ARTICLE

Supporting Information

Interfacial Modification by Multifunctional Octocrylene for High Efficiency and Stable Planar Perovskite Solar Cells

Yinyi Huang [a, §], Shina Li [b, §], Chaorong Wu [a], Shuo Wang [a], Chengyan Wang [a, c, e*] and RuiXin Ma [a, d*]

[a] *School of Metallurgical and Ecological Engineering, University of Science and Technology Beijing, Beijing 100083, China*

[b] *Tianjin Research Institute for Water Transport Engineering， M. O. T. Tianjin, 300000, China*

[c] *Beijing Key Laboratory of Rare and Precious Metals Green Recycling and Extraction, University of Science and Technology Beijing, Beijing 100083, China*

[d] *Beijing Key Laboratory of Special Melting and Preparation of High-End Metal Materials, University of Science and Technology Beijing, Beijing 100083, China*

[e] *Faculty of Materials Metallurgy and Chemistry， Jiangxi University of Science and Technology, Ganzhou 341000, China*

Corresponding author

Ruixin Ma, maruixin@ustb.edu.cn

Chengyan Wang, chywang@yeah.net

Author Contributions

§Yinyi Huang and Shina Li contributed equally to this work.

Materials preparation

The SnO_2 colloid precursor was mixed with deionized water at a volume ratio of 1:5 to prepare a SnO_2 solution. PbI_2 solution was prepared by dissolving 1.3 M PbI_2 and CsCl (1:0.03 molar ratio) in anhydrous DMF/ DMSO (95:5, v/v). FAI/MAI/MABr/MACl (40 mg/ 19 mg/ 6 mg/ 5 mg) was dissolved in 1 mL of isopropanol. The octocrylene was dissolved in isopropanol at concentrations of 2, 5 and 7 mg/mL without any further purification. The spiro-OMeTAD solution was prepared by dissolving 72.3 mg spiro-OMeTAD in 1 mL CB and 17.5 µl Li-TFSI solution (520 mg in 1 mL ACN) and 28.8 µl TBP.

Device fabrication

ITO glass substrates were cleaned with detergent, deionized water and absolute ethanol in sequence (20 minutes per step). And then use the flowing nitrogen gas to dry the glass. Then irradiated with UV-Ozone for 15 min. After that SnO_2 solution was spin-coated on the top of ITO substrate at 4000 rpm for 30 s. This layer was then annealed at 150 °C for 30 min. Then, PbI_2 (1.3M) was spin-coated on the top of SnO_2 at 2300 rpm for 30 s and then annealed at 70℃. After cooling to room temperature, The FAI/MAI/MABr/MACl solution was then spin-coated on the top of PbI_2 layer at 2000 rpm for 30 s, followed by annealing at 150 °C for 15 min in an ambient air condition (30-40% humidity). In our method, an interfacial layer was introduced between the perovskite layer and the hole layer, and a layer of octocrylene was spin-coated at a speed of 4500 rpm for 20 s. The film was annealed at 100 ℃ for 10 min. the spiro-OMeTAD was formed at 4000 rpm for 20 s to obtain the hole transporting layer. Finally, 80 nm of gold metal was thermally evaporated on top of the device to form the back contact.

Characterizations of photovoltaic properties

The scanning electron microscopy (SEM) images were obtained using a ZEISS SUPRA55 microscope, The X-ray diffraction (XRD) patterns were collected with a Smart Lab from Rigaku by using Cu-Ka radiation (λ = 0.15405 nm). Atomic force microscopy (AFM) images were measured with a 300HV scanning force microscope (SEIKO). The ultraviolet photoelectron spectroscopy (UPS) spectra were analyzed by using AC-2 gas detector (Riken Keiki, Japan). We recorded PV performance of PSC using Keithley 2400 light source instrument with AM 1.5G (100 mW/cm^2) illumination and solar simulator (Newport Oriel Sol3A class A, 64023A class simulator). Related electrochemical tests were performed using a chi660d electrochemical station. The external quantum efficiency (EQE) measurements were performed in the wavelength range of 300 to 900 nm using a DK240 monochromator. Steady state photoluminescence (PL) was measured by using FLS980 spectrometer (Edinburgh, England). The UV-vis light absorption measurement was performed by an ultraviolet-visible (UV-vis-IR) spectrophotometer (Lambda 950).

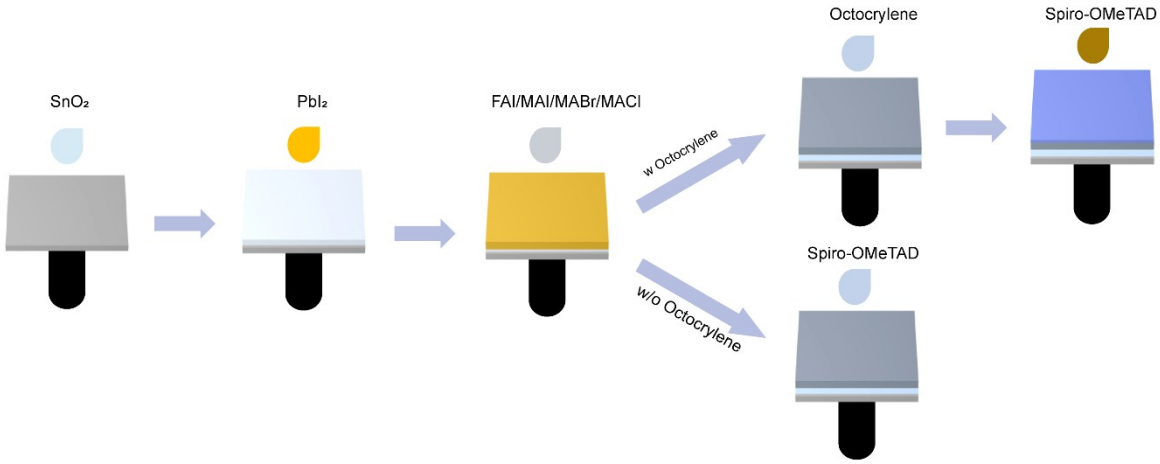

Fig. S1 Schematic representation of the manufacturing process for perovskite devices with and without octocrylene.

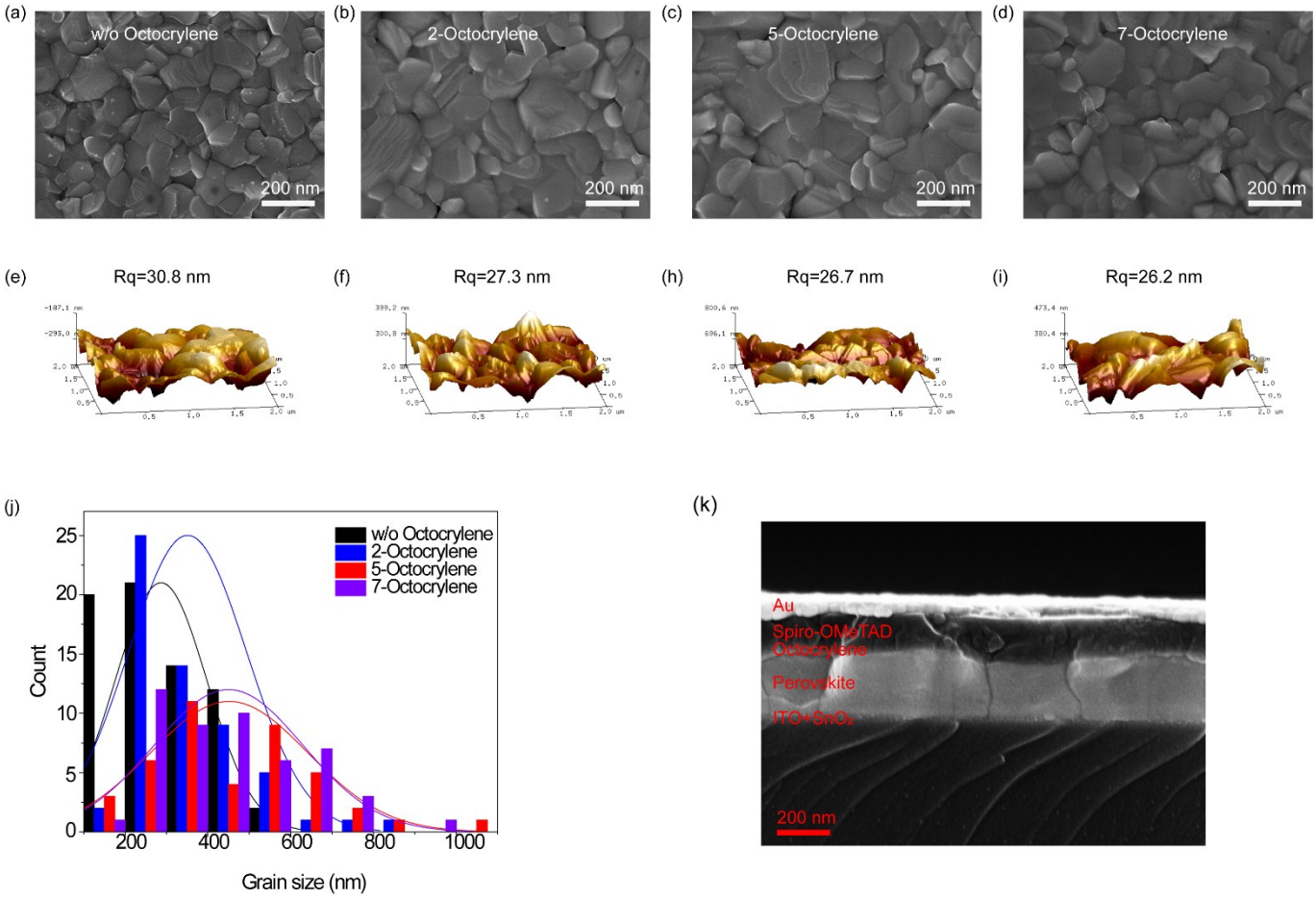

Fig. S2 The SEM and AFM images of the perovskite films (a) and (e) w/o octocrylene, (b) and (f) 2-Octocrylene, (c) and (h) 5-Octocrylene and (d) and (i) 7-Octocrylene. (j) Grain size distributions obtained from SEM images. (k) Cross-section image of the octocrylene device.

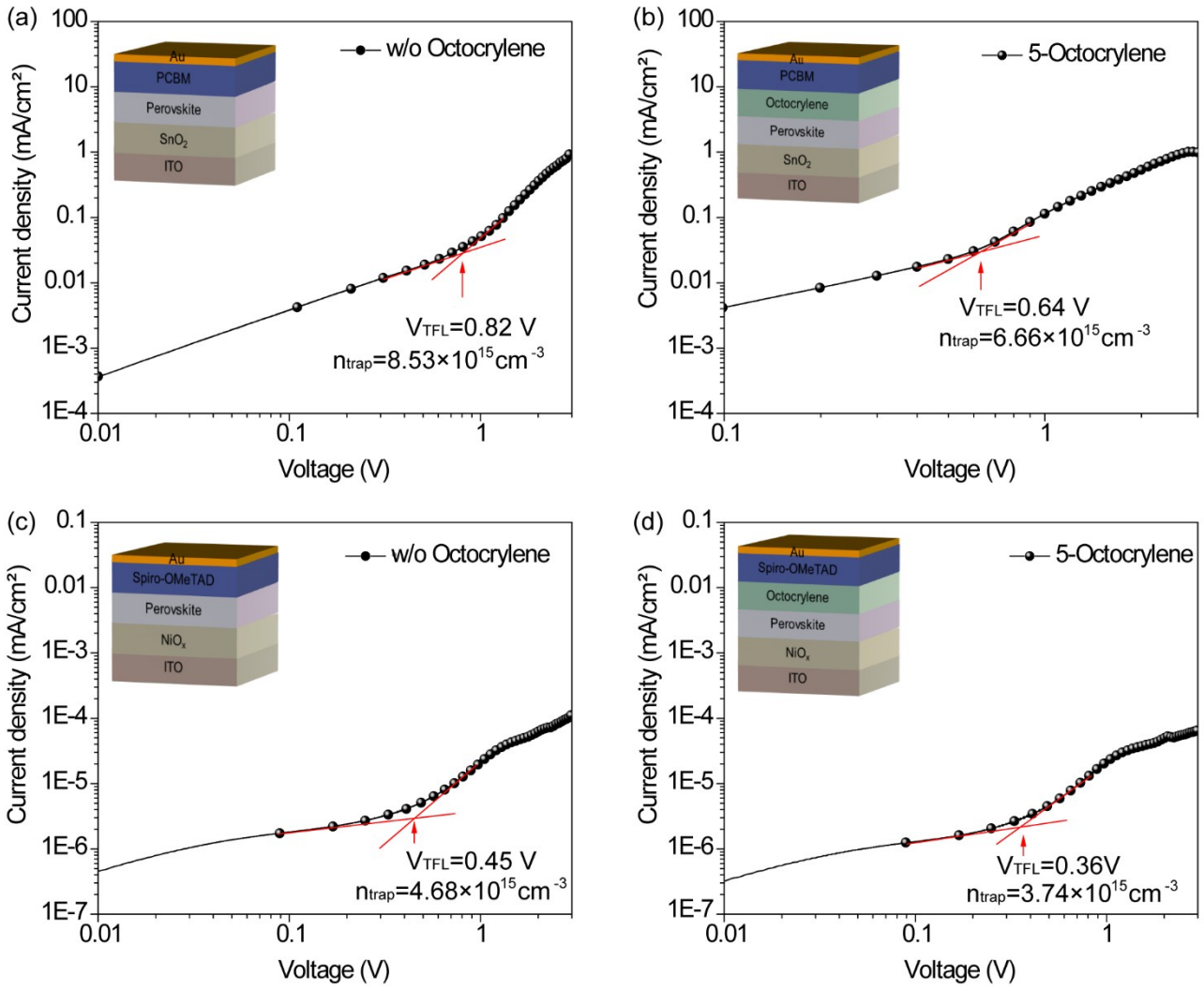

Fig.S3 Current–voltage curves and trap densities of (a and b) electron-only and (c and d) hole-only devices using the space-charge-limited current (SCLC) method (inset, device structure).

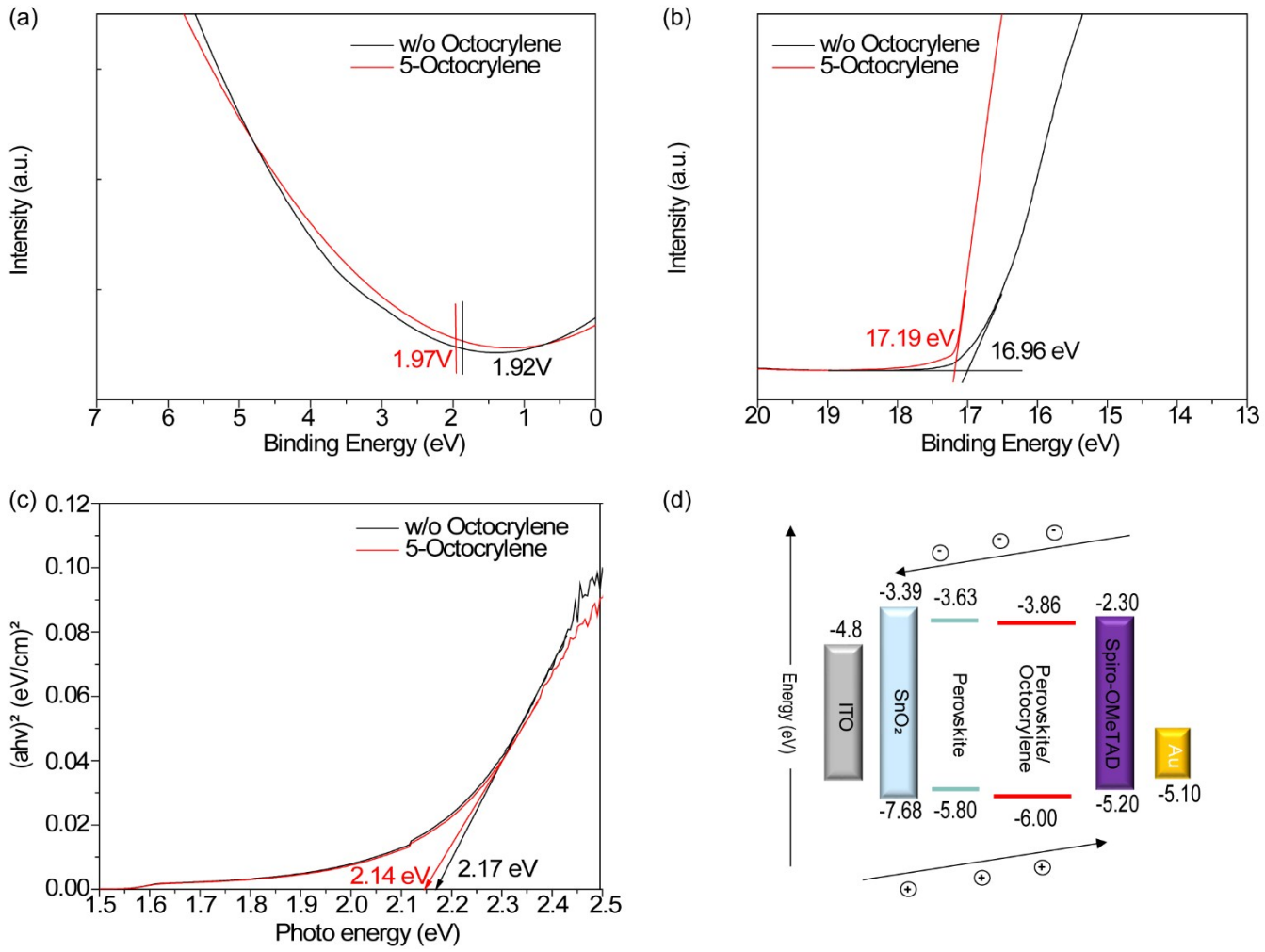

Fig.S4 (a) Valence band spectra. (b) The secondary electron cutoff (SEC) edge. (c) The band gap calculation using the Tauc plot. (d) Energy level diagram of the device.

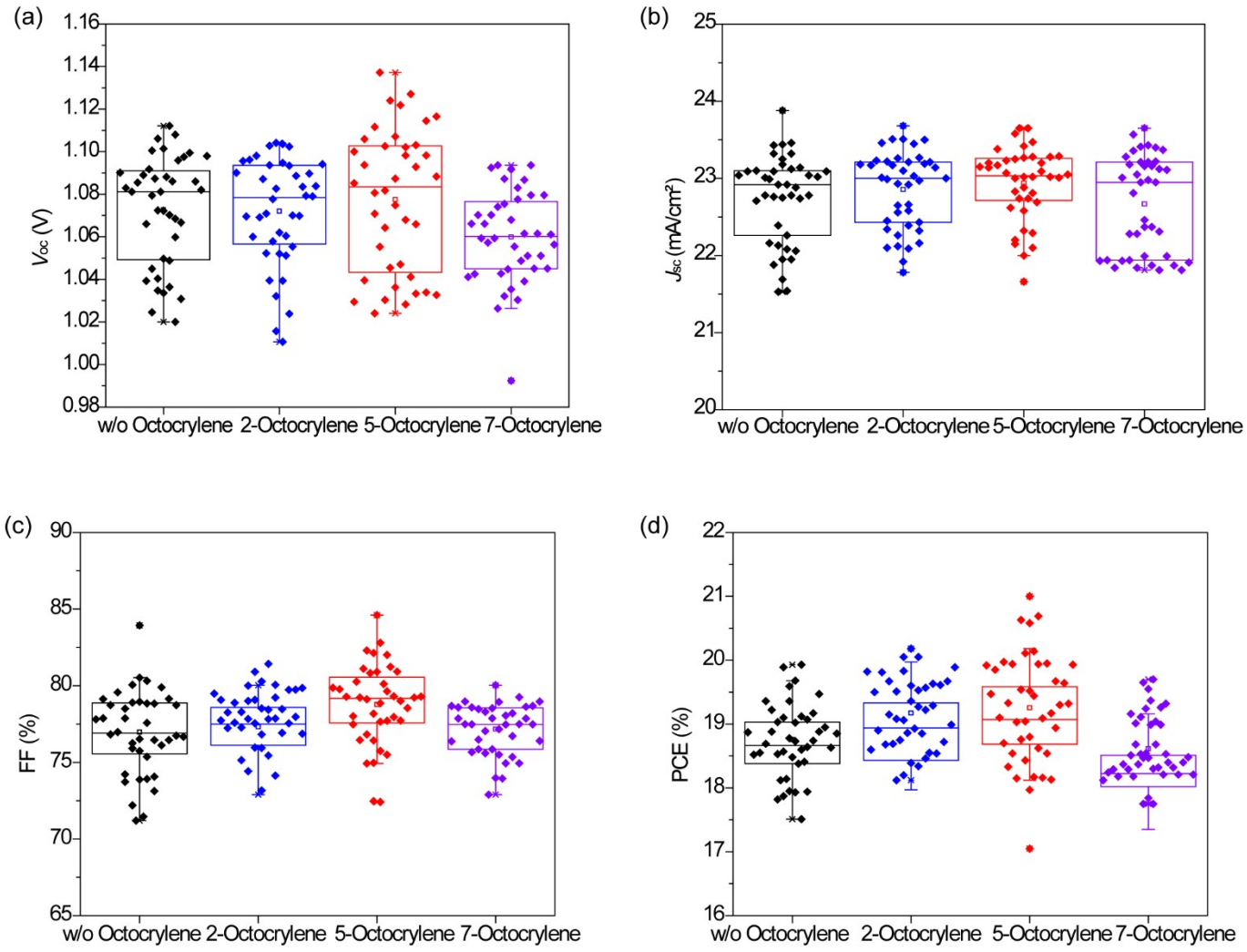

Fig.S5 Statistics on the distribution of (a) V_{oc}, (b) J_{sc}, (c) FF and (d) PCE of PSCs with different concentrations of octocrylene.

Table. S1 Device parameters in forward and reverse scans.

		J_{sc}(mA/cm^2)	V_{oc}(V)	FF(%)	PCE(%)	Hysteresis index
w/o Octocrylene	Reverse	22.06	1.080	83.50	19.89	9.10%
	Forward	22.15	1.067	80.76	18.08	
5-Octocrylene	Reverse	22.91	1.115	80.41	20.54	3.70%
	Forward	22.91	1.076	80.25	19.78	