Support information

Synergistic passivation with multi-dentate 2,6-pyridinedicarboxylic acid for high-performance perovskite solar cells

Yi-Lin Li,[#] Xing Liu,[#] Lei Jin, Jian Zhou*, and Wensheng Fu*

Chongqing Key Laboratory of inorganic functional materials, College of chemistry, Chongqing normal university, Chongqing, 401331, P.R. China

From the EIS data and the following equation, the defect state density of the device at different energies can be quantified:

$$C = -\frac{1}{\omega Z''}$$

$$N_t(E_\omega) = -\frac{V_{bi}}{eW}\frac{dC}{d\omega}\frac{\omega}{K_B T}$$

$$E_\omega = K_B T \ln\left(\frac{\omega_0}{\omega}\right)$$

Where C is the capacitance of the device, ω is the angular frequency, Z'' is the imaginary part of the impedance, N_t is the trap density, W is the depletion layer width, q is the elementary charge, K_B is the Boltzmann constant, T is the absolute temperature, ω_0 is the escape frequency ($\approx 10^{11}$ s^{-1}), and E_ω is the energy boundary.

The defect density of states (N_t) can be calculated by using the following formula:

$$N_t = 2\varepsilon_r\varepsilon_0 V_{TFL}/eL^2$$

Where V_{TFL} is the defect filling limiting voltage, ε_0 is the vacuum dielectric constant (8.854×10^{-14} F/cm, ε_r is the relative dielectric constant of $MAPbI_3$ (21.2), q is electron charge (1.6×10^{-19} C), and L is the thickness of perovskite film (about 353 nm). V_{TFL} can be found from the SCLC curve, and N_t can be calculated.

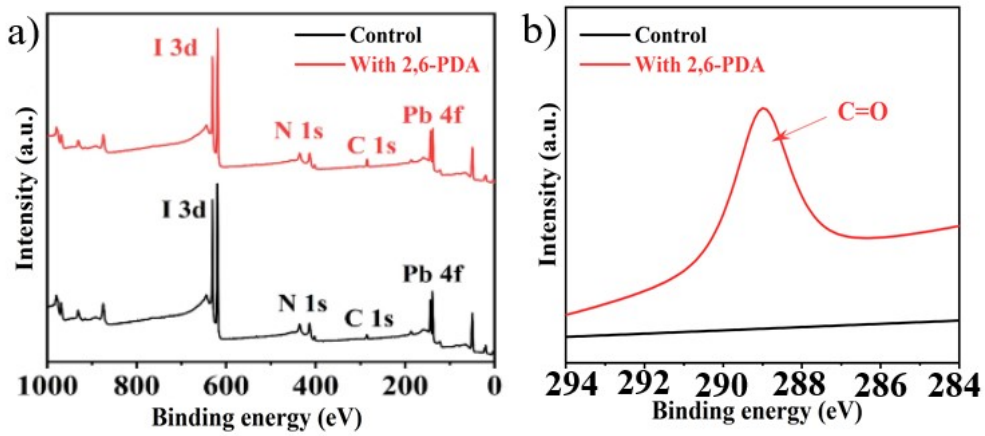

Fig. S1. a) XPS spectra of ITO/PTAA/$MAPbI_3$ and ITO/PTAA/$MAPbI_3$/2,6-PDA films. b) XPS C = O spectra of ITO/PTAA/$MAPbI_3$ and ITO/PTAA/$MAPbI_3$/2,6-PDA films.

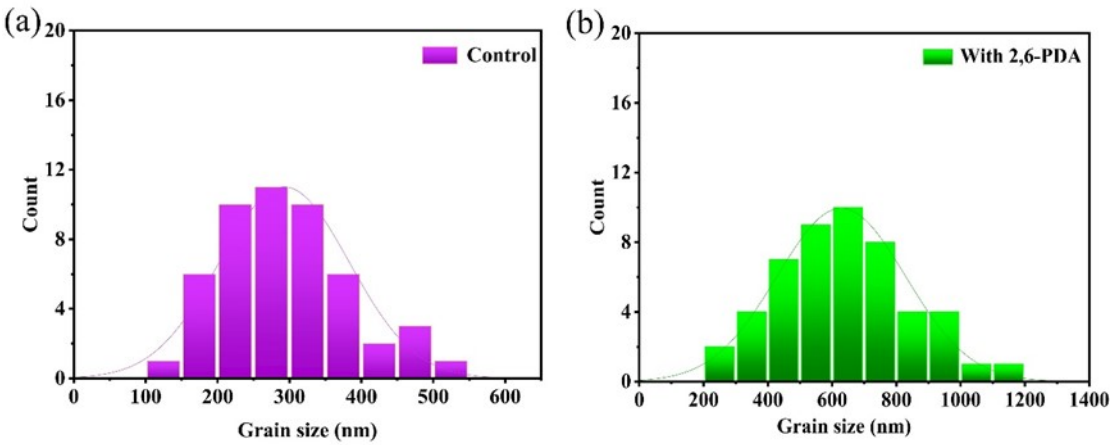

Fig. S2. The grain sizes of (a) ITO/PTAA/$MAPbI_3$ and (b) ITO/PTAA/$MAPbI_3$/2,6-PDA films.

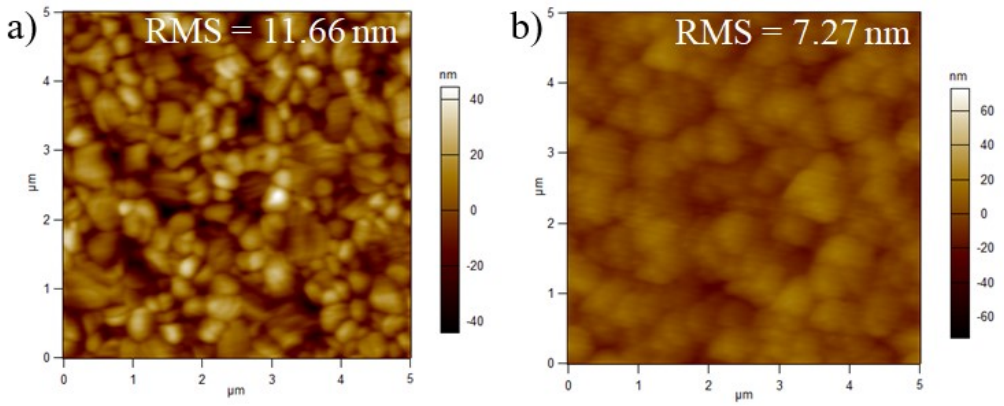

Fig. S3. The 2D AFM images of (a) ITO/PTAA/$MAPbI_3$ and (b) ITO/PTAA/$MAPbI_3$/2,6-PDA films.

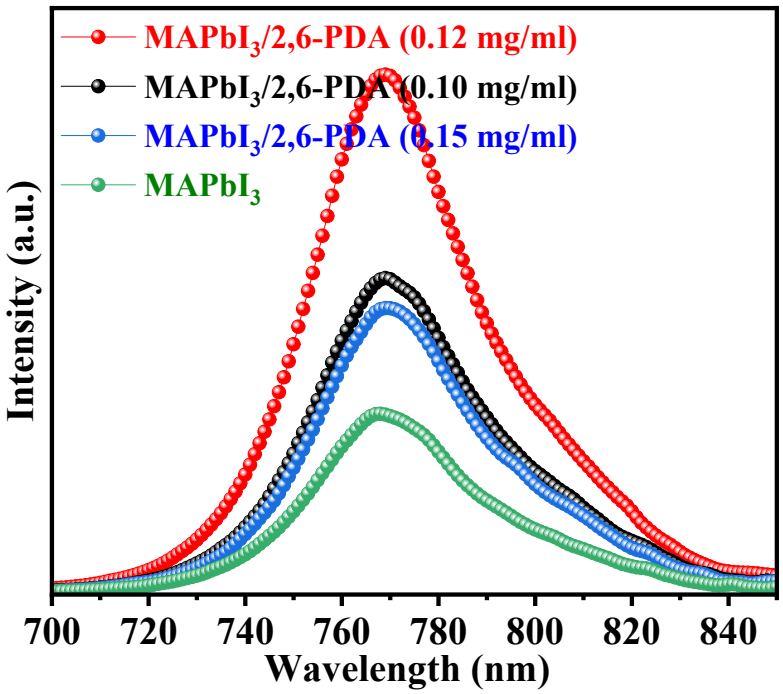

Fig. S4 The PL emission of the quartz/$MAPbI_3$/2,6-PDA film with the different 2,6-PDA concentration.

Table S1. Photovoltaic parameters of the device in different scanning directions

Sample	Direction	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)	HI	Average HI
2,6-PDA	Forward	1.10	23.37	80.26	20.57	0.17	0.14
	Reverse	1.11	23.31	79.24	20.50		
	Forward	1.10	21.83	81.58	19.64	0.10	
	Reverse	1.11	21.90	81.38	19.68		
	Forward	1.11	21.93	79.53	19.41	0.15	
	Reverse	1.11	21.99	79.45	19.47		
Control	Forward	1.10	21.93	79.28	19.19	1.24	1.05
	Reverse	1.10	21.92	77.64	18.72		
	Forward	1.09	21.80	76.51	18.21	0.84	
	Reverse	1.09	21.89	77.39	18.52		
	Forward	1.09	21.74	77.58	18.46	1.07	
	Reverse	1.10	21.57	79.91	18.86		

Table S2. TRPL fitting parameters for different films

Sample	τ_1 (ns)	A_1 (%)	τ_2 (ns)	A_2 (%)	T_{ave} (ns)
$MAPbI_3$	6.42	26.67	16.70	73.33	15.43
$MAPbI_3$/2,6-PDA	6.74	23.63	19.69	76.37	18.45
$MAPbI_3$/PCBM	1.61	96.84	4.41	3.16	1.84
$MAPbI_3$/2,6-PDA/PCBM	1.20	98.73	3.59	1.27	1.29

Table S3. EIS fitting parameters of control device and 2,6-PDA device

Sample	R_s	R_{rec}(Ω)	CPE1	R_{dr} (Ω)	CPE2
Control	10.02	6870	4.63×10^{-9}	23339	4.11×10^{-7}
2,6-PDA	12.90	10876	4.44×10^{-9}	26402	7.30×10^{-7}