Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C. This journal is © The Royal Society of Chemistry 2020

## **Electronic Supplementary Information**

## Green Solvent-Processed Organic Solar Cells Based on Low Cost Polymer Donor and Small Molecule Acceptor

He Huang<sup>a,b</sup>, Xiaojun Li<sup>a,b</sup>, Chenkai Sun<sup>a,b</sup>, Indunil Angunawela<sup>c</sup>, Beibei Qiu<sup>a,b</sup>, Jiaqi Du<sup>a,b</sup>, Shucheng Qin<sup>a,b</sup> Lei Meng<sup>b\*</sup>, Zhanjun Zhang<sup>a\*</sup>, Harald Ade<sup>c\*</sup>, Yongfang Li<sup>a,b,d\*</sup>

<sup>a</sup>School of Chemical Science, University of Chinese Academy of Sciences, Beijing 100049, China

<sup>b</sup>Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China

<sup>c</sup>Department of Physics and Organic and Carbon Electronics Lab (ORaCEL), North Carolina State University, Raleigh, North Carolina 27695, United States

<sup>d</sup>Laboratory of Advanced Optoelectronic Materials, College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou, Jiangsu 215123, China.

E-mail: menglei@iccas.ac.cn; zhangzj@ucas.ac.cn; hwade@ncsu.edu; liyf@iccas.ac.cn

## Materials

Unless otherwise stated, all the solvents and chemicals were purchased from TCI Chemical Co, J&K and Alfa Aesar. PTQ10, HO-IDIC-2F and PDINO were synthesized on the basis of literatures.

## **Device fabrication and characterization**

We fabricated the device with the usual structure of ITO/PEDOT: PSS/active layer /PDINO /Al. We deposited PEDOT:PSS aqueous solution on the clean ITO film at 3000 rpm and then annealing 15 minutes at 150 °C for drying the water in PEDOT:PSS film. The mixed solution of PTQ10:HO-IDIC-2F was prepared with a concentration of 14 mg mL<sup>-1</sup> in tetrahydrofuran (THF) solvent, where the weight ratio

of PTQ10:HO-IDIC-2F is 1:1. The active layer was spin-coated on the cooled surface of PEDOT:PSS layer in nitrogen glove box with a spin-coating rate of 2800 rpm. The separate concentration of PTQ10 and HO-IDIC-2F for the layer-by layer (LL) method in THF solvent is 4 mg mL<sup>-1</sup> and 8 mg mL<sup>-1</sup> respectively. For the active layer based on LL spin-coating, firstly, we spin-coated the PTQ10 solution with 1000 rpm, and then HO-IDIC-2F solution was spin-coated on the surface of PTQ10 layer with 2000 rpm. For the active layer based on the LL blade-coating, firstly, we blade-coated the PTQ10 layer with about 80 nm thickness through adjusting the temperature of baseplate and the height between blade and baseplate. Then, the HO-IDIC-2F layer was blade-coated on the surface of PTQ10 layer with the thickness of about 40 nm. It is worth mentioning that all layers based on LL coating are prepared in air without any thermal treatment. Then, the PDINO film from its methanol solution with a concentration of 1.0 mg ml<sup>-1</sup> was spin-coated on the surface of active layer with the thickness of 15 nm, which act as a cathode buffer layer. The last step is to evaporate Al in vacuum under a pressure of ca.  $5.0 \times 10^{-5}$  Pa. The current density-voltage (J-V) characteristics of the PSCs were measured in Glove box on a computer-controlled Keithley 2450 Source-Measure Unit. Oriel Sol3A Class AAA Solar Simulator (model, Newport 94023A) with a 450 W xenon lamp and an air mass (AM) 1.5 filter was used as the light source. The scanned scale of voltage is from -1.5 V to 1.5 V. The External Quantum Efficiency (EQE) was measured by Solar Cell Spectral Response Measurement System QE-R3-011 (Enli Technology Co., Ltd., Taiwan).

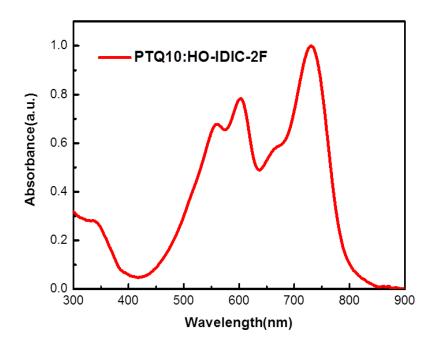


Fig. S1 Absorption spectra of the PTQ10:HO-IDIC-2F blend film.

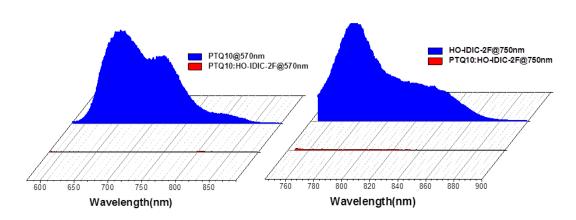


Fig. S2 Photoluminescence spectra of PTQ10, HO-IDIC-2F and their blend films.

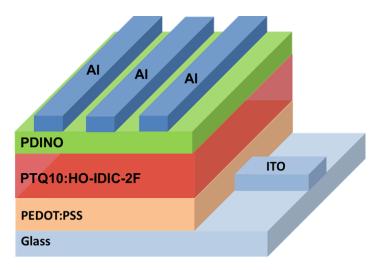
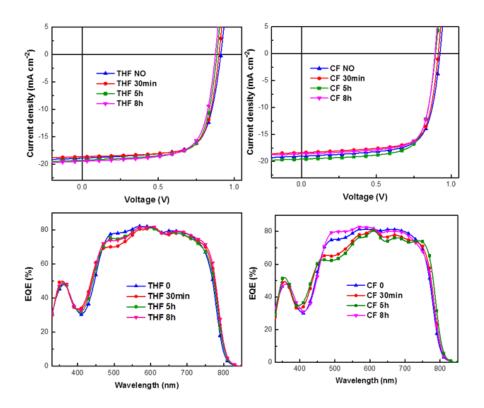
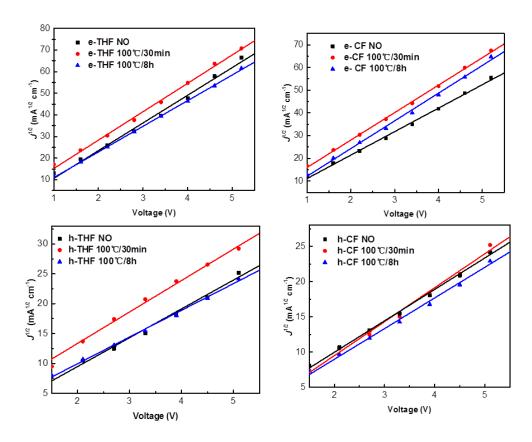


Fig. S3 The device structure used in this work.



**Fig. S4** The J-V plots and EQE curves of the PSCs with different thermal treatment time at 100 °C.



**Fig. S5** The plots of mobility measurements for the devices based on THF and CF solvent with different thermal treatment time.

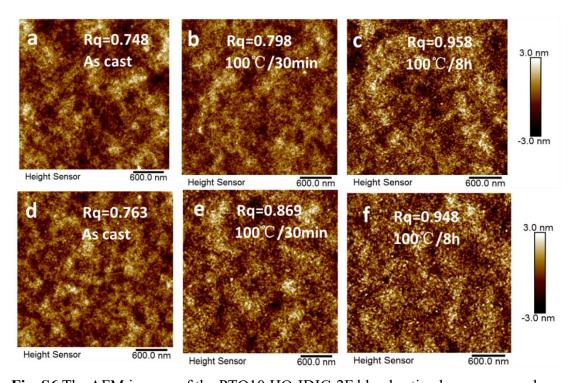
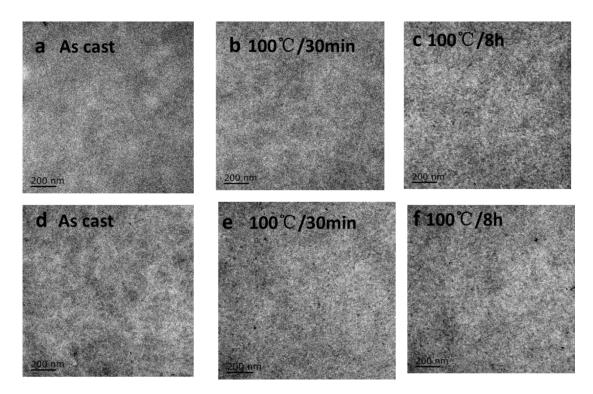
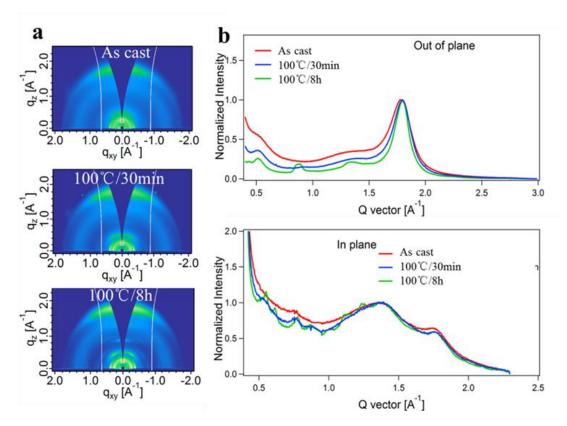


Fig. S6 The AFM images of the PTQ10:HO-IDIC-2F blend active layers prepared

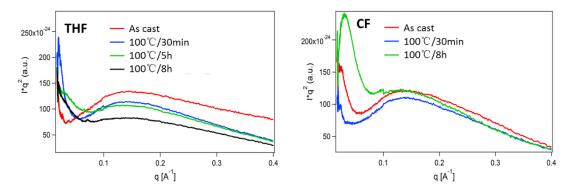
with (a-c) THF as solvent and (d-f) with CF as solvent, with different thermal treatment times.



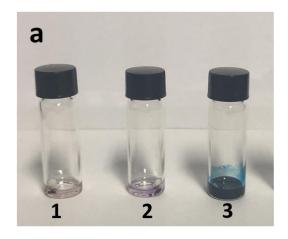
**Fig. S7** The TEM images of the of the PTQ10:HO-IDIC-2F blend active layers prepared with (a-c) with THF as solvent, (d-f) with CF as solvent, with different thermal treatment times.



**Fig. S8** a) The 2D GIWAXS patterns and b) the corresponding line cuts image of the PTQ10:HO-IDIC-2F blend active layers prepared with CF solvent with different thermal treatment times.



**Fig. S9** The RSoXS plots of blend films prepared with THF and CF solvent with different thermal treatment times.



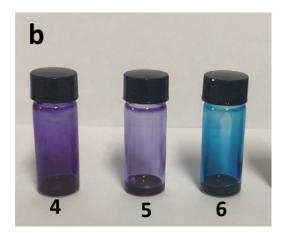


Fig. S10 The picture of monomer in solvent a) before stirring b) after stirring 12 hours with  $45^{\circ}$ C (1,4: PTQ10 in THF. 2,5: PTQ10 in CF. 3,6: HO-IDIC-2F in THF.)

Table S1. The photovoltaic performance of device with thermal treatment time

Solvent	Thermal	$V_{\rm oc}$	$J_{ m sc}$	$J_{ m cal}$	FF	PCE
	treatment	(V)	$(mA cm^{-2})$	$(mA cm^{-2})$	(%)	(%)
	$time(100^{\circ}C)$					
	0	0.91	18.95	18.52	70.77	12.20
THF	30 minutes	0.90	18.67	18.49	72.67	12.21
ТПГ	5 hours	0.89	19.28	18.45	71.14	12.14
	8 hours	0.88	19.32	18.89	71.37	12.13
	0	0.92	19.01	18.6	70.73	12.43
CF	30 minutes	0.914	18.33	18.15	72.98	12.23
	5 hours	0.904	18.83	18.18	73.29	12.48
	8 hours	0.89	19.28	18.85	71.80	12.32

**Table S2**. The mobility of device based on THF and CF solvent with different thermal treatment time.

Mobility	Annealing	Electron	Hole	$\mu_{\rm e}/\mu_{\rm h}$
		$(*10^{-3} \text{ cm}^2 \text{V}^{-1} \text{ s}^{-1})$	$(*10^{-4} \text{ cm}^2 \text{V}^{-1} \text{ s}^{-1})$	
THF	No	1.66	2.14	7.76
	100°C/30min	4.10	2.83	14.48
	100℃/8h	2.24	1.96	11.43
CF	No	1.33	1.10	12.09
	100°C/30min	2.12	1.35	15.70
	100°C/8h	1.43	1.12	12.77

**Table S3**. The data got from GIWAXS based on CF solvent with different thermal treatment time.

Solvent	Thermal treatment	$\pi$ -π distance (A <sup>0</sup> )	Coherence length (A <sup>0</sup> )	PCE (%)
	As-cast	3.55	18	12.20
THF	100°C/30min	3.54	19	12.21
	100℃/5h	3.54	22	12.14
	100°C/8h	3.53	23	12.13
CF	As-cast	3.56	19	12.37
	100°C/30min	3.55	19	12.23
	100°C/8h	3.56	20	12.32

**Table S4**. The data got from RSoXS based on THF and CF solvent with different thermal treatment time.

Solvent	Thermal	Long-Period (nm)	Normalized	FF(%)
	treatment		total ISI	
	NO	N/A	N/A	70.77
THF	100°C/30min	$48 \pm 0.7$	$0.96 \pm 0.04$	72.67
	100℃/5h	50±1.5	$0.96 \pm 0.05$	71.14
	100°C/8h	52±0.1	$0.94 \pm 0/03$	71.37
	NO	51±1.0	1.00	70.73
CF	100°C/30min	49± 1.3	$0.90\pm0.01$	72.98
	100°C/8h	$45\pm1.3$	$0.95 \pm 0.05$	71.80

**Table S5**. Photovoltaic performance of the device based on LL spin-coating and LL blade-coating with and without thermal annealing treatment.

Annealing	<i>V</i> <sub>oc</sub> (V)	$J_{ m sc}$ (mA cm $^{-2}$ )	$J_{ m cal}$ (mA cm $^{-2}$ )	FF (%)	PCE (%)
As cast	0.905	18.11	17.34	73.40	12.03
100℃ /10min	0.886	18.67	17.89	71.88	11.89
	0.000	40.50		<b>=</b> 0.60	44.0.
As cast	0.892	18.79	17.95	70.69	11.85
100℃ /10min	0.875	18.87	17.99	70.68	11.67
	As cast  100°C  /10min  As cast	(V)  As cast 0.905  100°C 0.886  /10min  As cast 0.892  100°C 0.875	(V)     (mA cm <sup>-2</sup> )       As cast     0.905     18.11       100℃     0.886     18.67       /10min     .892     18.79       100℃     0.875     18.87	(V)     (mA cm $^{-2}$ )     (mA cm $^{-2}$ )       As cast     0.905     18.11     17.34 $100^{\circ}$ C     0.886     18.67     17.89       /10min	(V)     (mA cm <sup>-2</sup> )     (mA cm <sup>-2</sup> )     (%)       As cast $0.905$ $18.11$ $17.34$ $73.40$ $100^{\circ}$ C $0.886$ $18.67$ $17.89$ $71.88$ /10min       As cast $0.892$ $18.79$ $17.95$ $70.69$ $100^{\circ}$ C $0.875$ $18.87$ $17.99$ $70.68$