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Restrained light-soaking and reduced hysteresis in perovskite solar cells employing a helical perylene diimide interfacial layer

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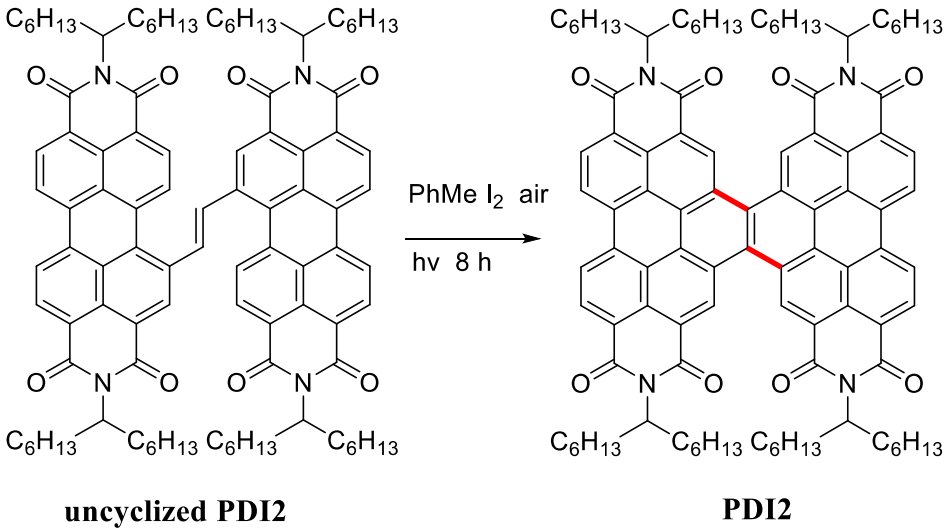

Fig. S1. The uncyclized PDI2 (500 mg, 0.326 mmol), which was synthesized by referring to previous literature procedure,[1,2] was dissolved in 300 mL toluene in a 500ml round bottom flask, and iodine (100 mg) was added. The reacting mixture solution was drawn into a home-built flow reactor (equipped with four 450 W-mercury lamps). The purple reaction mixture was turned to orange red after pumped through the flow reactor twice with a retention time of ~8 hours. The solvent was removed using vacuum rotary evaporator and the crude residue was washed with methanol to remove excessive iodine. The crude red solid was purified with silica gel (eluent: petroleum ether/dichloromethane) and recrystallization from hexane, then the final product PDI2 was obtained as a red solid (440 mg, 88%).

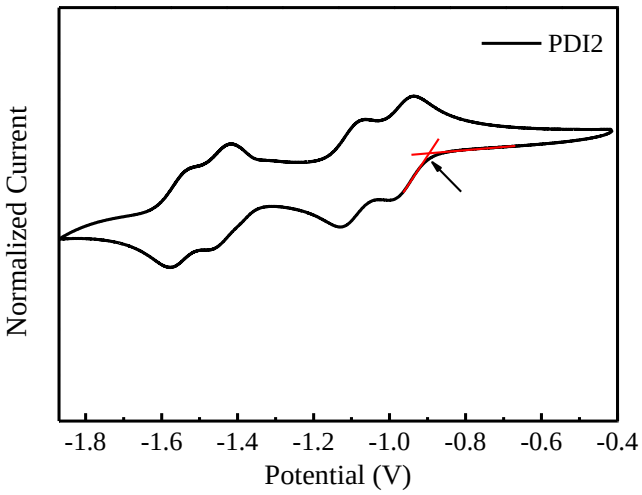

Fig. S2 Cyclic voltammograms (CVs) of PDI2 (versus Fc/Fc+). The LUMO levels were calculated by the following equations: $E_{LUMO} = -(E_{red} - E_{Fc} + 4.8)$ eV, where E_{red} results were obtained from the onset of reduction, respectively, while E_{Fc} was the half-wave potential of ferrocene. The optical bandgap was estimated from the onset positions of the absorption spectra and calculated by the equation: $E_g = 1240/\lambda_{onset}$. Where the λ_{onset} is 576 nm. So the calculated E_g is 2.15 eV. It was measured that the $E_{red} - E_{Fc} = -0.89$ eV. So the $E_{LUMO} = -(E_{red} - E_{Fc} + 4.8)$ eV = -3.91 eV, $E_{HOMO} = -6.06$ eV.

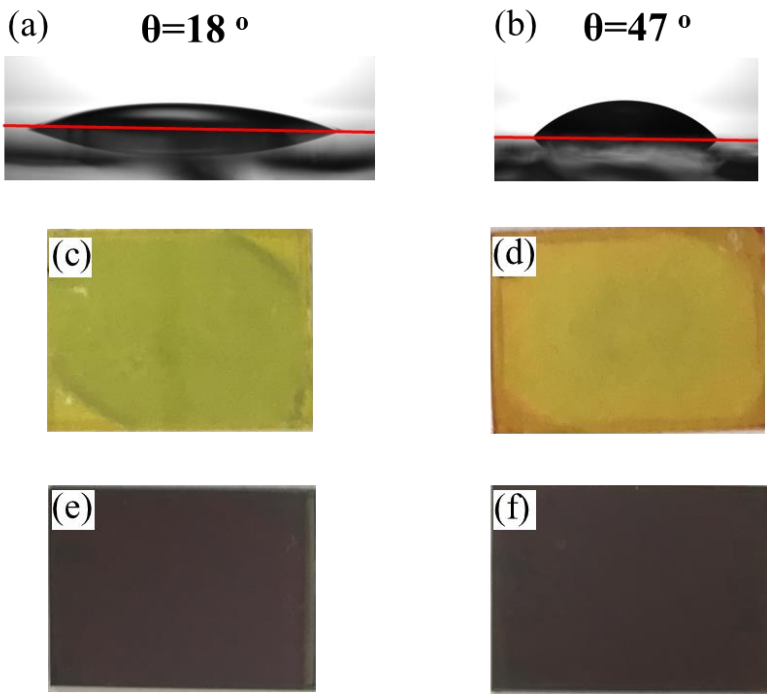

Fig. S3 The contact angle of mixed solvent of DMF and DMSO (9:1) on (a) TiO_2 and (b) TiO_2/PDI2 surfaces. The PbI_2 films cast on (c) TiO_2 and (d) TiO_2/PDI2 surfaces, and perovskite films on (e) TiO_2 and (f) TiO_2/PDI2 surfaces.

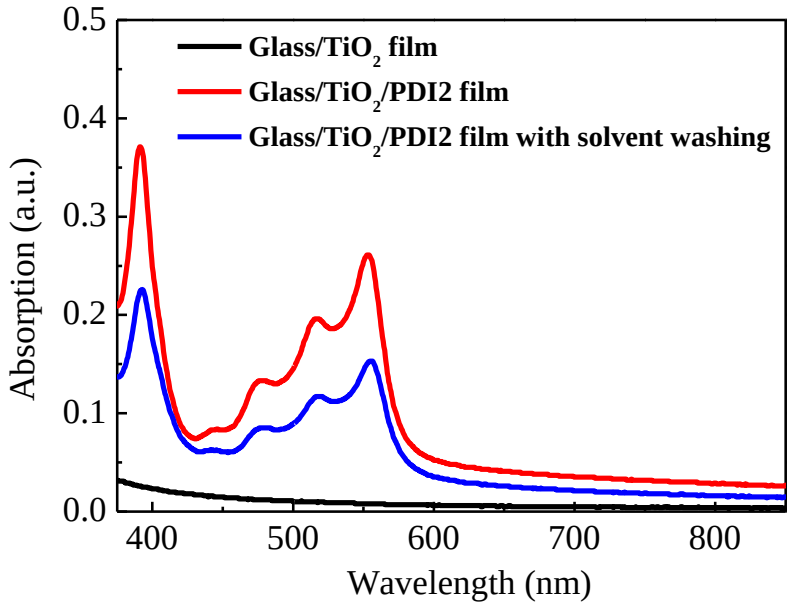

Fig. S4 The absorption of TiO_2 film on glass, and PDI2 film coated on glass/TiO_2 before and after washing with mixed solvents of DMF and DMSO (9:1)

Table S1 Device metrics of perovskite solar cells w/o PDI2 interlayer upon continuous illumination.

ETLs	Light soaking time (s)	Scan direction	PCE (%)	Jsc (mA/cm^2)	Voc (V)	FF (%)
TiO_2	0	Forward scan	10.38	23.27	0.93	48.15
	20		12.80	23.22	0.98	56.33
	40		12.87	23.17	0.99	55.90
	0	Reverse scan	16.40	23.30	1.04	67.77
	20		18.86	23.16	1.09	74.46
	40		19.33	23.25	1.09	75.93
TiO_2/PDI2	0	Forward scan	17.13	23.19	1.06	69.94
	20		17.28	23.18	1.06	70.63
	40		17.50	23.17	1.06	71.68
	0	Reverse scan	19.08	23.25	1.07	76.82
	20		19.76	23.32	1.07	79.21
	40		19.84	23.30	1.07	79.52

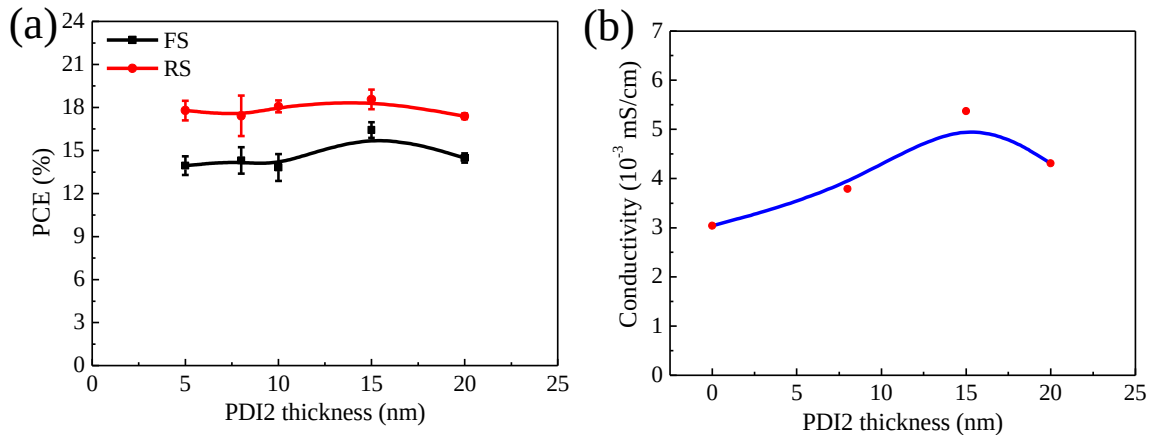

Fig. S5 (a) The PCE of perovskite solar cells with varying thickness of the PDI2 interlayer from forward and reverse scans. (b) PDI2 conductivity as a function of thickness. The electrical conductivity (σ) was determined from devices structure of ITO/TiO_2/PDI2/Ag, by using $J=\sigma L^{-1}V$, where L is the thickness.

References

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