Electro-optical modeling for the design of semitransparent mixed bromide-chloride PSCs

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***Abstract*—UV-selective absorbing perovskites have attracted significant interest due to their potential applications in innovative fields, such as building integration photovoltaics. This appeal arises from the possibility to tune the bandgap by simply varying their crystal composition. In this work we present electro-optical simulations to study the effect of Cl doping in $MAPb(Br_{1-x}Cl_x)_3$ based semi-transparent solar cells. The final purpose is to obtain important guidelines for the solar cell design in order to maximize the transparency and power conversion performance.**

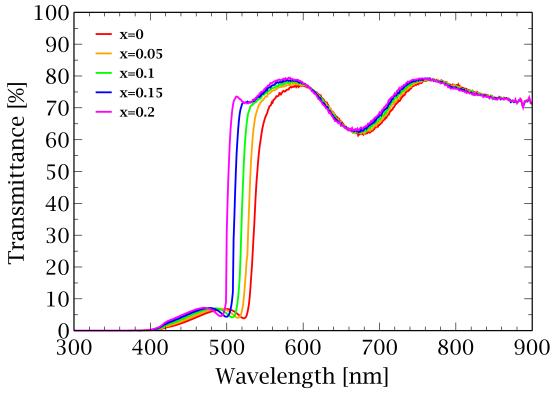
I. Introduction

Over the last decades, the fast increase of global energy demand made the development of Nearly Zero Energy Building (NZEB) solutions crucially important to reduce the effort required by terrestrial PV installations. Among all NZEB solutions, the Building Integration Photovoltaics (BIPV) for facade/window installation guarantees at same time in-situ production of electricity and transparency. Visible Transparent Photovoltaics (TPV) technologies are generally evaluated considering their average visible transmittance (AVT) and power conversion efficiency (PCE). Despite this, the light utilization energy (LUE=PCE$\times$AVT) figure of merit allows to compare different technologies against theoretical limits, furthermore indicating an overall system efficiency. [1] Among all emergent PV technologies for BIPV, perovskite solar cells (PSCs) have recently attracted the interest of the scientific community, due to the high PCE of 25.2% [2] recorded for opaque devices. This is due to their ability providing tunable UV-selective absorption useful for the simultaneous optimization of PCE and AVT.

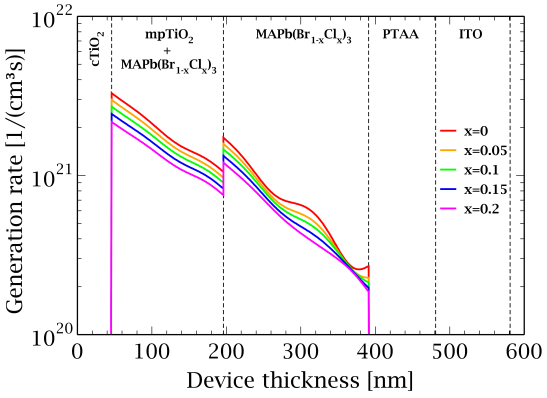
In this work we study the impact of Cl doping on the performance of $MAPb(Br_{1-x}Cl_x)_3$ based semi-transparent perovskite solar cell (ST-PSC). Using a proper electro-optical modeling we extract the guidelines useful for the optimization of the solar cell design.

II. Electro-optical modeling

Although optical calculations are very important for the simulation of solar cells, they can only provide an estimation on the upper limits of performance, in fact not considering all possible electrical losses affecting the power conversion. Therefore, a better approach is to calculate the charge transport considering the generation profile extracted by optical simulations. With this purpose electro-optical simulations have been performed by combining the transfer matrix method (TMM)[3] and drift-diffusion (DD)[4] approach. The TMM is used to calculate the electromagnetic field confinement through the 1D device structure and allows estimating the spectral transmittance and internal absorption profile (G). This is done using the complex refractive index of mediums $\widetilde{k} = 2\pi/\lambda_0\,(n - ik)$, where n and k indicate respectively the refractive index and the extinction coefficient. Performance parameters such as the short-circuit current density (J_{SC}), open-circuit voltage (V_{OC}), fill factor (FF) and PCE are estimated from the charge



(a)



(b)

Fig. 1. Transmittance (a) and internal generation profile (b) obtained with TMM calculations by varying the chlorine doping from 0 to 0.2.

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transport calculation with DD simulations.

III. Results and Discussion

We start our study considering a $MAPbBr_3$ based PSC with mesoporous architecture fabricated on FTO-glass substrate, and varying the Cl doping to tune the $MAPb(Br_{1-x}Cl_x)_3$ bandgap. The absorber layer consists of 150 nm thick mesoporous TiO_2 ($mpTiO_2$) with 195 nm thick emerging perovskite (PK). The full structure is completed by electron and hole transport layers, respectively made by compact TiO_2 (45 nm) and PTAA (90 nm), and 100 nm indium tin oxide (ITO) as bottom transparent contact.

Using proper complex refractive indices[5] we calculated the output transmittance $T(\lambda)$ in the wavelength range of 300-900 nm and the corresponding generation profile within the $mpTiO_2$+PK/PK absorber layers. The $mpTiO_2$+PK layer is considered as blend, therefore the resulting complex refractive index is calculated by effective medium approximation theory (EMA). Transmittance obtained in Figure 1(a) are used to calculate the AVT for the wavelength step $\Delta\lambda$ as follows

$$AVT\,[\%] = \frac{\sum_{\lambda=380}^{780} S_\lambda T(\lambda) V(\lambda) \Delta\lambda}{\sum_{\lambda=380}^{780} S_\lambda V(\lambda) \Delta\lambda}. \quad (1)$$

S_λ is the AM1.5 solar spectra distribution [2] while $V(\lambda)$ indicates the photopic eye sensitivity function. Differently, the internal absorption profiles in Figure 1(b) are used to interface the TMM and DD models. Considering the band alignment summarized in Table I, we performed DD simulations with the purpose to draw the different JV curves corresponding to the generation profile optically calculated. Electrical losses are accounted including recombinations at ETL,HTL/PK interfaces and in the bulk regions. In absorber layers we adopt a trap-assisted recombination model for which we set a trap density value of N_t=5×10^{16} cm^{-3} placed 0.1 eV below the CB, and radiative recombination with rate constant of 10^{-9} cm^3s^{-1}.

Figure 2(a) shows the comparison between experimental and calculated JV for $MAPbBr_3$, and curves simulated for different Cl doping. The perfect match obtained for the reference structure demonstrates the validity of the electro-optical modeling approach adopted. Results obtained for T(λ) and JV allow to conclude on the impact of the Cl doping in ST-PSC devices. Figure 2(b) summarizes the changing of PCE, AVT and LUE due to the increase of Cl doping in $MAPbBr_{1-x}Cl_x$. The most important result is definitely that despite of the gradual decrease of the PCE, the LUE still improves for x=0.05 and 0.1. Therefore, we conclude that the use of a weak Cl doping in $MAPb(Br_{1-x}Cl_x)_3$ perovskite can be successfully used to increase the light utilization efficiency of ST-PSCs.

TABLE I
Energy levels and bandgaps used in DD simulations.

Layer	Material	E_g[eV]	CB[eV]	VB[eV]
ETL	$cTiO_2$	3.30	-4.10	-7.40
Scaffold	$mpTiO_2$	-	-4.10	-
Absorber	$MAPbBr_3$	2.27	-3.63	-5.90
	$MAPbBr_{2.85}Cl_{0.15}$	2.31	-3.61	-5.92
	$MAPbBr_{2.7}Cl_{0.3}$	2.34	-3.60	-5.94
	$MAPbBr_{2.55}Cl_{0.45}$	2.38	-3.59	-5.97
	$MAPbBr_{2.4}Cl_{0.6}$	2.42	-3.57	-5.99
HTL	PTAA	3.35	-1.80	-5.15

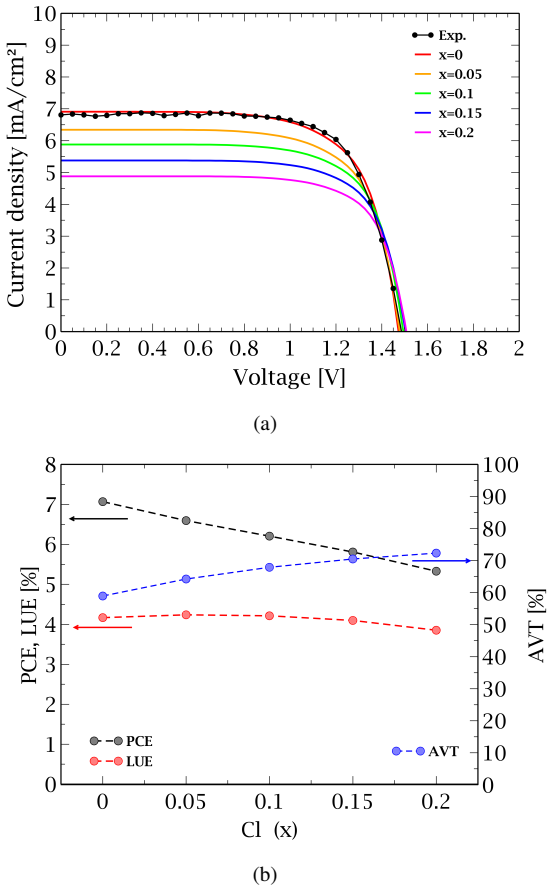

Fig. 2. (a) JV curves (full-lines) obtained with DD simulations by varying x; the dotted line represents the experimental curve considered as reference for the full study. (b) AVT, PCE and LUE obtained for Cl doping.

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