Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.
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Supporting Information

Evolution of Morphology and Open-circuit Voltage in Alloy-Energy Transfer Coexisted Ternary Organic Solar Cells

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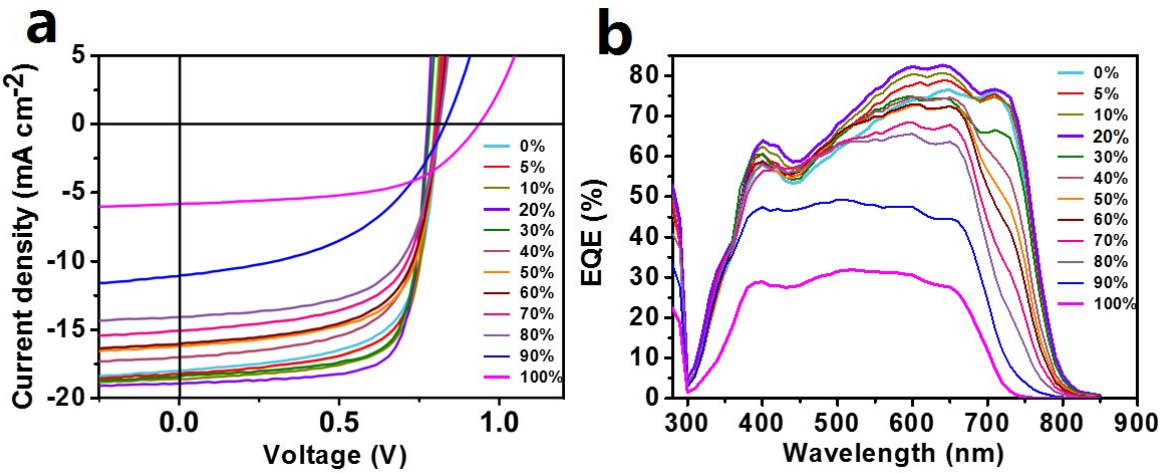

Figure S1. a) *J–V* curves of ternary organic solar cells with different weight ratios of PDT2FBT-ID under AM 1.5 G illumination (100 mW cm^{-2}). b) The corresponding EQE spectra of ternary organic solar cells.

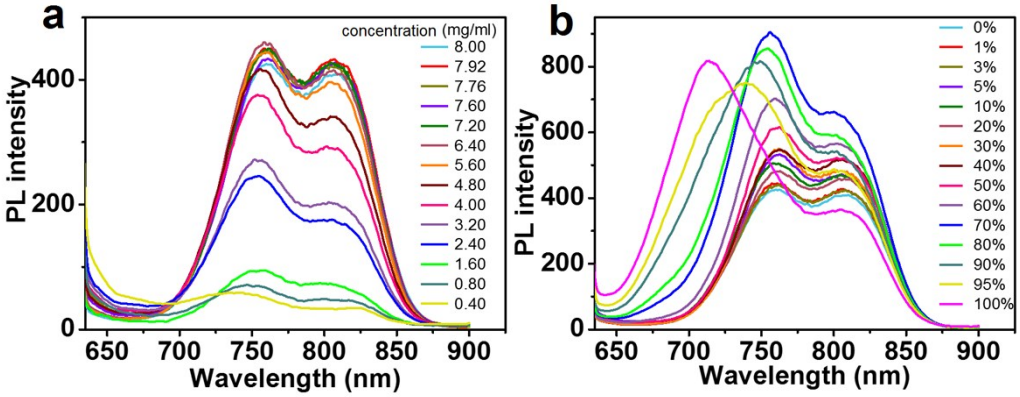

Figure S2. The photoluminescence properties of a) Referenced neat PTB7-Th films obtained from CB solution with different concentration. b) PTB7-Th/PDT2FBT-ID blend films obtained from CB solution with different doping ratio of PDT2FBT-ID, and the total concentration of PTB7-Th/PDT2FBT-ID is 8 mg/ml.

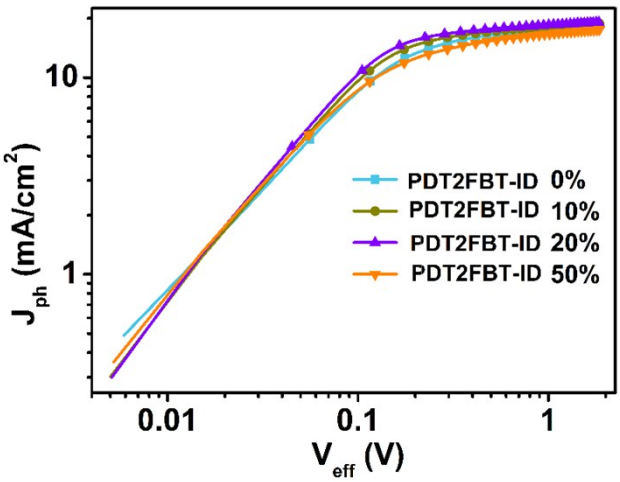

Figure S3. Photocurrent density (J_{ph}) versus effective voltage (V_{eff}).

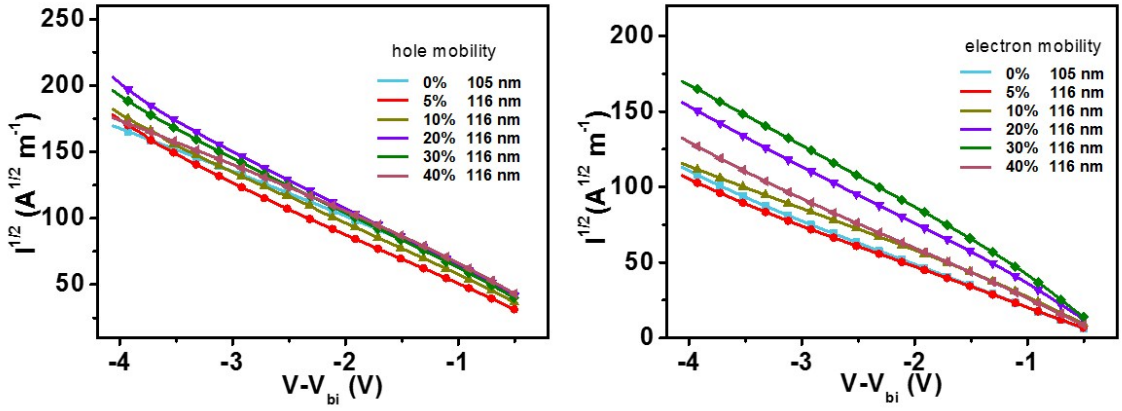

Figure S4. SCLC measured $J^{1/2}$—V-V_{bi} curves under dark condition for ternary active layers with different weight ratios of PDT2FBT-ID in CB solution, a) hole-only devices and b) electron-only devices.

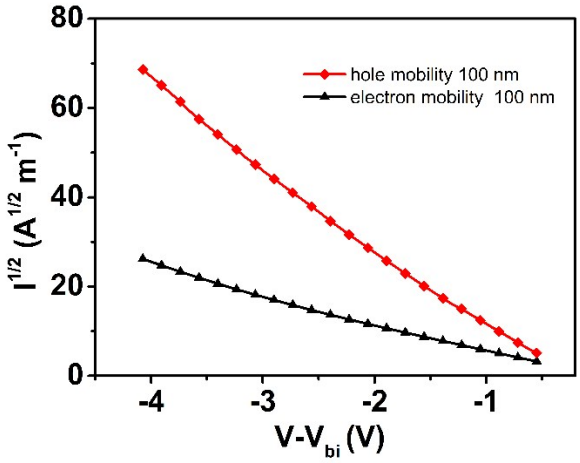

Figure S5. Hole and electron mobility of PDT2FBT-ID/$PC_{71}BM$ blend films from chloroform solution.

Table S1. Photovoltaic parameters of PTB7-Th:$PC_{71}BM$ binary and PTB7-Th: PDT2FBT-ID:$PC_{71}BM$ ternary organic solar cells with different D:A ratios under AM 1.5G illumination (100 mW/cm^2). Remarkably, the ternary devices shown good stability. The best PCEs could maintain 85%-90% in atmosphere environment without encapsulation after three days.

PTB7-Th: PDT2FBT-ID:$PC_{71}BM$	J_{sc} [mA cm^{-2}]	V_{oc} [V]	FF [%]	PCE_{max} (PCE_{ave})[a] [%]
100:0:100	16.69	0.792	61.73	9.07 (9.02)
100:0:130	17.04	0.783	68.28	10.12 (10.0)
100:0:150	16.48	0.789	71.52	10.32 (10.18)
100:0:170	16.1	0.778	70.79	9.86 (9.80)
80:20:100	16.83	0.775	74.20	10.75 (10.67)
80:20:120	16.74	0.765	74.97	10.77 (10.69)
80:20:130	17.20	0.762	74.07	10.76 (10.66)
80:20:140	16.65	0.750	72.48	10.61 (10.46)
80:20:150	16.88	0.756	73.82	10.43 (10.31)
80:20:170	15.94	0.753	75.63	10.08 (10.00)

[a] The average PCE is obtained from over 4-8 devices.

Table S2. Mobility parameters of ternary organic solar cells with different weight ratios of PDT2FBT-ID.

	0%	5%	10%	20%	30%	40%	100%
μ_h(cm^2 V^{-1} s^{-1})	4.78×10^{-4}	8.22×10^{-4}	8.18×10^{-4}	1.05×10^{-3}	9.38×10^{-4}	6.97×10^{-4}	1.09×10^{-4}
μ_e(cm^2 V^{-1} s^{-1})	3.35×10^{-4}	4.00×10^{-4}	4.43×10^{-4}	7.99×10^{-4}	9.52×10^{-4}	6.00×10^{-3}	1.36×10^{-5}

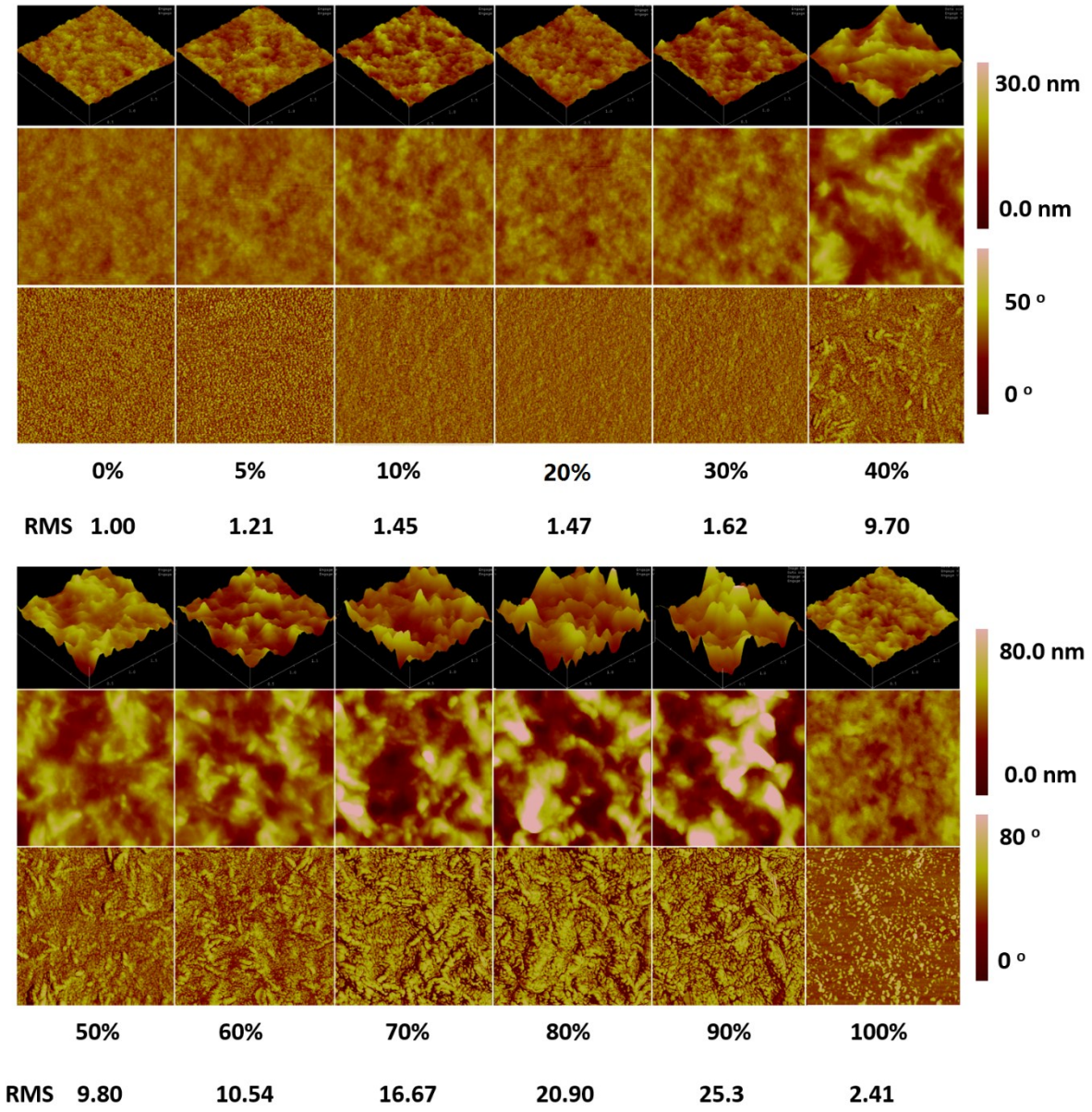

Figure S6. AFM topography images and phase images obtained in tapping mode of PTB7-Th:PDT2FBT-ID:$PC_{71}BM$ blend films with various weight ratio of PDT2FBT-ID.

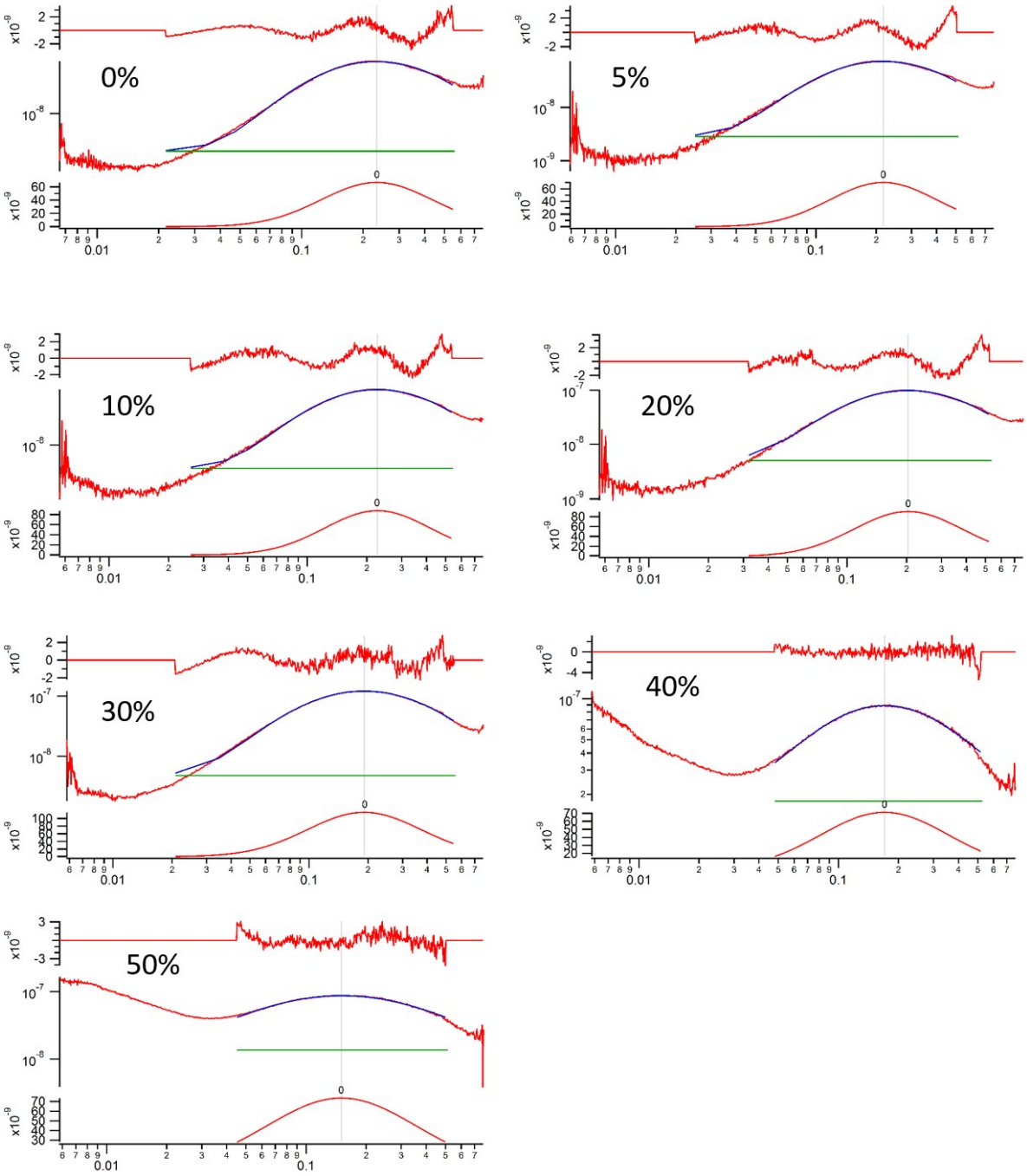

Figure S7. Fitting peaks of RSoXS with different weight ratios of PDT2FBT-ID.

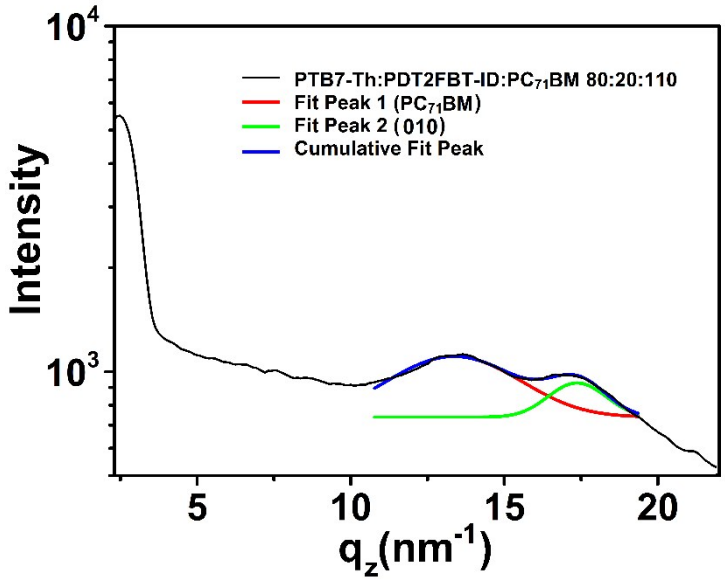

Figure S8. An example of Gaussian fitting for out-of-plane cut. The π-π stacking distance and the FWHM of the π-π stacking peak (010) were obtained from the fitting.

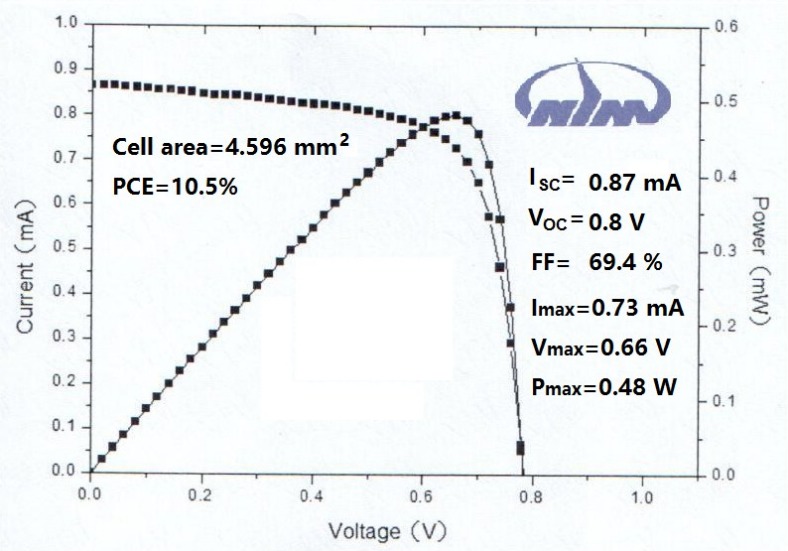

Figure S9. I-V curve and Power-V curve for certification.

中 国 计 量 科 学 研 究 院

校 准 证 书
Calibration Certificate

证书编号 GXtc2016-0895
Certificate No.

客户名称 Client	国家纳米中心 National Center for Nanoscience and Technology (NCNST)
器具名称 Instrument	三元有机太阳电池 (Tenary organic Solar Cells)
型号/规格 Type/Model	/
出厂编号 Serial No.	D6-2
生产厂家 Manufacturer	/
客户地址 Address	国家纳米中心 National Center for Nanoscience and Technology (NCNST)
校准日期 Date of calibration	2016-05-18

批准人：
Approved by

中国计量科学研究院 2 校准专用章

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证书编号 GXtc2016-0895
Certificate No.

中国计量科学研究院是国家最高的计量科学研究中心和国家级法定计量技术机构。1999 年授权签署了国际计量委员会（CIPM）《国家计量基(标)准和国家计量院签发的校准与测量证书互认协议》（CIPM MRA）。The National Institute of Metrology (NIM) is China's national metrology institute (NMI) and a state-level legal metrology institute. NIM is China's signatory to the Mutual Recognition of National Measurement Standards and of Calibration and Measurement Certificates Issued by National Metrology Institutes (CIPM MRA) which is arranged by the International Committee of Weights and Measures (CIPM).

中国计量科学研究院的质量管理体系符合 ISO/IEC17025 标准，通过中国合格评定国家认可委员会和亚太计量规划组织（APMP）联合评审的校准和测量能力（CMCs）在国际计量局（BIPM）关键比对数据库中公布。NIM's quality management system meets requirements of the ISO/IEC 17025. Its Calibration and Measurement Capabilities (CMCs) that are peer reviewed both by China National Accreditation Service for Conformity Assessment (CNAS) and the Asia Pacific Metrology Programme (APMP) are published in the International Bureau of Weights and Measures (BIPM) Key Comparison Database (KCDB).

2011 年，中国计量科学研究院和中国合格评定国家认可委员会就认可领域的技术评价活动签署了谅解备忘录，承认中国计量科学研究院的计量支撑作用和出具的校准/检测结果的溯源效力。NIM and CNAS signed a Memorandum of Understanding (MOU) for Recognition of Technical Assessment in Laboratory Accreditation Field in 2011, in which CNAS recognizing the technical supporting role of NIM in laboratory accreditation and the traceability of NIM's calibration / test results.

校准结果不确定度的评估和表述均符合 JJF1059 系列标准的要求。The evaluation and expression of uncertainty of the calibration results are in line with the requirements of JJF1059 series standards.

校准所依据的技术文件（代号、名称）Reference documents (Code,Name)

Measurement of photovoltaic current-voltage characteristics（IEC60904-1）

太阳电池校准规范：光电性能（NIM-ZY-GX-TT-402）(Calibration Specification of Solar Cells：Photoelectric Properties)

校准环境条件及地点 Calibration place and environment

温　度 Temperature：25　℃　　地　点 Location：光学楼 110 室

湿　度 Humidity：45　%RH　其　它 Others：/

校准使用的计量基（标）准装置(含标准物质)/主要仪器

Reference Standards（Including the Reference Material）/ Instruments used

名　称 Name	测量范围 Measurement Range	不确定度/准确度等级 Uncertainty/Accuracy	证书编号 Certificate No.	证书有效期至 Due Date (YYYY-MM-DD)
太阳电池光电性能校准装置 Measurement Standard	I_{sc}:（0.1-10）A V_{oc}: (0.1-200)V P_m:(0.01-500) W	I_{sc}: 1.5%（k=2） V_{oc}: 0.5% (k=2) P_m:1.6% (k=2)	[2015]国量标计证字第 286 号	2019-07-05
KG5-标准太阳电池 KG5-Reference	I_{sc}:（0-200）mA	1.2% (k=2)	GXtc2016-0080	2017-02-26

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证书编号 GXtc2016-0895
Certificate No.

校 准 结 果
Calibration Results

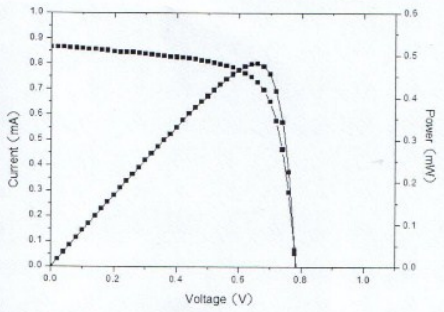
1. 校准条件 Calibration Conditions:

标准太阳电池：KG5-单晶硅；
Reference Solar Cell: KG5 filterd mono-Si;
标准太阳电池的标定值：38.9 mA；
CV of Reference Solar Cell：38.9 mA；
太阳模拟器等级：AAA 级；
Solar Simulator Classification：AAA 级；
温度传感器/控制系统：无。
Teperature Sensor/Control System: None。
扫描方向：正扫
Scan Direction: Forward

2. I-V 特性参数 I-V Characteristic parameters:

以上述标准太阳电池标定太阳模拟器辐照度至 1000 W/m^2，校准被测太阳电池的 I-V 特性曲线和参数如下：

By using the above reference solar cell to calibrate the solar simulator's irradiance to 1000 W/m^2, the I-V characterisitc curve and parameters as follows:



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证书编号 GXtc2016-0895
Certificate No.

校准结果
Calibration Results

有效面积 (mm^2)	短路电流 I_{sc}(mA)	开路电压 V_{oc}(V)	最大功率 P_{max}(mW)
4.596	0.87	0.80	0.48

最大功率电流 I_{max}(mA)	最大功率电压 V_{max}(V)	填充因子 FF (%)	转换效率 (PCE) η (%)
0.73	0.66	69.4	10.5

不确定度描述 Uncertainty:
I_{sc}：1.8%（k=2）； V_{oc}：1.2%（k=2）； P_{max}：2.2%（k=2）。

注 Note:
1. 太阳电池的有效面积为 4.596 mm^2（证书编号：CDjc2016-3318）。
The certificated cell area is 4.596mm^2 (Certificate No.: CDjc2016-3318).
2. 此数据仅对被测样品当时状态有效。
The data apply only at the time of the test for the sample.

建议 Suggestion:
根据客户要求和校准文件的规定，通常情况下 12 个月校准一次。
According to the client or the calibration documents, the recommended calibration cycle is 12 months.

声明 Statement:
1.我院仅对加盖“中国计量科学研究院校准专用章”的完整证书负责。
NIM is ONLY responsible for the complete certificate with the calibration stamp of NIM.
2.本证书的校准结果仅对所校准的计量器具有效。
The certificate is ONLY valid for the calibrated instrument.
3.本证书用中英文两种语言表达，准确含义以中文为准。
The certificate is reported in both English and Chinese, with the Chinese version as standard.

校准员： 核验员：

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Figure S10. Detail information of certification.