

## Supporting Information

# Hybrid sequential processing of mixed Sn-Pb Narrow-Bandgap Perovskite Solar Cells

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## Experimental

*Materials.* All chemicals were purchased from Sigma-Aldrich, TCI, Merck KGaA, Luminescence Technology Corp, Greatcell Solar and used without further purification.

*Evaporation of inorganic seed layers.* Pre-patterned ITO substrates were cleaned with detergent, DI water and isopropanol, respectively, in an ultrasonic bath. A 20 min UV/O<sub>3</sub> treatment was performed on the cleaned substrates. The substrates were either used as HTM-free or coated with PEDOT:PSS or PTAA prior to seed layer deposition. For the samples with PEDOT:PSS, following the UV/O<sub>3</sub> treatment, the substrates were spin coated with PEDOT:PSS with 4000rpm, for 30s. Then the films were annealed at 150°C for 10 mins. For the samples employing PTAA, 1.5mg/ml PTAA was dissolved in toluene and applied on the substrates with 3000rpm, for 30s. Then the films were annealed at 100°C for 10 mins. The prepared substrates were transferred to a vacuum chamber confined within a nitrogen-filled glovebox for inorganic layer deposition. The sublimation is initiated once the pressure of the evaporation chamber is  $2 \times 10^{-6}$  mbar. PbI<sub>2</sub>, SnI<sub>2</sub> and SnF<sub>2</sub> were co-evaporated simultaneously and the rates were set according to the desired composition. For Pb<sub>0.5</sub>Sn<sub>0.5</sub>I<sub>2</sub> the rates were kept as  $0.5 \text{ \AA s}^{-1}$ ,  $0.5 \text{ \AA s}^{-1}$  and  $0.03 \text{ \AA s}^{-1}$  for PbI<sub>2</sub>, SnI<sub>2</sub> and SnF<sub>2</sub>, respectively. The evaporation rates were monitored through individual QCM sensors for each of the three sources. The typical evaporation temperatures for PbI<sub>2</sub>, SnI<sub>2</sub> and SnF<sub>2</sub> were 250°C, 180°C and 170°C, respectively.

The tooling factors are primarily determined by the source–QCM–substrate geometry. Our vacuum chamber is equipped with four evaporation sources and four dedicated QCM sensors, arranged in a centro-symmetric configuration with respect to the substrate holder. As a result, the tooling factors are effectively equivalent for all sources and are dictated by the fixed chamber geometry rather than by the individual materials. Each precursor was calibrated independently at its specific source/QCM position. To target a desired stoichiometry, the deposition rates were not interpreted directly as molar ratios but were converted into molar fluxes by accounting for the molecular weight and bulk density of each material (assuming a deposition area of  $1 \text{ cm}^2$ , for simplicity). The evaporation rates were then adjusted accordingly. As an illustrative example, for the Pb<sub>0.5</sub>Sn<sub>0.5</sub>I<sub>2</sub> absorber with SnF<sub>2</sub> as a minor additive, PbI<sub>2</sub> and SnI<sub>2</sub> were deposited at identical thickness rates ( $0.5 \text{ \AA s}^{-1}$ ) which, after correction for molecular weight and density, correspond to comparable molar deposition rates, while SnF<sub>2</sub> was introduced at a significantly lower molar flux. The corresponding parameters are summarized below:

PbI<sub>2</sub>: (MM = 461 g mol<sup>-1</sup>; d = 6.16 g cm<sup>-3</sup>) for  $r = 0.5 \text{ \AA s}^{-1}$ ,  $r_{\text{mol}} \approx 0.07 \text{ nmol s}^{-1}$

SnI<sub>2</sub>: (MM = 373 g mol<sup>-1</sup>; d = 4.97 g cm<sup>-3</sup>) for  $r = 0.5 \text{ \AA s}^{-1}$ ,  $r_{\text{mol}} \approx 0.07 \text{ nmol s}^{-1}$

SnF<sub>2</sub>: (MM = 157 g mol<sup>-1</sup>; d = 4.57 g cm<sup>-3</sup>) for  $r = 0.03 \text{ \AA s}^{-1}$ ,  $r_{\text{mol}} \approx 0.01 \text{ nmol s}^{-1}$

*Perovskite Film Preparation.* The inorganic seed layers were transferred to another N<sub>2</sub> glovebox for solution processing. A mixed cation solution of FAI, MAI and MACl (60 mgml<sup>-1</sup>, 6 mgml<sup>-1</sup>, and 6 mgml<sup>-1</sup>, respectively) in iso-propanol or ethanol spin coated dynamically (40 s, 3500 rpm) on the evaporated Pb<sub>x</sub>Sn<sub>(1-x)</sub>I<sub>2</sub> films. After spin coating, the substrates were annealed at 100°C for 1 min in the glovebox.

*Device Fabrication.* After perovskite conversion process, 20 nm of C60 and 7 nm of BCP were deposited in another evaporator with  $0.5 \text{ \AA s}^{-1}$  (~390°C) and  $0.2 \text{ \AA s}^{-1}$  (~130°C), respectively. Ag contacts (100nm) were evaporated within a metal evaporator using Ag pellets by applying currents ranging from 2.0-2.2 A. The fabricated devices were encapsulated with 30 nm of Al<sub>2</sub>O<sub>3</sub> through atomic layer deposition in an Arradiance reactor at 40 °C in accordance with a published protocol.<sup>[1]</sup>

*Measurements.* Absorption spectroscopy measurements were performed with fiber optics based Avantes Avaspec2048 Spectrometer. For photoluminescence measurements, the films were illuminated with a diode laser of Integrated Optics, emitting at 515 nm and the spectra was obtained by Avantes Avaspec2048 spectrometer. The film thickness was measured by using a profilometer (Ambios, XP1). J–V characteristics were measured under AM 1.5G light (100 mW cm<sup>-2</sup>) using a Wavelabs Sinus 70 LED solar simulator. Prior to measurements light intensity was calibrated using a calibrated Si reference diode. A Keithley 2612A source meter was used to record J-V curves, in a -0.2 and 0.8V voltage range, with 0.01 V steps and integrating the signal for 20 ms after a 10 ms delay, corresponding to a scan speed of  $\approx 0.3 \text{ V s}^{-1}$ . Masks with 0.05 cm<sup>2</sup> aperture area were placed on top of the cells during all measurements. The crystalline structure of films was studied by X-ray diffraction (XRD) and the data were collected in Bragg-Brentano geometry on an Empyrean PANalytical powder diffractometer with a copper anode operated at 45 kV and 40 mA. SEM images were taken using the Zeiss Gemini SEM 500 at 4 kV and 0.4 nA. Measurements of external quantum efficiency, internal quantum efficiency and reflection were made using the QE-R system by Enlitech<sup>®</sup>. For calibration of the EQE system, a silicon calibrated device is used (range from 300-1100nm), while for IQE, an integrating sphere is used, which allows to measure the

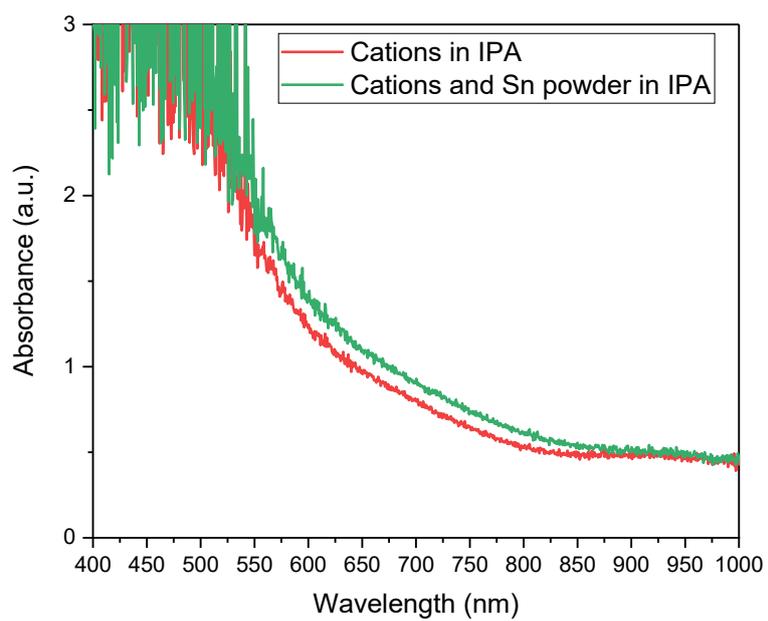
reflection of the sample, which is later used to calculate the internal quantum efficiency IQE

by the formula 
$$IQE = \frac{EQE}{1 - R}$$
.

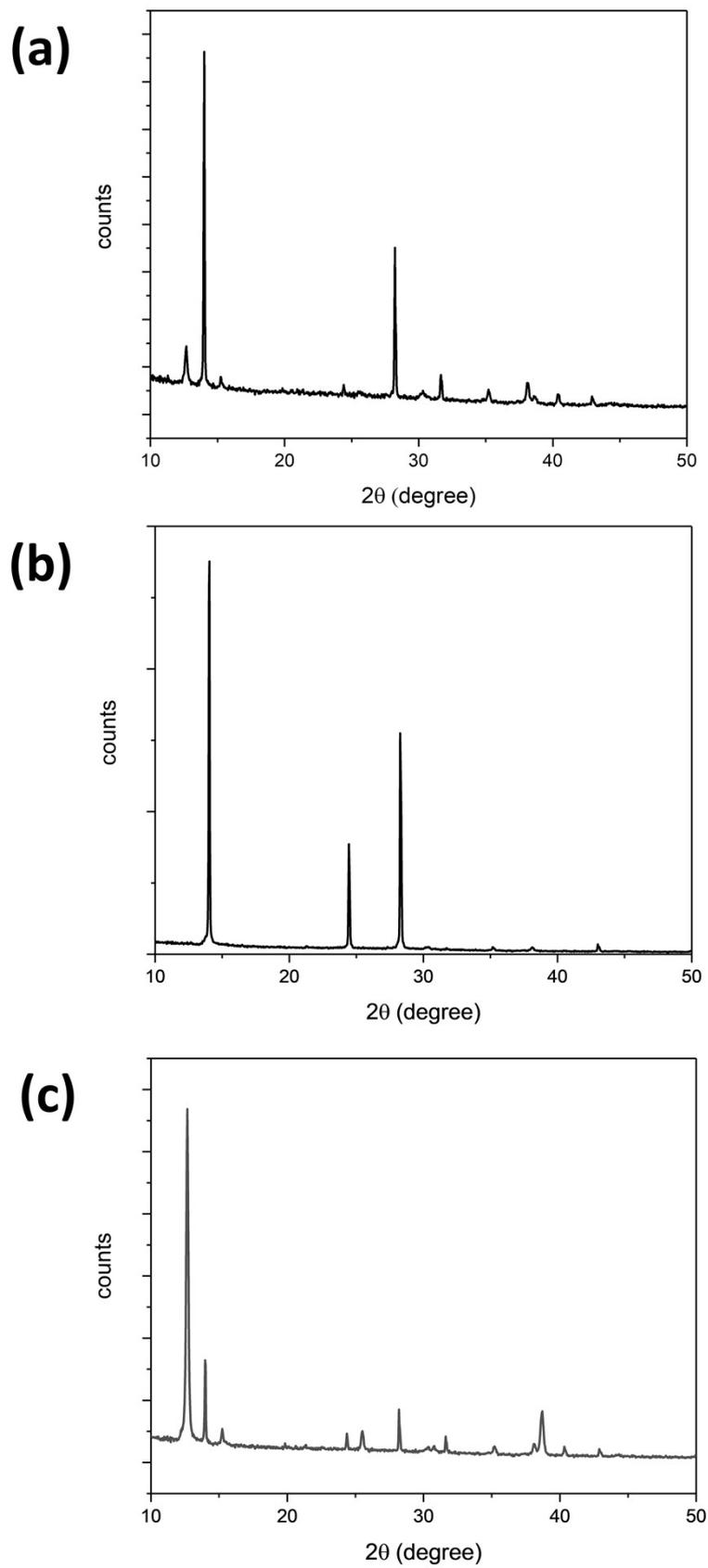
*Diffusion length measurements.* SSPG technique was measured using a configuration similar to the one reported.<sup>[2]</sup>The main idea of the technique is to measure a small change in sample conductivity (at a given voltage) in the presence of an optical grating, which is created by the division of a laser (633nm and 15mW of power in our case) by means of a beam splitter. The measurement is conducted under illumination of two beams I1 being the stronger one (95% of the total illumination) that sets the generation rate, and I2, that's is being chopped serving as a probe beam. The change in conductivity is directly measured on the sample using a lock-in amplifier for two configurations: when the two beams have orthogonal polarization states and therefore do not interfere (homogeneous illumination), followed by aligned polarization states, creating a periodic optical grating. The grating period  $\Lambda$  can be controlled by changing the angle between the two beams, which in our case is done by controlling a motorized linear stage which contains a mirror that redirects the weaker beam into 9 different mirrors, giving us a range of grating period  $\Lambda$  that goes from 0.9  $\mu\text{m}$  up to 27  $\mu\text{m}$ . The current generated is passed through a current/voltage amplifier and then sent to a Lock-In amplifier. The  $\beta$  parameter is then calculated as the ratio between the average of the measures with polarization and without it. Then the curve  $\beta$  vs  $\Lambda$  can be fitted using the formula:

$$\beta = 1 - \frac{2\vartheta}{(1 + (2\pi L_{diff})^2)^2}$$

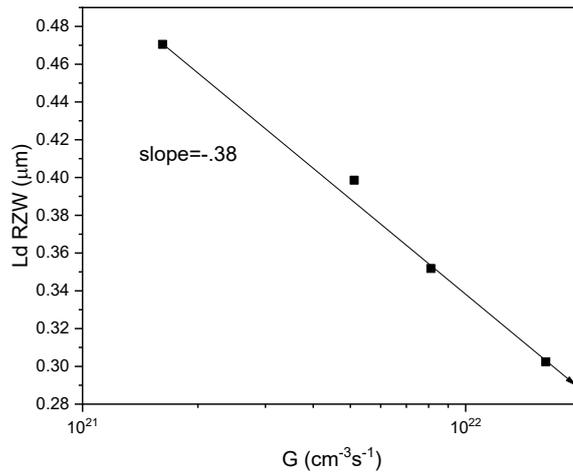
Which gives the diffusion length ( $L_{diff}$ ) and the constant  $\vartheta$  associated with the interference quality.



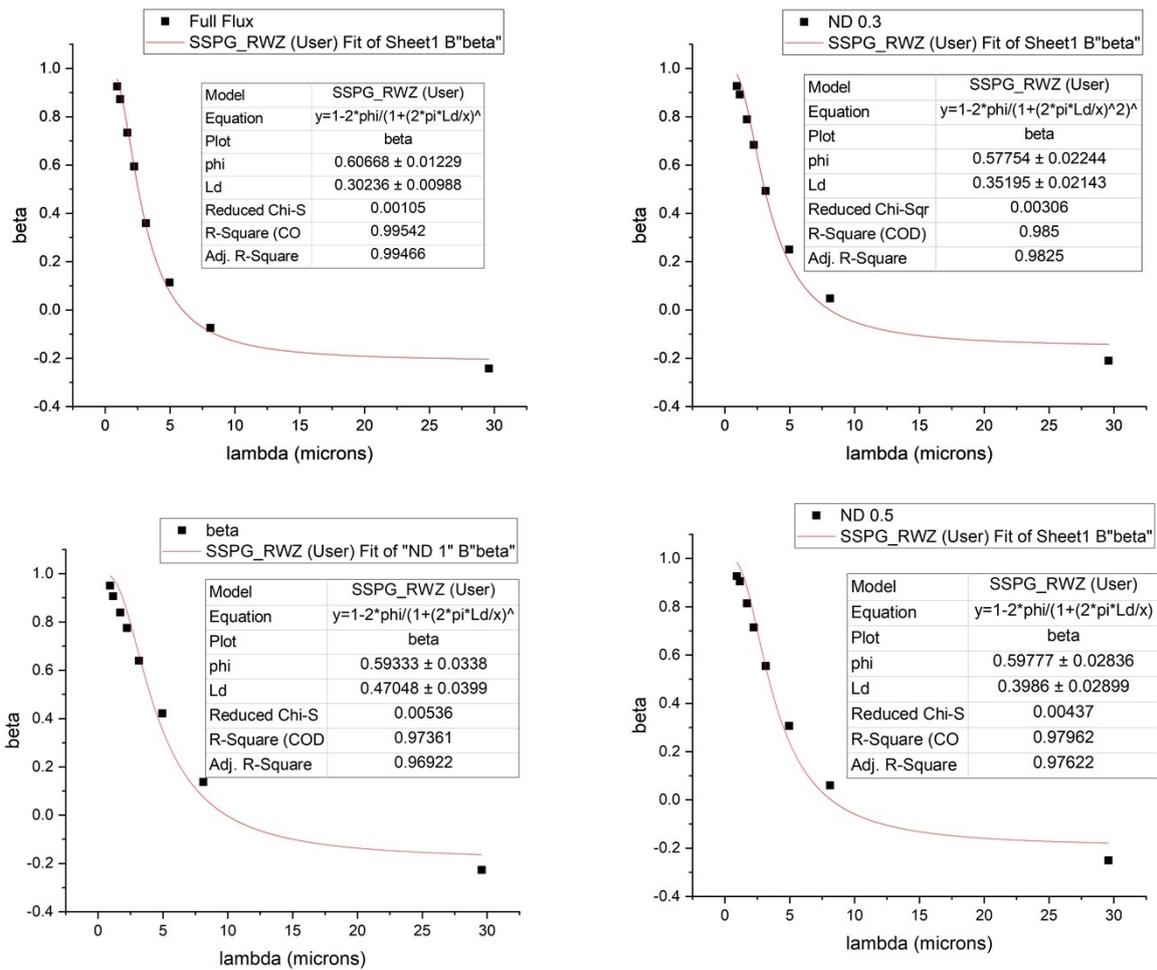
**Figure S1** UV-vis spectra of the fabricated perovskite films.



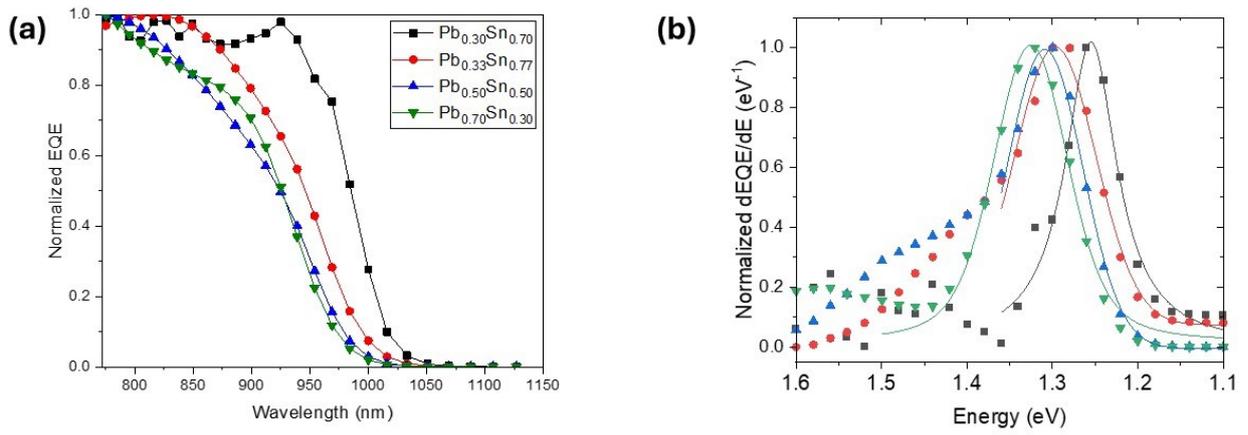
**Figure S2** XRD data of  $\text{FA}_{0.7}\text{MA}_{0.3}\text{Pb}_{0.5}\text{Sn}_{0.5}\text{I}_3$  perovskite on (a) ITO, (b) PEDOT:PSS, (c) PTAA substrates.



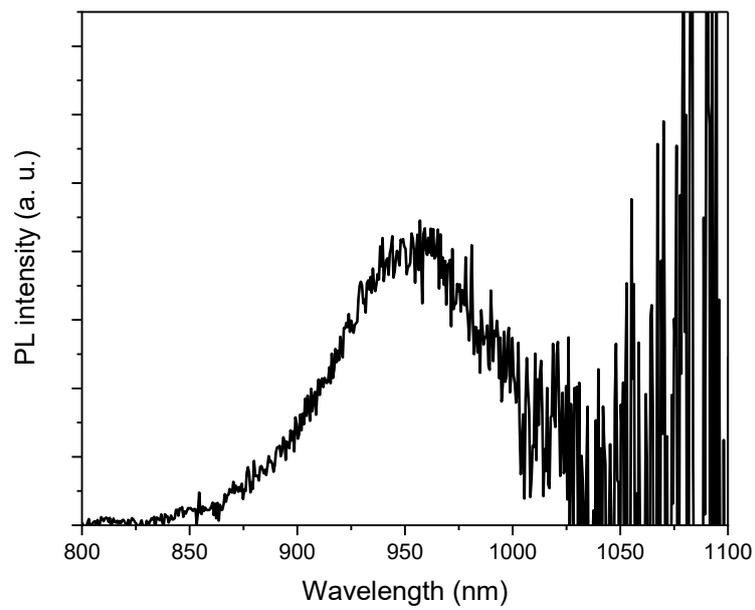
**Figure S3** Change in diffusion lengths according to carrier generation.



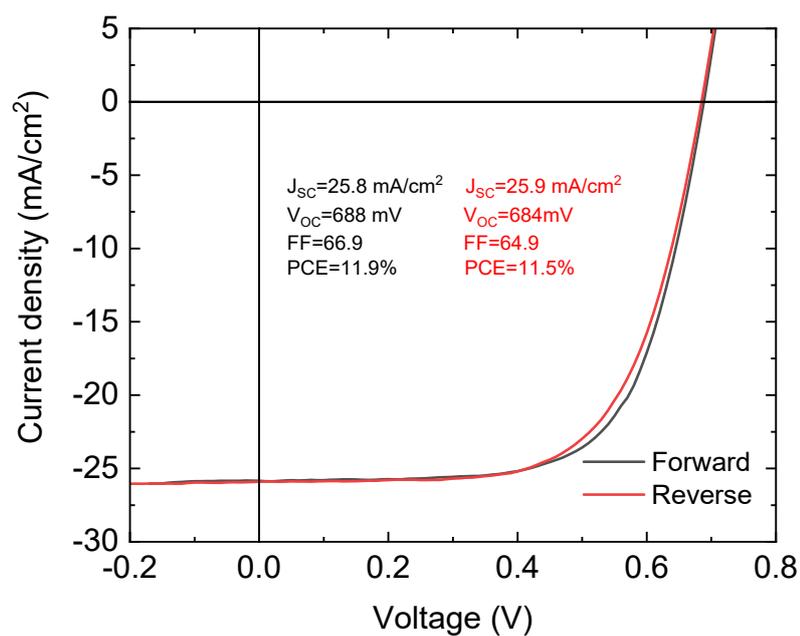
**Figure S4** SSPG Analysis.



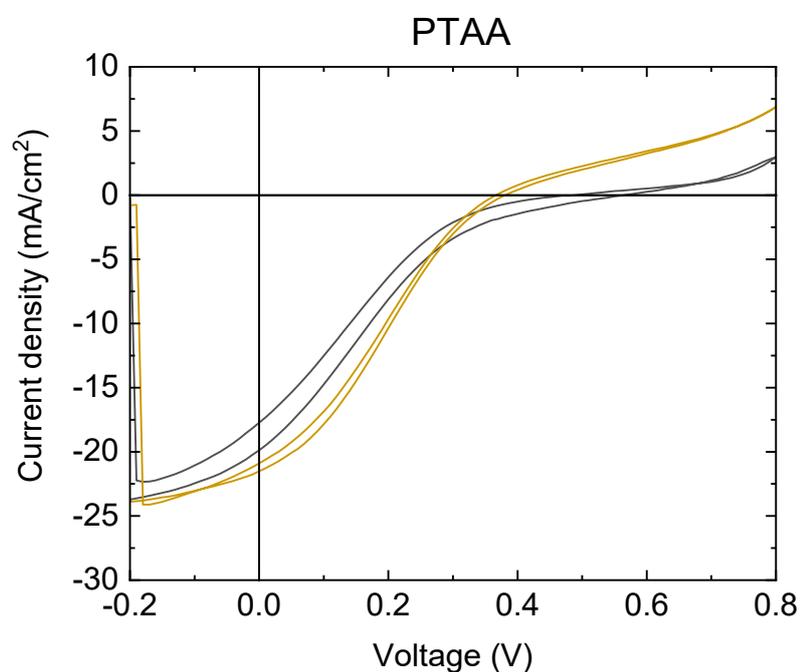
**Figure S5** (a) Normalized EQE spectra at low energy region for different perovskites obtained by conversion of inorganic precursors with different compositions (b) Derivative of the normalized EQE spectrum



**Figure S6** A typical PL image of a fabricated perovskite film.



**Figure S7** Photocurrent density vs voltage curves measured under standard AM 1.5G illumination for the champion device employing PEDOT:PSS as HTM.

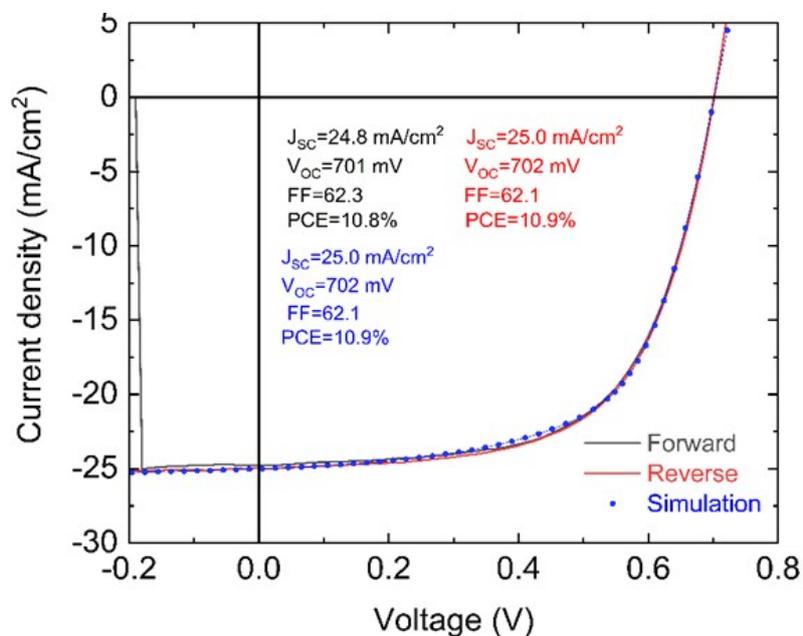


**Figure S8** Photocurrent density vs voltage curves measured under standard AM 1.5G illumination for typical devices employing PTAA as HTM.

## SCAPS-1D Simulations

In order to better elaborate on the changes in PV parameters with respect to the nominal Sn/Pb ratios, we simulated the J-V characteristics of the solar cells using  $\text{FA}_{0.7}\text{MA}_{0.3}\text{Pb}_{0.3}\text{Sn}_{0.7}\text{I}_3$ ,  $\text{FA}_{0.7}\text{MA}_{0.3}\text{Pb}_{0.5}\text{Sn}_{0.5}\text{I}_3$ , and  $\text{FA}_{0.7}\text{MA}_{0.3}\text{Pb}_{0.7}\text{Sn}_{0.3}\text{I}_3$  perovskites on ITO, using SCAPS-1D.<sup>[3]</sup> In the course of the simulations, bandgap values were those derived from EQE measurements, whereas other parameters were gathered from literature. Electron affinity ( $\chi$ ) and acceptor density ( $N_A$ ) values were taken from the absolute energy-level measurements for tin and lead based perovskites<sup>[4]</sup> and from self-doping/redox trends,<sup>[5, 6]</sup> respectively. Interface-trap density ( $D_{it}$ ) values were derived from perovskite/electron transport layer (ETL)<sup>[7]</sup> interface studies, and shunt resistance ( $R_{sh}$ ) values were extracted by means of PSC modeling and standard J-V analysis methods<sup>[8, 9]</sup> to ensure that the simulated and experimental data aligns well (**Figure S9**). The set values for the parameters and the device metrics obtained through the simulations are given in **Table S1** (the information regarding the Global SCAPS settings, contact properties, layer profiles, and interface properties are provided in **Table S2-S4**). Our simulations reveal that higher  $J_{SC}$  values can be attributed to the lower acceptor density  $N_A$  and interface-trap density  $D_{it}$  values, with  $N_A$  having the stronger influence. In wider band gap compositions, the optical penalty is compensated by reduced recombination. Our simulations suggest that enhancement in  $V_{OC}$  values with increasing Pb content is predominantly resulting from the reduction of interface traps. Additionally, fill factor decreases mainly when the shunt resistances and acceptor densities are lower, indicating that higher leakage currents and weaker charge transport outweigh the positive effects of fewer interface traps. The device with 1.3 eV band gap shows slightly improved FF values, due to higher acceptor density and shunt resistance compared to the wider band gap device. The device with the lowest bandgap (1.26 eV) suffers from significant charge collection and recombination

losses resulting in markedly reduced  $J_{SC}$  and  $V_{OC}$  values but higher  $R_{sh}$  value allows better FF values.



**Figure S9** Measured and Simulated J-V Curves

**Table S1:** The parameters used for SCAPS-1D simulation and the resulting J-V metrics.

	$Pb_{0.3}Sn_{0.7}I_2$	$Pb_{0.5}Sn_{0.5}I_2$	$Pb_{0.7}Sn_{0.3}I_2$
Band gap $E_g$ (eV)	1.26	1.30	1.32
Electron affinity ( $\chi$ ) (eV)	4.30	4.39	4.11
Acceptor doping ( $N_A$ ) ( $cm^{-3}$ )	$4.68 \times 10^{17}$	$4.79 \times 10^{16}$	$1.20 \times 10^{15}$
Perovskite/ETL ( $D_{it}$ ) ( $cm^{-2}$ )	$2.29 \times 10^{12}$	$9.00 \times 10^{11}$	$1.00 \times 10^9$
Shunt resistance ( $R_{sh}$ ) ( $\Omega.cm^2$ )	$7.44 \times 10^2$	$2.91 \times 10^2$	$2.00 \times 10^2$
Device metrics			
$J_{SC}$ ( $mA.cm^{-2}$ )	14.0	22.7	25.1
$V_{OC}$ (V)	0.65	0.70	0.72
FF (%)	67.2	59.4	55.2
PCE (%)	6.15	9.37	9.90

**Table S2** Global SCAPS settings and contacts

Geometry, Scan, Illumination	
Illumination	From left (ITO/perovskite side), AM1.5G, 1 sun, 300K. <sup>[10]</sup>
Series / Shunt ( $\Omega.cm^2$ )	Rs=3.67; Rsh=Variable <sup>[8]</sup>
Contact optical filters	Transmission value = 0.82 (used as a flat front-side loss proxy). <sup>[11]</sup>
SCAPS contact mapping	
Left contact (front)	ITO/Glass; Flatband. <sup>[3]</sup> $S_n = 1 \times 10^2 cm.s^{-1}$ , $S_p = 1 \times 10^7 cm.s^{-1}$ <sup>[3]</sup>
Right contact (Rear)	Ag; Work function $\Phi_m = 4.3 eV$ <sup>[12]</sup> $S_n = 1 \times 10^7 cm.s^{-1}$ , $S_p = 1 \times 10^3 cm.s^{-1}$ <sup>[3]</sup>

**Table S3** Layer Profiles

Layer parameter	<i>Perovskite</i>	$C_{60}$ (ETL)	<i>BCP</i>
Thickness (nm)	430	20	7
Bandgap $E_g$ (eV)	Variable	2.30 <sup>[13]</sup>	3.50 <sup>[14]</sup>
Electron affinity $\chi$ (eV)	Variable	4.50 <sup>[15]</sup>	4.50 *
Dielectric permittivity $\epsilon_r$ (relative)	20 <sup>[16]</sup>	4 <sup>[17]</sup>	3 <sup>[17]</sup>
Density of states $N_C = N_V$ ( $cm^{-3}$ )	$1 \times 10^{18}$ <sup>[18]</sup>	$1 \times 10^{19}$ <sup>[19]</sup>	$1 \times 10^{19}$ <sup>[19]</sup>
Thermal velocities $v_{th}$ ( $cm.s^{-1}$ )	$1 \times 10^7$ (n,p) <sup>[18]</sup>	$1 \times 10^7$ (n,p) <sup>[18]</sup>	$1 \times 10^7$ (n,p) <sup>[18]</sup>

Mobilities ( $cm^2.V^{-1}.s^{-1}$ )	$\mu_n = 2$ $\mu_p = 2$ [20]	$\mu_n = 1$ $\mu_p = 1 \times 10^{-3}$ [15]	$\mu_n = 1 \times 10^{-4}$ $\mu_p = 1 \times 10^{-8}$ [14]
Doping ( $cm^{-3}$ )	$N_A = Variable$ $N_D = 1 \times 10^{14}$ [6]	$N_A = 0$ $N_D = 1 \times 10^{16}$ [19]	$N_A = 0$ $N_D = 1 \times 10^{15}$ [19]
Radiative $K_{rad}$ ( $cm^3.s^{-1}$ )	$1 \times 10^{-10}$ [21]	Default	Default
Bulk SRH density of recombination: $N_t$ ( $cm^{-3}$ )	$8 \times 10^{14}$ [22]	$1 \times 10^{14}$ [19]	$1 \times 10^{16}$ [19]
Bulk SRH cross sections: $\sigma_n \sigma_p$ ( $cm^2$ )	$\sigma_n = 1 \times 10^{-15}$ $\sigma_p = 1 \times 10^{-15}$ [23]	$\sigma_n = 1 \times 10^{-15}$ $\sigma_p = 1 \times 10^{-15}$ [23]	$\sigma_n = 1 \times 10^{-15}$ $\sigma_p = 1 \times 10^{-18}$ [23]
Bulk SRH defect energy level: $E_t$ (eV)	0.60 above $E_V$ [23]	0.30 above $E_V$ [23]	0.50 above $E_V$ [23]
Absorption model $\alpha_0$ value (1/cm)	$1.027 \times 10^5$ [24]	Default	Default
Sub-gap tail energy $E_0$ (eV)	0.0025 [25]	Default	Default

Note: “variable” in the perovskite column indicates composition-dependent values reported in main file **Table 1**.

\*: BCP electron affinity ( $\chi_{BCP}$ ) was fixed to 4.50 eV as a numerical convenience to enforce an ohmic Ag/BCP/ $C_{60}$  contact and to avoid convergence errors [3]; this value is not claimed physically (physical value reported typically as  $\sim 3$  eV [26]) and does not affect the composition-dependent trends, which are governed by the perovskite/ $C_{60}$  junction.

**Table S4** Interface profile

	<b>Perovskite/<math>C_{60}</math></b>	<b><math>C_{60}</math>/BCP</b>
Energy reference $E_t$	single at 0.60 eV (above highest $E_V$ ) [23]	single at 0.60 eV (above highest $E_V$ ) [23]
Capture cross-	$\sigma_p = \sigma_n = 6 \times 10^{-16}$ [19, 23]	$\sigma_p = 1 \times 10^{-17} / \sigma_n = 1 \times 10^{-15}$

sections (cm <sup>2</sup> )		[19, 23]
Defect density $D_{it}$ (cm <sup>-2</sup> )	<i>Variable</i>	$3 \times 10^{10}$ [19]

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