Research article

Computational analysis of mixed cation mixed halide-based perovskite solar cell using SCAPS-1D software

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ABSTRACT

Standard MAPbI_3 (MAPI) perovskite suffers from stability and toxicity problems. In this numerical simulation study using SCAPS-1D software, we propose a hybrid perovskite (MA_1−xFA_xPb_1−ySr_yI_3) to reduce these effects; thus, the influence of the mixture of formamidinium (NH_2CHNH_3+), strontium (Sr), methylammonium (CH_3NH_3+ (MA+)) and lead (Pb) on the electrical parameters of a hybrid perovskite-based solar cell is studied. This simulation was performed through modeling the perovskite absorber band gap depending on x and y proportions. This mixture leads to increase the crystallinity or stability by decreasing MA+ proportion by FA+, while the toxicity is reduced by decreasing Pb2+ proportion by Sr2+. We show that the substitution of 90% MA and 15% Pb (MA_0.1FA_0.9Pb_0.85Sr_0.1I_3) to the standard MAPI radically changes the electrical parameters of the material and the performance of the solar cell. A maximum efficiency of 29% (J_sc = 24.2 mA/cm², V_oc = 1.37 V, FF = 87.49%) is obtained in this simulation of the hybrid perovskite-based solar cell. These results are obtained after optimizing the hybrid perovskite band gap (Eg = 1.60 eV), layer thicknesses (0.400 μm for hybrid perovskite, 0.250 μm for TiO_2, ETL, and 0.150 μm for CaO HTL), absorber bulk defect density (10¹¹ cm⁻³), and perovskite/TiO_2 interface defects density (10¹² cm⁻²). Our results show that the composition of MA, FA, Pb, and Sr in the MA_1−xFA_xPb_1−ySr_yI_3 hybrid perovskite may be a way to obtain new perovskites with interesting physical properties for application in solar cells.

1. Introduction

Organic-inorganic perovskites have received considerable attention in recent years. This is due to their great potential as new optoelectronic materials for devices that could be processed with simple and cheap techniques on large surfaces and flexible substrates (Docampo et al., 2013; Hu et al., 2014) and to the modulation of their intrinsic properties (i.e. by changing the composition of AMX, lattice, where A+ is an organic and/or inorganic cations (Cs+, methylammonium (CH3NH3+=MA+), formamidinium (HC(NH2)2+=FA+)), M²⁺ is a metal cation, and X⁻ is a halide anion (Cl⁻, Br⁻, I⁻)). The discovery of their optoelectronic properties has led to the synthesis of many lead halide perovskite materials (APbX₃). A large number of mixed perovskites, i.e., with a mixture of homovalent organic and/or inorganic cations (McMeekin et al., 2016; Pellet et al., 2014; Saliba et al., 2016) and/or a mixture of homovalents anions, have also been successfully synthesized. These perovskite materials have been developed to improve the performance and stability of photovoltaic devices using these types of materials as an absorber layer. However, lead toxicity remains a major issue for the further development of halogenated perovskite-based photovoltaic devices (Yin et al., 2014). Indeed, the degradation of materials in the presence of humidity leads to the release of Pb²⁺ in aqueous medium, posing serious health and environmental problems. Thus, many studies have focused on the substitution of homovalent Pb²⁺ cation by Sn²⁺ cation (Eperon et al., 2016; Noel et al., 2014), since it belongs to the same group in the periodic table and therefore materials with similar properties are expected; but, Sn²⁺ easily oxidizes to Sn⁴⁺ when exposed to air (Adjokate et al., 2019), which compromises the stability of perovskite materials and renders them unusable. Therefore, the identification of alternative divalent metal cations to Pb²⁺ and Sn²⁺ and allowing to preserve the excellent optoelectronic properties of perovskite, to reduce its toxicity without further altering its stability, remains to be explored. Thus, compositional engineering and doping are commonly employed strategies, which are viable means to control the crystal growth, structural stability, and light conversion properties of most perovskite materials (Lau et al., 2017; Zhou et al., 2018). Stron-

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tium (Sr$^{2+}$) is one of the metal dopants with multiple functions such as improving the stability of the host perovskite and the device performance; in addition, its oxidation state (+2) allows the doping of the crystal structure of Sn-based perovskites to stabilize and tune their optoelectronic properties. Moreover, strontium is very abundant and environmentally friendly (Adjokatse et al., 2019). Its ionic radius (1.18 Å) is close to that of Pb$^{2+}$ (1.19 Å) (Kour et al., 2019), which favors an excellent substitution of lead while maintaining the intrinsic properties of the host (Gualdrón-Reyes et al., 2021). However, pure Sr halide perovskite has a very wide band gap (3.6 eV for MAPbI$_3$ (Pérez-del-Rey et al., 2016)) which is not suitable for the absorber layer in single n-p junction solar cells, as their band gap limit is 1.60 eV (Polman et al., 2016).

It is also necessary to remedy the crystallinity problem caused using the organic cation MA$^+$ in the perovskite and in this case, formamidinium (HC(NH$_2$)$_2$$^+$ = FA$^+$) is used to promote a more stable perovskite structure (Mateen et al., 2020). However, the implementation of the device with FAPbI$_3$ as absorber being very restrictive (Mozaffari et al., 2018), and the resulting performances are often lower than those of the MAPbI$_3$-based solar cell. To solve these problems, composition engineering suggests the mixing of MA$^+$ and FA$^+$ cations as in the structure proposed by He et al. (MA$_{1-x}$FA$_x$PbI$_3$) (He et al., 2017). In this simulation study via SCAP-1D software, we employ compositional engineering through the hybrid perovskite structure MA$_{1-x}$FA$_x$Pb$_{1+3y}$Sr$_{1+y}$I$_3$ to propose a solution to both crystallinity and toxicity problems; while optimizing the electrical parameters of the cell. First, we determine the correlation between the band gap and the different proportions x and y. Then, we solve the equation obtained by varying these different ratios to obtain different values of the band gap. Finally, we run simulations with these different band gaps to see their impact on the performance of the device. In practice, the implementation of the partial x and y substitutions of the cations can be done by a combination of different techniques such as the two-step spin coating used by He et al. (2017), doping engineering used by Gualdrón-Reyes et al. (2021) and Adjokatse et al. (2019) for y proportions. Furthermore, the formation of AMX$_3$ halide perovskites depends on:

(i) The stability of the BX$_6$ octahedra, which can be predicted by the octahedral factor $\mu_o$.
(ii) The ionic radii of A, B, and X must satisfy the Goldschmidt tolerance factor $t$.

According to Hoefler et al. (2017), Travis et al. (2016), Jacobsson et al. (2015), both of these criteria are satisfied by the perovskite absorber used in our device. Based on the band gap limit and the available experimental data on strontium (Sr), we show that the suitable absorber perovskite layer is MA$_{1-x}$FA$_x$Pb$_{0.35}$Sr$_{0.15}$I$_3$, with a band gap of 1.60 eV. The optimal electrical parameters of the solar cell based on this perovskite absorber layer are: $J_{sc} = 24.2$ mA/cm$^2$, $V_{oc} = 1.37$ V, FF = 87.49%, and PCE = 29%.

2. Modeling and structure of the solar cell

2.1. Numerical modeling

The concept of the numerical simulation of a solar cell is based on the resolution of the differential equations of Poisson and continuity in semiconductors (Abena et al., 2022; Nguopo et al., 2021). These equations are nonlinearly coupled differential equations for both electrons and holes and are position dependent. In view of the size of the cells, of the order of a few micrometers for the largest, a one-dimensional numerical resolution of these equations is realistic enough to produce convincing results. In this work, we have adopted a one-dimensional description of the perovskite-based solar cell, using the simulation code SCAPS-1D, developed by Burgelman et al. (2000).

2.2. SCAPS input parameters

The structure of our basic solar cell is Glass/SnO$_2$:F/TiO$_2$/MA$_{0.5}$ FA$_{0.5}$PbI$_3$/CuI/CuO/Au, as we presented and explained in our previous work (Abena et al., 2022). However, to propose a solution to the crystallinity and toxicity problems of perovskite, the absorber layer MA$_{0.5}$ FA$_{0.5}$PbI$_3$ is replaced by MA$_{1-x}$FA$_x$Pb$_{1+y}$Sr$_{1+y}$. The optical absorption coefficient of the absorber is calculated using the following relationship $a(E) = A_x (hv - E_g)^{0.5}$ (Gamal et al., 2021), where the pre-factor $A_x$ is $10^5$ cm$^{-1}$eV$^{-0.5}$. This absorption coefficient is thus affected by the band gap which varies with x and y. When the band gap increases, the absorption coefficient decreases and this is illustrated in Fig. 1. The input parameters of the solar cell are presented in Table 1.

3. Results and discussion

Firstly, we correlate the x and y proportions with the band gap Eg. Thus, by solving the equation Eg(x, y) obtained, we simultaneously obtain the rates of MA and Pb which can be substituted, and the corresponding band gap value. Subsequently, we perform simulations of this Glass/SnO$_2$:F/TiO$_2$/MA$_{0.5}$ FA$_{0.5}$Pb$_{0.35}$Sr$_{0.15}$I$_3$/CuI/CuO/Au solar cell using the SCAPS-1D software to determine the optimal photovoltaic parameters.

3.1. Effect of formamidinium (FA) and strontium (Sr) proportions on the perovskite solar cell performance

Shockley and Queisser showed that the band gap (Eg) of the absorber material used in solar cells strongly influences the photovoltaic performance (Shockley and Queisser, 1961). However, Eg often varies nonlinearly with the composition (x) of ternary alloys (A$_x$B$_{1-x}$) (J. Xu et al., 2011), and as a first approximation, its variation is quadratic (Equation (1)) (Swafford et al., 2006; Venugopal et al., 2006; Wang et al., 2007).

$$E_g (A_xB_{1-x}) = xE_g (AC) + (1 - x)E_g (BC) - bx(1 - x)$$

(1)

where $b$ is a curvature parameter, describing the extent of the nonlinearity.

In this numerical study, by applying the band gap variation law (Equation (1)) to the work of Ono et al. (2017), Gualdrón-Reyes et al. (2021) and Navas et al. (2015), we respectively obtain the variation of the band gaps of the perovskite absorbers MA$_{1-x}$FA$_x$PbI$_3$ (Equation (2)), FAPb$_{1-x}$Sr$_{1+y}$ (Equation (3)) MAPb$_{1-x}$Sr$_{1+y}$ (Equation (4)), with a (x) FA content and (y) Sr content.

$$E_g (eV) = 0.074x^2 - 0.155x + 1.54$$

(2)
with $x \in [0; 1]$, 

$$E_g(eV) = 1.98y^2 + 0.43y + 1.59$$

with $y \in [0; 0.12]$. 

$$E_g(eV) = 7y^2 - 1.43y + 1.57$$

with $y \in [0; 0.15]$. 

Thus, the application of Equations (1) to (4) to the hybrid perovskite MA$_{1-x}$FA$_x$Pb$_{1-y}$Sr$_y$I$_3$ leads to the following band gap variation law:

$$E_g(eV) = 0.074x^2 + 7y^2 - 5.02xy^2 + 1.86xy - 0.05x - 1.43y + 1.57$$

(5)

with $x \in [0; 1]$ and $y \in [0; 0.15]$. 

Fig. 2 shows, according to Equation (5), the influence of the proportions of FA and Sr on the hybrid perovskite band gap. It can be observed that the band gap decreases when the strontium concentration ($y$) increases and the formamidinium concentration ($x$) decreases. The ideal is to decrease the band gap, it is thus beneficial to substitute MA by FA because as $x$ increases, the band gap decreases. On the other hand, the band gap increases as $y$ increases, despite the fact that it is necessary to substitute Pb by Sr. It is probably through this joint substitution that the negative effect of the partial replacement of lead is reduced. This shows that the smaller the band gap, the higher the electrical parameters. However, for an FA content greater than or equal to 0.9 (90%), and whatever the proportion of Sr, the band gap is less than or equal to 1.60 eV (Fig. 2), which corresponds to the Shockley-Queisser limit, in the case of the perovskite absorber for n-p single junction solar cells (Polman et al., 2016). For an adequate substitution of lead (Pb) by strontium (Sr) and in agreement with the above-mentioned band gap limit, 15% of Sr is the optimal proportion, which allows the perovskite absorber MA$_{1-x}$FA$_x$Pb$_{0.85}$Sr$_{0.15}$I$_3$ to be obtained. This perovskite structure could be obtained by improving the quality and method of deposition. The choice of the band gap value at 1.60 eV, corresponding to 90% FA and 15% Sr, is confirmed by Fig. 3, which illustrates the dependence of the electrical parameters on the proportions $x$ and $y$. 

Fig. 3 shows that for a proportion $x$ greater than or equal to 90%, and whatever the concentration $y$, the electrical parameters of $J_{sc}$ (Fig. 3.a), $FF$ (Fig. 3.c), and $PCE$ (Fig. 3.d) are optimal. Thus, we can reasonably choose $y = 0.15$ which is the highest value proportion of Sr in this study. This corresponds to a band gap less than or equal to 1.60 eV as mentioned previously. On the other hand, only $V_{oc}$ presents a variation contrary to the other electrical parameters according to the proportions $x$ and $y$ (Fig. 3.b), and similar to that of $E_g$ (Fig. 2). This suggests a correlation between the band gap and the open circuit voltage; it is a linear correlation justified by Fig. 4 and Equation (6). This equation is obtained by linear fitting. Many studies have also shown that there is a linear correlation between Voc and band gap, among these are Yang et al. (2017), Vandewal et al. (2008), and Scharber et al. (2006).

$$V_{oc} = 0.879 \times E_g - 0.0368$$

(6)
phenomena leads to a decrease of $V_{oc}$ (Equation (8) Rai et al., 2020). The decrease of PCE is due to the joint decrease in $J_{sc}$ and $V_{oc}$ according to Equation (9). $FF$ decreases with increasing ETL thickness (Fig. 5.c) due to the increase of charge recombination.

$$V_{oc} = \frac{n k T}{q} \ln \left[ \frac{J_{sc}}{J_0} + 1 \right]$$

(8)

Where $\frac{k T}{q}$ is the thermal voltage and $n$ is a factor due to the increase in series resistance.

$$PCE = \frac{V_{oc} \times J_{sc} \times FF}{P_{in}}$$

(9)

Furthermore, we observe a slight increase of $J_{sc}$ with the increase of the thickness of the absorber (Fig. 5.a). This result is explained by a slight increase in the thickness of the space charge region ($W$) with the absorber thickness, which increases the photocurrent through Equation (10) (Abega et al., 2021); and thus causes $J_{sc}$ to increase through Equation (7).

$$J_{ph} = q \times G \times (I_a + W + L_p)$$

(10)

Where $I_a$ and $L_p$ are the electron and hole diffusion lengths, respectively, $W$ is the width of the space charge region, $q$ is the elementary charge, and $G$ is the carrier generation rate.

The decrease of $V_{oc}$ with increasing absorber thickness (Fig. 5.b), is a result of the increase of the recombination phenomenon (Cho and Park, 2017; Jeyakumar et al., 2020) represented by $J_0$ in Equation (8). Fig. 5.c shows that increasing perovskite layer thickness induces a decline of FF from 88.14% to 81.74%, this is explained by the relation between $FF$ and $V_{oc}$ (equation (11) (Guirdjebaye et al., 2019); thus, the increase in the recombination rate and series resistance with this thickness induces a decrease in the $FF$. 

Fig. 3. Variation of electrical parameters as a function of proportions (x) and (y). (a) $J_{sc}$, (b) $V_{oc}$, (c) $FF$, and (d) efficiency (PCE).

Fig. 4. Variation of $V_{oc}$ as a function of the band gap of the MA$_{1-x}$FA$_x$Pb$_{1-y}$Sr$_y$I$_3$ absorber.
Fig. 5. Variation of electrical parameters as a function of absorber and ETL thicknesses. (a) J_{sc}, (b) V_{oc}, (c) FF, and (d) efficiency (PCE).

\[ FF = \frac{V_{oc} - \ln (V_{oc} + 0.72)}{V_{oc} + 1} \]  
(11)

Where \( V_{oc} = \frac{q V_{oc}}{K T} \).

Moreover, as the absorber thickness increases, the charge carriers have also to cover a greater distance to reach the electrodes, increasing the probability of electron recombination with the minority carriers (holes); on the other hand, the low mobility of electrons in the TiO_{2} layer accentuates this effect. Consequently, the efficiency of the cell decreases (Fig. 5.d) and is accentuated by the decrease of \( V_{oc} \) and \( FF \). The maximum efficiency of 29.18% is obtained for absorber and ETL thicknesses equal to 0.400 \( \mu \)m and 0.250 \( \mu \)m, respectively. We therefore choose these thickness values for the rest of our work.

### 3.3. Influence of absorber defect density

To estimate the optimal defect concentration in the absorber for optimal electrical parameters, a simulation was realized, varying the defect density from \( 10^{11} \) cm\(^{-3} \) to \( 10^{17} \) cm\(^{-3} \), as in the work of Shahariar et al. (2020). The J-V characteristic curve (Fig. 6) illustrates how the device parameters decrease significantly when the defect concentration in the absorber is greater than \( 10^{13} \) cm\(^{-3} \). Thus, to obtain a better efficiency, the defects in perovskite must be reduced to \( 10^{13} \) cm\(^{-3} \), as in the work of Slami et al. (2019). This could be done by improving the crystal structure and the processing method. A promising \( FF \) and \( PCE \) of 87.49% and 29.00% were obtained at a defect density of \( 10^{13} \) cm\(^{-3} \).

A higher defect density leads to a higher recombination rate in the perovskite layer, which reduces the carrier lifetime as well as the diffusion length (\( L_D \)) of the charge carriers. This provides a theoretical explanation for the mechanisms that cause the reduction of the electrical parameters of the solar cell.

\[ \tau_{\text{life time}} = \frac{1}{N_i \delta \upsilon_{\text{th}}} \]  
(12)

\[ L_D = \frac{\mu_{\text{e,h}} \mathbb{R} T}{q \tau_{\text{life time}}} \]  
(13)

where, \( N_i, \delta, \upsilon_{\text{th}}, L_D, \mu_{\text{e,h}}, \mathbb{R}, T, q, \) and \( \tau_{\text{life time}} \) are, respectively, the defect density, electron and hole capture cross-section, thermal velocity of the carrier, diffusion length, electron and hole mobility, Boltzmann constant, temperature, charge, and carrier lifetime.

Based on Equations (8) and (14), we can conclude that increasing defect density can increase the recombination current and lead to a decrease in \( V_{oc} \). This is in agreement with the results of Chowdhury et al. (2020), MarisSoucase et al. (2016), and Jamal et al. (2019).
more, the decrease in the internal quantum efficiency (IQE) is due to the increasing of the diffusion length \( L_D \), according to Equation (15) (Geist, 1979); this has a negative effect on the \( J_s \) (Fig. 6).

\[
J_0 \approx q \frac{Dn^2}{L_0N_i} \tag{14}
\]

\[
IQE = 1 - \alpha t - \frac{B}{aL_D^2} \tag{15}
\]

where \( \alpha \), \( t \), and \( B \) are, respectively, the spectral absorption coefficient, the distance to the perovskite material, and the thickness of the perovskite.

### 3.4. Effect of perovskite/TiO₂ interface defect density on PV parameters of PSC

The structural incompatibility of two different materials leads to the occurrence of interfacial defects. The quality of the junction is therefore essential for the performance of the photovoltaic device. In this simulation study, the defect densities at the perovskite/TiO₂ interface vary from \( 10^{10} \) cm\(^{-2} \) to \( 10^{17} \) cm\(^{-2} \) and Fig. 7 shows the effects of this variation on the device performance. It can be seen that for a defect density of \( 10^{10} \) cm\(^{-2} \) to \( 10^{12} \) cm\(^{-2} \), the device parameters vary little; but beyond \( 10^{12} \) cm\(^{-2} \), they start to decrease due to the fact that interface defects behave as recombination centers (Ahmed et al., 2021). Moreover, the largest generation of electron-hole pairs occurs at the perovskite/TiO₂ interface; which is also accompanied by a higher recombination rate (Sengar et al., 2021). We choose an optimal defect density equal to \( 10^{12} \) cm\(^{-2} \) and this leads to the following electrical parameters: \( J_s = 24.2 \) mA/cm\(^2\), \( V_{oc} = 1.37 \) V, \( FF = 87.49\% \); and \( PCE = 29\% \).

Comparing our simulation results with the experimental ones found in the literature (Table 2), we can observe that our results are better than those of the experiment. This is due to the fact that numerical simulation allows to reach unexplored limits by experiment. Thus, numerical simulation is a promising strategy for investigating the properties of photovoltaic devices to improve their performance. The partial substitution of lead by strontium (up to 15%) is a strategy to improve the open-circuit voltage and the fill factor of the hybrid perovskite-based solar cell.

### 3.5. Effect of temperature on solar cell performance

Solar cells are largely governed by their operating temperature. To determine the temperature dependence of our device’s performance, we performed the solar cells parameters using the SCAPS-1D solar simulator, at ambient temperatures (\( T \)) ranging from 25 °C to 105 °C with a 10 °C increment, under 1 sun irradiation as in our previous work (Abena et al., 2022). The value of the temperature coefficient (TC) can be expressed as follows (Krajangsang et al., 2014):

\[
TC(\text{par}/°C) = \frac{1}{Z} \times \left( \frac{\delta Z}{\delta T} \right)_{T_s=25°C}
\]

where \( Z \) means solar cell parameters such as efficiency (PCE), open circuit voltage \( (V_{oc}) \), short circuit current \( (J_s) \), and fill factor \( (FF) \). With a standard temperature \( (T_s) \) equal to 25 °C, corresponding to the standard measurement of the test solar cells.

The normalized electrical parameters obtained are shown in Fig. 8. A slight increase in \( J_s \) is observed before reaching saturation. This increase is due to a decrease in the band gap with the temperature gradient \( (\text{Equation (17)}) \) and an increase in the number of charge carriers generated (Chander et al., 2015), and consequently, to a higher band-to-band absorption coefficient throughout the spectrum associated with the increased temperature (Sameera et al., 2022).

\[
E_s(T) = E_s(0) - \frac{aT^2}{T + \beta}
\]

The effect of temperature on \( V_{oc} \) is due to the growth of the recombination process (Green, 2005; Jhuma et al., 2019). The \( FF \) and efficiency of the solar cell decrease with the increasing operating temperature due to the significant reduction of \( V_{oc} \). Furthermore, based on the temperature coefficients of the efficiency curves, we established that the solar cell structure \( \text{Glass/SnO}_2:F/TiO_2/MA_0.9FA_0.1 Pb_0.65Sr_0.15I_2/Cu_2/O/Au} \) obtained in this work is more stable than the \( \text{Glass/SnO}_2:F/TiO_2/MA_0.9FA_0.1 Pb_0.65Sr_0.15I_2/Cu_2/O/Au } \) solar cell structure obtained by Abena et al. (2022), because the \( TC \) of \(-0.00107/°C \) calculated by Equation (16) in the cell with the MA\(_{0.1}\)FA\(_{0.9}\)Pb\(_{0.65}\)Sr\(_{0.15}\)I\(_2\) absorber is lower than that \((-0.0014/°C \) of the cell with the MA\(_{0.3}\)FA\(_{0.7}\)Pb\(_{1}\) absorber in absolute value.

### 4. Conclusions

In this study, to improve the stability and reduce the toxicity of the MAPb\(_1\) absorber, we proceeded with a partial cation substitution of MA\(^+\) using FA\(^+\) and Pb\(^2+\) using Sr\(^2+\) to form the hybrid perovskite \( (\text{MA}_{1-x}\text{FA}_x\text{Pb}_1\text{Sr}_1\text{I}_2) \). To realize this study by numerical simulation using the SCAPS-1D software, we first established and solved the correlation equation of the \( \text{MA}_{1-x}\text{FA}_x\text{Pb}_1\text{Sr}_1\text{I}_2 \) absorber band gap with \( x \) and \( y \) proportions. Therefore, several configurations are possible for each band gap value. However, the choice of our absorber \( (\text{MA}_{0.1}\text{FA}_{0.9}\text{Pb}_{0.65}\text{Sr}_{0.15}\text{I}_2\text{, } E_g = 1.60 \text{ eV}) \) was based on several criteria such as: the optimal substitution of MA and Pb, the maximum electrical parameters, the maximum limitation of the band gap according to the Shockley-Queisser limit for simple n-p junction perovskite, and the difficulty in practice to realize the structures with 100% FA. Thus, the simulations realized on the different interest parameters of the structure \( \text{Glass/SnO}_2:F/TiO_2/MA_0.1FA_0.9Pb_{0.65}Sr_{0.15}I_2/Cu_2/O/Au } \) lead to the maximum efficiency of 29.0% \((J_{sc} = 24.2 \text{ mA/cm}^2, V_{oc} = 1.37 \text{ V}, \text{ and } FF = 87.49\% )\), which is a 2.33% gain compared to the initial structure with \( \text{MA}_{0.3}\text{FA}_0\text{Pb}_1 \) as an absorber. Finally, the study of the effect of operating temperature suggests that the device having \( \text{MA}_{0.1}\text{FA}_{0.9}\text{Pb}_{0.65}\text{Sr}_{0.15}\text{I}_2 \) as absorber is slightly more stable \( (TC = -0.00107/°C) \) than having \( \text{MA}_{0.3}\text{FA}_0\text{Pb}_1 \) as absorber \( (TC = -0.0014/°C) \). In this study, although progress has been achieved in lead reduction, its substitution by more than 15% strontium cannot be performed due to the limitation of the experimental data available to develop the band gap equation model of the perovskite absorber.
Fig. 7. Variation of $J_{sc}$, $V_{oc}$, $FF$, and efficiency (PCE) as a function of perovskite/TiO$_2$ interface defects. (a) $V_{oc}$ and $J_{sc}$, (b) PCE and $FF$.

Table 2. Comparison of the performance of photovoltaic devices based on different perovskite absorbers.

| Strategy          | Perovskite absorber                  | $J_{sc}$ (mA/cm$^2$) | $V_{oc}$ (V) | $FF$ (%) | PCE  |
|-------------------|--------------------------------------|-----------------------|--------------|----------|------|
| Simulation        | MA$_3$FA$_3$Pb$_3$S$_7$I$_3$          | 24.2                  | 1.37         | 87.49    | 29   |
|                   | (This work)                           |                       |              |          |      |
| Experimental      | MA$_3$FA$_3$Pb$_3$S$_7$I$_3$          | 31.4                  | 0.83         | 81       | 21.1 |
| (R. Lin et al., 2019) |                                    |                       |              |          |      |
|                   | MA$_3$FA$_3$Sn$_2$Pb$_3$I$_3$        | 30.5                  | 0.83         | 81       | 20.5 |
| (Tong et al., 2019) |                                    |                       |              |          |      |
|                   | FA$_3$MA$_3$Cs$_3$Pb$_3$Sn$_2$I$_3$  | 30.2                  | 0.85         | 79       | 20.3 |
| (Yang et al., 2019) |                                    |                       |              |          |      |
|                   | Cs$_8$H$_{16}$FA$_3$MA$_3$Sn$_2$Pb$_3$I$_3$ | 33.14              | 0.81         | 76       | 20.4 |
| (Kapil et al., 2019) |                                    |                       |              |          |      |
|                   | MA$_3$FA$_3$Pb$_3$Sn$_2$I$_3$        | 25.69                 | 0.78         | 70       | 14.01|
| (X. Xu et al., 2017) |                                    |                       |              |          |      |
|                   | FA$_{33}$MA$_{33}$Pb$_{33}$Sn$_2$I$_3$ | 26.45                 | 0.87         | 79       | 18.21|
| (Z. Zhu et al., 2019) |                                    |                       |              |          |      |
|                   | FA$_{33}$MA$_{33}$Sn$_2$I$_3$Ge$_{33}$I$_3$ | 19.5                 | 0.42         | 55       | 4.48 |
| (Ito et al., 2018) |                                    |                       |              |          |      |

Fig. 8. Normalized electrical parameters of the optimized solar cell as a function of operating temperature.

Declarations

Author contribution statement

Aimé Magloire Ntouga Abena; A. Teyou Ngoupo, Dr.: Conceived and designed the experiments; Performed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

J.M.B. Ndjaka, Pr.: Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data.

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Declaration of interests statement

The authors declare no conflict of interest.

Additional information

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