Electronic Supplementary Information (ESI)

Stable PbS Quantum Dots Ink for Efficient Solar Cells by Solution-Phase Ligand Engineering

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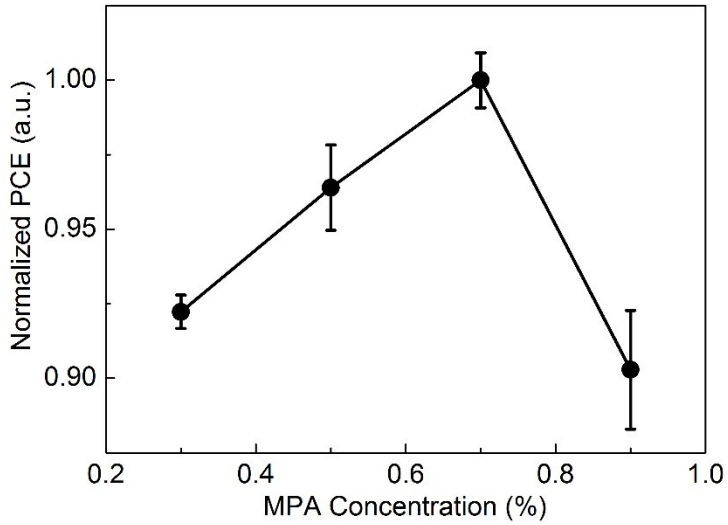

Figure S1. Optimization of the MPA concentration in butylamine (v/v) on device performance.

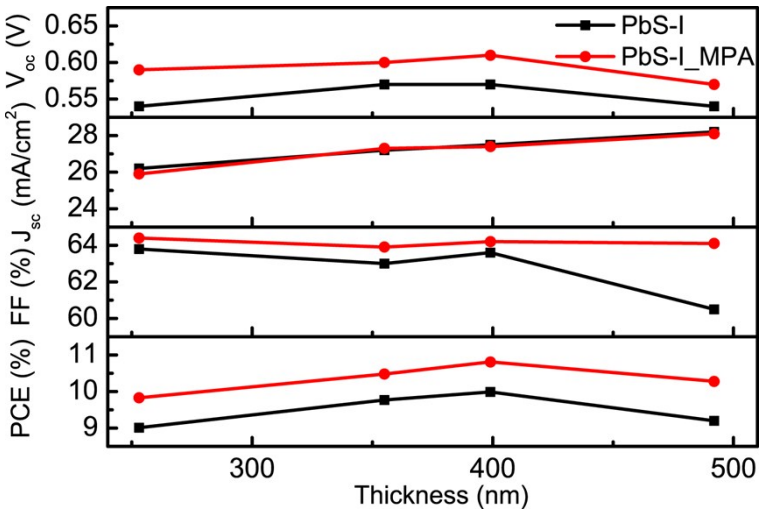

Figure S2. The effect of active layer thicknesses on device performances.

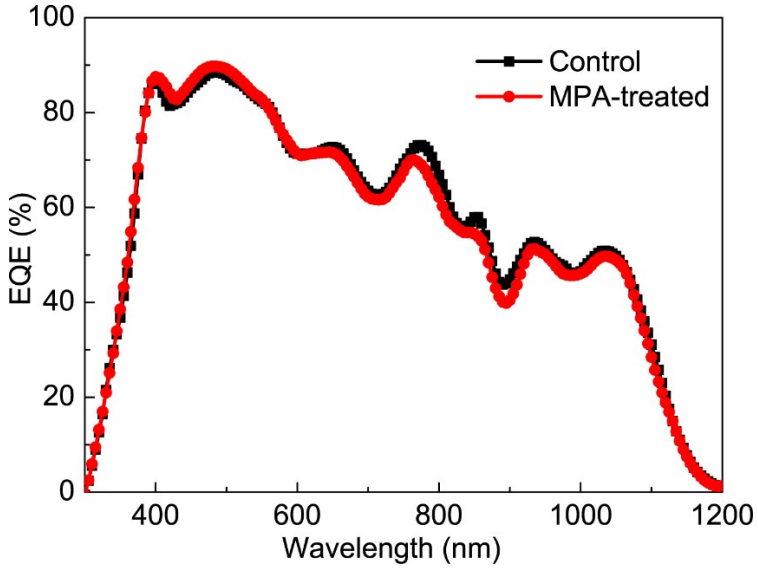

Figure S3. External quantum efficiency (EQE) spectra of control and MPA-treated QD devices.

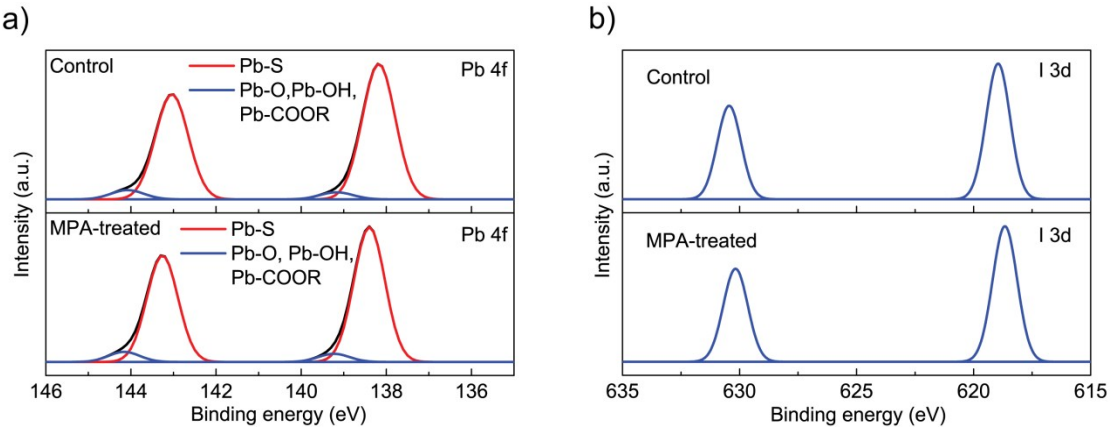

Figure S4. High-resolution a) Pb 4f and b) I 3d XPS spectra of control and MPA-treated QD films.

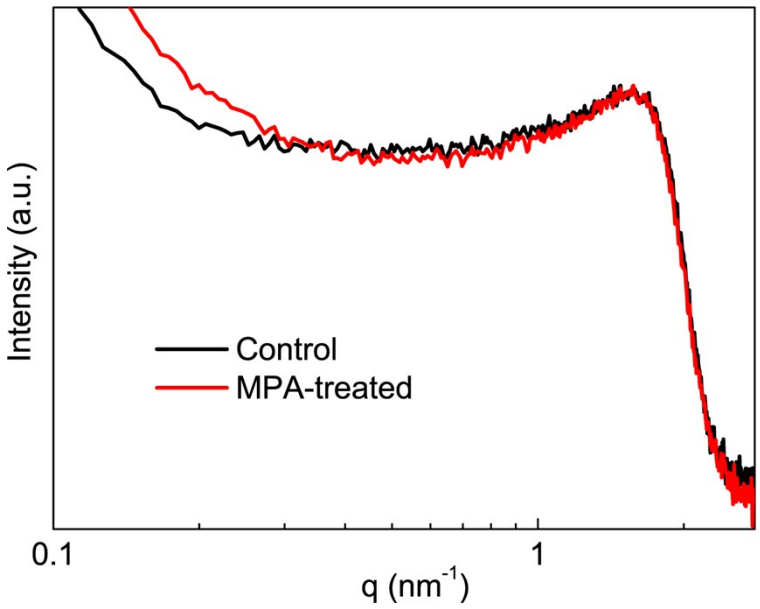

Figure S5. The small-angle x-ray scattering (SAXS) of control and MPA-treated QD films.

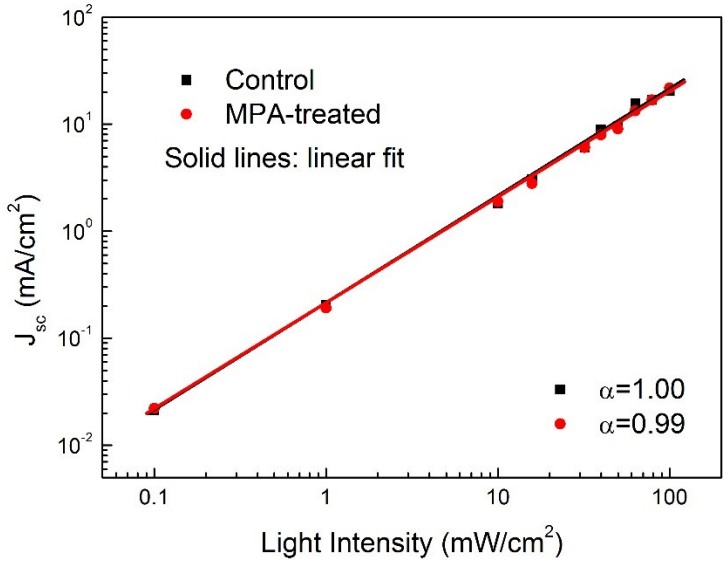

Figure S6. Light-intensity dependence of J_{sc} (solid lines: linear fits) of control and MPA-treated QD devices.

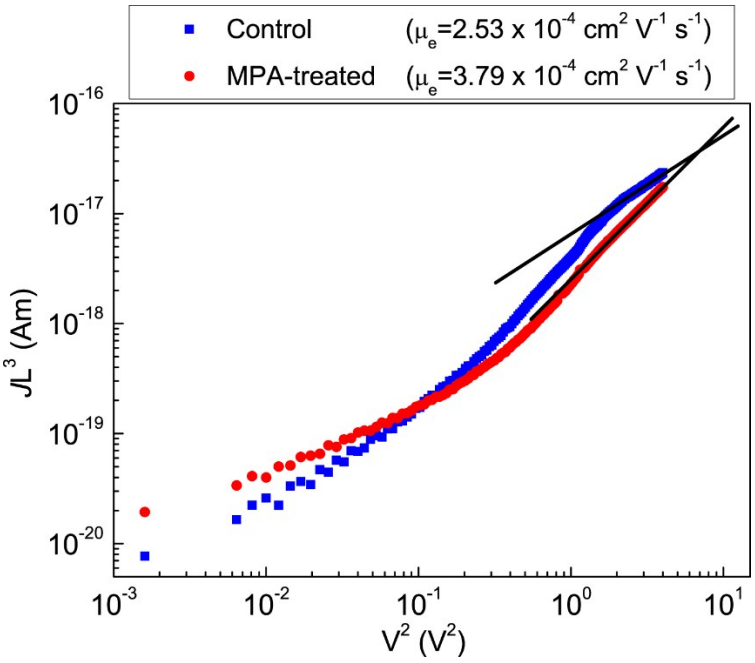

Figure S7. SCLC electron only devices analysis result, faster charge extraction in MPA-treated QDs-ink devices is revealed.

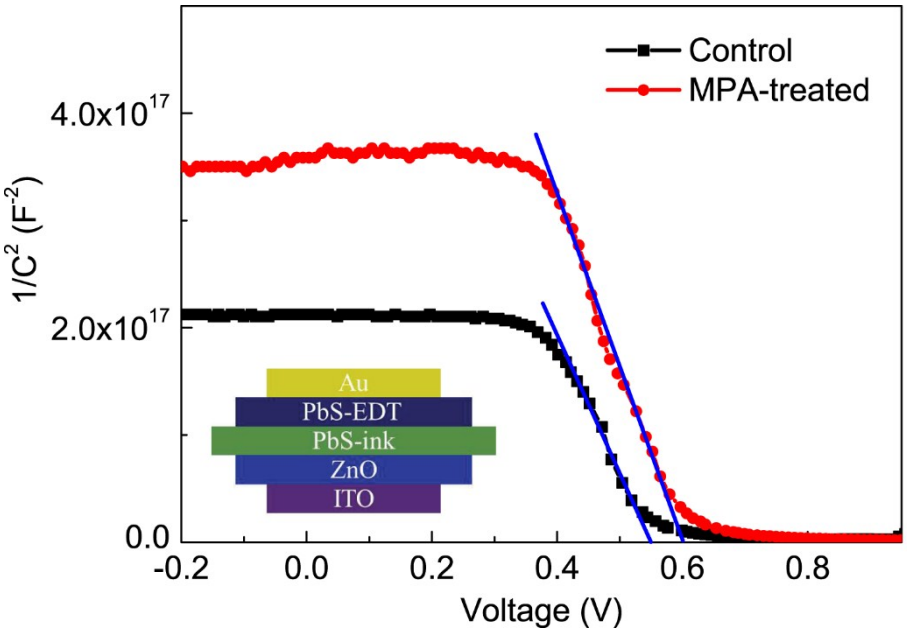

Figure S8. Capacitance-voltage measurement of the built-in potential in control (0.55 eV) and MPA-treated (0.60 eV) devices.

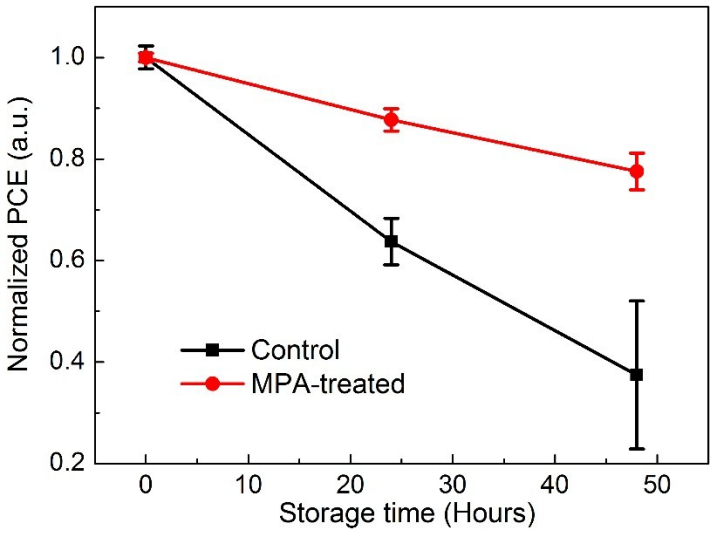

Figure S9. The effect of the storage time of control and MPA-treated QD inks on device performances. The QD inks were stirred for 5 min before fabricated devices.

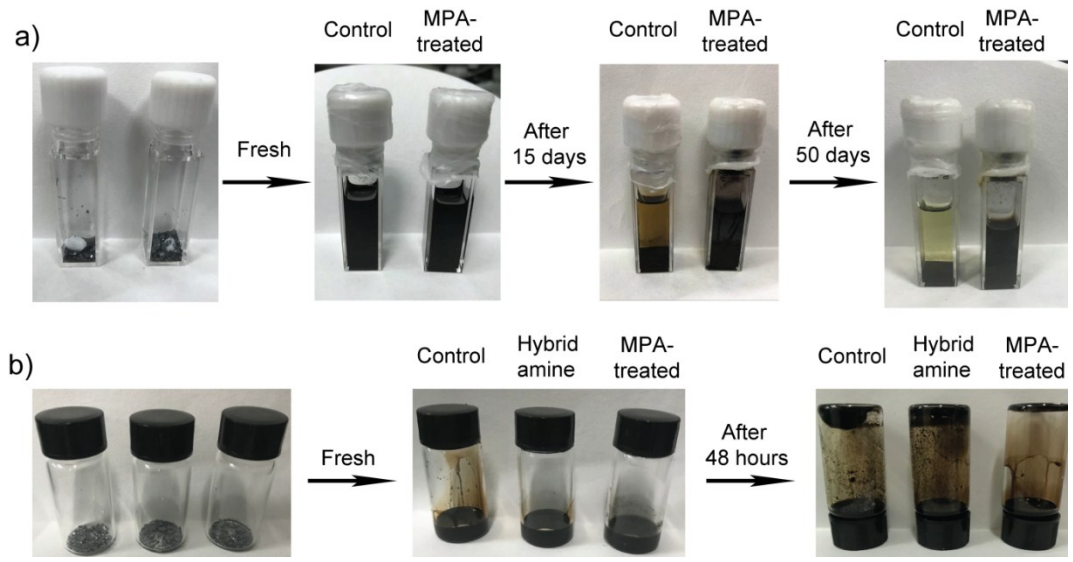

Figure S10. a) Solution-stability of control and MPA-treated QD inks in BA after 50 days. b) Solution-stability of control QD inks in BA and hybrid amine (BA, amylamine and hexylamine), and MPA-treated QD inks in BA. The vials were centrifuged (8000 r.p.m for 3min) and inverted to highlight the precipitation on the bottom.

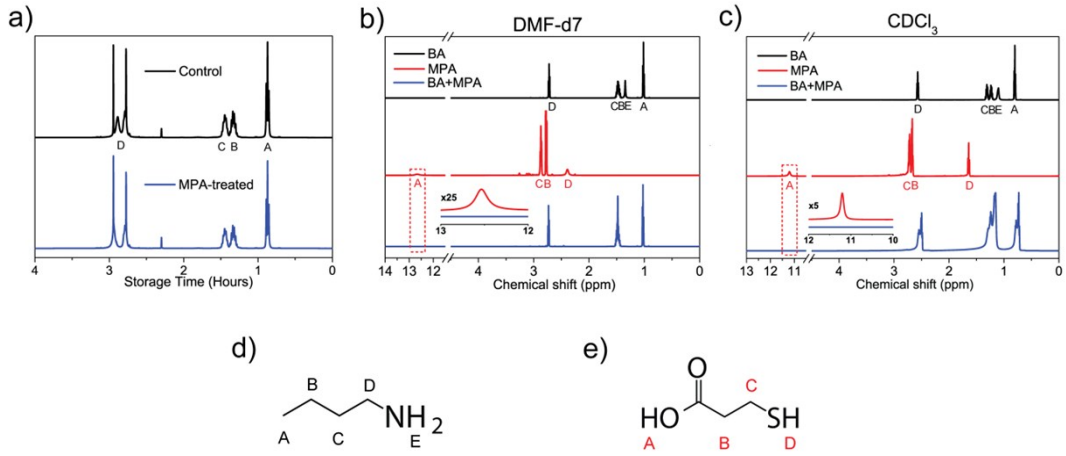

Figure S11. a) ^{1}H NMR spectra of control and MPA-treated QDs in BA:DMF-d7 = 0.1:1 (v/v). ^{1}H NMR spectra of BA, MPA and BA+MPA (MPA:BA=0.007:1) in b) DMF-d7 and c) $CDCl_3$. Chemical structures of d) BA and e) MPA.

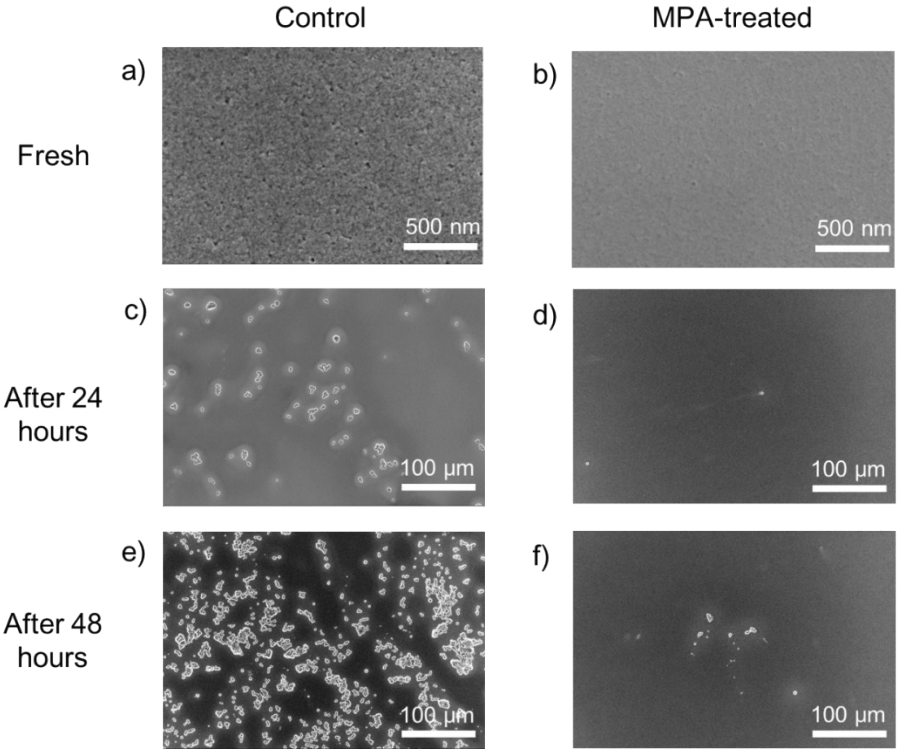

Figure S12. SEM images for control and MPA-treated QD films fabricated by using QDs ink solution after stored for different times.

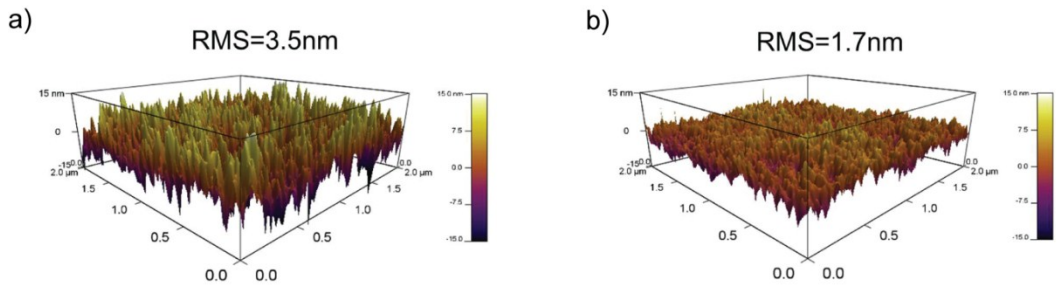

Figure S13. Topographic AFM morphology images of control and MPA-treated QD films, respectively.

Table S1. Fitting parameters and quantitative analysis of XPS spectra for Control and MPA-treated films in Figure 2 and Figure S4.

Elements	Species	Control	Peak (eV)	MPA-treated	Peak (eV)
Pb	Total	1.00	-	1.00	-
	Pb-S	0.93	138.2/143	0.96	138.4/143.3
	Pb-O, Pb-OH, Pb-COOR	0.07	139.2/144.1	0.04	139.2/144.2
S	Total	0.54	-	0.75	-
	S-Pb	0.54	160.6/161.8	0.57	160.7/161.9
	S_bound thiol	0.00	-	0.11	161.5/162.2
	S_unbound thiol	0.00	-	0.07	163.1/164.2
O	Total	0.44	-	0.39	-
	O-Pb	0.03	530.5	0.02	530.8
	Pb-OH	0.29	531.7	0.06	531.8
	$-COO^-$, CO_2	0.12	532.8	0.20	532.8
	Free COOH	0.00	-	0.10	533.8
I	-	0.67	618.9/630.4	0.66	618.7/631.2

Table S2. Different thickness of PbS QD film by changing the QDs concentration.

QDs concentration (mg/mL)	Film thickness (nm)
200	253
300	355
350	399
400	492