholes in the perovskite layer of devices with the back-contact architecture is not as detrimental as in PSCs with

* Corresponding author.

E-mail address: askhat.jumabekov@nu.edu.kz (A.N. Jumabekov).

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the sandwich architecture [9–15].

Various designs of back-contact architecture for BC-PSCs have been proposed in recent years [4–8]. Based on the design of back-contact electrodes (BCEs), BC-PSCs can be classified into three main categories: 1) BC-PSCs with quasi-interdigitated electrodes (hereon indicated as quasi-interdigitated back-contact (QIBC) PSCs) [4,10–22], 2) BC-PSCs with flat-interdigitated electrodes (hereon indicated as flat-interdigitated back-contact (FIBC) PSCs) [6,11], and 3) BC-PSCs with interdigitated electrodes (hereon indicated as interdigitated back-contact (IBC) PSCs) [5,6,23]. The principal difference between these three different designs of BC-PSCs is in the structural arrangement of the anode and cathode layers of BCEs. Scheme 1a shows a schematic design of QIBC PSCs. In this design, a microstructured anode layer (metallic contacts (denoted as ‘+’) with their HTL) of BC-PSC is located on top of a continuous cathode layer (metallic layer (denoted as ‘-’) with its ETL) and separated by a thin insulating layer. Hence, the anode and cathode layers are not on the same plane. The contact between the perovskite layer and the cathode layer is achieved through the gaps between the microstructured anode layer. Scheme 1b shows a schematic design of FIBC PSCs. In this design, the interdigitated anode and cathode layers are located on the same plane and separated from each other by the insulating gap layers. Here, both the top and bottom side of the perovskite layer is flat due to the flat surface of FIBC BCEs. This is entirely different to the QIBC design, in which the bottom interface of the perovskite layer is structured due to a structured surface of QIBC BCEs. Scheme 1c shows a schematic design of IBC PSCs. In this design, the interdigitated anode and cathode layers are also on the same plane; however, the gaps between the neighboring anode and cathode units are not filled with an insulating material. Thus, the surface of BCEs with the IBC design is not flat, making it a hybrid between the QIBC and FIBC designs.

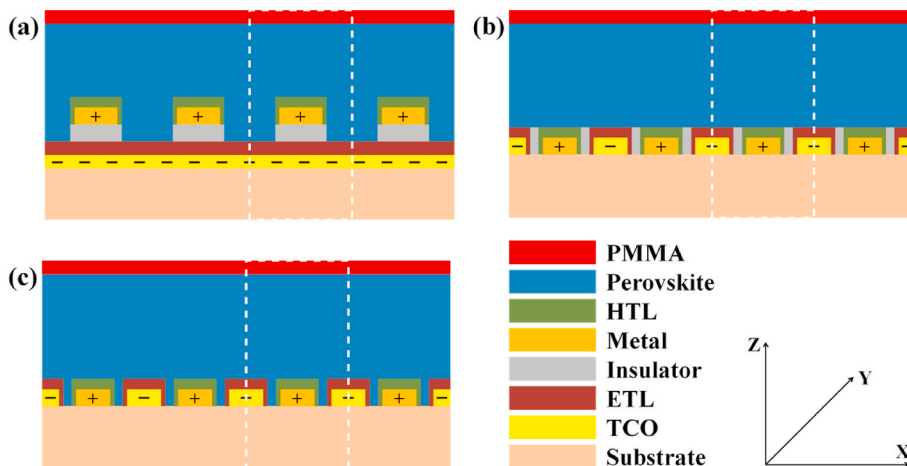
First experimental demonstration of QIBC PSCs was reported by Jumabekov et al. [4] in 2016, which is also the first example of PSCs with the back-contact architecture. Currently, this design for BC-PSCs has been investigated more or less in detail, both experimentally [4, 16–22] and theoretically [10,12–15], by several research groups. The fabrication of BCEs for QIBC PSCs requires microfabrication for the top anode layer, which involves a single step lithography process on substrates with the cathode layer followed by vacuum deposition of the anode layer with subsequent lift-off and annealing of the electrodes. The perovskite layer is then deposited via solution-processed deposition methods to finish device fabrication. The highest reported *PCE* value for QIBC PSCs up to date is around 11 % [22]. However, in our previous report, we conducted a detailed comparative analysis of the device physics, behavior, and performance of QIBC PSCs and sandwich-structured planar PSCs [15]. By employing a commonly used

standard drift-diffusion model [10–14] and calculation of the exact optical response of devices [12,13,15], we showed that it is possible to obtain *PCE* values for QIBC PSCs well above 25.5 %. Here, SnO_2 or TiO_2 were selected as the ETL layer, whereas Cu_2O was selected as the HTL layer. The corresponding sandwich-structured planar PSCs showed a *PCE* value of only around 22 %, which is significantly smaller (by ~ 10 %) than the one for QIBC PSCs [15]. Similar findings have also been reported by Yang et al. [13] for PSCs with SnO_2 and NiO as the ETL and HTL layers, respectively. Moreover, in the same report, the authors demonstrate that by employing antireflective coating and accounting for the photon recycling process, it is possible to increase the *PCE* values of QIBC PSCs up to 29.9 % [13].

An experimental demonstration of FIBC PSCs was reported recently by Song et al. [6], in which the interdigitated cathode (gold contacts with their ETL) and anode (gold contacts only) were deposited directly onto a pre-synthesized single crystal of perovskite photo-absorber layer. Here, devices have both semiconductor-semiconductor (ETL/perovskite) and semiconductor-metal (perovskite/Au) junctions. The highest *PCE* value obtained with FIBC PSC devices and reported by Song et al. [6] is also around 11 %. However, theoretical studies reported by Ma et al. [11] predict the *PCE* values around 22.7 % for FIBC PSCs with TiO_2 and NiO as the ETL and HTL layers, correspondingly. The *PCE* values of the corresponding sandwich-structured planar PSCs, according to the findings of Ma et al. [11], is only around 19.9 %. Thus, the *PCE*s of FIBC PSCs can be higher than the *PCE*s of sandwich-structured planar PSCs by a factor of ~ 1.14 .

The first experimental demonstration of IBC PSCs was reported by Pazos-Outón et al., in 2016 [5]. Currently, the highest recorded *PCE* value with IBC PSCs is around 3 % [7]. To date, a comparative study for IBC PSCs and sandwich architecture PSCs has not been reported. However, it can be speculated that similar findings as for QIBC and FIBC PSCs are possible considering that BC-PSCs are inherently superior to sandwich-structured planar devices in terms of their optical properties.

The advantages of BC-PSCs over conventional sandwich-structured planar PSCs have been demonstrated explicitly in a number of reports by other groups [10–13] as well as in our previous reports [14,15]. However, in terms of various designs of back-contact architecture for PSCs, one of the important questions remaining unexplored is: “which one of these three aforementioned designs has a greater potential for developing high-efficiency devices, and how the specific design contributes to achieving the desired *PCE* values?” Answering this question can help to direct research efforts in BC-PSCs and develop novel experimental strategies, which are specifically tailored to a particular type of back-contact architecture design, that yielding devices with the best performance. With this in mind, this work aims to conduct a comparative analysis of device performance of BC-PSCs with QIBC, FIBC



Scheme 1. Cross-section diagram of QIBC (a), FIBC (b), and IBC (c) PSCs (shown in *xz*-plane). The simulation experiments are performed using the base unit areas (enclosed with dashed white rectangles), imposing periodic boundary conditions along the *x*-direction. The widths of the base unit areas (along *x*-direction) for QIBC, FIBC and IBC PSC are 2 μm , 2.2 μm , and 2.2 μm , respectively. The length of the base unit areas (along *y*-direction) for QIBC, FIBC and IBC PSC are 1 μm , 0.909 μm , and 0.909 μm , respectively. The heights of the base unit areas (along *z*-direction) are determined by the thickness of the device layers along *z*-direction.

and IBC designs, and explore the influence of some of the key device and material parameters on the performance of devices. The device structures for BC-PSCs with the QIBC, FIBC and IBC designs investigated in this work are illustrated in Scheme 1. Exact optical responses of BC-PSCs for each type of back-contact architecture designs are calculated to accurately obtain the charge carrier generation rates in devices. Charge carrier recombination rates in the perovskite layer of devices are calculated considering the major recombination pathways. The effects of charge carrier lifetime, charge carrier diffusion length, bulk and interfacial defects in the perovskite layer on the performance of QIBC, FIBC and IBC PSCs are investigated to examine the behavior of devices for various changes in the perovskite material properties. A discussion of the device fabrication process is provided to highlight the main advantages and disadvantages of each type of BC-PSCs designs considered in this work.

2. Results and discussion

Numerical simulation of the optical and electrical properties of BC-PSCs are undertaken as follows. The optical response i.e., charge generation rate in the perovskite photo-absorber layer, of the considered BC-PSCs is obtained using a multi-dimensional model reported by Li et al. [24]. This model allows determination of the exact electromagnetic (EM) response of devices (see equations S1–S4 in Supporting Information). The main idea here is to calculate the power flow (Poynting vector, P_s) within the devices, which is a key factor that connects the EM and electronic parts. Li et al. [24] as well as Yang et al. [12,13] have demonstrated that this approach is more accurate than the typical Lambert-Beer optical absorption approximation as it allows more adequate description of the spatial optical processes taking place in the device body [12–15,24]. This is particularly important when the optical properties of BC-PSCs are considered since the textured surface of BCEs, which, depending on the geometry and design of BCEs, can result in different optical response of devices. For electrical stimulation of BC-PSCs, the standard drift-diffusion model is employed (see equations S (5)–(21) in Supporting Information) [13–15]. More details about the method can be found in our previous reports [14,15].

In order to achieve a fair comparison between devices for various device parameters investigated, the volume per unit area ($0.6 \mu\text{m}^3 \mu\text{m}^{-2}$) of the perovskite layer ($\text{CH}_3\text{NH}_3\text{PbI}_3$ (MAPbI₃)) and widths (along x-direction) of the ETL (SnO_2) and HTL (Cu_2O) layers in contact with the perovskite layer are kept identical in all devices. With this, the widths of the base unit areas along x-direction are equal to $2 \mu\text{m}$ for QIBC PSC, and $2.2 \mu\text{m}$ for FIBC and IBC PSCs (see the areas enclosed with dashed white rectangles in Scheme 1). The lengths of the base unit areas along y-direction are equal to $1 \mu\text{m}$ for QIBC PSC, and $0.909 \mu\text{m}$ for FIBC and IBC PSCs. The heights (along z-direction) of the perovskite layers in QIBC, FIBC and IBC PSCs are equal to 690 nm (measured from the top surface of the perovskite layer till the surface of the ETL layer), 600 nm (measured from the top surface of the perovskite layer till the surface of both the ETL and HTL layers), and 672.73 nm (measured from the top surface of the perovskite layer till the surface of substrate), respectively. The values for the width of the base unit area and the volume per unit area of the perovskite layer for QIBC PSCs are chosen based on the optimized values reported in our previous studies [14,15], and these parameters are imposed on PSCs with the FIBC and IBC designs. The geometrical dimensions of different functional layers of QIBC, FIBC and IBC PSCs are presented in Table S1 in Supporting Information. The material selection for the ETL and HTL layers is based on the findings of our previous report [15], in which SnO_2 as ETL and Cu_2O as HTL are shown to be the best material combination in yielding high PCEs for BC-PSC. The details of the physical parameters used in simulation experiments are given in Table S2 in Supporting Information.

Fig. 1 shows the spatial two-dimensional (2D) charge generation profile maps for QIBC, FIBC and IBC PSCs. As expected, generation of charge carriers close to the top surface of the perovskite layer is the

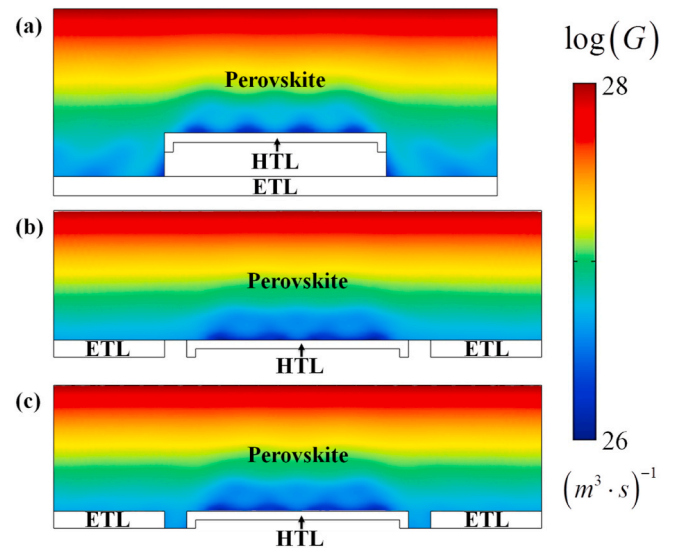


Fig. 1. Two-dimensional carrier generation profile maps (shown in xz-plane) for the perovskite layer of QIBC (a), FIBC (b), and IBC (c) PSCs. All device designs have the same perovskite area ($1.2 \mu\text{m}^2$) in the xz-plane to ensure the same volume of the perovskite layer per unit area ($0.6 \mu\text{m}^3 \mu\text{m}^{-2}$).

highest due to absorption of most of the incident light in these regions. Close to the bottom of the perovskite layer, carrier generation dissipates due to a somewhat exponential decrease of the photons as the incident light travels further down the absorber layer. All three designs show a peculiar, wave-like pattern of the carrier generation distributions over the HTL layers. This originates from the constructive and destructive interference of the incident light with the light that is reflected from the Cu metal electrodes underneath the HTL layer. While the general trends in the charge generation profile maps for all three designs of BC-PSCs appear similar, there are also subtle differences between them due to the following reasons: 1) the specific shapes of BCEs, 2) the equal widths of the ETL and HTL layers, and 3) the identical values of the perovskite layer volume per unit area.

The thicknesses of the perovskite layers over the HTL layers of BC-PSCs with the QIBC, FIBC and IBC designs are close to each other (510 nm , 600 nm , and 592.73 nm , respectively). Hence, the profile maps of charge carrier generation rate at the regions above the HTL layers in all three device designs are comparable. The situation is different when the charge generation profile maps are compared for the regions above the ETL layers. For FIBC and IBC PSCs, the charge generation profile maps over the ETL layers are similar due to comparable thickness of the perovskite layers (600 and 592.73 nm , respectively). However, due to a thicker perovskite layer over the ETL part, the charge generation profile map over the ETL layer of QIBC PSCs is taller (along z-direction) than in BC-PSCs with the FIBC and IBC designs. This enables QIBC PSCs to absorb more photons in the vertical direction than in BC-PSCs with the FIBC and IBC designs. However, the widths of FIBC and IBC PSCs are larger than the width of QIBC PSCs by 200 nm . Thus, FIBC and IBC PSCs absorb more photons in the lateral direction compared to QIBC PSCs.

Fig. 2 depicts the averaged charge generation rate profiles for QIBC, FIBC and IBC PSCs along z-direction from the top to the bottom surfaces of the perovskite layer (obtained from averaging the profile maps of carrier generation rate along x-direction). The FIBC and IBC designs have almost identical trends in the charge generation rate profiles from the top surface of the perovskite layer to the surface of the anode and cathode layers of the devices. However, it is noted that devices with the IBC design have an additional feature between 592.73 nm and 672.73 nm , which is attributed to light absorption by the perovskite layer located between the anode and cathode layers (see Scheme 1c). As for QIBC PSCs, the values for the carrier generation rate profile up to ~ 500

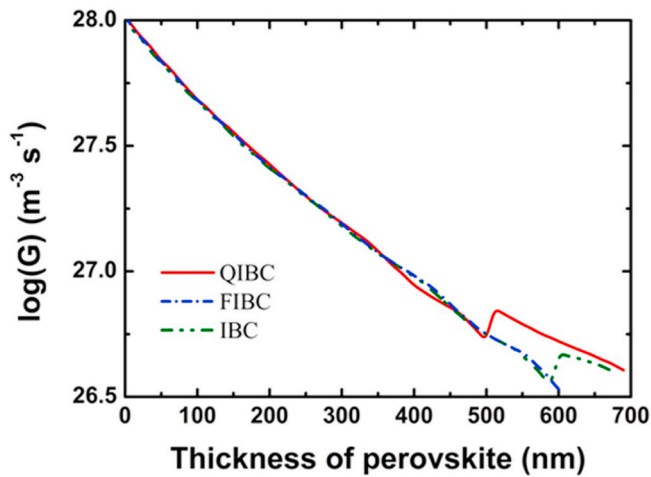


Fig. 2. Comparison of the averaged charge generation rate profiles across the perovskite layer in PSC devices with QIBC (red), FIBC (blue), and IBC (olive) designs. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

nm is similar to those in FIBC and IBC PSCs. However, a clear dominance of the carrier generation rate profile in the region between ~ 500 nm and 690 nm is observed for QIBC PSCs. This is due to larger thickness (longer penetration depth for more photon absorption) of the perovskite layer over the ETL part of QIBC PSCs than in FIBC and IBC PSCs. The estimation of the space charge density from the carrier generation rates results in 38.957 C cm^{-3} , 22.823 C cm^{-3} , and 25.278 C cm^{-3} for QIBC, FIBC and IBC PSCs, respectively, which is consistent with trends in the charge generation rate profiles shown in Fig. 2. Overall, this comparative analysis indicates that among these three designs, QIBC PSCs have the highest, whereas FIBC PSCs have the lowest light harvesting abilities.

Recombination of photogenerated charge carriers in the active layer of devices is another important parameter that can be influenced by the electrode design of BC-PSCs. Fig. 3 shows the spatial distributions of charge carrier recombination in the perovskite layer of QIBC, FIBC and IBC PSCs at the short-circuit (SC), maximum power (MP), and open-circuit (OC) conditions. Here, the total recombination rate includes Shockley-Read-Hall recombination (R_{SRH}), the Auger (R_{Aug}), radiative (R_{rad}), and surface (R_{sur}) recombinations (see Equations (S18–S21) in Supporting Information) [11,13–15,25–29]. At the SC condition (see Fig. 3a, d, and g), recombination losses are the strongest close to the top surface of the perovskite layer, and mostly over the HTL regions in all three designs of BC-PSCs. There are also some noticeable recombination losses over the ETL regions at the SC condition in all three designs of

BC-PSCs. At the MP condition (see Fig. 3b, e, and 3h), recombination losses become more severe in all three devices. The recombination losses are the strongest near the top surface of the perovskite layer with a gradual reduction over the regions of HTL and ETL towards the bottom of devices. At the OC condition (see Fig. 3c, f, and 3i), photogenerated charge carriers are not extracted from devices and lost completely due to recombination.

Quantification of the charge carrier recombination rate can provide information on what fraction of photogenerated charge carriers contributes to photocurrent in PSC devices. For this reason, the averaged profiles of charge carrier recombination rates along the depth of the perovskite layer are estimated using the 2D recombination loss distributions shown in Fig. 3. Fig. 4 shows a comparison of the averaged profiles of charge carrier recombination rates along the depth of the perovskite layer in QIBC, FIBC, and IBC PSCs at the SC and MP conditions. Fig. 4a shows that at SC, the highest recombination rate is in QIBC PSCs. The recombination rates in FIBC and IBC PSCs coincide with each other up to 592.73 nm of the perovskite layer (the entire thickness of the perovskite layer in the FIBC design). The additional tail of the recombination rate in IBC PSCs from 592.73 nm to 672.73 nm is due to the perovskite layer located between the anode and cathode layers (see Scheme 1c). As for the MP condition (see Fig. 4b), the recombination rates in FIBC PSCs is the same as in QIBC and IBC PSCs up to 400 nm along the depth of the perovskite layer; then, it lies slightly higher than in QIBC PSCs up to ~ 500 nm, and also slightly higher than in IBC PSCs up to 600 nm. The recombination rates in QIBC and IBC PSCs coincide up to ~ 500 nm along the depth of the perovskite layer. However, between ~ 500 nm and ~ 640 nm, the recombination rates in QIBC PSC are more substantial than in IBC PSCs.

Analysis of these findings in relation to the carrier generation rates discussed above indicate that even though QIBC PSCs, in general, can harvest more light and produce more photogenerated charge carriers (38.957 C cm^{-3}) for the same volume of the perovskite layer per unit area, the amount of charge carriers lost due to recombination in QIBC PSCs is larger relative to FIBC and IBC PSCs. As for FIBC and IBC PSCs, the space charge density in IBC PSCs (25.278 C cm^{-3}) is slightly higher than in FIBC PSCs (22.823 C cm^{-3}), and IBC PSCs have a somehow lower recombination rate for the same depth of the perovskite layer. However, charge recombination in the perovskite layer between the anode and cathode layers in IBC PSCs (tails of the green curves (see region between 510 and 690 nm) in Fig. 4) reduces the overall number of charge carriers that contribute to photocurrent in these devices. These competing factors in IBC PSCs, results in some small disparity between the photocurrent values in FIBC and IBC PSCs.

Fig. 5 shows the dependence of photovoltaic parameters of QIBC, FIBC and IBC PSCs on bulk defect density (N_t) in the perovskite photo-absorber layer. Bulk defect density is expressed as $N_t = 1/(\sigma_{np} \nu_{th} \tau_{np})$,

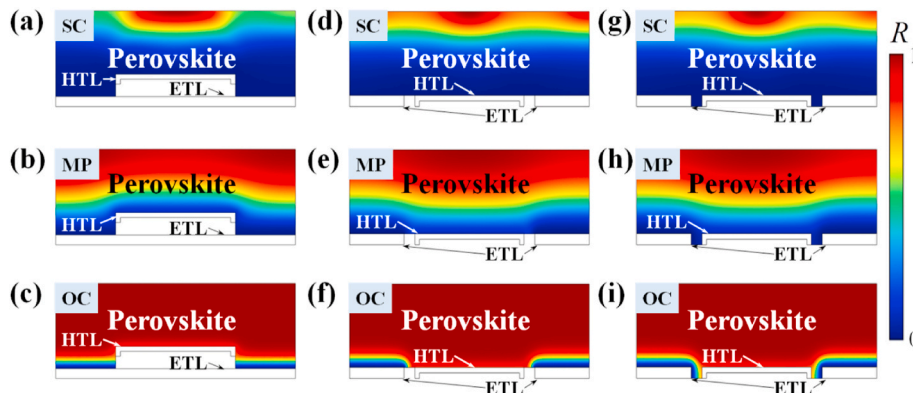


Fig. 3. Normalized recombination loss distributions (shown in xz-plane) within the perovskite regions at the (a, d, g) SC, (b, e, h) MP, and (c, f, i) OC conditions for QIBC (a–c), FIBC (d–f), and IBC (g–i) PSCs. The values for S_{np} , A_{np} , and B_{rad} equal to 1 cm s^{-1} , $2 \times 10^{-29} \text{ cm}^6 \text{ s}^{-1}$, and $3 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$, respectively.

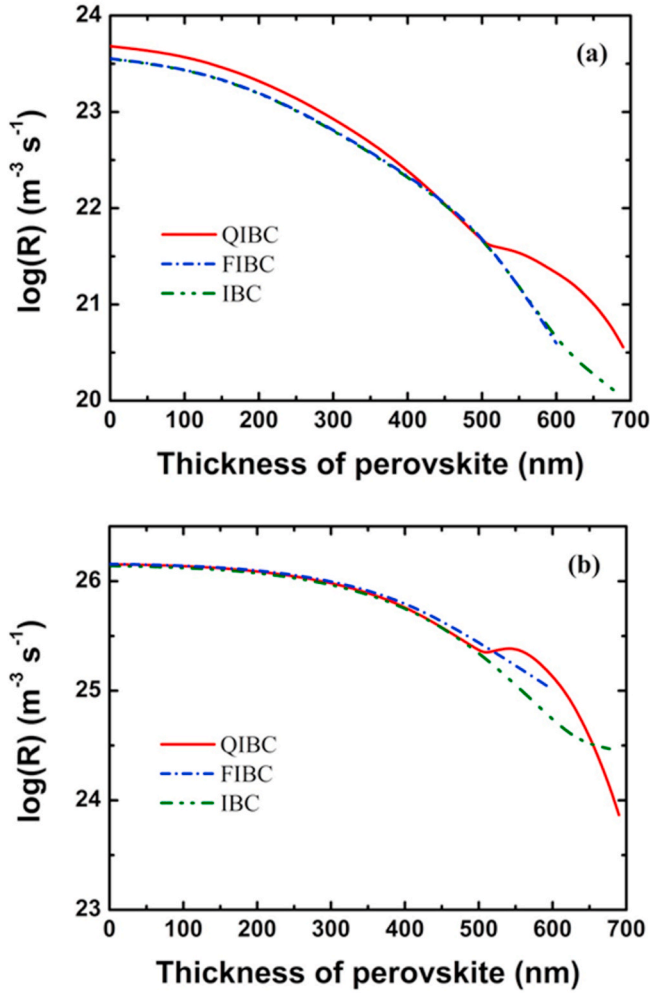


Fig. 4. Comparison of averaged recombination rate profile across the perovskite layer in devices with QIBC (red), FIBC (blue), and IBC (olive) architectures at SC (a) and MP (b) conditions. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

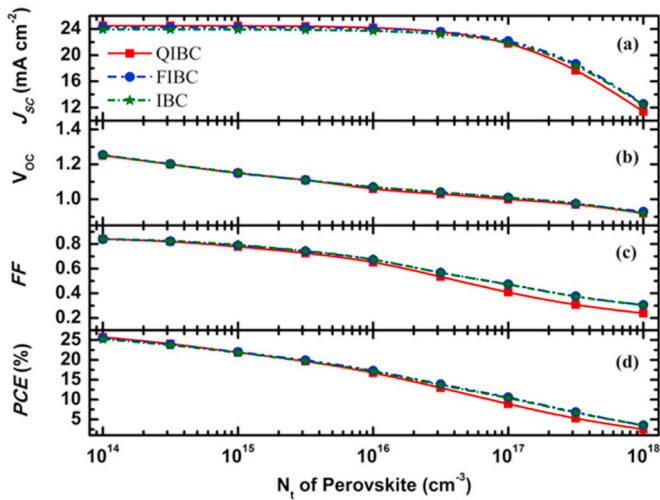


Fig. 5. J_{sc} (a), and V_{oc} (b) FF (c), and PCE (d) as a function of bulk defect density (N_t) of QIBC (red line with solid squares), FIBC (blue line with solid circles), and IBC (olive line with solid stars) PSCs. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

where σ_{np} is the electron/hole capture cross section, v_{th} is the thermal velocity of charge carriers, and τ_{np} is the electron/hole lifetime [13]. Fig. 5a shows that the J_{sc} values of devices remain rather stable even if the values of N_t increase by two orders of magnitude from 10^{14} to 10^{16} cm^{-3} . Beyond that point, the J_{sc} values of all three devices plummet down, decreasing by about 50 % from their initial values. The J_{sc} values of QIBC PSCs remain a bit higher than in FIBC and IBC PSCs for the N_t values ranging from 10^{14} to 3×10^{16} cm^{-3} . At $N_t = 10^{17}$ cm^{-3} , the J_{sc} of all three types of devices coincide with each other. At N_t values higher than 10^{17} cm^{-3} , the J_{sc} of QIBC PSCs become a bit smaller than they are in FIBC and IBC PSCs. Fig. 5b shows that the dependence of V_{oc} on N_t is almost identical in all three types of devices. The V_{oc} values of device degrade by ~ 30 % when N_t become as large as 10^{18} cm^{-3} . The FF values in all three devices decrease rather slowly when the values of N_t increase from 1×10^{14} cm^{-3} to 1×10^{16} cm^{-3} (see Fig. 5c). Then, the FF values decrease with a slightly faster pace as the N_t values increase further. It appears that, starting from about $N_t = 10^{16}$ cm^{-3} , the FF of QIBC PSCs becomes smaller than in FIBC and IBC PSCs, and this disparity becomes even more apparent as the values of N_t increase further. Due to the continuous decreasing trends in V_{oc} and FF with the increasing N_t values, the PCE s of devices also degrade as the values of defect density in the perovskite layer increase (see Fig. 5d). At the highest value of N_t (10^{18} cm^{-3}) considered in this work, the PCE values in all three types of devices degrade by about 90 % or higher compared to their initial values at $N_t = 10^{14}$ cm^{-3} . We note that for the N_t values between 10^{14} and 10^{16} cm^{-3} , the PCE s of all devices coincide with each other. Below this range ($<10^{16}$ cm^{-3}), QIBC PSCs perform slightly better than FIBC and IBC PSCs, whereas above this range ($>10^{16}$ cm^{-3}), FIBC and IBC PSCs perform a bit better than QIBC PSCs. The crossing of the PCE vs. N_t curves for QIBC PSCs with the ones for FIBC and IBC PSCs suggests that the performance of QIBC PSCs has a slightly higher sensitivity to variations in defect density than in FIBC and IBC PSCs.

Fig. 6 shows the dependence of photovoltaic parameters of QIBC, FIBC and IBC PSCs on interface trap density (D_{it_HTL}/D_{it_ETL}) at the ETL/perovskite as well as at the HTL/perovskite interfaces. The interface trap density for electrons and holes is expressed by the relation $D_{it_HTL}/D_{it_ETL} = S_{np}\sigma_{np}v_{th}$, where S_{np} is the surface recombination velocity for electrons and holes, σ_{np} is the electron/hole capture cross section, and v_{th} is the thermal velocity of charge carriers [29]. Fig. 6a shows that for the considered range of D_{it_HTL}/D_{it_ETL} values (from 10^8 to 10^{12} cm^{-2}), the J_{sc} values in all three types of devices remain unchanged up to the

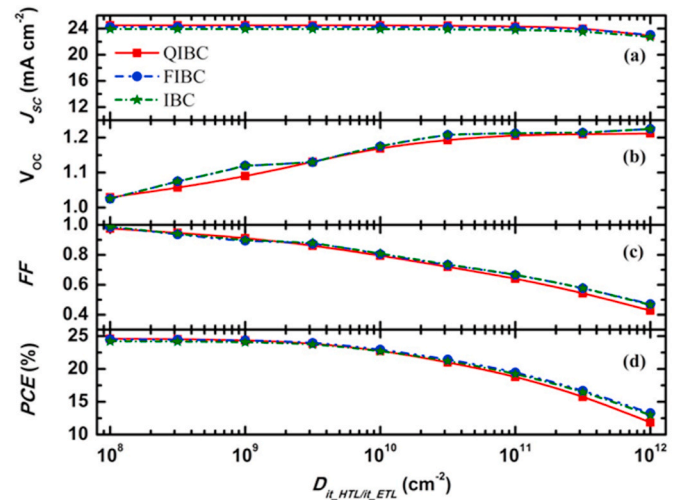


Fig. 6. J_{sc} (a), V_{oc} (b), FF (c), and PCE (d) as a function of interface trap density (D_{it_HTL}/D_{it_ETL}) of QIBC (red line with solid squares), FIBC (blue line with solid circles), and IBC (olive line with solid stars) PSCs. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

point that the value of D_{it_HTL}/D_{it_ETL} become $\sim 3 \times 10^{11} \text{ cm}^{-3}$. A further increase of the D_{it_HTL}/D_{it_ETL} values results in slight decrease of the J_{SC} values in all three devices. Fig. 6b shows that with the increase in the values of interface trap density, the V_{OC} of devices also increase, and start saturating when the D_{it_HTL}/D_{it_ETL} values become $3 \times 10^{10} \text{ cm}^{-3}$ or higher. For the considered range of the D_{it_HTL}/D_{it_ETL} (from 10^8 to 10^{12} cm^{-3}), the V_{OC} values of all three devices more or less coincide with each other except for the range between 1×10^8 to $3 \times 10^{10} \text{ cm}^{-3}$. Changes in the interface trap density seem to affect FF of devices significantly (Fig. 6c). The increase in the D_{it_HTL}/D_{it_ETL} from 10^8 to 10^{12} cm^{-3} reduces the FF in all three devices by about 50 % compared to its initial values. At the lower values of D_{it_HTL}/D_{it_ETL} , the FF s of all three devices are roughly the same. However, at the larger values of D_{it_HTL}/D_{it_ETL} , the FF of QIBC PSCs becomes smaller than that of FIBC and IBC PSCs. With such dependence of V_{OC} , J_{SC} , and FF on D_{it_HTL}/D_{it_ETL} , the PCE in all three devices decrease with the increase in D_{it_HTL}/D_{it_ETL} values. Fig. 6d shows that when the D_{it_HTL}/D_{it_ETL} change from 10^8 to 10^{12} cm^{-3} , the PCE of QIBC, FIBC, IBC PSCs decrease by about 50 % from their initial values. We note that at lower values of D_{it_HTL}/D_{it_ETL} ($< 10^9 \text{ cm}^{-3}$), QIBC PSCs show only a slightly higher PCE than FIBC and IBC PSCs. For the D_{it_HTL}/D_{it_ETL} values between 10^9 and $3 \times 10^{11} \text{ cm}^{-3}$, the PCE s of all three devices more or less coincide with each other. Above this range ($> 3 \times 10^{11}$), FIBC and IBC PSCs show a bit higher PCE values than in QIBC PSCs. Similar to the response of BC-PSCs towards the bulk defect density, the crossing of the PCE vs. D_{it_HTL}/D_{it_ETL} curves for QIBC PSCs with the ones for FIBC and IBC PSCs suggests that the performance of QIBC PSCs have a slightly higher sensitivity to variations in interface trap density compared to FIBC and IBC PSCs.

The results discussed above indicate that the performances of considered BC-PSC types are functions of charge carrier lifetime (see Fig. 5) and the surface recombination velocity (see Fig. 6). The

performance of BC-PSCs is also a function of charge carrier mobility [11, 13–15]. Hence, we also investigated the dependence of photovoltaic parameters of QIBC, FIB and IBC PSCs on charge carrier mobility (see Fig. S1 in Supporting Information). The PCE s of all three devices designs gradually improve (mainly due to increase in the J_{SC} and FF values) with the increase in charge carrier mobility values. The photovoltaic parameters of QIBC, FIB and IBC PSCs show more or less similar values and trends with the change in charge carrier mobility. This suggests that the influence of the device design on charge carrier mobility in the perovskite layer is small or negligible. From the practical point of view, it is useful to know how the PCE values of devices vary when all three parameters (charge carrier lifetime (τ_{np}), charge carrier mobility (μ_{np}), and the surface recombination velocity of electrons/holes (S_{np})) are combined. Fig. 7 shows the variation of the PCE s of QIBC, FIBC, and IBC PSCs with different combinations of charge carrier diffusion length (L_d) and S_{np} in the perovskite layer. L_d combines μ_{np} and τ_{np} into a single parameter through the following relation $L_d = ((\mu_{np}\tau_{np}k_B T)/q)^{1/2}$, in which k_B is the Boltzmann's constant, T is the absolute temperature, and q is the elementary charge. The subfigures (Fig. 7a–c) shown in Fig. 7 indicate that the conditions at which the surface recombination is small and charge carrier diffusion length is large are favorable for obtaining BC-PSCs with high performance. The PCE values around 20 % can be obtained with all three types of BC-PSCs already when the L_d values as small as $\sim 3 \mu\text{m}$, and S_{np} values as large as $\sim 10 \text{ cm s}^{-1}$. However, for the PCE values above 25 %, L_d and S_{np} values must be an order of magnitude higher and lower, correspondingly. Fig. 7d shows the profile of PCE variation as a function of S_{np} when $L_d = 8 \mu\text{m}$ (see white dashed line in Fig. 7a–c). At the lower values of S_{np} ($< 1.5 \times 10^2 \text{ cm s}^{-1}$), the PCE values of QIBC PSCs are slightly higher than that of FIBC and IBC PSCs, whereas at the higher values of S_{np} ($> 3 \times 10^3 \text{ cm s}^{-1}$), the PCE s of

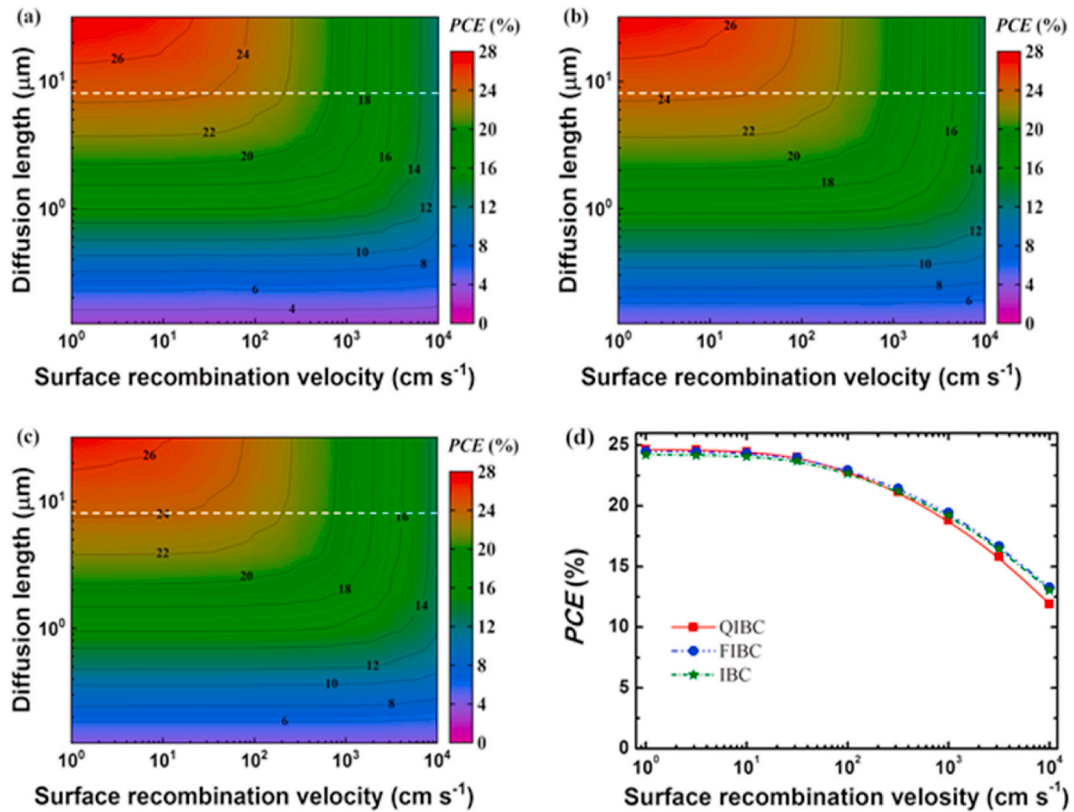


Fig. 7. PCE maps for QIBC (a), FIBC (b), and IBC (c) PSCs as the function of charge carrier diffusion length and the surface recombination velocity of electrons/holes in the perovskite layer. (d) Dependence of PCE s of QIBC (red line with solid squares), FIBC (blue line with solid circles), and IBC (olive line with solid stars) PSCs on surface recombination velocity of electrons/holes in the perovskite layer when charge carrier diffusion length in the perovskite layer is equal to $8 \mu\text{m}$ (see white dashed line in (a)–(c)). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

FIBC and IBC PSCs are higher than that of QIBC PSCs. For the S_{np} values between 1.5×10^2 and $3 \times 10^3 \text{ cm s}^{-1}$, the PCE s of all three BC-PSC types coincide with each other as in Fig. 6d.

Generally, the perovskite layer in typical solution processed planar PSCs has a polycrystalline nature and already possesses a high surface to volume ratio due to grain boundaries. This implies that surface recombination (R_{sur}) plays a key role in determining the performance of PSCs [13,15,30]. This can be more crucial for BC-PSCs with micro- or nano-structured BCEs as the textured surface of electrodes increases the overall surface to volume ratio of the perovskite layer. For the designs of BC-PSCs considered in this work, the textured surface of QIBC and IBC BCEs makes it even more challenging to deposit a perovskite layer with uniform grain sizes and low degree of polycrystallinity [7,16,23]. Additionally, during the deposition stage, the surface chemistry of both the anode and cathode layers simultaneously influences the perovskite crystal formation (relevant to all BC-PSC designs). Such a fact affects further the uniformity of the resulting perovskite film. All of these can significantly increase electron/hole surface trap state concentrations (n_{ts} and p_{ts}) and S_{np} , resulting in high values for R_{sur} and D_{it_HTL}/D_{it_ETL} . Recently, Yang et al. [13] and in our previous report [15], it was shown that if the S_{np} values are higher than 10^2 cm s^{-1} , the performance of QIBC PSCs become significantly lower than the performance of corresponding traditional sandwich-structured planar PSCs. Similar findings have also been reported by Ma et al. [11] for FIBC PSCs. This suggests that in order to fully utilize the optical advantage of BC-PSCs, the quality of the perovskite layer needs to be high i.e., highly crystalline, with large grain sizes, and low concentration of defects. Also, an additional surface passivation of the perovskite layer trap states is also required to achieve high-performance BC-PSCs [21,31–33].

Fig. 8 shows the simulated J - V curves for QIBC, FIBC and IBC PSC obtained with the consideration of calculated charge generation rates, recombination losses, and optimum values for, bulk defect density (N_t), charge carrier lifetime (τ_{np}), charge carrier mobility (μ_{np}), and interface trap density (D_{it_HTL}/D_{it_ETL}). Here, the values for the electron/hole Auger recombination coefficient A_{np} , the radiative recombination coefficient B_{rad} , and electron/hole surface recombination velocity S_{np} are taken equal to $2 \times 10^{-29} \text{ cm}^6 \text{ s}^{-1}$, $3 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$, and 1 cm s^{-1} , correspondingly. The values for μ_{np} and τ_{np} are taken equal to $50 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, $1 \times 10^{-6} \text{ s}$ ($L_d = 11.2 \text{ }\mu\text{m}$), whereas the values for N_t and D_{it_HTL}/D_{it_ETL} are taken equal to 10^{14} cm^{-3} and 10^8 cm^{-2} , respectively. The photovoltaic parameters for three different device architectures are summarized in Table 1. The obtained results solely show the impact of

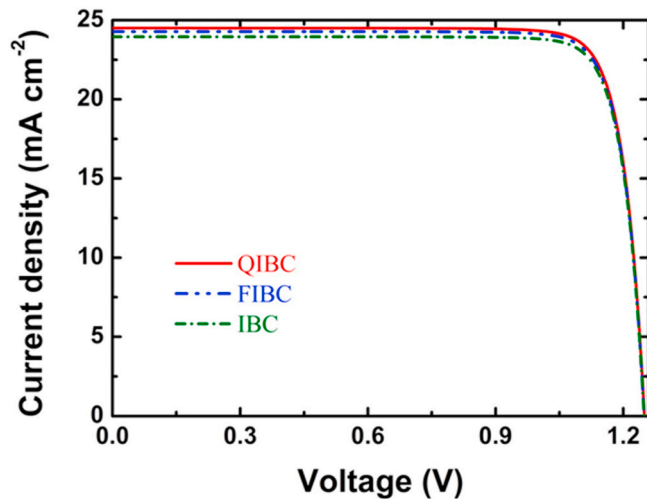


Fig. 8. Comparison of the J - V curves of QIBC (red), FIBC (blue), and IBC (olive) PSCs. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

Table 1

Solar cell parameters of QIBC, FIBC, and IBC PSCs.

Type	J_{SC} (mA cm^{-2})	V_{OC} (V)	FF	PCE (%)
QIBC	24.504	1.250	0.848	25.98
FIBC	24.284	1.249	0.847	25.72
IBC	23.957	1.249	0.849	25.42

different charge generation and recombination rates originated from various designs of back-contact device architectures on the J - V characteristics. QIBC PSCs exhibit a PCE of 25.98 %, which is the highest among these three types of designs. FIBC PSCs yield a PCE of 25.72 %, which is only slightly higher than the PCE of 25.42 % for IBC PSC devices. The major contributing factor to the higher value of PCE for QIBC PSC is the J_{SC} value, which is higher than the J_{SC} values for FIBC and IBC PSCs by around ~ 0.9 % and ~ 2.2 %, respectively. The enhanced value for J_{SC} is attributed to a better net charge generation ability (see Fig. 2) in QIBC PSCs. It is noteworthy to mention that the V_{OC} value of $\sim 1.25 \text{ V}$ and the FF value of ~ 0.84 are achieved for all three types of BC-PSCs. These indicate that the difference in charge generation and recombination rates do not cause significant changes in these photovoltaic parameters, regardless of the designs of BC-PSCs.

Fig. 9 shows the external quantum efficiency (EQE) spectra of different designs of BC-PSCs. The obtained results reveal the ratio of the collected charge carriers externally from the devices to the incident photons at different wavelengths for QIBC, FIBC and IBC PSCs. The absorption edge of PSCs is at 800 nm as the bandgap of the perovskite used in this work is 1.55 eV. Throughout the considered spectral range (from 300 nm to 800 nm), the EQE values for QIBC PSCs are the highest, whereas for IBC PSCs are the lowest. The EQE values for FIBC PSCs are slightly higher than that for IBC PSCs. This correlates well with the J_{SC} values in the J - V curves shown in Fig. 8 and indicated in Table 1.

The analysis of the optical and device properties shown above indicates that for the same volume of the perovskite layer per unit area, QIBC PSCs possess a better light harvesting ability than FIBC and IBC PSCs. However, FIBC and IBC PSCs have a better tolerance for imperfections in material properties of the perovskite layer (e.g., small charge carrier diffusion length and high surface recombination rates in the perovskite layer). An additional criterion that is worth mentioning is the challenges associated with the device manufacturing, especially when considering which of these three types of BC-PSC designs are better

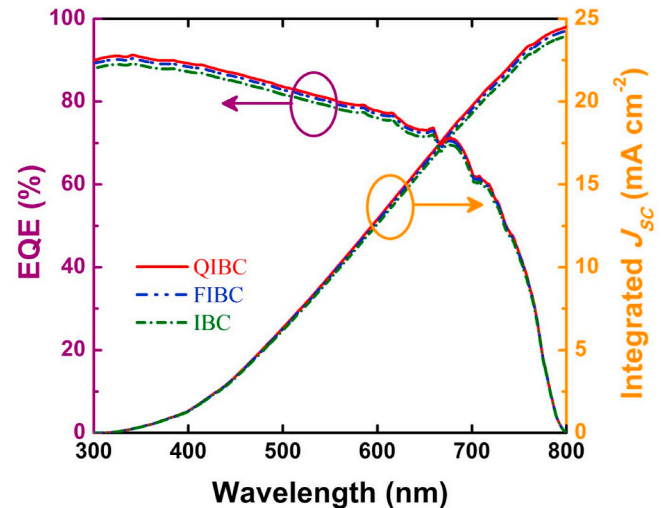


Fig. 9. External quantum efficiency (EQE) spectra of QIBC (red), FIBC (blue), and IBC (olive) PSCs and integrated short-circuit current density for each device type, obtained from integration of the corresponding EQE spectra. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

suited for experimental studies. The BCEs with the traditional IBC design typically involve a two-step lithography process and vacuum deposition of the electrode functional layers to fabricate the interdigitated anode and cathode layers. Alternatively, it is also possible to employ a one-step lithography process to fabricate the interdigitated metallic contacts, and then deposit the ETL and HTL layers on them [5,7,23,34]. The resulting IBC electrodes are suitable for solution-processed deposition of the perovskite layer. From the manufacturing point of view, the IBC design for BCEs is rather challenging because of the two-step lithography processing and small distances (~ 100 nm) between the anode and cathode contacts, which requires more sophisticated and, perhaps, expensive lithography tools. As for IBC electrodes made with only a one-step lithography process, challenges arise during the deposition of the ETL and HTL layers. Here, the ETL and HTL layers can be deposited via electrochemical methods [5,7,23,34]. However, due to small distances (~ 100 nm) between the anode and cathode contacts, deposition of the high-quality ETL and HTL layers to their respective electrodes might also be challenging. Hence, a well-controlled selective deposition of the ETL and HTL materials to their respective metallic contacts must be ensured to avoid cross-contamination [7].

Fabrication of FIBC PSCs can be even more complex than IBC PSCs. In this case, FIBC electrodes can be fabricated on top of a pre-synthesized single-crystal perovskite layer as was demonstrated by Song et al. [6], or FIBC electrodes can be fabricated first, and then the perovskite layer is deposited on top of FIBC electrodes to complete the device fabrication process. Either way, the fabrication of BCEs with the FIBC design involves two-step lithography processing and vacuum deposition of device functional layers. However, the advantage of the FIBC design over the IBC design is that the former is suitable for both, the pre-synthesized perovskite layers (e.g., single-crystal) or the perovskite layer deposited on top of pre-fabricated FIBC electrodes (e.g. using various solution-processing methods) in the final step of device fabrication. We also note that the width of the insulating gap between the anode and cathode contacts is also small (~ 100 nm). Hence, as in IBC BCEs, manufacturing of FIBC BCEs may also require more sophisticated and expensive lithography tools.

Finally, fabrication of QIBC PSCs involves a single-step lithography process and vacuum deposition of the device functional layers to fabricate BCEs with the QIBC design, and deposition of the perovskite layer (e.g. using various solution-processing methods) to complete the device fabrication process [4,16,17,19,21,22]. Hence, BCEs with the QIBC design, due to their textured surface, may not be suitable for a perovskite layer that is made of a single-crystal. In this sense, QIBC PSCs are similar to IBC PSCs. However, unlike the FIBC and IBC designs, BCEs with QIBC design can be made by using non-traditional lithographic methods that are more affordable and do not require expensive lithographic techniques and facilities. For instance, Jumabekov et al. [17] has shown that BCEs for QIBC PSCs can be fabricated using microsphere lithography, which is a cost-effective and scalable method to fabricate these electrodes. Thus, from the practical point of view, the QIBC design for BC-PSCs has a bigger advantage over the FIBC and IBC designs. This becomes more apparent when the gap layer between the anode and cathode layers in FIBC and IBC PSCs is considered. Ma et al. showed that if the gap between the anode and cathode layers in FIBC PSCs is increased, the PCE of devices drops quickly [11]. Similar outcome can be anticipated for the IBC design as well. Additionally, as was mentioned above, experimental fabrication of small (~ 100 nm) gap layers between the anode and cathode contacts is extremely challenging, and it is usually achieved with expensive lithography tools such electron beam lithography or thermal scanning probe lithography. This might become an issue when the cost-effectiveness and scalability of FIBC and IBC PSCs are considered. While the PCEs of FIBC and IBC PSCs exceed the PCEs of QIBC PSCs only by a small percentage when there are some electronic imperfections in the perovskite layer (see Figs. 5–8), it may not be as challenging to reduce these electronic imperfections in the perovskite layer by optimizing the deposition process for the perovskite layer.

Hence, it can be cautiously suggested that the QIBC design might have a better application potential than the FIBC and IBC designs if the appropriate protocols for deposition of high-quality perovskite layers on QIBC BCEs are devised.

3. Conclusions

In conclusion, numerical simulation methods are employed to investigate and compare optical and electrical properties of BC-PSCs with the QIBC, FIBC and IBC designs. It is found that BC-PSCs with the QIBC design possess a superior light harvesting ability, whereas the FIBC and IBC designs showed comparable results. Estimation of the charge recombination rates indicate that the lowest recombination loss is found in FIBC PSCs, whereas the highest is found in QIBC PSCs. The effect of the perovskite layer material parameters on the behavior of devices revealed that BC-PSCs with the QIBC design show the best photovoltaic performance at optimal conditions. However, BC-PSCs with the FIBC and IBC designs are more tolerant to certain electronic imperfections in the perovskite layer, and can even produce higher PCEs than QIBC PSCs at such conditions. The QIBC design seems to have a better application potential compared to the FIBC and IBC designs in developing high-performance BC-PSCs due to more cost-effective, scalable, and easy manufacturing possibilities. Overall, our findings presented in this work give insights into the optical and electrical properties of BC-PSCs with the QIBC, FIBC and IBC designs, which are the BCE designs proposed in the literature for developing high-performance PSCs. The findings of this work provide a certain perspective and direction for future development of experimental research in BC-PSCs.

CRediT authorship contribution statement

Erik O. Shalenov: Investigation, Visualization, Writing – original draft, preparation. **Yeldos S. Seitkozhanov:** Investigation, Visualization. **Constantinos Valagiannopoulos:** Methodology, Investigation, Writing – review & editing. **Annie Ng:** Methodology, Writing – review & editing. **Karlygash N. Dzhumagulova:** Methodology, Writing – review & editing. **Askhat N. Jumabekov:** Funding acquisition, Supervision, Conceptualization, Methodology, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.solmat.2021.111426>.

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