

# Interfacial engineering eliminates energy loss at perovskite/HTL junction

Yingke Ren,<sup>a</sup> Hongyang Fu,<sup>a</sup> Yun Li,<sup>a</sup> Zhaoqian Li<sup>\*b</sup> Cong Li,<sup>c</sup> and Xingtao An<sup>\* a</sup>

<sup>a</sup>Hebei Key Laboratory of Photoelectric Control on Surface and Interface, College of Science, Hebei University of Science and Technology, Shijiazhuang 050018, China.

<sup>b</sup>Key Laboratory of Photovoltaic and Energy Conservation Materials, CAS, Institute of Solid State Physics, Hefei Institutes of Physical Science, Chinese Academy of Sciences, Hefei, Anhui, 230031, China.

<sup>c</sup>School of Advanced Materials and Nanotechnology, Xidian University, Xi'an 710126, China

\*Corresponding author

E-mail: anxt2005@163.com (X An)

E-mail: zqli@rntek.cas.cn (Z Li)

## EXPERIMENTAL SECTION

### Film Fabrication (TiO<sub>2</sub>)

Fluorine-doped tin oxide (FTO, Pilkington, TEC15) glass was etched with HCl aqueous and Zn powder. The obtained glass was then cleaned with detergent, distilled water and ethanol, respectively. The blocking TiO<sub>2</sub> layers (bl-TiO<sub>2</sub>) were deposited on the as-prepared FTO through spray pyrolysis method followed by calcining at 510 °C for 30 min. The mesoporous TiO<sub>2</sub> (mp-TiO<sub>2</sub>) films were deposited on the above bl-TiO<sub>2</sub> layer by means of spin-coating the TiO<sub>2</sub> paste (Dyesol 30NR-T). The obtained

layers were following by heating at 510 °C for 20 min.

### **Solar Cell Fabrications (FAPbI<sub>3</sub>)**

The PbI<sub>2</sub> solution (600 mg of PbI<sub>2</sub> and 93 μL of DMSO in 1 mL of DMF) was spin-coated on the TiO<sub>2</sub>/ITO substrate. The obtained films were annealed at 70 °C for 10 min. Then 100 μL of the FAI solutions (80 mg of FAI and 10 mg of MAI in 1 mL of isopropanol) were immediately spin-coated on the PbI<sub>2</sub> films at 5000 rpm for 20s. The intermediate films were immediately annealed at 150 °C for 20 minutes to form various perovskite films. The spiro-OMeTAD solution (25 μL), which consists 73 mg of spiro-OMeTAD, 28 μL of 4-tert-butyl pyridine and 17.5 μL of lithium bis (trifluoromethanesulfonyl) imide (Li-TFSI) solution (520 mg of Li-TFSI in 1 mL of acetonitrile) in 1 mL of CBZ, was spin-coated on the perovskite film at 3000 rpm for 20 s. Finally, Au electrode with a thickness of 60 nm was deposited by using thermal evaporation under vacuum at a constant evaporation rate of 0.6 nm s<sup>-1</sup>.

### **Passivation Layer (BAI)**

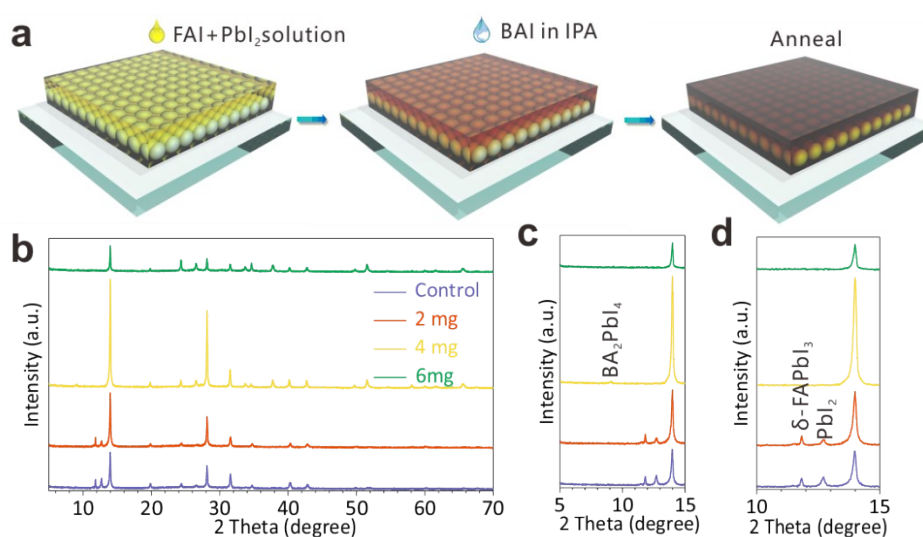
To introduce a passivation layer, 40 μL solution of BAI (4mg) dissolved in the IPA (1 mL) was dropped on the as prepared film. Subsequently, the as-prepared films were heated at 100 °C for 15 min.

### **Characterization**

Field emission scanning electron microscope (SEM) was used to study the top-morphology of the prepared film (FEI Sirion 200, Netherland). The crystal phase was obtained with X-ray diffraction (XRD) using Cu K $\alpha$  beam (X'Pert Pro, Netherland).

The current-voltage curve was measured under one sun illumination (AM 1.5G) with

a solar simulator (94043A, USA) equipped with Keithley 2400 source meter. XPS spectra were collected using a Thermo-Scientific Ka X-ray Photoemission Spectrometer operating at a base pressure of  $5 \times 10^{-8}$  mbar and using an Al anode at a power of 72 W, a hemispherical analyzer, and pass energy of 20 eV. No flood gun was used as all samples are fabricated on the FTO substrate with decent electrical conductance. Ultraviolet-visible (UV-vis) absorption spectroscopy was measured using the spectrophotometer (SOLID3700, Shimadzu Co. Ltd, Japan). Incident photon-to-electron conversion efficiency (IPCE) spectra were measured using a 300 W xenon lamp with a spectral resolution of 5 nm equipped with order sorting filters (Newport/Oriel). Steady PL, TRPL and confocal PL mapping were recorded with a laser confocal Raman spectrometer (Princeton Instruments, Acton Standard Series SP-2558) and a 405 nm laser (OBIS LX-405) using a home-built confocal microscope on a  $10 \times 10 \mu\text{m}^2$  sample area.



**Figure S1** (a) Schematic illustration of the spin-coating with BAI passivation layer for fabricating perovskite layers. (b-d) XRD patterns of annealed formamidinium-based perovskites films fabricated based on different concentrations of BAI precursor

solution.

**Table S1** The detailed  $\tau_1$  and  $\tau_2$  fitting from TRPL of n-type FAPbI<sub>3</sub>.

	$\tau_1$ (ns)	$\tau_2$ (ns)	Average $\tau$ (ns)
n-FAPbI <sub>3</sub>	8.01	25.83	16.87
Rel. (%)	50.3	49.7	