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Supporting Information

Towards understanding the initial performance improvement of PbS quantum dot solar cells upon short-term air exposure

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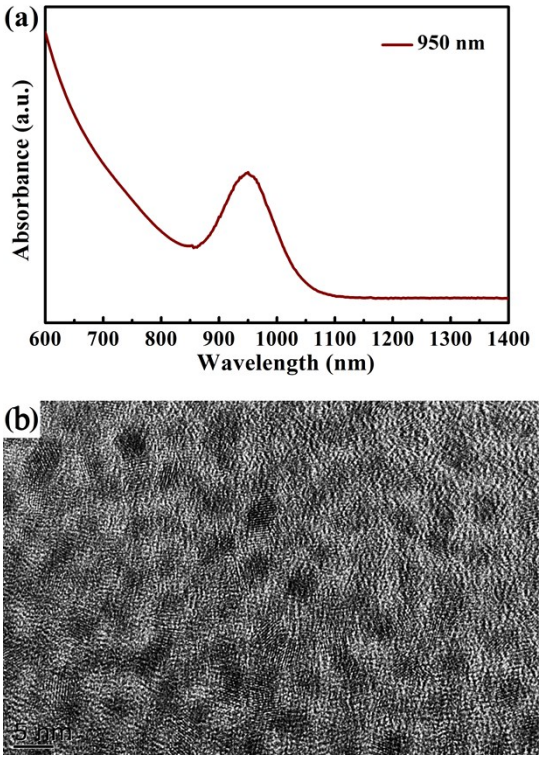

Fig. S1 (a) The absorption spectrum of the PbS quantum dot solution in octane used in the work. (b) A TEM image of the PbS quantum dots synthesized in the work.

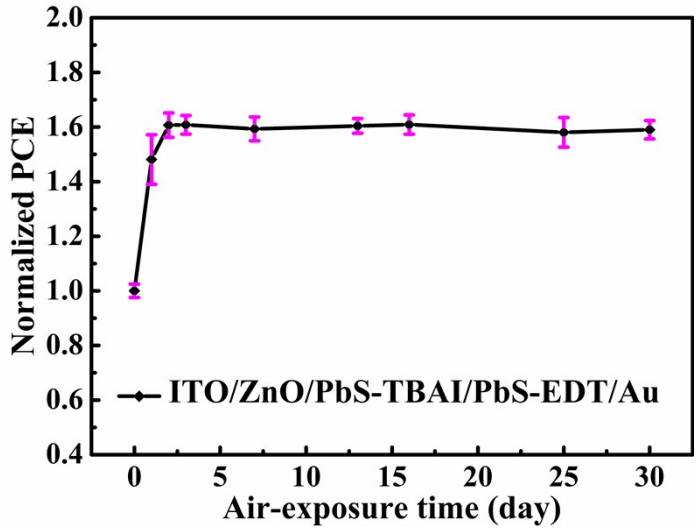

Fig. S2 The typical performance evolution of PbS quantum dot solar cells with TBAI and EDT bi-ligands upon air-exposure.

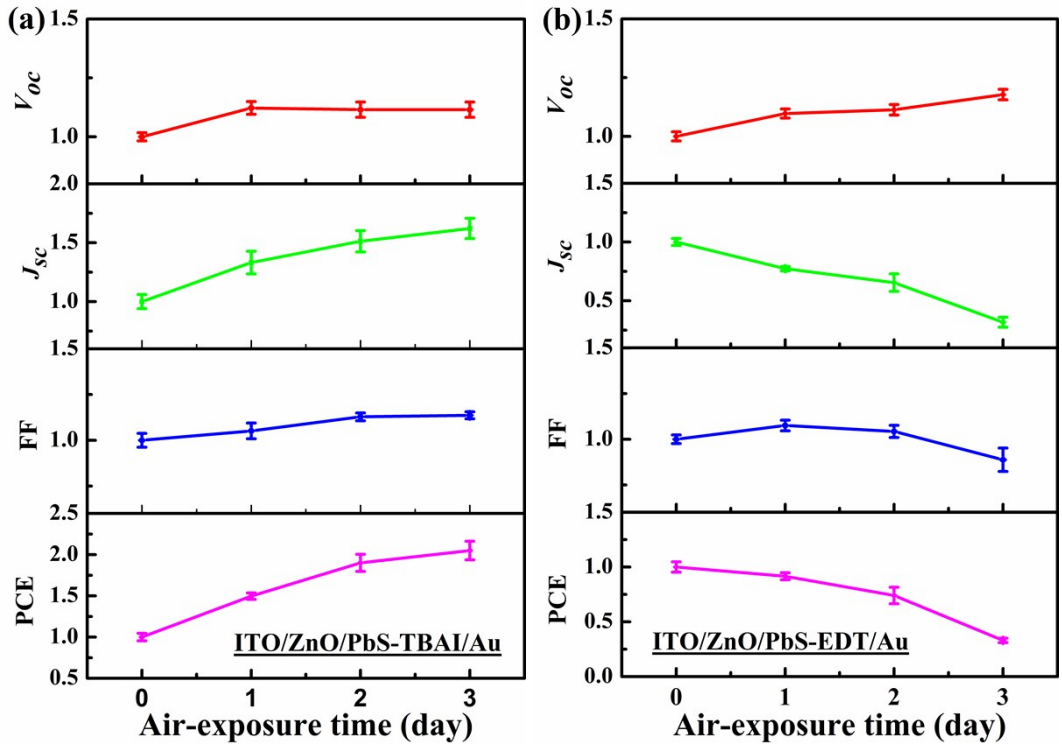

Fig. S3 The evolution of normalized performance parameters of (a) the devices based on PbS QD-films treated by TBAI only, (b) the devices based on PbS QD-films treated by EDT only.

Table S1 The parameters used for deconvolution of the O1s core level spectra of the PbS-TBAI and PbS-EDT films.

The PbS-TBAI film

component	peak (eV)	FWHM (eV)
Pb-O	529.3	1.4
Pb-OH	531.2	1.5
COO,C=O,CHO	532.2	1.5
OH	533.7	1.5

The PbS-EDT film

component	peak (eV)	FWHM (eV)
Pb-O	529.3	2
Pb-OH	531.2	1.5
COO,C=O,CHO	532.2	1.5
OH	533.7	1.5

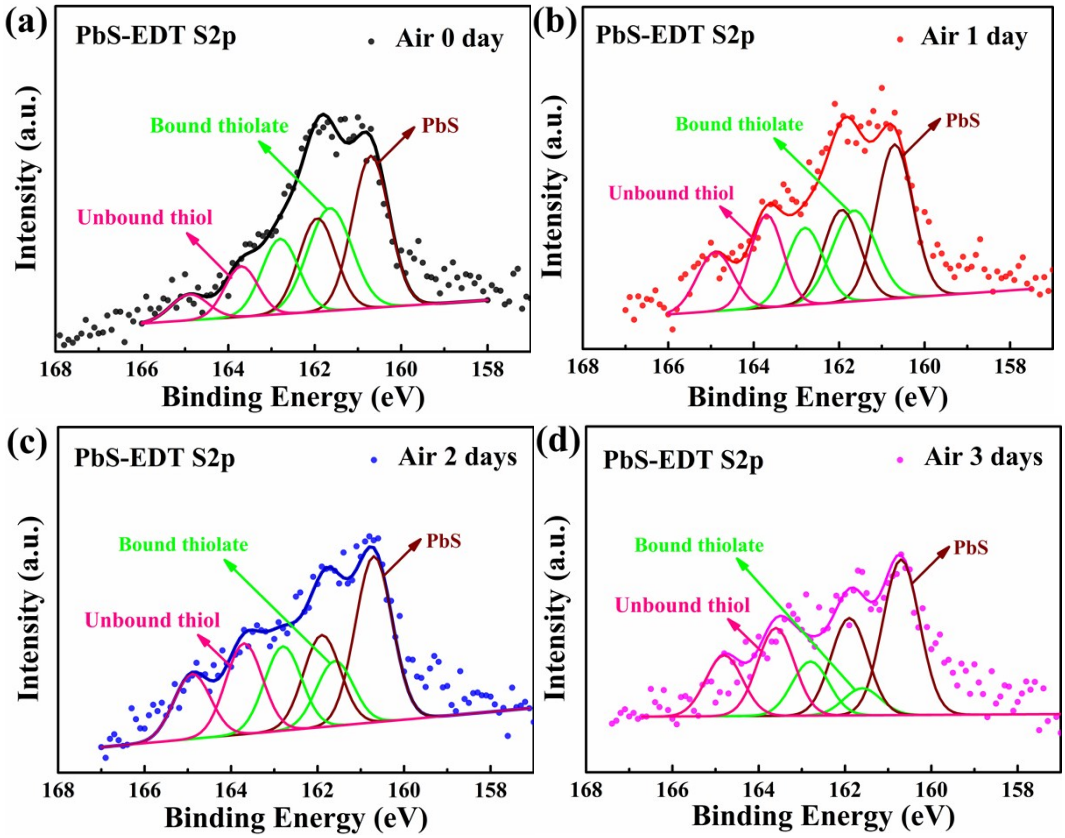

Fig. S4 Deconvoluted XPS spectra of the S2p core level of the PbS-EDT film with different air-exposure time.

Table S2 The parameters used for deconvolution of the S2p core level spectra of the PbS-EDT film.

component	peak (eV)	FWHM (eV)
PbS	160.7	1.2
	161.8	1.2
bound thiolate	161.6	1.4
	162.8	1.4
unbound thiol	163.6	1
	164.8	1

Extraction of diode ideality factors

According to the diode model, the dark *J-V* equation is:

$$J_d = J_0 \left[exp \left(\frac{qV}{nk_0T} \right) - 1 \right] \approx J_0 \, exp \left(\frac{qV}{nk_0T} \right) \qquad (1)$$

Where q is the elementary charge, k_0T the thermal energy, J_d the dark current density, J_0 the saturation dark current intensity, n the ideality factor. By taking natural logarithm of the equation (1), equation (2) can be obtained, as follows,

$$ln(J_d) = ln(J_0) + \frac{qV}{nk_0T} \qquad (2)$$

Equation (2) displays the linear relationship between $In(J_d)$ and V, where q/nk_0T is the slope of the curve, q/k_0T is a constant (38.46 at room temperature). According to the slope of equation (2), the ideality factor (n) can be extracted directly.

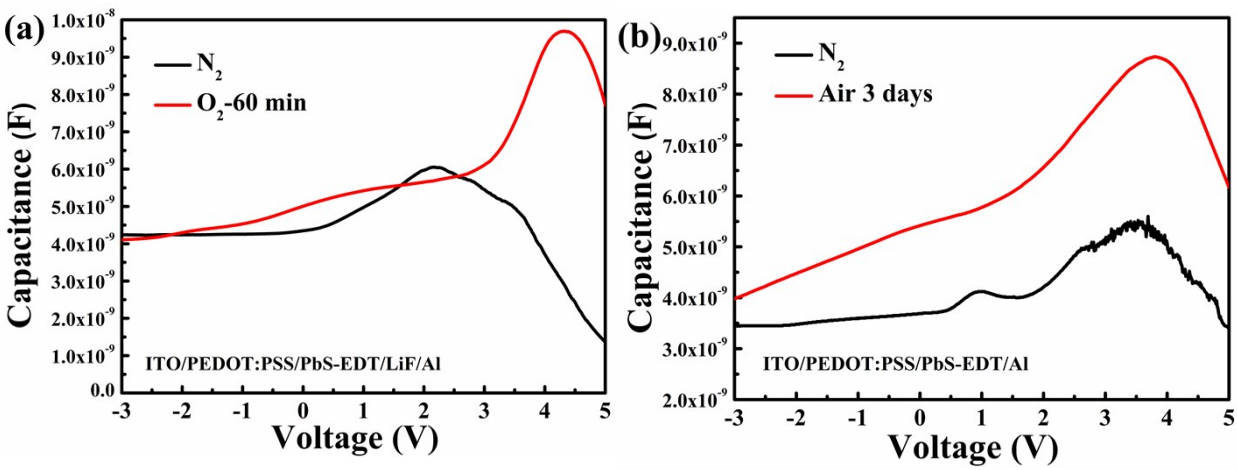

Fig.S5 (a) Capacitance-Voltage curves of the device with a structure of ITO/PEDOT:PSS/PbS-EDT/LiF/Al before air exposure and after one hour of oxygen exposure. (b) Capacitance-Voltage curves of the device with a structure of ITO/PEDOT:PSS/PbS-EDT/Al before and after air exposure.