ADVANCED MATERIALS

Supporting Information

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Over 20% Efficient Water-Based Layer-by-Layer Organic Solar Cells with High Thickness Tolerance Enabled by Surfactant Promoted Electrostatic Interaction

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Over 20 % efficient water-based layer-by-layer organic solar cells with high thickness tolerance enabled by surfactant promoted electrostatic interaction

Experimental section

Materials: PM6 (Mn = 45,000, Mw = 97,000), L8-BO, BTP-eC9 were purchased from Solarmer Materials Inc. Sodium dodecyl sulfate (SDSO4), sodium dodecyl sulfonate (SDSO3), dodecyl trimethylammonium bromide (DTAB), dodecyl pyridinium bromide (DPB), 1-dodecyl-3-methylimidazolium bromide (DMMB) were purchased from Aladdin. Sodium dodecyl phosphate (SDP) was purchased from TCI. All the solvents were purchased from Sigma-Aldrich and used as received.

Density Functional Theory (DFT) Calculations: All electrostatic potential (ESP) calculations were performed using density functional theory at the B3LYP/6-31G(d,p) level, as implemented in Gaussian 09. Following full geometry optimizations, the molecular electrostatic potentials were mapped onto the respective molecular surfaces. We then evaluated a series of derived ESP metrics to quantify the polarity, charge distribution, and potential reactivity of each system.

ESP analysis was performed using the Multiwfn 3.7(dev) program[1,2]. For any given molecule, the electrostatic potential at a point $\boldsymbol{r}$ in the surrounding space arises from both the nuclei and electrons, and can be rigorously expressed as:

$$V(r) = \sum_A (Z_A/|\boldsymbol{r} - R_A|) - \int (\rho(\boldsymbol{r}')/|\boldsymbol{r} - \boldsymbol{r}'|) d\boldsymbol{r}' \quad (1)$$

Here, Z_A and R_A denote the nuclear charge and position vector of atom A, respectively, and $\rho(\boldsymbol{r}')$ is the electron density. To compactly characterize the molecular polarity and the variation in the ESP, a set of integral measures over the molecular surface (S) was employed.

The Molecular Polarity Index (MPI), defined as:

$$MPI = (1/A) \iint \iint_S |V(r)|\, dS \quad (2)$$

provides a measure of the overall magnitude of the electrostatic potential averaged over the molecular surface. Here, A represents the total molecular surface area. Regions of positive and negative ESP were delineated, and the mean positive ($\bar{V}_S^+$) and mean negative ($\bar{V}_S^-$) potentials were computed from discrete sampling points $\{\boldsymbol{r_i}\}$ on those respective domains:

$$\bar{V}_s^+ = (1/m)\sum_{i=1}^{m} V(\boldsymbol{r_i}) \quad (3)$$

$$\bar{V}_s^- = (1/n)\sum_{j=1}^{n} V(\boldsymbol{r_j}) \quad (4)$$

where m and n are the numbers of sampling points in the positive and negative domains, respectively. The overall average ESP, $\bar{V}_s$, was taken over the entire set of t points encompassing both domains.

To quantify the internal charge separation or local polarity, we employed the parameter Π :

$$\Pi = (1/t)\sum_{k=1}^{t} |V(\boldsymbol{r_k}) - \bar{V}_s| \quad (5)$$

Moreover, the variance of the ESP, σ_{tot}^2 , was decomposed into positive and negative contributions to elucidate the extent to which the molecule's surface potential is non-uniform. The total variance:

$$\sigma_{tot}^2 = \sigma_+^2 + \sigma_-^2 = (1/m)\sum_{i=1}^{m}[V(\boldsymbol{r_i}) - \bar{V}_s^+]^2 + (1/n)\sum_{j=1}^{n}[V(\boldsymbol{r_j}) - \bar{V}_s^-]^2 \quad (6)$$

reflects the range and unevenness of the ESP distribution. Larger variances (σ_+^2 or σ_-^2) correspond to more pronounced polarity features and thus stronger tendencies for intermolecular interactions.

Nanoparticle preparation: PM6 5 mg were dissolved in 1mL chloroform and stirred at 50 °C for 3h. Then the solution was added to 10 mL 10 mg mL^{-1} aqueous solution of surfactant and stirred at 40 °C for 1h. The formed micro-emulsion dispersion was ultrasonicated using a SCIENTZ-IID ultrasonic finger (200 watt, 5 min) in an ice-water bath. The miniemulsion system was heated at 40 °C while constant stirring until chloroform was completely eliminated. The excess surfactant from the particle solution was removed using Amicon® ultra-15 centrifuge filter (cutoff 30K). The dispersion was placed into the filter and centrifuged at 4000 rpm for 20 min. The retentate was raised to 15 mL with water and then centrifuged again. This process was repeated for 5 several times until surface tension of the filtrate reached 38 ± 2 mN m^{-1}. The retentate was filtered by a 0.45 μm filter before the last centrifugation.

Solar cells fabrication and characterization: Solar cell devices were fabricated in the conventional structure of ITO/2PACZ/Active layer/PNDIT-F3N/Ag. The pre-structured ITO/glass were cleaned with acetone and isopropyl alcohol in an ultrasonic bath for 10 min each. After drying, the 2PCAz (0.3 mg·mL^{-1} in ethanol) was spin-coated at 5000 rpm onto 10 minutes plasma-treated substrates outside, and then dried on a heating plate at 150 °C for 10 min. The samples were then transferred into a dry nitrogen glove box. For BHJ devices processed by toluene, the active layer PM6:L8-BO solution with polymer concentration of 8 mg mL^{-1} (D:A = 1:1.2, 0.5% DIO) was spin-coated on 2PACZ at 4000 rpm. For LBL devices, a 9 mg mL^{-1} PM6 solution was firstly deposited at 1800 rpm on 2PACZ, followed by deposing 10 mg mL^{-1} L8-BO solution at 2000 rpm. In mn-LBL devices, an aqueous donor NP ink of 20 mg mL^{-1} was spin-coated onto a heated substrate (80 °C) at 1250 rpm for 1 min in air. To remove remaining surfactant, the substrate was spin-rinsed with pure ethanol at 2000 rpm for 3 times. Then the substrate was immediately placed into a N_2-filled glovebox and stored overnight. After thermal annealing, the L8-BO solution of 8 mg mL^{-1} was spin-coated at 2000 rpm. The substrate was then annealed at 100 °C for 5 min.

To be detailed, for thick mn-LBL devices, the 200, 300 and 400 nm thickness were given by aqueous PM6 ink of 35 mg mL^{-1}, 60 mg mL^{-1} and 80 mg mL^{-1}, respectively. The concentration of acceptor was 12, 16 and 20 mg mL^{-1} for 200, 300 and 400 nm films, respectively. For other solvents processed devices, the chloroform solution of PM6 was fixed to 7 mg mL^{-1}. The concentration for chloroform solution of L8-BO is 7 mg mL^{-1} and 10 mg mL^{-1} for o-xylene, respectively.

After active layer deposition, a 0.5 mg mL^{-1} methanol solution of PNDIT-F3N was deposited at 3000 rpm for 30s in nitrogen atmosphere, followed by thermal evaporation of 100 nm of silver through a shadow mask with a 6 mm^2 active area opening under a vacuum of approximately 1×10^{-6} mbar. The current–voltage characteristics of the solar cells were measured under AM 1.5 G irradiation on a Newport solar simulator (Taiwan, China). The light source was calibrated using a silicon reference cell. All the cells were tested under an inert atmosphere. EQEs were measured using an Enlitech QE−S EQE system (Taiwan, China) that was equipped with a standard Si diode. Monochromatic light was generated from a Newport 300 W lamp source.

TPC, TPV, Photo-CELIV, CE, impedance and Mott-Schottky measurements are measured by Paios setup from FLUXiM AG.

FTPS-EQE and EL-EQE measurements: FTPS-EQE was measured using a integrated system (PECT-600, Enlitech), where the photocurrent was amplified and modulated by a lock-in instrument. EL-EQE measurements were performed by applying external voltage/current sources through the devices (REPS-Pro, Enlitech). All of the devices were prepared for EL-EQE measurements according to the optimal device fabrication conditions. EL-EQE measurements were carried out from 0 to 1.8 V.

Characterizations: Particle size and distribution were determined by dynamic light scattering (DLS) using a Malvern Zetasizer Nano ZS90 from Malven Panalytical (Malvern, UK). UV/Vis absorption, transmittance and reflectance spectra were measured using an UV-Vis-NIR spectrometer (Lambda 1050, from Perkin Elmer, Waltham, MA, USA). SEM results were obtained from the field emission scanning electron microscopy (FESEM) GeminiSEM 300 (Carl Zeiss Microscopy Ltd., Jena, Germany). AFM measurements were performed by Cypher S from Oxford Instruments Asylum Research, Inc. in contact mode. UPS experiments was performed on the Thermo Scientific XPS Escalab Xi+ using He I as the excitation source and its source energy was 21.21 eV. Contact angle measurements were carried out by an Attention Theta Flex meter, using water and diiodomethane by sessile drop analysis in open ambient atmosphere. EPR measurements were performed using an EPR200M spectrometer (Guoyi Quantum Technology Co., Ltd., China). Fourier transform infrared (FT-IR) measurements were performed using a Thermo Fisher Scientific iS500 spectrometer.

Film-depth-dependent light absorption: Film-depth-dependent light absorption spectra were acquired by an in-situ spectrometer (PU100, Shaanxi Puguang Weishi Co. Ltd.) (Shaanxi, China) equipped with a soft plasma-ion source. The power-supply for generating the soft ionic source was 100 W 39with an input oxygen pressure ~10 Pa. The film surface was incrementally etched by the soft ion source, without damage to the materials underneath the surface, which was in situ monitored by a spectrometer. From the evolution of the spectra and the Beer–Lambert's Law, film-depth-dependent absorption spectra were extracted. The exciton generation contour is numerically simulated upon inputting sub-layer absorption spectra into a modified optical transfer-matrix approach. The detailed experimental and numerical method are available elsewhere.[3,4]

The exciton formation of FLAS measurement is expressed by absorption coefficient. The absorption coefficient can be obtained according to

$$\alpha = 4\pi k/\lambda \quad (7)$$

$$I \approx I_0 e^{-\alpha(\lambda)d} \quad (8)$$

$$A(\lambda) = \lg(I_0/I) = -\lg(e^{-4\pi kd/\lambda}) \quad (9)$$

The real part (n) of complex index of refraction is set to be 2 for clarity, while the imaginary part (k) of complex refraction is from absorption coefficient (α) and absorbance (A). λ and d are wavelength and film thickness. k is related to film-depth. The detailed model is illustrated in elsewhere.[5]

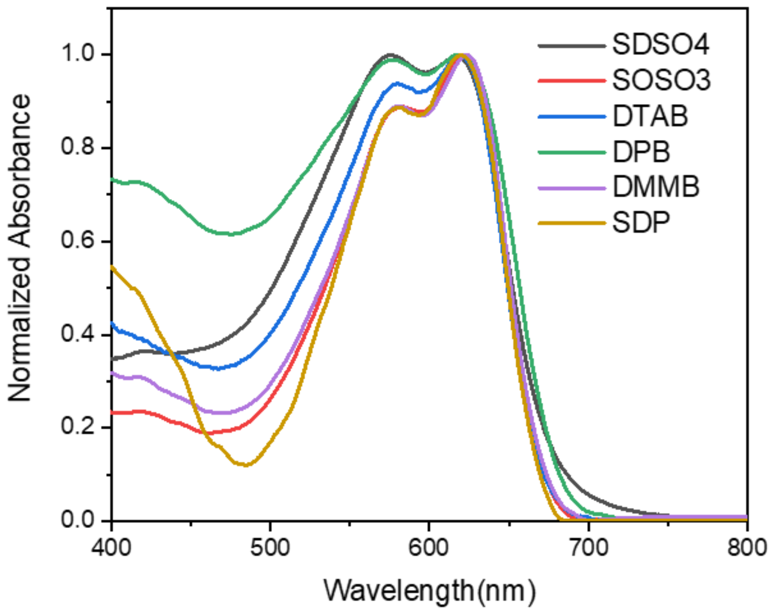

Figure S1. UV-vis absorption spectra of PM6 NPs processed films with various surfactants.

Table S1. Molecular surface area, MPI, extreme value of ESP and total average ESP of PM6, L8-BO and various surfactants (Isosurface = 0.001 au).

Material	Overall surface area (Å^2)	MPI	Minimal value (Kcal/mol)	Maximal value (Kcal/mol)	Overall average value (Kcal/mol)
PM6	1270.80	5.33	-31.12	17.02	-0.59
L8-BO	1434.27	7.92	-34.00	30.16	3.90
SDSO4	1280.94	2.44	-126.46	-12.95	-56.23
SDSO3	1244.19	2.44	-133.16	-13.06	-56.30
DTAB	1285.66	2.71	18.49	118.55	62.53
DPB	1333.22	2.66	17.96	113.70	61.28
DMMB	1378.76	2.63	17.44	119.76	60.72
SDP	1328.59	4.76	-210.40	-55.25	-109.85

Table S2. Other ESP indicators of PM6, L8-BO and various surfactants at ground state.

Material	Π^a (Kcal mol^{-1})	σ^2_{tot}^{b} (Kcal^2 mol^{-2})	σ^2_+^{c}(Kcal^2 mol^{-2})	σ^2_-^{d} (Kcal^2 mol^{-2})	ν^e
PM6	5.34	40.48	13.46	27.03	0.22
L8-BO	6.53	96.97	26.06	70.91	0.20

SDSO4	32.49	1429.97	0.00	1429.97	1.00
SDSO3	32.97	1515.86	0.00	1515.86	1.00
DTAB	28.54	971.25	971.25	0.00	1.00
DPB	27.44	895.30	895.30	0.00	1.00
DMMB	27.59	911.94	971.94	0.00	1.00
SDP	49.55	3126.94	0.00	3126.94	1.00

[a] the average deviation over the surface;

[b] the total ESP variance;

[c] the positive ESP variance;

[d] the negative ESP variance;

[e] the charge balance factor, which can be described by the following equations:

$\nu = \sigma^2_+ \sigma^2_- / (\sigma^2_{tot})^2$.

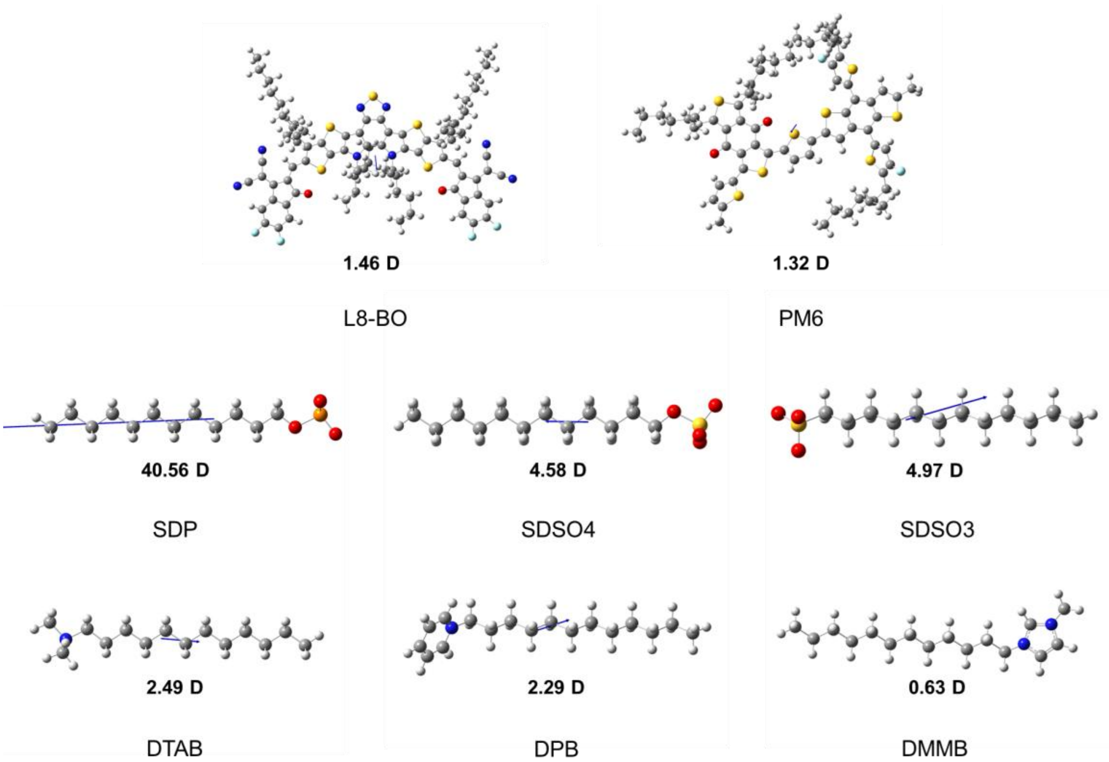

Figure S2. The calculated dipole moments of PM6, L8-BO and different surfactants.

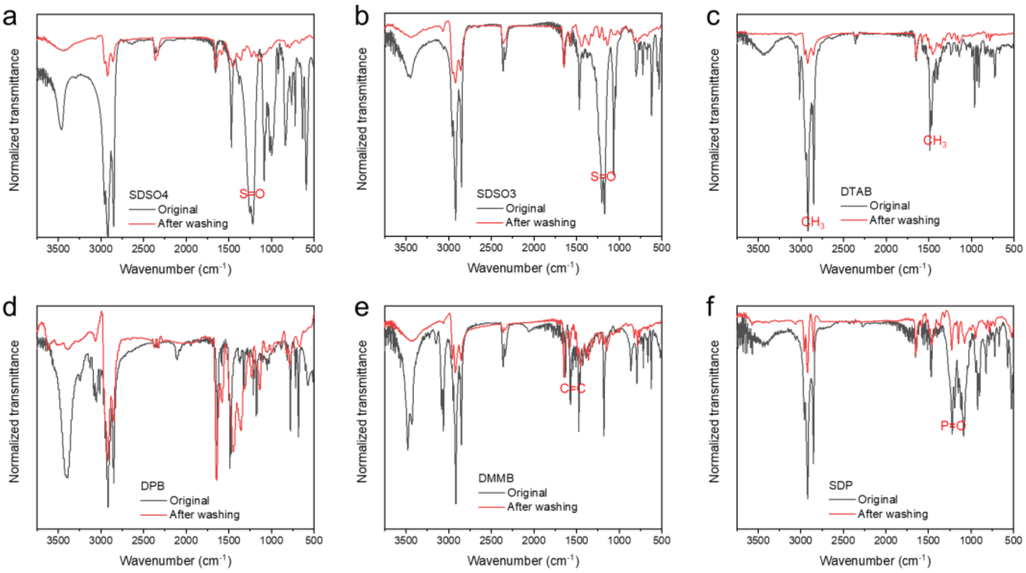

Figure S3. FT-IR spectra of PM6 NPs with (a) SDSO4, (b) SDSO3, (c) DTAB, (d) DPB, (e)DMMB, (f) SDP as surfactant before and after washing process.

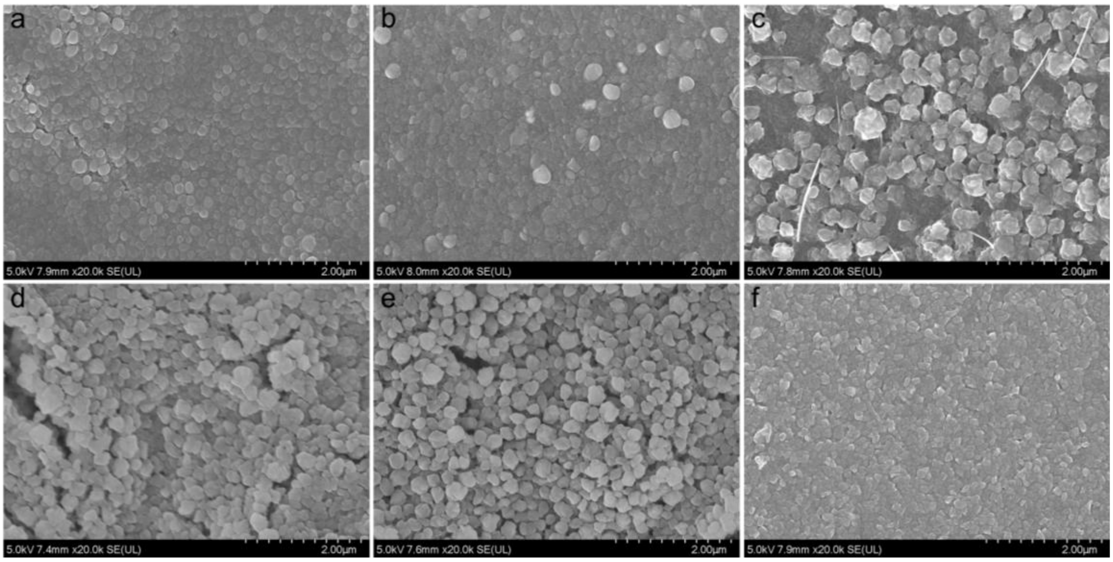

Figure S4. SEM of PM6 films processed from NPs with (a) SDSO4, (b) SDSO3, (c) DTAB, (d) DPB, (e)DMMB, (f) SDP as surfactant.

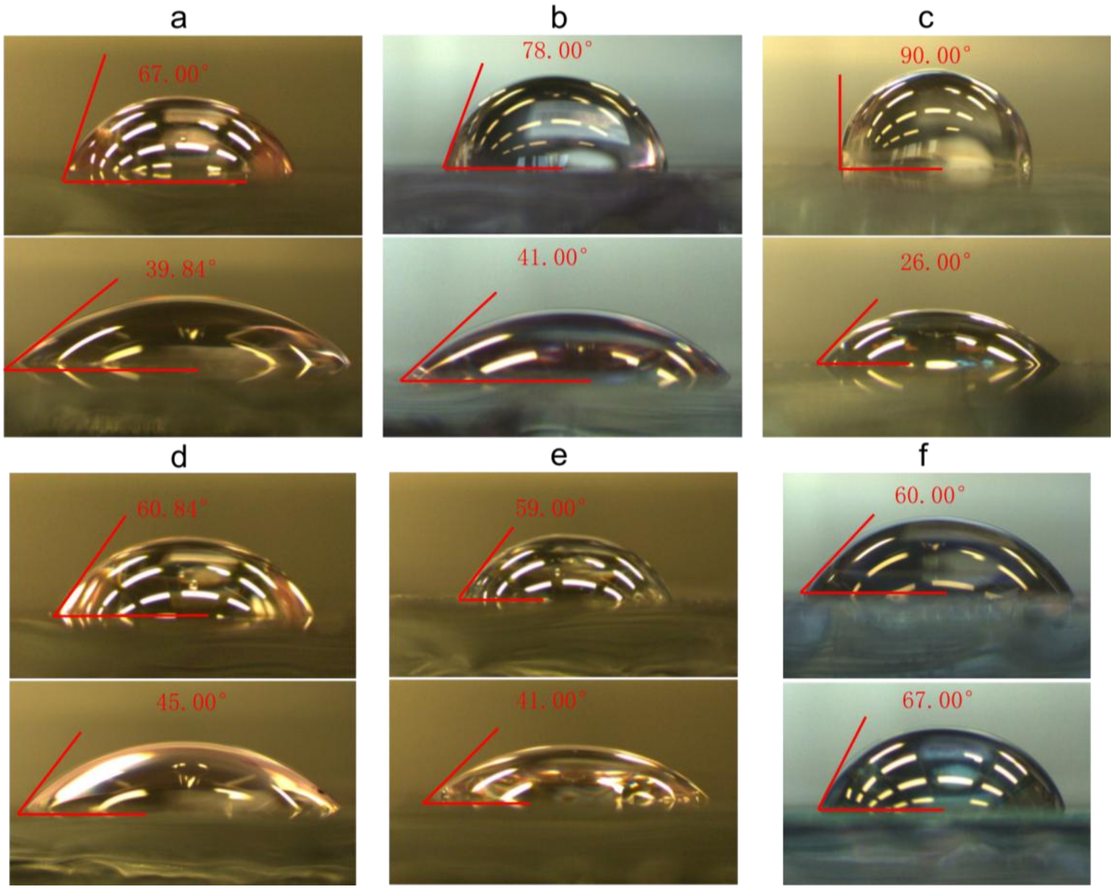

Figure S5. Contact angle image of water (top) and CH2I2 on top of mesostructured PM6 film.

Table S3. Contact angle results, surface energy and interaction paramenter values calculated according to Owens, Wendt, Rabel and Kaelble (OWRK) method.

Material	Water contact Angle	DIM contact Angle	Surface energy (mN/m)	Interaction parameter
L8-BO	89.9	39.0	41.0	-
PM6	101.0	48.0	32.4	0.506
PM6 NP (SDSO4)	67.0	39.8	48.5	0.315
PM6 NP (SDSO3)	78.0	41.0	43.4	0.034
PM6 NP (DTAB)	90.0	26.0	46.2	0.155
PM6 NP (DPB)	60.8	45.0	49.0	0.356
PM6 NP (DMMB)	59.0	41.0	50.3	0.475
PM6 NP (SDP)	60.0	67.0	44.0	0.053

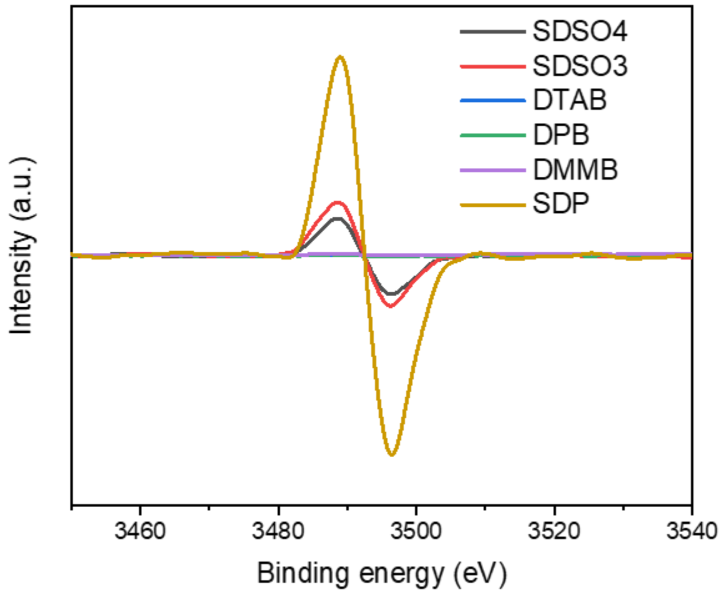

Figure S6. EPR spectra of PM6 NP films with different surfactants.

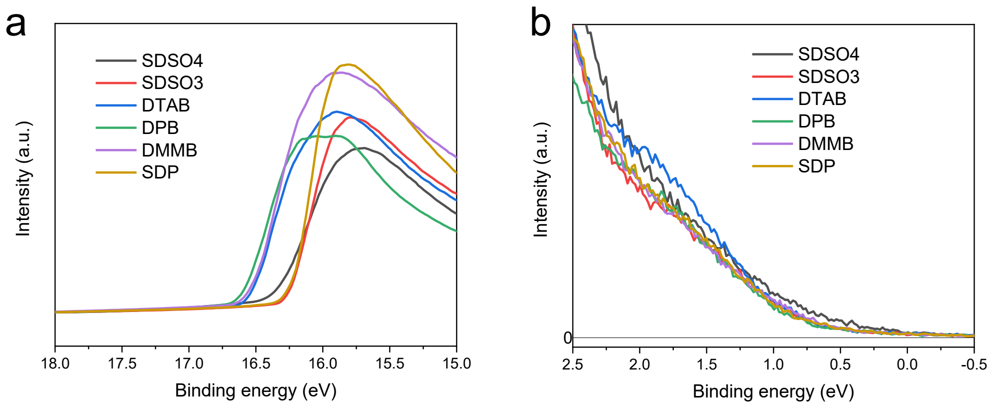

Figure S7. UPS spectra of PM6 NP films with different surfactants.

Table S4. The energy of secondary electron cutoff edge (E_{SE}), the valence band energy (E_{VB}), calculated HOMO energy level (E_{HOMO}) and work functions of PM6 NP films incorporating different surfactant.

Surfactant	E_{SE} (eV)	E_{VB} (eV)	E_{HOMO} (eV)	Work function (eV)
Neat	16.55	0.87	-5.52	4.65
SDSO4	16.37	0.78	- 5.61	4.83
SDSO3	16.27	0.74	- 5.67	4.93
DTAB	16.54	0.84	- 5.50	4.66
DPB	16.61	0.90	-5.49	4.59
DMMB	16.65	0.90	- 5.45	4.55
SDP	16.25	0.77	-5.72	4.95

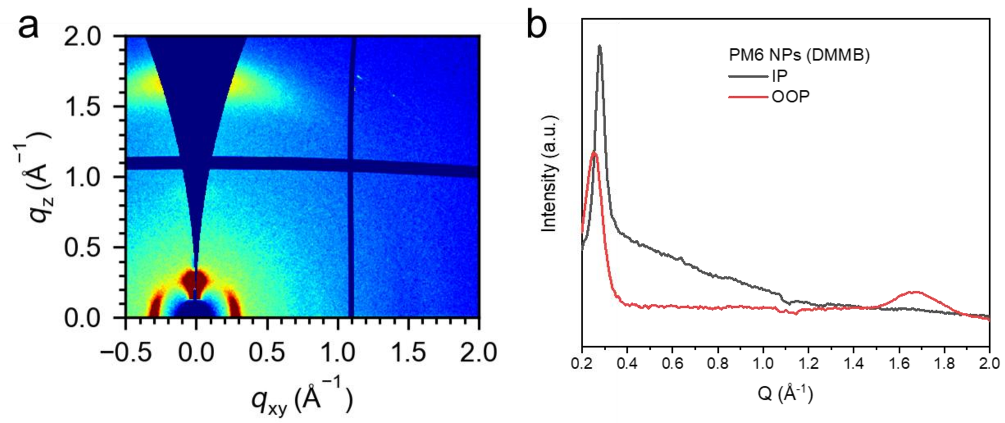

Figure S8. (a) 2D GIWAXS pattern and (b) its corresponding in-plane and out-of-plane line-cuts of PM6 NP film with DMMB as surfactant.

Table S5. The peak positions, d-spacings, FWHMs and CCLs of PM6 and PM6:L8-BO films processed with PM6 NPs.

Film	IP				OOP			
	q ($Å^{-1}$)	d-spacing(Å)	FWHM ($Å^{-1}$)	CCL(Å)	q ($Å^{-1}$)	d-spacing (Å)	FWHM ($Å^{-1}$)	CCL (Å)
Neat PM6	0.278	22.64	1.017	55.62	1.645	3.820	0.257	21.97
PM6 NP (DMMB)	0.278	22.64	0.641	88.25	1.641	3.825	0.216	26.22
PM6 NP (SDP)	0.275	22.85	0.558	101.4	1.662	3.779	0.226	25.02
BC	0.285	22.05	0.818	69.15	1.678	3.746	0.351	16.09
c-LBL	0.283	22.24	0.702	80.50	1.685	3.729	0.343	16.46
mn-LBL (DMMB)	0.278	22.64	0.607	93.14	1.685	3.729	0.341	16.56
mn-LBL (SDP)	0.278	22.64	0.641	88.24	1.700	3.696	0.336	16.81

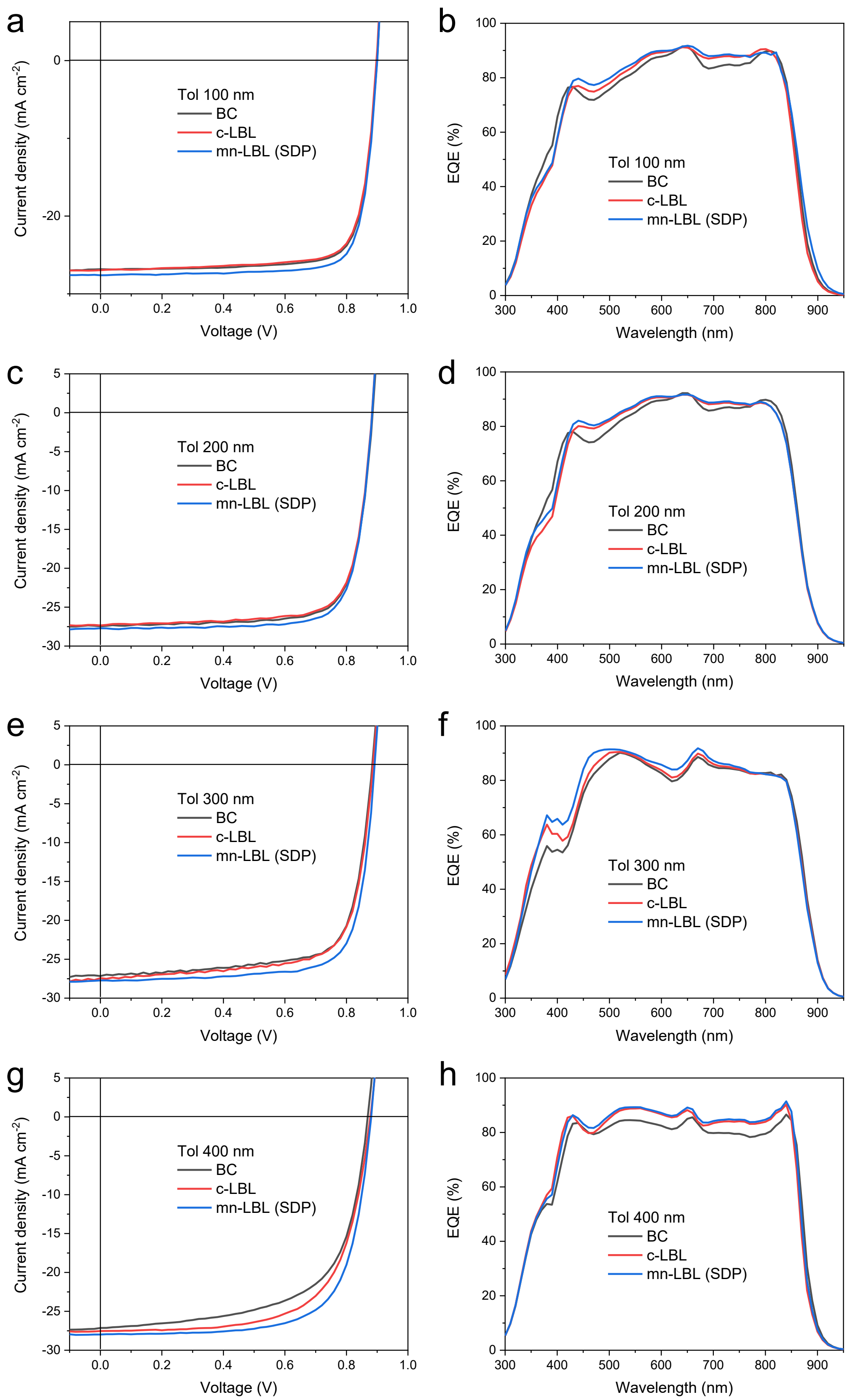

Figure S9. (a, c, e, g) J-V curves and (b, d, f, h) EQE spectra of toluene-based PM6:L8-BO devices prepared by different processing strategies with a thickness of (a, b) 100 nm, (c, d) 200 nm, (e, f) 300 nm and (g, h) 400 nm, respectively.

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第 1 页 page 1
共 4 页 This report includes 4 page

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TIANJIN INSTITUTE OF METROLOGICAL SUPERVISION AND TESTING
ELECTRONIC &INSTRUMENTAL LABORATORY

检测报告
TEST REPORT

报告编号： TDYF 字第 240010-WT 号
ReportNo

产品名称： 太阳电池
Name Solar cells

规格型号： OPV-normal
Model

委托单位： 深圳技术大学 新材料与新能源学院
Applicant Shenzhen Technology University, College of New Materials and New Energy

生产单位： 深圳技术大学 新材料与新能源学院
Manufacturer Shenzhen Technology University, College of New Materials and New Energy

检验检测专用章
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电话 Tel：022-81264268 传真 Fax：022-28326590 电邮 Email：tjpvtc@163.com
网址 Web：http://www.tjelab.com

Figure S10. First page of the certification report of PM6:L8-BO device with a thickness of 100 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.

中国合格评定国家认可委员会认可证书：№.CNAS L0921 号

Certificate approved by CNAS：№.CNAS L0921 号

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Figure S11. Second page of the certification report of PM6:L8-BO device with a thickness of 100 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.

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Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory

检测报告

TEST REPORT

№：TDYF 字第 240010-WT　　　　共 4 页 第 2 页

委托单位 Applicant	深圳技术大学新材料与新能源学院 Shenzhen Technology University, College of New Materials and New Energy	单位地址 Address	广东省深圳市坪山区深圳技术大学 B2 新材料与新能源学院 Shenzhen Technology University B2, College of New Materials and New Energy, Shenzhen,Guangdong
产品名称 Name	太阳电池 Solar cells	商　标 Trademark	—
规格型号 Model	OPV-normal	生产日期 Date	—
产品编号 Number	SZTU-SL202402	检测类别 Sort	委托检测 Request examination
检测依据 Reference documents for the test	IEC 60904-1:2020《光伏器件 第 1 部分：光伏电流-电压特性的测量》 Photovoltaic devices – Part 1: Measurement of photovoltaic current-voltage characteristics		
样　品 Sample	样品来源 Source: 送样 Sample delivery	样品状态 Condition	外观良好 Normal
	样品数量 Quantity: 1 片	收样日期 Date of receiving	2024 年 Year 01 月 Month 12 日 Day
检测地点 Place	天津市河西区五号堤路 18 号 106 室 Room 106,No.18 WuHao Di Road,Hexi Distric,Tianjn		
环境条件 Environment	温度 Temperature 25°C	相对湿度 Relative humidity 35%	气压 Pressure —
检测自 Test begin from	2024 年 Year 01 月 Month 12 日 Day	至 To	2024 年 Year 01 月 Month 12 日 Day
主　检 Inspector	[illegible]		
审　核 Examiner	[illegible]		
批　准 Approver	杨学毫 [illegible]		
		签发日期 Date of issue	2024 年 Year 01 月 Month 12 日 Day
备注： Remarks	—		

Figure S12. Third page of the certification report of PM6:L8-BO device with a thickness of 100 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.

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Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory

检测报告

TEST REPORT

№：TDYF 字第 240010-WT 共 4 页 第 3 页

检测用主要仪器设备一览表 Equipments for Test					
序号 №	仪器设备名称 Name	规格型号 Model	设备编号 Serial №	证书有效期 Valid date of verification	备注 Remarks
1	电池片 I-V 特性测试仪 I-V Tester for Solar Cells	VS-6831S	21VJ002	2024.09.10	—
2	红外测温仪 Infrared thermometers	562	51350514WS	2024.03.12	—
3	Keithley 2400 Standard Series Sourcemeter	2400	4463530	2024.08.31	—

样品信息 Information for Samples		
样品编号 Sample Number	规格型号 Sample Type	产品编号 Serial Number
240010-1	OPV-normal	SZTU-SL202402

Figure S13. Fourth page of the certification report of PM6:L8-BO device with a thickness of 100 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.

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检 测 报 告

TEST REPORT

№：TDYF 字第 240010-WT　　　　　　　　　　共 4 页 第 4 页

检测内容：Test content　　光伏电流-电压特性 *I-V* Characteristic

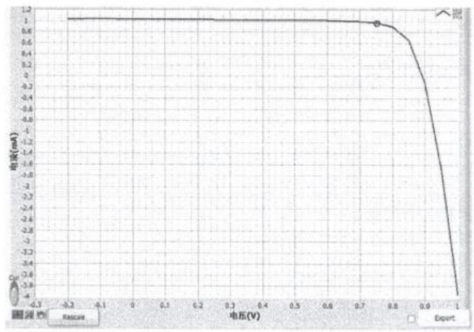
序号 №	项目 Item	技术要求 Requirement	检测结果 Test result
1	光伏电流-电压特性 *I-V* Characteristic	—	见下表 As follows

测试时间 Date	2024. 01. 12
测试条件 Condition	使用稳态 AAA 级太阳模拟器，在 AM1. 5G，1000W/m²，25. 0℃条件下测试 Sample was tested under the condition of AM1.5G, 1000W/m², 25.0°C with a steady-state class calibrated AAA solar simulator
有效面积 Active area	0. 0375cm² 备注：器件的有效面积是由带固定孔径的薄金属掩膜板量化 Remark: Designated area defined by thin metal aperture mask.

样品编号 №	V_{oc} (V)	I_{sc} (mA)	J_{sc} (mA/cm²)	P_{max} (mW)	V_{Pmax} (V)	I_{Pmax} (mA)	FF (%)	η (%)
240010-1	0. 893	1. 031	27. 50	0. 730	0. 750	0. 973	79. 27	19. 46

测试程序 Test program settings		
	起始电压：Starting voltage:	-0. 20V
	终止电压：Termination voltage:	+1. 00V
	扫描间隔：Scan interval:	0. 05V
	延迟时间：Delay time:	0. 1s

I-V 曲线图 *I-V* curve



本报告结束 **The end of the report**

Figure S14. Fifth page of the certification report of PM6:L8-BO device with a thickness of 100 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.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第1 页 page 1
共4 页 This report includes 4 page

天津市计量监督检测科学研究院
电子仪表实验所
TIANJIN INSTITUTE OF METROLOGICAL SUPERVISION AND TESTING
ELECTRONIC &INSTRUMENTAL LABORATORY

检测报告
TEST REPORT

报告编号: TDYF 字第 240009-WT 号
ReportNo

产品名称: 太阳电池
Name Solar cells

规格型号: PM6/L8-BO
Model

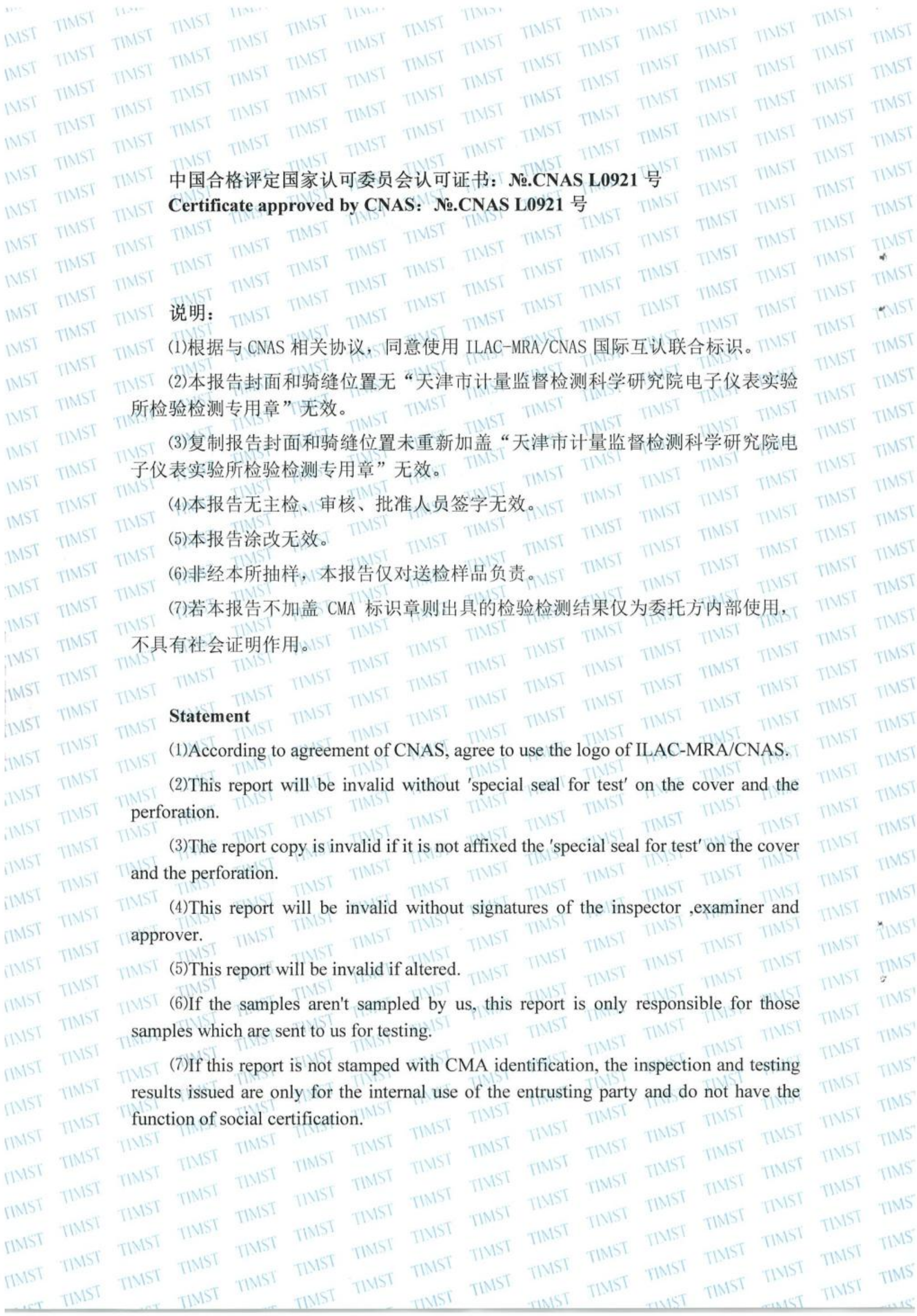
委托单位: 深圳技术大学 新材料与新能源学院
Applicant Shenzhen Technology University, College of New Materials and New Energy

生产单位: 深圳技术大学 新材料与新能源学院
Manufacturer Shenzhen Technology University, College of New Materials and New Energy

检验检测专用章
stamp

地址 Add: 天津市河西区五号堤路18号№.18WuHaoDi Road Hexi District Tianjin
电话 Tel: 022-81264268 传真 Fax: 022-28326590 电邮 Email: tjpvtc@163.com
网址 Web: http://www.tjelab.com

Figure S15. First page of the certification report of PM6:L8-BO device with a thickness of 300 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.



中国合格评定国家认可委员会认可证书：**№.CNAS L0921 号**
Certificate approved by CNAS：№.CNAS L0921 号

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Figure S16. Second page of the certification report of PM6:L8-BO device with a thickness of 300 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.

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Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory

检 测 报 告

TEST REPORT

№: TDYF 字第 240009-WT 共 4 页 第 2 页

委托单位 Applicant	深圳技术大学新材料与新能源学院 Shenzhen Technology University, College of New Materials and New Energy	单位地址 Address	广东省深圳市坪山区深圳技术大学B2 新材料与新能源学院 Shenzhen Technology University B2, College of New Materials and New Energy, Shenzhen,Guangdong
产品名称 Name	太阳电池 Solar cells	商 标 Trademark	—
规格型号 Model	PM6/L8-BO	生产日期 Date	—
产品编号 Number	SZTU-XC202403	检测类别 Sort	委托检测 Request examination
检测依据 Reference documents for the test	IEC 60904-1:2020《光伏器件 第 1 部分：光伏电流-电压特性的测量》 Photovoltaic devices – Part 1: Measurement of photovoltaic current-voltage characteristics		

样 品 Sample	样品来源 Source	送样 Sample delivery	样品状态 Condition	外观良好 Normal
	样品数量 Quantity	1 片	收样日期 Date of receiving	2024 年 Year 01 月 Month 12 日 Day

检测地点 Place	天津市河西区五号堤路 18 号 106 室 Room 106,No.18 WuHao Di Road,Hexi Distric,Tianjn
环境条件 Environment	温度 Temperature 25°C 相对湿度 Relative humidity 35% 气压 Pressure —
检测自 Test begin from	2024 年 Year 01 月 Month 12 日 Day 至 To 2024 年 Year 01 月 Month 12 日 Day
主 检 Inspector	[illegible] [illegible]
审 核 Examiner	[illegible]
批 准 Approver	杨学毫 [illegible]
	签发日期：2024 年 Year 01 月 Month 12 日 Day Date of issue
备注： Remarks	—

Figure S17. Third page of the certification report of PM6:L8-BO device with a thickness of 300 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.

天津市计量监督检测科学研究院电子仪表实验所
Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory

检测报告
TEST REPORT

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共 4 页 第 3 页

检测用主要仪器设备一览表 Equipments for Test					
序号 №	仪器设备名称 Name	规格型号 Model	设备编号 Serial №	证书有效期 Valid date of verification	备注 Remarks
1	电池片 I-V 特性测试仪 I-V Tester for Solar Cells	VS-6831S	21VJ002	2024. 09. 10	—
2	红外测温仪 Infrared thermometers	562	51350514WS	2024. 03. 12	—
3	Keithley 2400 Standard Series Sourcemeter	2400	4463530	2024. 08. 31	—

样品信息 Information for Samples		
样品编号 Sample Number	规格型号 Sample Type	产品编号 Serial Number
240009-1	PM6/L8-BO	SZTU-XC202403

Figure S18. Fourth page of the certification report of PM6:L8-BO device with a thickness of 300 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.

天津市计量监督检测科学研究院电子仪表实验所

Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory

检测报告

TEST REPORT

№：TDYF 字第 240009-WT

检测内容：Test content	光伏电流-电压特性 *I-V* Characteristic		
序号 №	项目 Item	技术要求 Requirement	检测结果 Test result
1	光伏电流-电压特性 *I-V* Characteristic	—	见下表 As follows

测试时间 Date	2024.01.12
测试条件 Condition	使用稳态 AAA 级太阳模拟器，在 AM1.5G，1000W/m²，25.0℃条件下测试 Sample was tested under the condition of AM1.5G, 1000W/m², 25.0°C with a steady-state class calibrated AAA solar simulator
有效面积 Active area	0.0375cm² 备注：器件的有效面积是由带固定孔径的薄金属掩膜板量化 Remark: Designated area defined by thin metal aperture mask.

样品编号 №	V_{oc} (V)	I_{sc} (mA)	J_{sc} (mA/cm²)	P_{max} (mW)	V_{Pmax} (V)	I_{Pmax} (mA)	FF (%)	η (%)
240009-1	0.886	1.037	27.66	0.687	0.750	0.916	74.74	18.32

测试程序 Test program settings		
	起始电压：Starting voltage:	-0.20V
	终止电压：Termination voltage:	+1.00V
	扫描间隔：Scan interval:	0.05V
	延迟时间：Delay time:	0.1s

I-V 曲线图 *I-V* curve

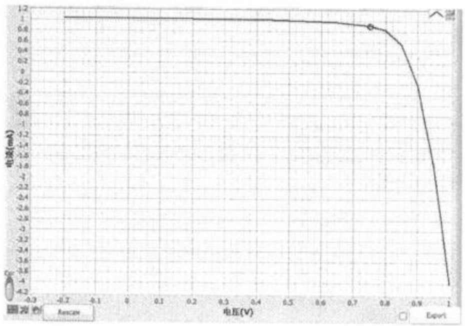

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Figure S19. Fifth page of the certification report of PM6:L8-BO device with a thickness of 300 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.

Table S6. Classification of representative OSCs with thick active layer.

NO.	Year	Active layer	Thickness (nm)	PCE (%)	URL
1	2020	Si25-H2:IEICO-4F	210	11.58	https://doi.org/10.1039/d0ta01340d
			250	12.02	
			320	13.2	
			380	12.79	
2	2020	PT2:TTPTTT-4F:IDIC	200	11.8	https://doi.org/10.1002/solr.202000476
			300	12.1	
			400	12.2	
3	2020	PBDB-T-2Cl:BP-4F:$PC_{61}BM$	200	15.3	https://doi.org/10.1007/s11426-019-9556-7
			300	14.3	
4	2020	D18:Y6:$PC_{61}BM$	200	16.63	https://doi.org/10.1016/j.scib.2020.08.027
			270	16.51	
			300	16.32	
			350	16.19	
5	2020	PBDB-TF:BTP-4Cl	328	15	https://doi.org/10.1021/acsami.0c05172
			545	13.8	
			1020	12.1	
6	2020	PM7:MF2	197	13.39	https://doi.org/10.1002/adfm.201908336
			251	12.89	
			308	12.34	
			373	11.58	
7	2020	PBDB-T-2Cl:BP-4F:MF1	200	15.04	https://doi.org/10.1039/C9EE04020J
			300	14.7	
			380	13.38	
8	2020	PM6:Y6:BTP-M	200	15.15	https://doi.org/10.1039/C9EE03710A
			300	14.23	
			400	13.48	
9	2020	PBT(E)BTz :PBDB-TF:BTP-4Cl	200	15.21	https://doi.org/10.1002/adfm.201910466
			250	14.61	
			300	14	
10	2020	P2FEhp:Y6	210	11.4	https://doi.org/10.1007/s10118-020-2355206-3
			520	10.5	
11	2021	PM6:BTP-eC9	300	16.25	https://doi.org/10.1038/s41467-017.4821-25148-8
			400	15.12	
			500	14.37	
12	2021	PM6:FCC-Cl	200	12.3	https://doi.org/10.1016/j.joule.2021.03.020
			300	10.9	
			400	9.0	
13	2021	PM6: BP4T-4F:	200	16.89	https://doi.org/10.1002/s

		BP3T-4F	250	16.58	olr.202100365
			300	16.03	
14	2022	PM6:BTP-4F-12:IT-M	200	17.08	https://doi.org/10.1016/j.cej.2021.129276
			250	15.89	
			300	15.34	
15	2022	PM6:Y7-BO:Y6-1O	200	17.57	https://doi.org/10.1002/adfm.202200807
			250	17.10	
			300	16.61	
			360	16.23	
			400	15.71	
16	2022	PM6:BTP-eC9:L8-BO-F	300	17.31	https://doi.org/10.1038/s41467-022-29803-6
			500	15.21	
17	2023	PM6:L8-BO:DY-TF	300	18.23	https://doi.org/10.1002/adma.202304225
			400	17.25	
			500	15.91	
18	2024	PM6:BTP-eC9	250	18.19	https://doi.org/10.1039/D4EE00068D
			400	17.22	
19	2024	PM6:L8-BO:PS	300	18.15	https://doi.org/10.1002/adma.202313532
			500	16.00	
20	2025	D18:L8-BO:IDIC	300	18.84	https://doi.org/10.1002/adma.202413125
21	2025	D18:Cl:N3:AT-β2O	250	19.15	https://doi.org/10.1038/s41563-024-02062-0
			400	17.93	
22	2025	PM6:L8-BO	200	19.07	This work
			300	18.87	
			400	17.30	

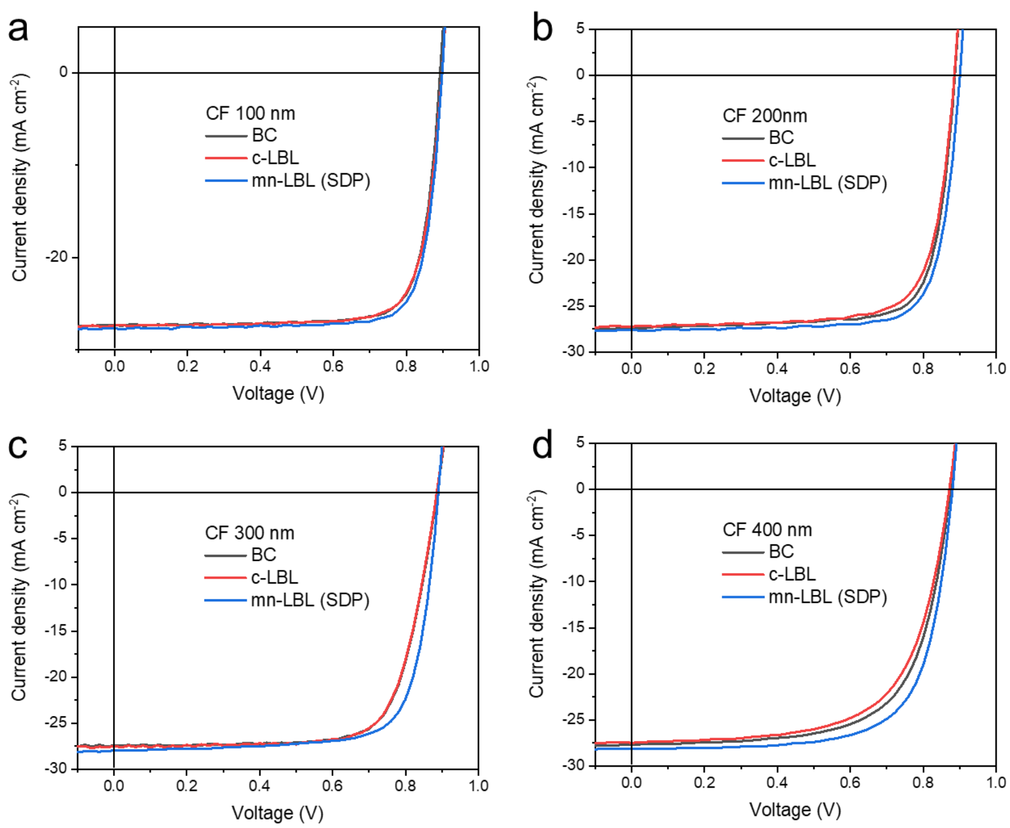

Figure S20. (a, c) J-V curves of chloroform-based PM6:L8-BO devices prepared by different processing strategies with a thickness of (a) 100 nm, (b) 200 nm, (c) 300 nm and (d) 400 nm, respectively.

Table S7. Summary of photovoltaic parameters of chloroform processed PM6:L8-BO solar cells with different thicknesses and processing methods.

Thickness (nm)	Processing method	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE[b] (%)
100 ± 10	BC	0.890	27.35	79.70	19.40 (19.19 ± 0.21)
	c-LBL	0.895	27.39	78.87	19.34 (19.09 ± 0.25)
	mn-LBL[c]	0.895	27.71	80.37	19.94 (19.66 ± 0.28)
200 ± 20	BC	0.884	27.41	77.20	18.71 (18.51 ± 0.20)
	c-LBL	0.883	27.26	75.21	18.11 (17.96 ± 0.15)
	mn-LBL[c]	0.899	27.65	77.86	19.34 (19.02 ± 0.32)
300 ± 20	BC	0.886	27.47	73.62	17.92 (17.55 ± 0.37)
	c-LBL	0.885	27.56	73.25	17.87 (17.50 ± 0.27)
	mn-LBL[c]	0.888	28.12	75.50	18.87 (18.62 ± 0.25)
400 ± 30	BC	0.872	27.51	67.02	16.08 (15.66 ± 0.42)
	c-LBL	0.870	27.31	65.06	15.46 (15.13 ± 0.33)
	mn-LBL[c]	0.878	27.91	70.53	17.29 (17.00 ± 0.29)

[a] Calculated from EQE;

[b] Average values with standard deviation were obtained from 20 devices;

c Processed from PM6 NPs with SDP as surfactant.

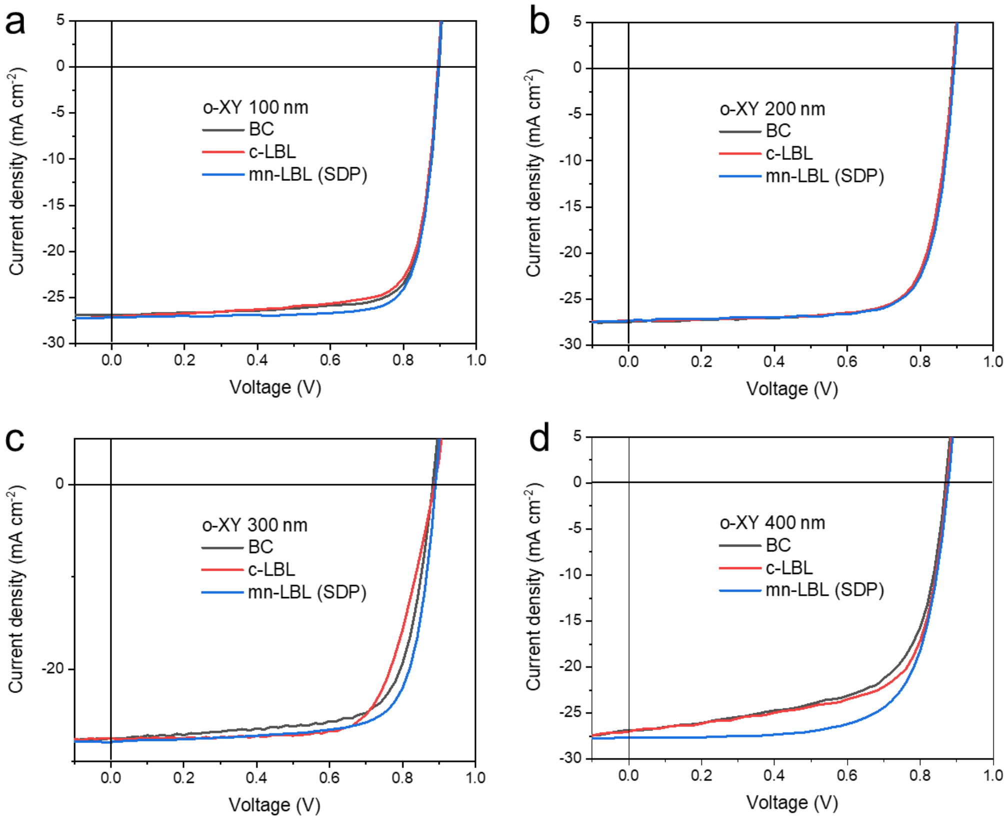

Figure S21. (a, c) J-V curves of O-xylene-based PM6:L8-BO devices prepared by different processing strategies with a thickness of (a) 100 nm, (b) 200 nm, (c) 300 nm and (d) 400 nm, respectively.

Table S8. Summary of photovoltaic parameters of O-xylene processed PM6:L8-BO solar cells with different thicknesses and processing methods.

Thickness (nm)	Processing method	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE[a] (%)
100 ± 10	BC	0.895	26.97	78.41	18.93 (18.68 ± 0.25)
	c-LBL	0.892	27.20	76.38	18.53 (18.19 ± 0.34)
	mn-LBL[b]	0.893	27.29	79.99	19.49 (19.12 ± 0.37)
200 ± 20	BC	0.887	27.46	76.22	18.56 (18.29 ± 0.27)
	c-LBL	0.888	27.30	76.09	18.44 (18.17 ± 0.27)
	mn-LBL[b]	0.891	27.40	76.67	18.71 (18.52 ± 0.19)
300 ± 20	BC	0.882	27.64	71.72	17.48 (17.11 ± 0.37)
	c-LBL	0.886	27.64	71.31	17.46 (17.12 ± 0.34)
	mn-LBL[b]	0.888	27.75	74.52	18.37 (18.04 ± 0.33)
400 ± 30	BC	0.867	27.18	63.84	15.04 (14.68 ± 0.46)
	c-LBL	0.871	27.27	66.08	15.70 (15.24 ± 0.46)
	mn-LBL[b]	0.875	27.83	70.34	17.13 (16.61 ± 0.52)

[a] Average values with standard deviation were obtained from 20 devices;

[b] Processed from PM6 NPs with SDP as surfactant.

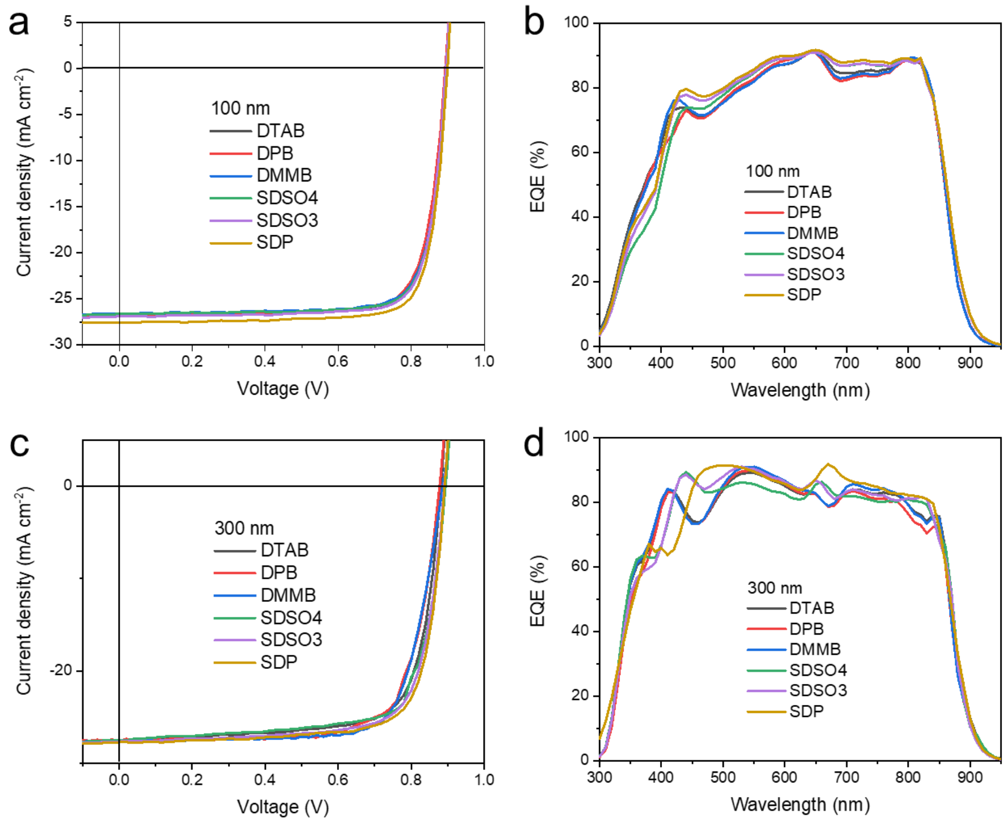

Figure S22. (a, c) J-V curves and (b, d) EQE spectra of mn-LBL PM6:L8-BO devices prepared by various surfactants with a thickness of (a, b) 100 nm and (c, d) 300 nm, respectively.

Table S9. Summary of photovoltaic parameters of toluene processed mn-LBL PM6:L8-BO solar cells with different surfactant.

Surfactant	Thickness (nm)	V_{OC} (V)	J_{SC} (mA cm^{-2})	J_{SC}[a] (mA cm^{-2})	FF (%)	PCE[b] (%)
SDSO4	100	0.893	26.75	26.15	79.99	19.11 (18.99 ± 0.12)
	300	0.892	27.50	26.39	74.61	18.35 (18.07 ± 0.28)
SDSO3	100	0.892	27.01	26.37	80.07	19.30 (19.11 ± 0.19)
	300	0.889	27.64	26.61	74.98	18.42 (18.14 ± 0.28)
DTAB	100	0.891	26.74	25.74	79.21	18.88 (18.65 ± 0.23)
	300	0.880	27.52	26.21	73.95	17.96 (17.50 ± 0.46)
DPB	100	0.891	26.72	25.64	79.08	18.83 (18.61 ± 0.22)
	300	0.876	27.59	26.09	73.88	17.86 (17.54 ± 0.32)
DMMB	100	0.896	26.60	25.77	79.34	18.91 (18.74 ± 0.17)
	300	0.886	27.74	26.34	74.20	18.23 (17.92 ± 0.31)
SDP	100	0.897	27.69	26.70	80.41	19.97 (19.58 ± 0.38)
	300	0.889	27.80	27.07	76.20	18.87 (18.54 ± 0.31)

[a] Calculated from EQE;

[b] Average values with standard deviation were obtained from 20 devices.

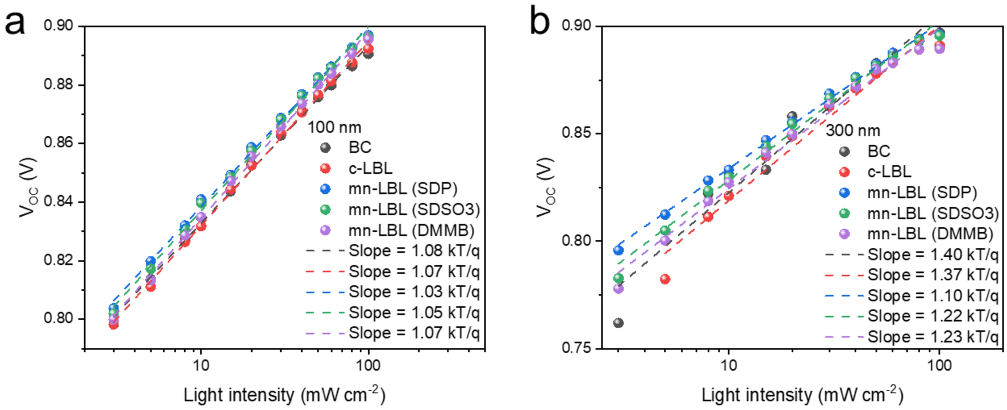

Figure S23. Voc as a function of light intensity of mn-LBL PM6:L8-BO devices prepared by various surfactants with a thickness of (a) 100 nm and (c) 300 nm, respectively.

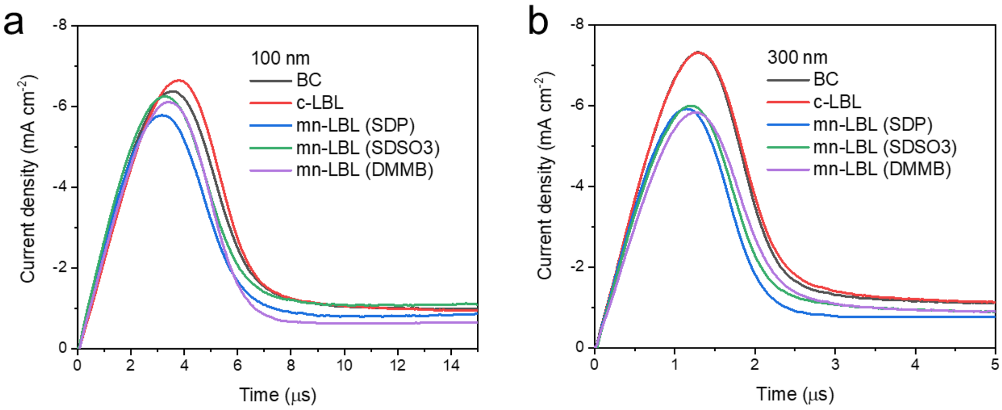

Figure S24. Photo-CELIV curves of mn-LBL PM6:L8-BO devices prepared by various surfactants with a thickness of (a) 100 nm and (c) 300 nm, respectively.

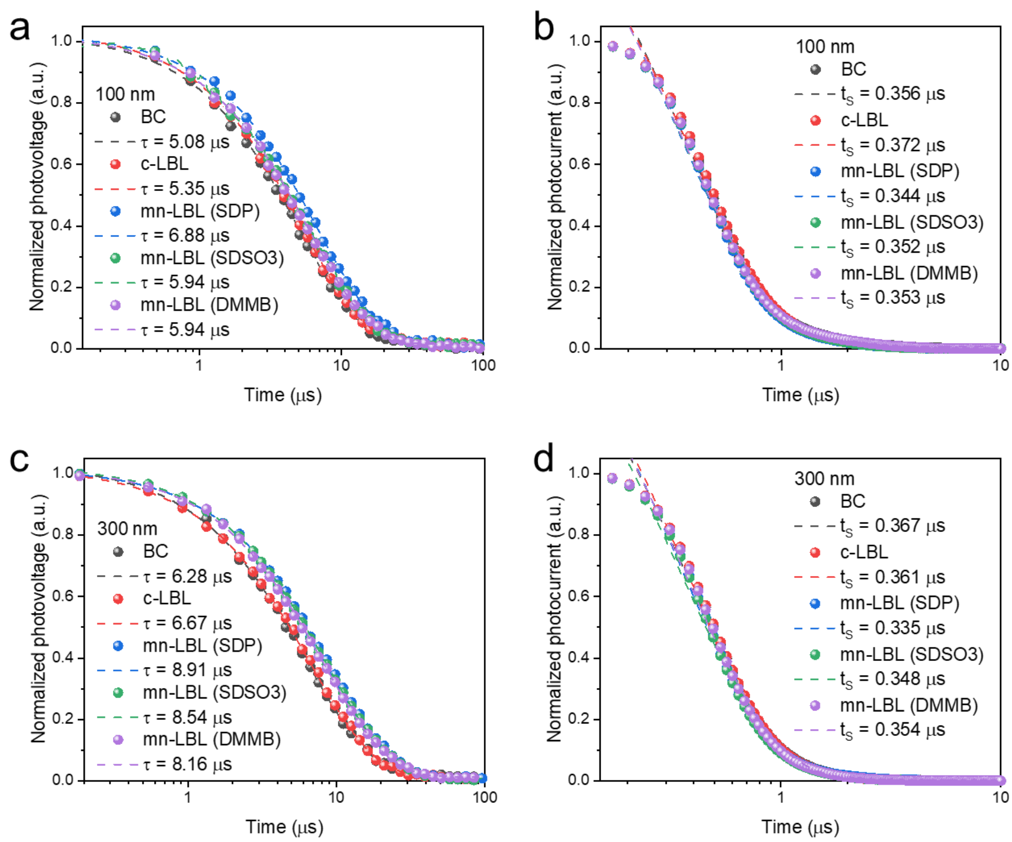

Figure S25. (a, c) TPV and (b, d) TPC curves of mn-LBL PM6:L8-BO devices prepared by various surfactants with a thickness of (a, b) 100 nm and (c, d) 300 nm, respectively.

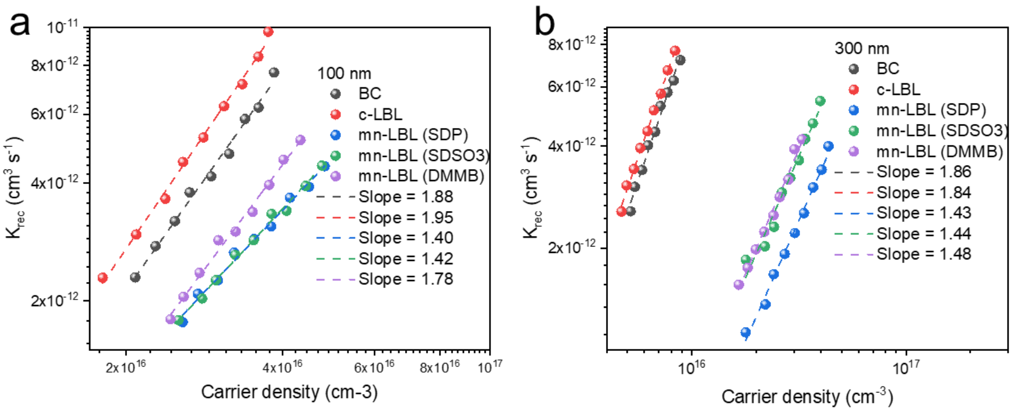

Figure S26. Bimolecular recombination rate constant (Krec) as a function of carrier density of mn-LBL PM6:L8-BO devices prepared by various surfactants with a thickness of (a) 100 nm and (c) 300 nm, respectively.

Table S10. Summary of calculated device physics parameters of PM6:L8-BO-based binary OSCs with different HTLs.

Thickness	Active layer	μ^a ($cm^2 V^{-1}s^{-1}$)	τ^b (μs)	$t_S{}^c$ (μs)	$K_{rec}{}^d$ ($cm^3 s^{-1}$)	n^e (cm^{-3})	$L_S{}^f$ (nm)
100 nm	BC	1.03×10^{-4}	5.08	0.36	2.30×10^{-12}	2.08×10^{16}	10.11
	c-LBL	9.09×10^{-5}	5.35	0.37	2.29×10^{-12}	1.80×10^{16}	10.21
	mn-LBL (SDP)	1.34×10^{-4}	6.88	0.34	1.76×10^{-12}	2.57×10^{16}	8.33
	mn-LBL (SDSO3)	1.29×10^{-4}	5.94	0.35	1.78×10^{-12}	2.52×10^{16}	8.62
	mn-LBL (DMMB)	1.12×10^{-4}	5.94	0.35	1.79×10^{-12}	2.43×10^{16}	9.38
300 nm	BC	8.86×10^{-5}	6.28	0.37	2.57×10^{-12}	5.17×10^{15}	51.16
	c-LBL	8.55×10^{-5}	6.67	0.36	2.56×10^{-12}	4.69×10^{15}	52.01
	mn-LBL (SDP)	1.12×10^{-4}	8.91	0.34	1.13×10^{-12}	1.78×10^{16}	44.53
	mn-LBL (SDSO3)	9.99×10^{-5}	8.54	0.35	1.85×10^{-12}	1.79×10^{16}	45.49
	mn-LBL (DMMB)	9.49×10^{-5}	8.16	0.35	1.56×10^{-12}	1.66×10^{16}	48.26

[a] Carrier mobility values from phto-CELIV measurements. [b] Charge carrier lifetime from TPV measurement, [c] sweeping out time from TPC measurement. [d] Bimolecular recombination rate constant. [e] Charge carrier density. [f] The width of the space-charge region from Mott-Schottky analysis.

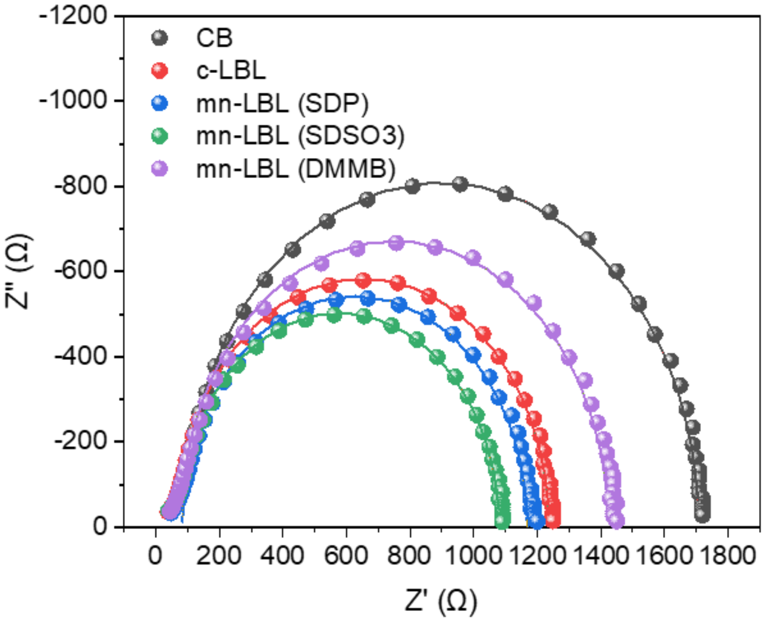

Figure S27. Nyquist plots of mn-LBL PM6:L8-BO devices prepared by various surfactants with a thickness of (a) 100 nm

Table S11. Fitting parameters for OPVs from Nyquist plots.

PM6 percentage in HTL	Rs (Ω)	Rp (Ω)	C_1 (nF)
BC	88.59	1619	12.41
c-LBL	83.52	1085	13.95
mn-LBL (SDP)	69.34	1167	12.46
mn-LBL (SDSO3)	74.37	1005	12.35
mn-LBL (DMMB)	77.83	1345	9.90

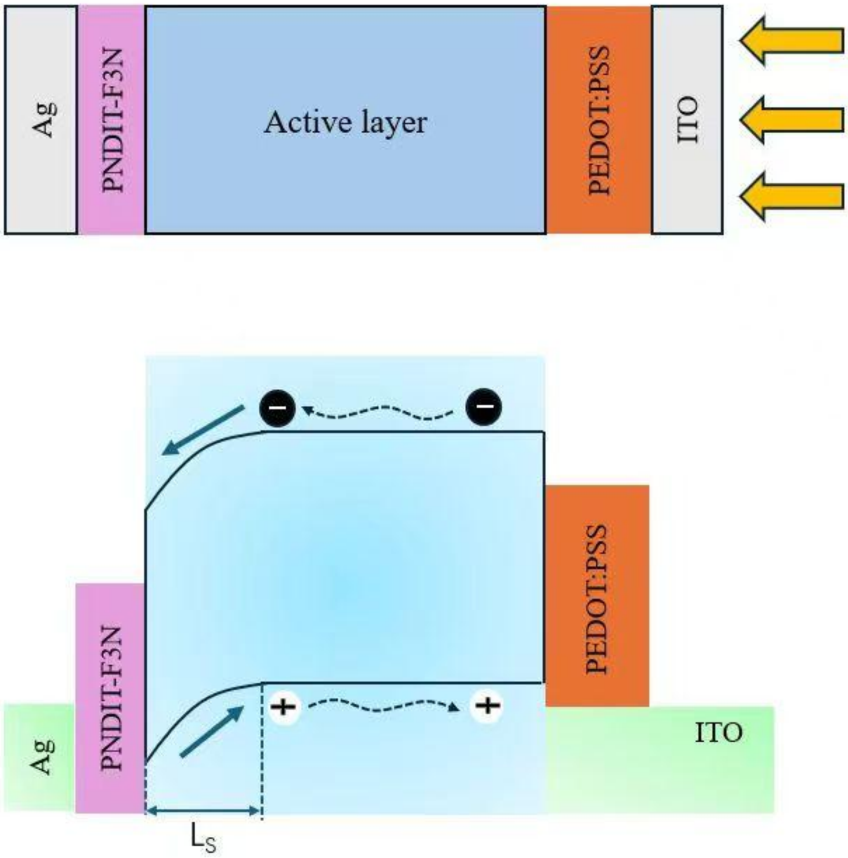

Figure S28. Device structure (top) and schematic illustration of energy bands in the active layer (bottom)

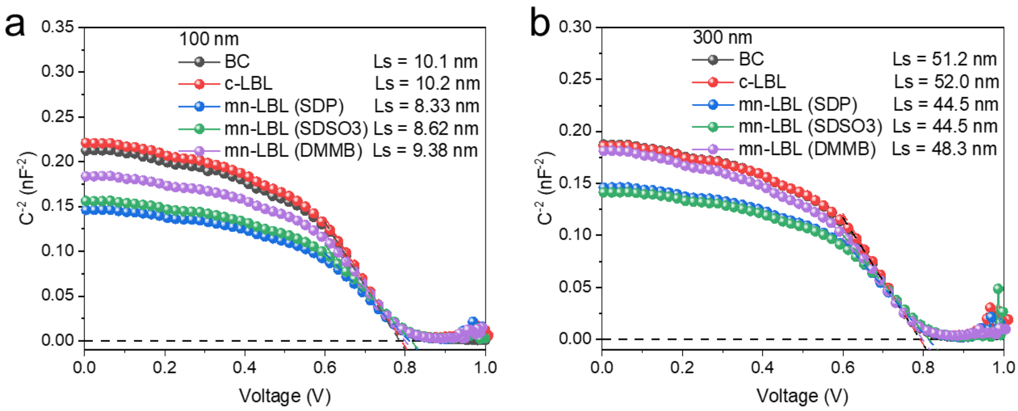

Figure S29. Mott-Schottky plots of mn-LBL PM6:L8-BO devices prepared by various surfactants with a thickness of (a) 100 nm and (c) 300 nm, respectively.

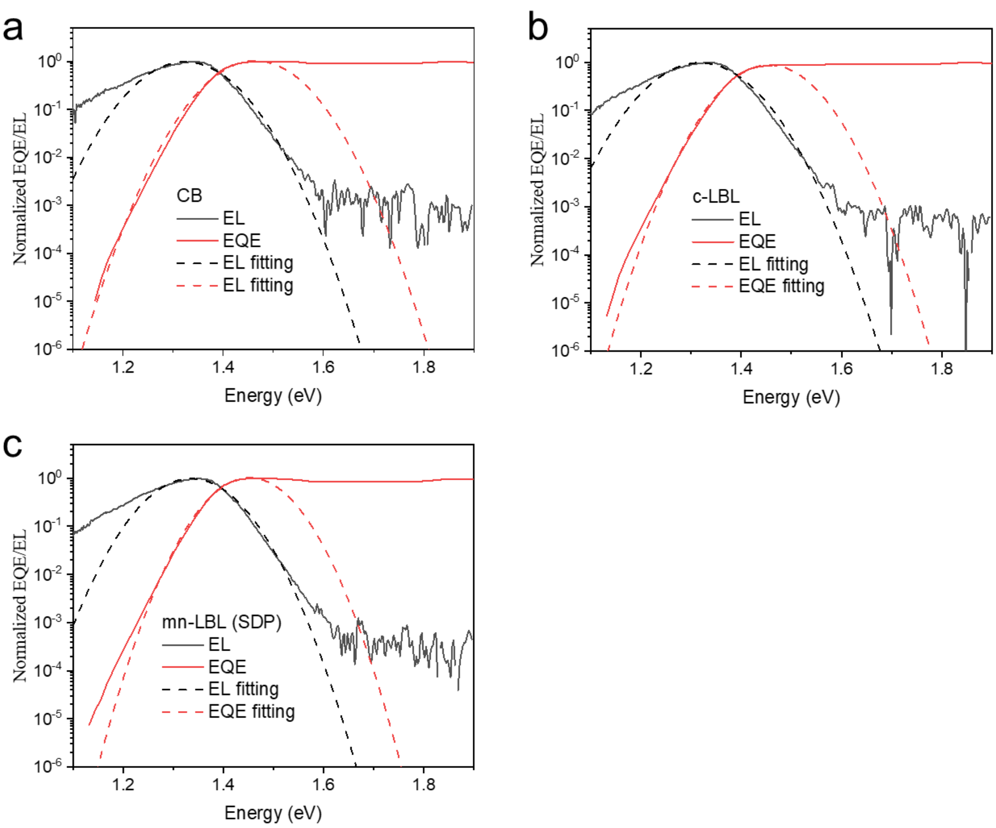

Figure S30. FTPS-EQE and EL spectra of of mn-LBL PM6:L8-BO devices prepared by various surfactants with a thickness of (a) 100 nm

Table S12. Summary of energy loss data of PM6:L8-BO devices with different HTL

HTL	Eg (eV)	$qV_{OC,SQ}$ (eV)	$qV_{OC,Rad}$ (eV)	EQE_{EL} ($\times10^{-4}$)	ΔE_1 (eV)	ΔE_2 (eV)	ΔE_3 (eV)	E_{loss} (eV)
BC	1.446	1.158	1.104	1.380	0.288	0.054	0.228	0.570
c-LBL	1.446	1.160	1.106	1.502	0.286	0.054	0.226	0.566
mn-LBL (SDP)	1.446	1.165	1.115	2.367	0.281	0.051	0.215	0.546

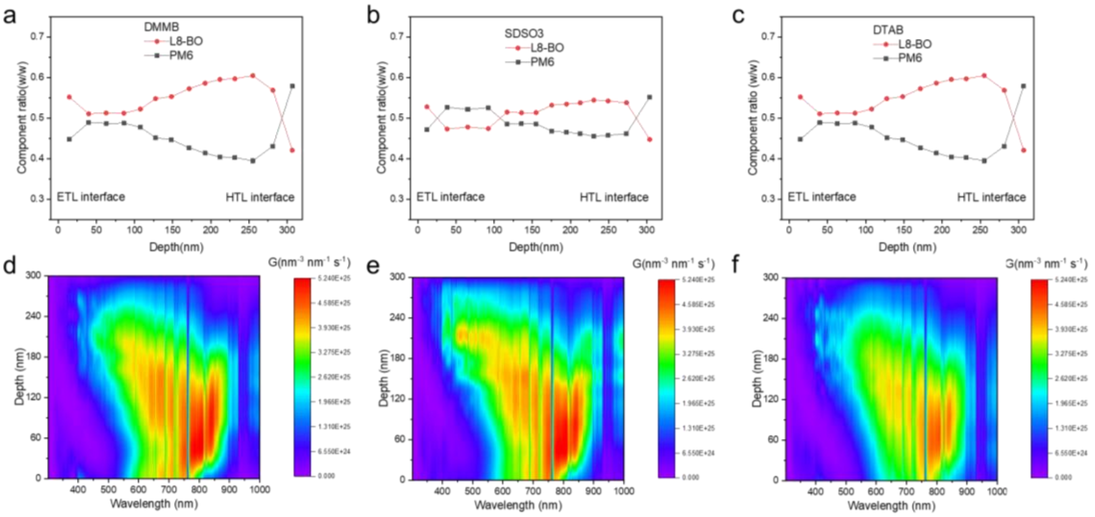

Figure S31. (a, b, c) Composition ratio in the vertical direction and (d, e, f) exciton generation contours of the PM6:L8-BO mn-LBL films with (a, d) DMMB, (b, e) SDSO3 and (c, f) DTAB as surfactant.

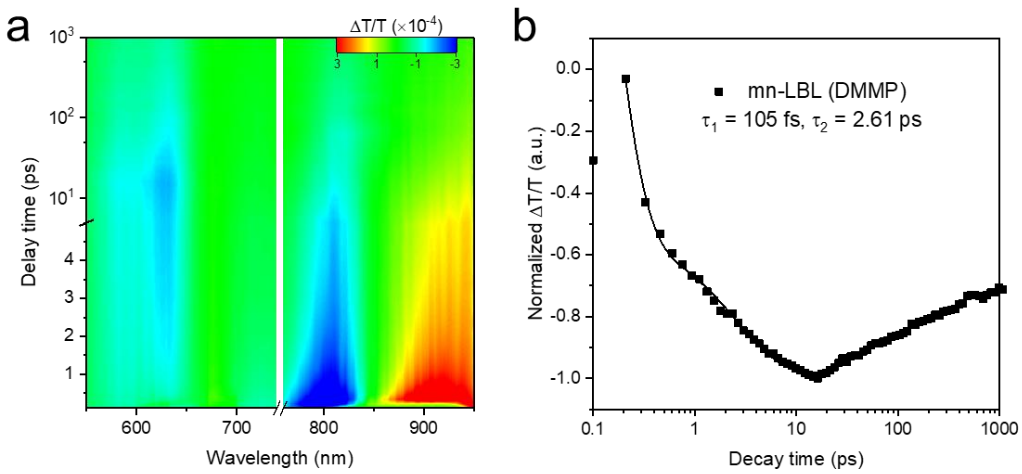

Figure S32. 2D fs-TA contour and decay dynamics probed at 625 nm of PM6:L8-BO films processed by mn-LBL (DMMB) techniques.

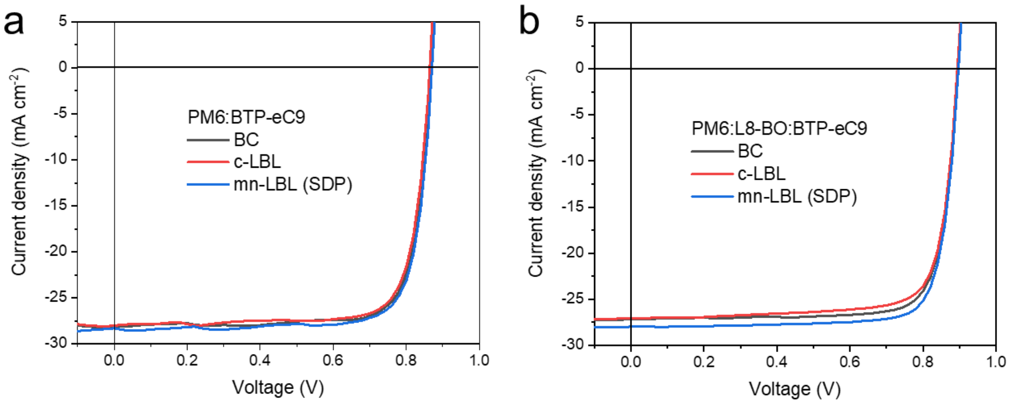

Figure S33. J-V curves of (a) PM6:BTP-eC9 and PM6:L8-BO:BTP-eC9 devices prepared by different processing strategies with a thickness of 100 nm.

Table S13. Summary of photovoltaic parameters of toluene processed solar cells with different active layer materials.

Active layer	Processing method	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE[a] (%)
PM6:BTP-eC9	BC	0.864	28.09	79.14	19.20 (18.98 ± 0.22)
	c-LBL	0.862	27.89	78.91	18.97 (18.86 ± 0.11)
	mn-LBL[b]	0.868	28.26	79.40	19.47 (19.18 ± 0.29)
PM6:L8-BO-BTP-eC9	BC	0.893	27.18	79.99	19.42 (19.25 ± 0.17)
	c-LBL	0.891	27.05	78.54	18.94 (18.68 ± 0.26)
	mn-LBL[b]	0.895	27.98	80.86	20.30 (20.00 ± 0.31)

[a] Average values with standard deviation were obtained from 20 devices;

[b] Processed from PM6 NPs with SDP as surfactant.

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CNAS L0641

210220110107

检 测 报 告

Test Report

报告编号：
Report No. JLY20250078W

样 品 名 称 Sample Name	L8-X
委 托 单 位 Name of Client	深圳技术大学
生产单位 Manufacturer	深圳技术大学

天津市计量监督检测科学研究院
Tianjin Institute of Metrological Supervision and Testing

Figure S34. First page of the certification report of PM6:L8-BO:BTP-eC9 device with a thickness of 100 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.

注 意 事 项

Attention

1. 检测报告和骑缝处未加盖“检验检测专用章”无效。
   The report is invalid without test report special stamp in report and the riding seam.

2. 检测只对来样及当时状态负责。
   The report just be responsible for the sample and Status at the time.

3. 检测报告无编制、审核、批准人员签字无效
   The report is invalid without signature of the compile, censor and approver.

4. 检测报告涂改无效。
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Figure S35. Second page of the certification report of PM6:L8-BO:BTP-eC9 device with a thickness of 100 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.

天津市计量监督检测科学研究院

Tianjin Institute of Metrological Supervision and Testing

检测报告

Test Report

报告编号：JLY20250078W 共 4 页 第 1 页

Report No. Page No. 4-1

样品名称 Sample Name	L8-X				
规格型号 Specification Type	N1	商标/出厂编号 Brand/Serial Number	/ 001	生产日期/批号 Produce Date/ Serial Number	/
样品等级 Sample Grade	/	样品描述 Sample Description	外观良好，无明显可见缺陷	样品接收时间 Sample receive time	2025-01-16
委托日期 Delivery Date	2025-01-16	送样人员 Delivered by	谢谌	样品数量 Sample Quantity	1块
委托单位名称及联系电话 Name of Client	深圳技术大学/18079428696				
生产单位名称 Manufacturer	深圳技术大学				
检测时间 Test Time	2025-01-16	检测地点 Test Location	本院五号堤路院区光伏产业计量部106室	检测环境 Test Condition	温度：25.2℃ 相对湿度：21.6%
检测依据 Test Standard	IEC 60904-1:2020《光伏器件 第1部分：光伏电流-电压特性的测量》				
检测结论 Test Conclusion	/ （检验检测专用章）（Stamp of Test Institution） 签发日期：2025-01-23 Issue Date: Y M D				
备注 Remark	/				

编制：Compiled by 审核：Checked by 批准：Approved by

Figure S36. Third page of the certification report of PM6:L8-BO:BTP-eC9 device with a thickness of 100 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.

天津市计量监督检测科学研究院

Tianjin Institute of Metrological Supervision and Testing

检测报告

Test Report

报告编号：JLY20250078W 共 4 页 第 2 页

Report No. Page No.4-2

检 测 仪 器 设 备					
序号 No.	仪器设备名称 Instrument	型号/规格 Type	设备编号 Instrument No.	证书有效期 Expiry Date	证书编号 Certificate No.
1	电池片 I-V 测试系统 I-V measurement system for solar cell	VS-6831S	21VJ002	2025.08.16	CGFg124070291

Figure S37. Fourth page of the certification report of PM6:L8-BO:BTP-eC9 device with a thickness of 100 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.

天津市计量监督检测科学研究院

Tianjin Institute of Metrological Supervision and Testing

检测报告

Test Report

报告编号：JLY20250078W　　　　共 4 页　第 3 页

Report No.　　　　Page No.4-3

受 检 样 品 信 息

样品编号 Sample Number	规格型号 Sample Type	产品编号 Product No.	产品序列号 Serial Number
20250078-1	N1	001	—

Figure S38. Fifth page of the certification report of PM6:L8-BO:BTP-eC9 device with a thickness of 100 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.

天津市计量监督检测科学研究院

Tianjin Institute of Metrological Supervision and Testing

检测报告

Test Report

报告编号：JLY20250078W　　　　共 4 页　第 4 页

Report No.　　　　Page No.4-4

检 测 项 目 及 结 果

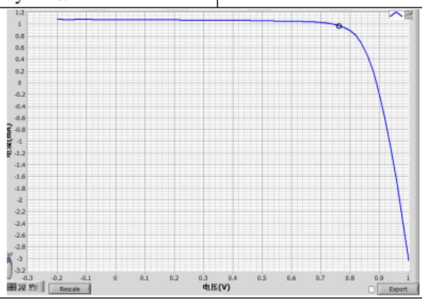
测试时间 Date	2025.01.16							
测试条件 Condition	使用稳态 AAA 级太阳模拟器，在 AM1.5G，1000W/m^2，25.0℃条件下测试 Sample was tested under the condition of AM1.5G, 1000W/m^2, 25.0℃ with a steady-state class calibrated AAA solar simulator							
有效面积 Active area	0. 0382cm^2 备注：器件的有效面积是由带固定孔径的薄金属掩膜板量化，由客户提供。 Remark: Designated area defined by thin metal aperture mask , provided by the customer.							
样品编号 №	V_{oc} (V)	I_{sc} (mA)	J_{sc} (mA/cm^2)	P_{max} (mW)	V_{Pmax} (V)	I_{Pmax} (mA)	FF (%)	η (%)
20250078-1	0.890	1.060	27.78	0.758	0.763	0.993	80.35	19.86
测试程序 Test program settings	起始电压： Starting voltage:				-0.2V			
	终止电压： Termination voltage:				+1.0V			
	扫描间隔： Scan interval:				0.02V			
	延迟时间： Delay time:				0.02s			
I-*V* 曲线图 *I*-*V* curve								
备注 Remark	—							

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Figure S39. Sixth page of the certification report of PM6:L8-BO:BTP-eC9 device with a thickness of 100 nm from the Tianjin Institute of Metrological Supervision and Testing Electronic & Instrumental Laboratory.

References

[1] T. Lu, F. Chen, *J. Comput. Chem.* **2012**, *33*, 580.
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[4] L. Bu, S. Gao, W. Wang, L. Zhou, S. Feng, X. Chen, D. Yu, S. Li, G. Lu, *Adv. Electron. Mater.* **2016**, *2*, 1600359.
[5] X. Feng, Y. Wang, T. Xiao, Z. Shen, Y. Ren, G. Lu, L. Bu, *Front. Chem.* **2020**, *8*, 1.