Electronic Supplementary Information

Correlated alkyl chain length to defect passivation efficacy in perovskite solar cells

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Experimental section

Device fabrication

The patterned ITO glass substrates were washed with detergent, deionized water, isopropanol and acetone baths for 30 min successively, followed by a UV-ozone (UVO) treatment for 15 min. A ~20 nm thick poly[bis(4-phenyl)(2,4,6-trimethylphenyl)amine] (PTAA) layer was spin-coated onto the ITO glass according to previous report.[1] The perovskite layers were fabricated via a blade-coating method.[2] The $Cs_{0.05}FA_{0.70}MA_{0.25}PbI_3$ perovskite ink (1.2 M) was prepared by dissolving PbI_2, FAI, MAI and CsI with designed stoichiometric ratio in dimethylformamide (DMF). A series of UAAs, i.e. methylamine (MA), n-butylamine (BA), hexylamine (HA) and octylamine (OA), were dissolved in DMF separately, then added to the as-prepared perovskite ink at an optimized concentration of 0.025 wt%. After coating, the perovskite films were annealed at 100 °C for 10 min. Finally, 25 nm of C_{60} (Nano-C), 8 nm of bathocuproine (BCP), and 80 nm of Cu electrode were sequentially deposited by thermal evaporation to assemble a complete PSC device.

Device characterization

XRD patterns were measured with a Bruker D8 Discover diffractometer with Cu Kα radiation (1.5406 Å). Scanning electron microscopy (SEM) images were investigated by a field emission scanning electron microscope (FE-SEM, Quanta 200F FEI). The *J-V* curves of the devices were recorded with a Keithley 2400 source-meter under simulated AM 1.5G irradiation produced by a Xenon lamp based solar simulator

(Oriel Sol3A, Class AAA Solar Simulator). The light intensity was calibrated by a silicon reference cell equipped with a Schott visible color KG5 glass filter (Newport 91150V). A non-reflective shadow mask was used to define a 0.16 cm^2 active area of the PSCs. Transient photovoltage (TPV) were taken using a pump pulse generated by a 450 nm laser and background illumination of white LED.

Table S1. The physical properties of different UAAs.

UAAs	Formula	Molecular weight (g/mol)	Boiling point (℃)
Methylamine (MA)	CH_5N	31.06	-6.3
n-Butylamine (BA)	$C_4H_{11}N$	73.14	78
Hexylamine (HA)	$C_6H_{15}N$	101.19	131-132
Octylamine (OA)	$C_8H_{19}N$	129.24	175-177

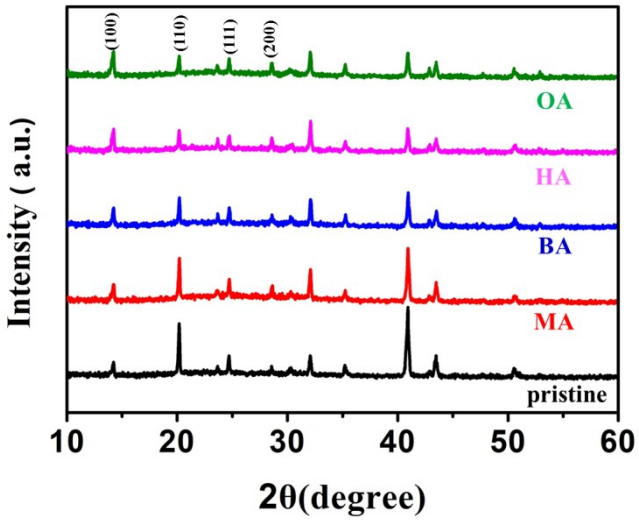

Fig. S1. XRD patterns of perovskite films modified with or without UAAs.

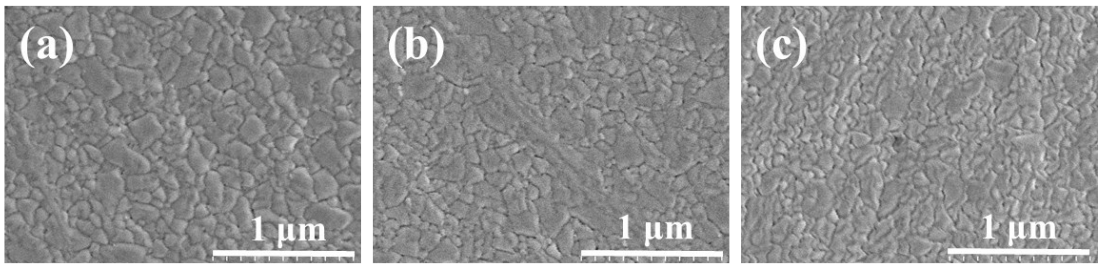

Fig. S2. Surface SEM images of the perovskite film modified with (a) MA, (b) BA and (c) HA.

Table S2. Detailed photovoltaic parameters of PSCs based on perovskite films modified with or without UAAs.

Devices	J_{SC} **(mA cm^{-2})**	V_{OC} **(V)**	**PCE (%)**	***Average* PCE(%)**	***FF* (%)**
Pristine	22.0	1.08	18.4	17.1±1.3	77.5
MA	22.1	1.10	19.1	18.2±0.9	78.6
BA	22.2	1.12	19.9	18.8±1.1	80.0
HA	22.5	1.14	20.9	20.1±0.8	81.5
OA	22.6	1.16	21.5	20.8±0.7	82.0

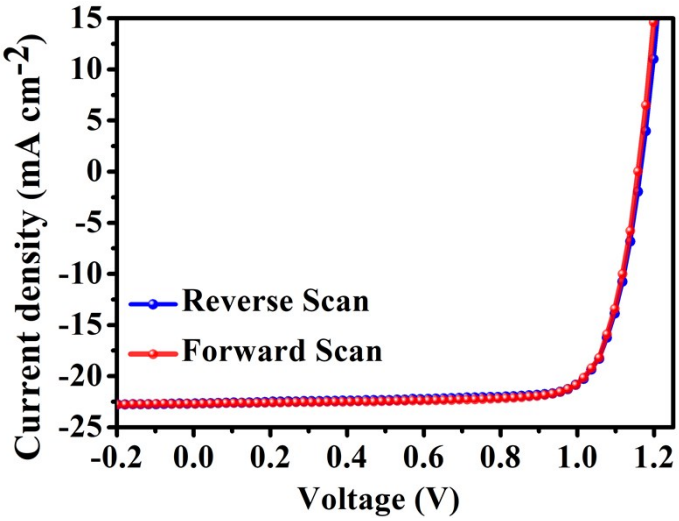

Fig. S3. *J-V* curves of the OA-passivated device measured under reverse and forward scanning direction.

Reference

1. Y. Deng, X. Zheng, Y. Bai, Q. Wang, J. Zhao and J. Huang, *Nat. Energy*, 2018, **3**, 560-566.
2. W.-Q. Wu, Z. Yang, P. N. Rudd, Y. Shao, X. Dai, H. Wei, J. Zhao, Y. Fang, Q. Wang, Y. Liu, Y. Deng, X. Xiao, Y. Feng and J. Huang, *Sci. Adv.*, 2019, **5**, eaav8925.