

Supporting information

Zwitterionic Polymer as an Interfacial Layer for Efficient and Stable Perovskite Solar Cells

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SI 1. The absorption spectrum of the Dex-CB-MA thin film

SI 2: Atomic force microscopy images of the Dex-CB-MA thin films

SI 3: The photocurrent hysteresis of perovskite solar cells

SI 4: The stability of perovskite solar cells testing in air

SI 1. The absorption spectrum of the Dex-CB-MA thin film

Fig. S1 shows the UV-visible absorption spectrum of Dex-CB-MA thin film. The optical bandgap is estimated to be 3.4 eV, according to $E_g = 1240 / \lambda_{\text{edge}}$,¹ where E_g is bandgap of Dex-CB-MA and λ_{edge} is absorption edge. The bandgap estimated by absorption spectrum is consistent well with the bandgap from HOMO and LUMO energy levels.

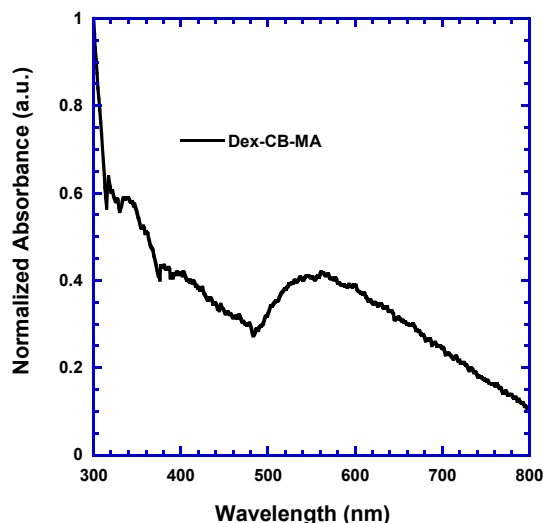


Fig. S1 UV-visible absorption spectrum of the Dex-CB-MA thin film.

SI 2: Atomic force microscopy images of the Dex-CB-MA thin films

Fig. S2 shows the atomic force microscopy (AFM) images of the Dex-CB-MA thin films on the top of PEDOT:PSS thin layer. The thicknesses of the Dex-CB-MA thin films were tuned by spin-speeds. The surface roughness was tested by the software for the whole testing area ($5\mu\text{m}\times 5\mu\text{m}$). Roughness and thickness of Dex-CB-MA thin layers were summarized in Table S1. The thicknesses of Dex-CB-MA thin films were decreased while the roughness increased with the high spin-speed. The high-speed during spin-coating process caused a thin thickness of the Dex-CB-MA thin films, which could not cover the PEDOT:PSS layers entirely, so it made no

contributions to smoothing the PEDOT:PSS surface. On the contrary, the Dex-CB-MA layer of 1 nm increased the roughness of the PEDOT:PSS/Dex-CB-MA hole extraction layer. As the thickness of the Dex-CB-MA thin films gradually increased, the surface of PEDOT:PSS layer was modified and smoother the PEDOT:PSS/Dex-CB-MA HTLs could be expected.

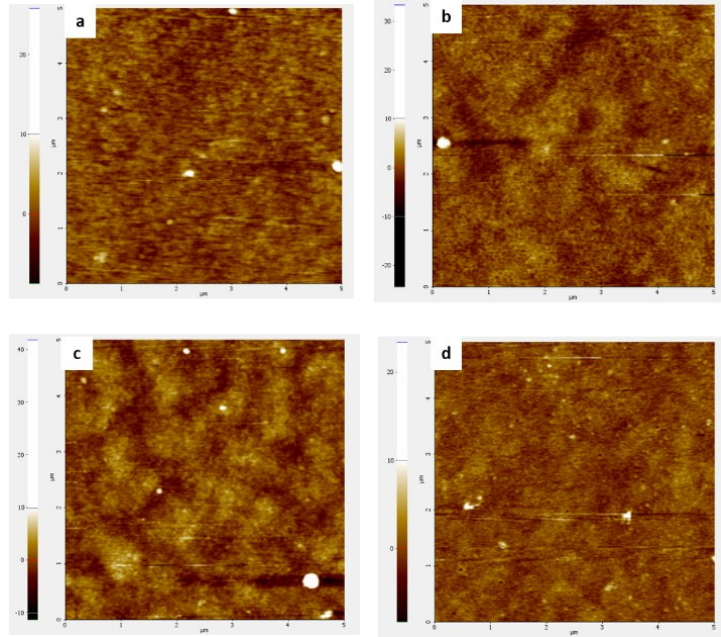


Fig. S2. AFM images of the surfaces of (a) PEDOT:PSS (b) PEDOT:PSS/Dex-CB-MA (5 nm), (c) PEDOT:PSS/Dex-CB-MA (2 nm), (d) PEDOT:PSS/Dex-CB-MA (1 nm).

Table S1. Roughness and thickness of Dex-CB-MA on PEDOT:PSS obtained from different spin rate.

Spin-speed (RPM)	RMS roughness (nm)	Thickness (nm)
0	1.645	0
1500	1.405	5
2500	3.042	2
3500	4.310	1

SI 3: The photocurrent hysteresis of perovskite solar cells

The hysteresis index can be calculated by the equation: $HI = (PCE_{reverse} - PCE_{forward}) / PCE_{reverse}$. At the scan rate of 0.5 V/s, the PSCs fabricated on PEDOT:PSS HTL possesses a HI of 0.098; whereas the PSCs fabricated on PEDOT:PSS/ DEX-CB-MA HTL possesses a HI of 0.049. Two times lower HI values indicate that the DEX-CB-MA plays a positive role in thin-film interface modification.

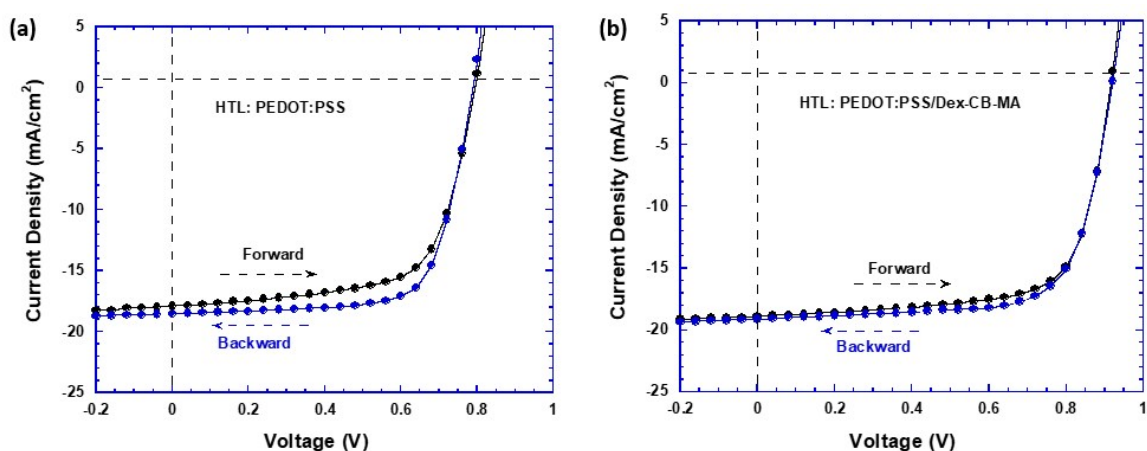


Fig. S3 The J-V characteristics of studied PSCs under different scanning direction. Scanning rate: 0.5 V/s

Table S2. The performance of studied PSCs under different scanning direction

Studied HTL	Direction	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE (%)	Hysteresis index
PEDOT:PSS	Forward	0.80	17.88	66.0	9.44	0.098
	Backward	0.80	18.51	70.7	10.46	
PEDOT:PSS/Dex-CB-MA	Forward	0.92	18.87	70.2	11.85	0.049
	Backward	0.92	19.11	70.9	12.47	

SI 4: The stability of perovskite solar cells testing in air

Fig. S5 presents the stability of PSCs with the PEDOT:PSS HEL and the PEDOT:PSS/ Dex-CB-MA HEL, respectively, where PSCs are unencapsulated and tested in air. It is clear that after 6 days, PCE of PSCs with the PEDOT:PSS/Dex-CB-MA HEL drops to 90% value of its initial value, but PSCs with the PEDOT:PSS HEL does not work at all. Thus, introduction of Dex-CB-MA interfacial layer can efficiently enhance the stability of PSCs.

In order to understand enhanced device stability, perovskite thin-film upon the PEDOT:PSS HTL the the PEDOT:PSS/Dex-CB-MA were tested in air. As presented in Fig. S5, the perovskite thin-film upon PEDOT:PSS HTL decay to PbI_2 after 2 weeks, but the thin film upon PEDOT:PSS/Dex-CB-MA only loss 20% absorption in the visible region. These results indicate that the perovskite thin-film upon PEDOT:PSS possess a faster decay compared to that upon PEDOT:PSS/Dex-CB-MA, due to the cross-linkable ability of zwitterionic polymer Dex-CB-MA.

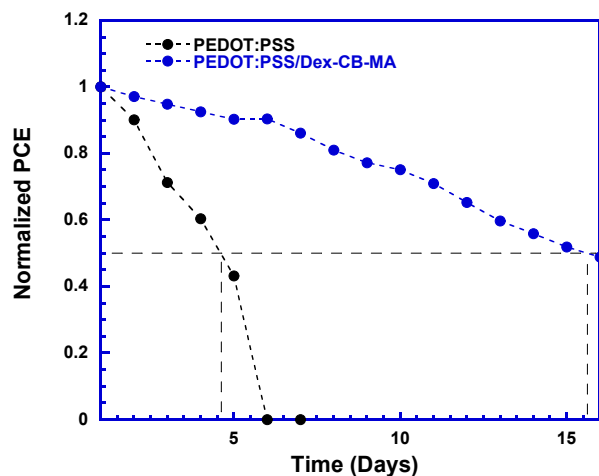


Fig. S4. The stability of PSCs with the PEDOT:PSS HEL and the PEDOT:PSS/ Dex-CB-MA HEL, respectively, where PSCs are unencapsulated and tested in air.

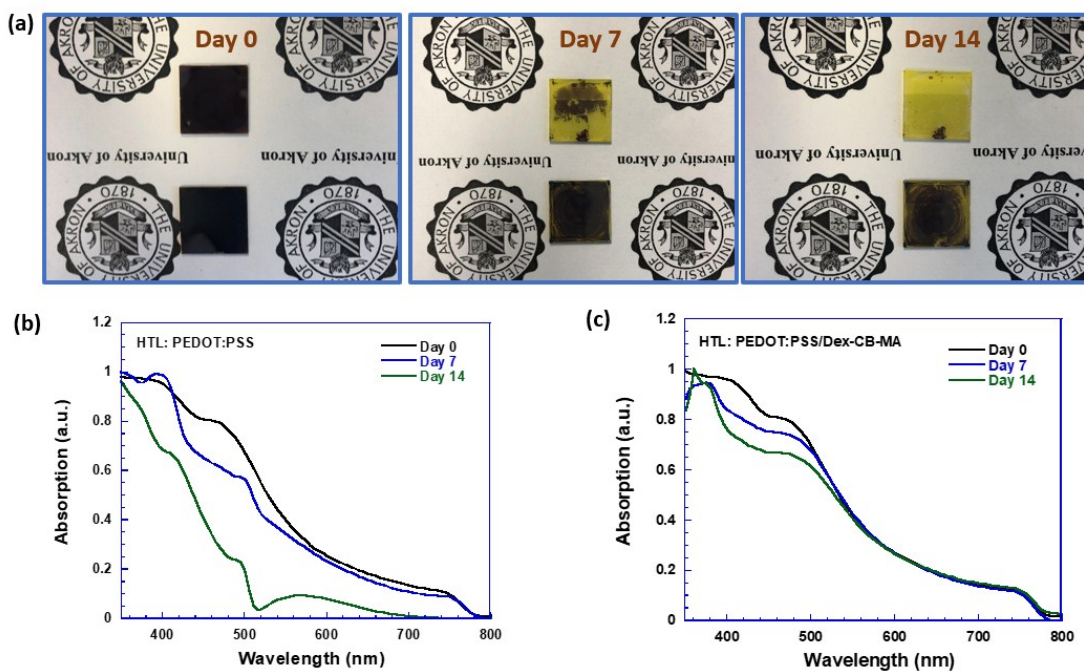


Fig. S5. (a) The images of decay process of perovskite thin films upon the PEDOT:PSS HEL (Top three) and the PEDOT:PSS/Dex-CB-MA HEL (Bottom three). The absorption spectra of perovskite thin film upon (b) the PEDOT:PSS HEL and (c) the PEDOT:PSS/Dex-CB-MA.

Notes and references

1. L. Leonat, G. Sbârcea and I. V. Branțoi, *UPB Sci. Bull. Ser. B Chem. Mater. Sci.* 2013, **75**, 111–118.
2. K.-L. Zhang, C.-M. Liu, F.-Q. Huang, C. Zheng and W.-D. Wang, *Appl. Catal. B Environ.* 2006, **68**, 125–129.