

## Supporting Information

### **Heterojunction Lithiation Engineering and Diffusion-Induced Defects Passivation for Highly Efficient Sb<sub>2</sub>(S,Se)<sub>3</sub> Solar Cells**

*Cong Liu,<sup>\*a</sup> Anweng Gong,<sup>a</sup> Chen Zuo,<sup>a</sup> Tao Liu,<sup>\*a</sup> Xiaoyang Liang,<sup>b</sup> Donglou Ren,<sup>a</sup> Kai Shen,<sup>c</sup> Jianzha Zheng,<sup>d</sup> Qifan Xue,<sup>e</sup> Zhiqiang Li,<sup>b</sup> Ruud E.I. Schropp,<sup>c</sup> Bingsuo Zou,<sup>\*a</sup> and Yaohua Mai<sup>\*c</sup>*

<sup>a</sup> State Key Laboratory of Featured Metal Materials and Life-cycle Safety for Composite Structures, School of Resources, Environment and Materials, Guangxi University, Nanning 530004, China

<sup>b</sup> National-Local Joint Engineering Laboratory of New Energy Photoelectric Devices, College of Physics Science and Technology, Hebei University, Baoding 071002, China

<sup>c</sup> Institute of New Energy Technology, College of Information Science and Technology, Jinan University, Guangzhou 510632, China

<sup>d</sup> Institute of Applied Physics and Materials Engineering, University of Macau, Macao, Macao SAR 999078, China

<sup>e</sup> State Key Laboratory of Luminescent Materials and Devices, Institute of Polymer Optoelectronic Materials and Devices, School of Materials Science and Engineering, South China University of Technology, Guangzhou 510640, China

\* E-mail: [congliu@gxu.edu.cn](mailto:congliu@gxu.edu.cn) (Cong Liu); [liutaozhx@gxu.edu.cn](mailto:liutaozhx@gxu.edu.cn) (Tao Liu); [zoubs@gxu.edu.cn](mailto:zoubs@gxu.edu.cn) (Bingsuo Zou); [yaohuamai@jnu.edu.cn](mailto:yaohuamai@jnu.edu.cn) (Yaohua Mai)

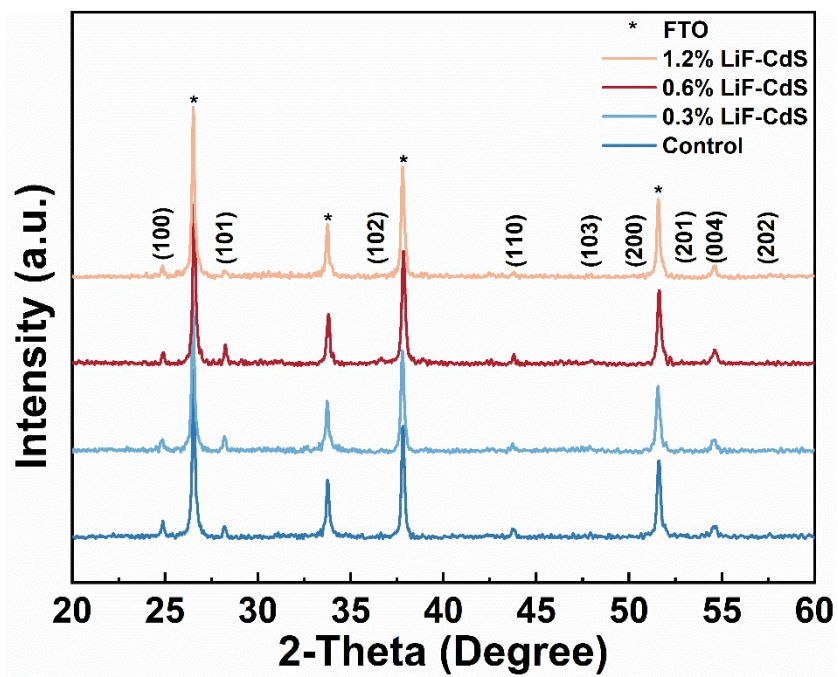
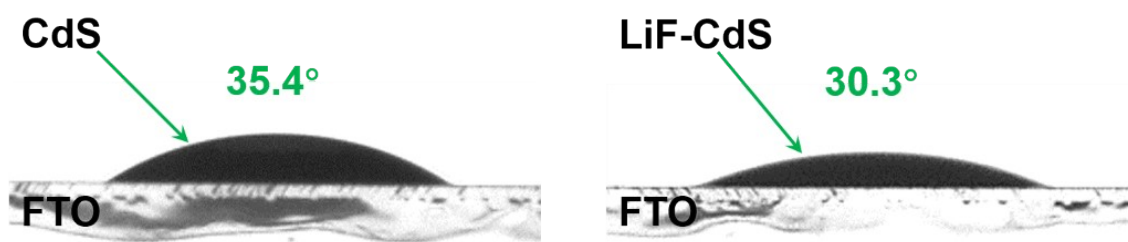
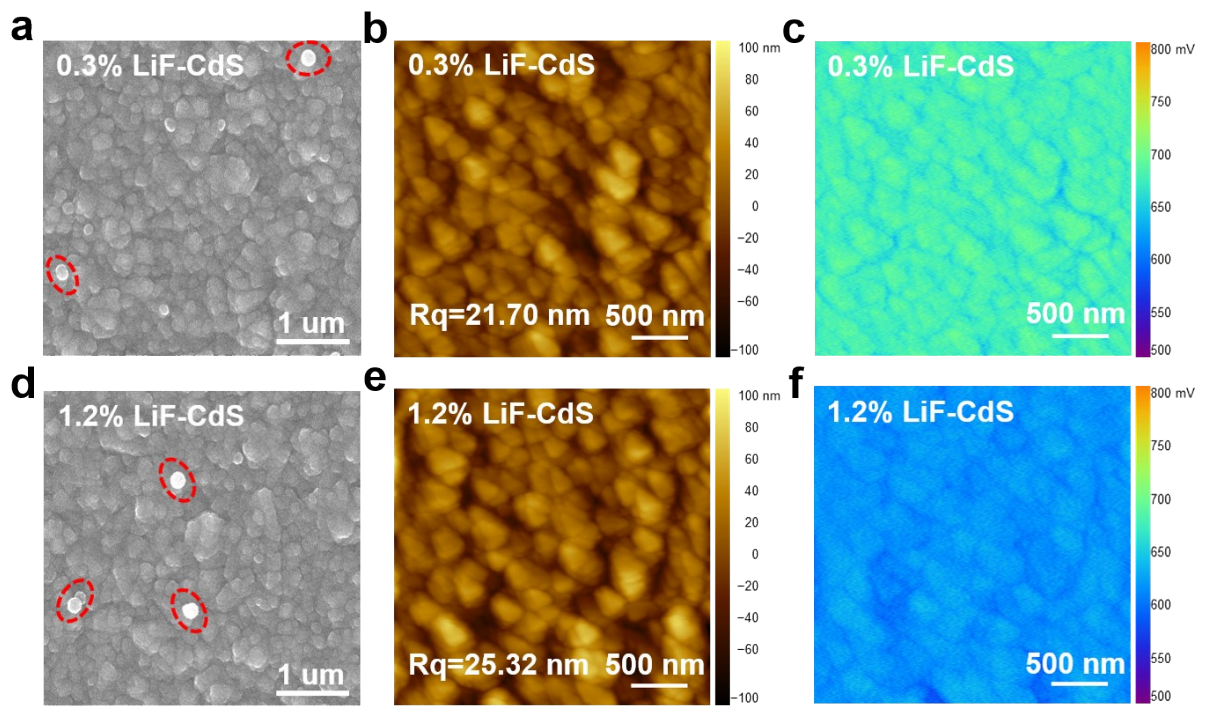


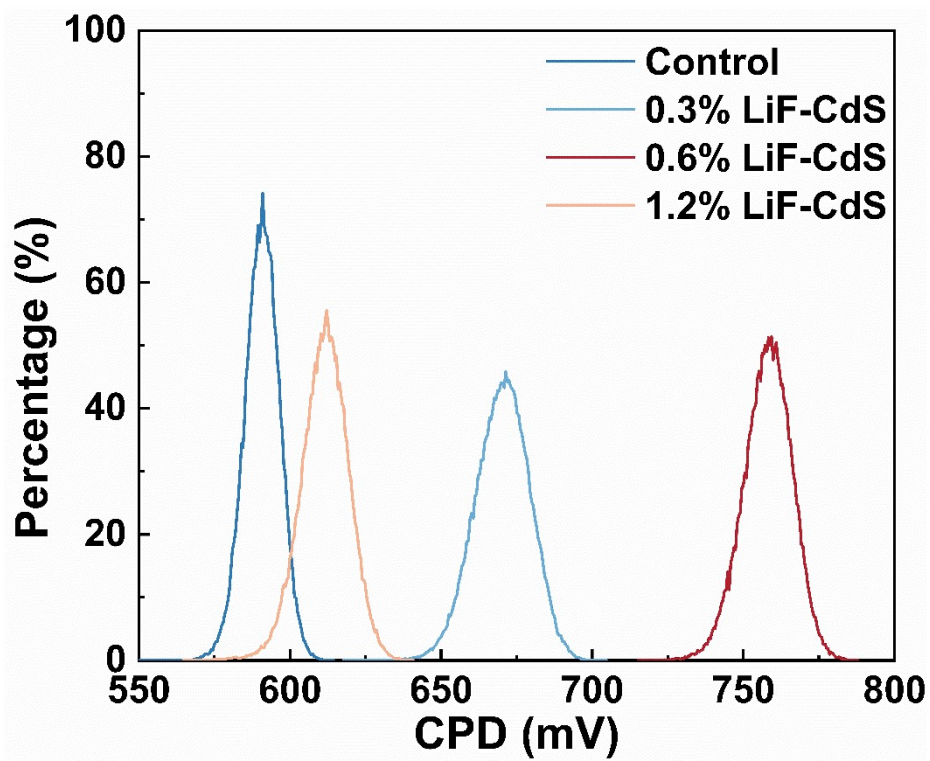
Fig. S1 XRD patterns of control, 0.3% LiF-CdS, 0.6% LiF-CdS and 1.2% LiF-CdS films.



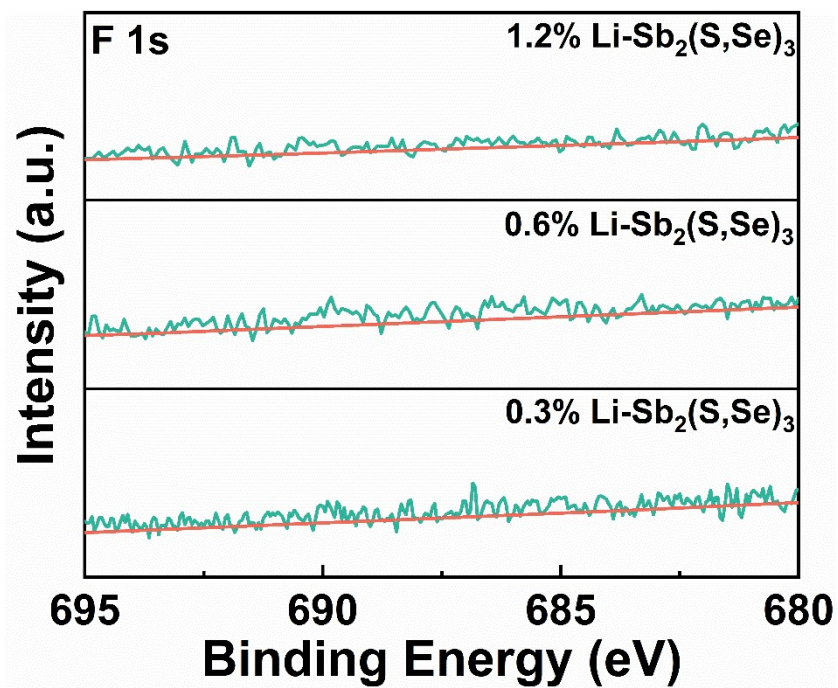
**Fig. S2** Contact angle measurements of FTO substrates with pure CdS and LiF-CdS solutions.



**Fig. S3** Surface morphology and potential characterization of CdS films. (a, d) SEM, (b, e) AFM, (c, f) KPFM of the 0.3% LiF-CdS and 1.2% LiF-CdS films, respectively.



**Fig. S4** Surface contact potential difference of control, 0.3% LiF-CdS, 0.6% LiF-CdS and 1.2% LiF-CdS films.



**Fig. S5** F 1s XPS spectra of 0.3%, 0.6% and 1.2% Li-Sb<sub>2</sub>(S,Se)<sub>3</sub> films.

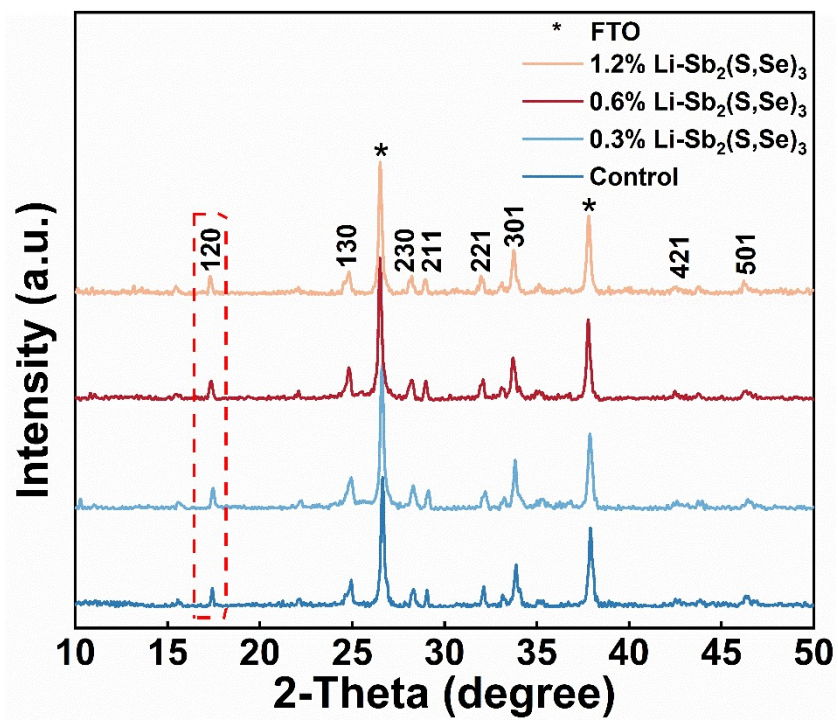
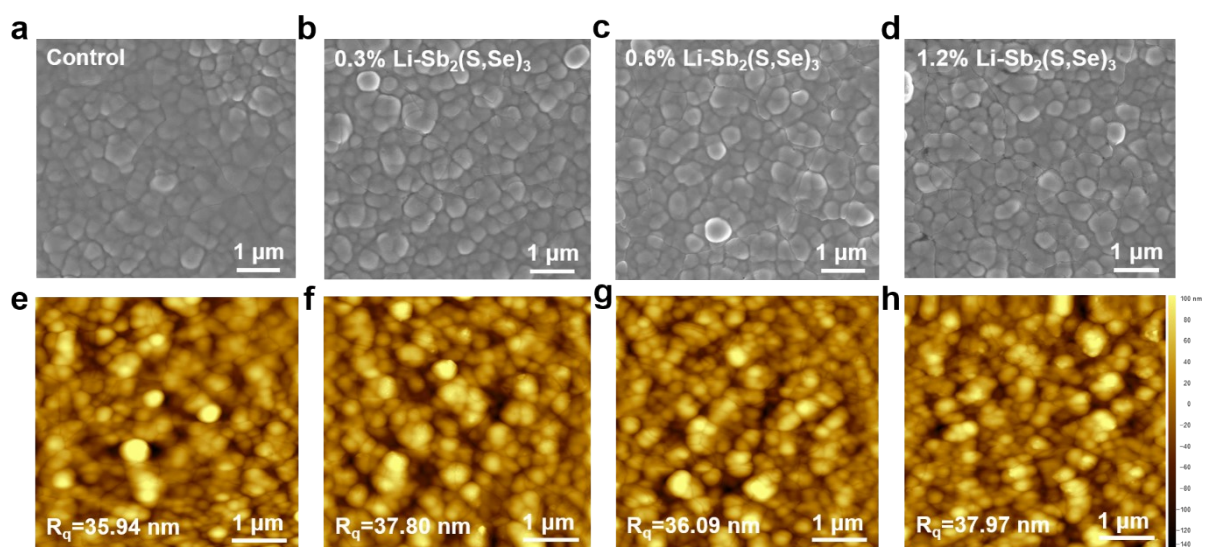


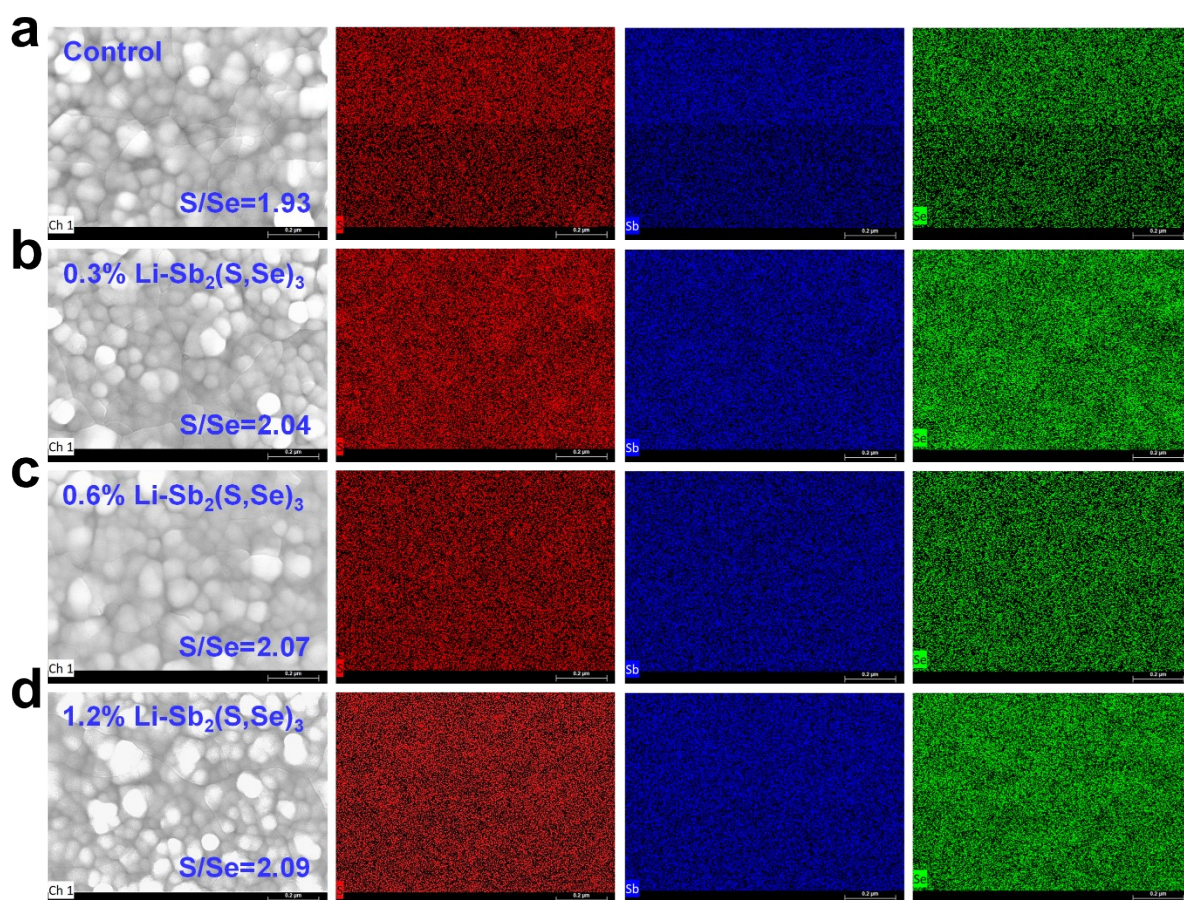
Fig. S6 XRD patterns of the control, 0.3%, 0.6% and 1.2% Li-Sb<sub>2</sub>(S,Se)<sub>3</sub> films.



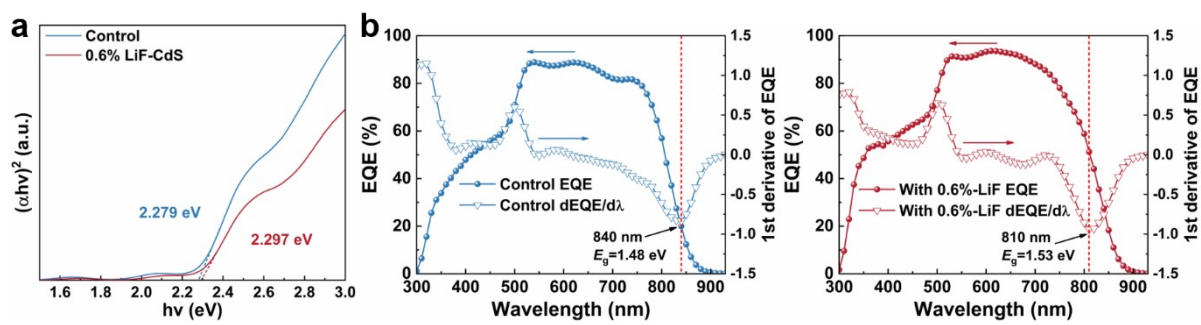


**Fig. S7** Surface morphology and AFM images of  $\text{Sb}_2(\text{S,Se})_3$  films. (a-d) SEM and (e-h) AFM of the control, 0.3%, 0.6% and 1.2%  $\text{Li-Sb}_2(\text{S,Se})_3$  films, respectively.

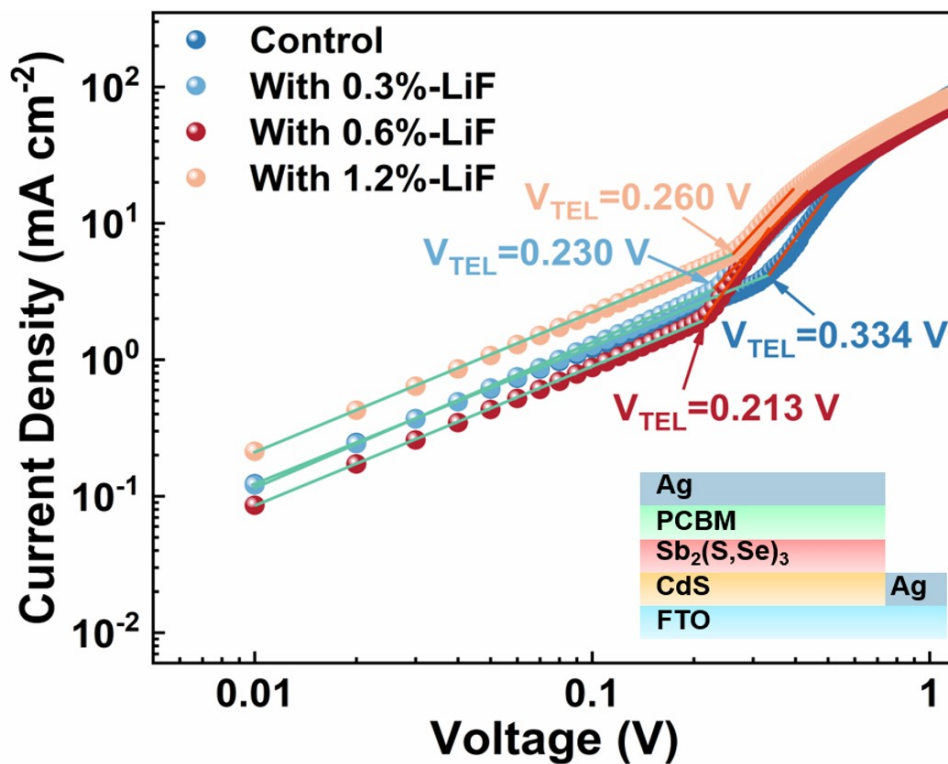




**Fig. S8** SEM-EDS analysis of the different Sb<sub>2</sub>(S,Se)<sub>3</sub> films.



**Fig. S9** Band gap characterization of CdS and  $\text{Sb}_2(\text{S,Se})_3$ . (a) Tauc plots of the control and 0.6% LiF-CdS films. (b) EQE spectra and the first derivatives of  $d\text{EQE}/d\lambda$  for the control and 0.6% LiF incorporated devices.



**Fig. S10**  $J$ - $V$  curves plotted using the space charge limited current (SCLC) model for the control and LiF incorporated devices.



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SOUTH CHINA NATIONAL CENTER OF METROLOGY  
GUANGDONG INSTITUTE OF METROLOGY

## 校准证书

CALIBRATION CERTIFICATE

证书编号: NY1202300558 第 1 页, 共 4 页  
Certificate No. Page of

委托方: 广西大学/华南理工大学  
Client: Guangxi University/South China University of Technology

委托方联络信息: 广西南宁市大学东路100号/广东省广州市天河区五山路381号  
Contact Information: 100 University East Road/Nanning, Guangxi 381 Wusheng Road/Guangzhou

计量器具名称: 砷化镓太阳能电池  
Description: Antimony arsenide/solar cell

型号/规格: 砷化镓太阳能电池  
Model/Type

制造厂: 广西大学/华南理工大学  
Manufacturer: Guangxi University/South China University of Technology

出厂编号: 20 设备管理编号: \_\_\_\_\_  
Serial No. Equipment No.

接收日期: 2023 年 10 月 08 日  
Date of Receipt: Y M D

结果: 见校准结果  
Results: Shows in the results of calibration

校准日期: 2023 年 10 月 08 日  
Date of Calibration: Y M D

批准人: 周军红  
Approved Signatory

校 准: 林洪波  
Reviewed by

校 准: 梅开明  
Calibrated by

扫一扫查真伪

实验室地址: 广东省东莞市石排镇东园大道南路段1号 邮政编码: 523343  
电话: (0620)96994172 传真: (0620)9699743 咨询电话: (0620)3661232 E-mail: scm@scm.com.cn  
Add. No. 1, Mianhuangyuan Section, Dongguan Road South, Shiqi Town, Dongguan, Guangdong  
Post Code: 523343 Tel: (0620)96994172 Fax: (0620)9699743 Complaint Tel: (0620)3661232  
证书真伪查询: www.scn.com.cn/105-00300102 Certificate Authority Identity: www.scn.com.cn/105-00300102

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**DIRECTIONS**

- 本中心是国家市场监督管理总局华南地区设立的国家法定计量检定机构, 本中心的质量管理体系符合 ISO/IEC 17025:2017 标准的要求。  
This laboratory is the National Legal Metrological Verification Institution in southern China set up by the State Administration for Market Regulation. The quality system is in accordance with ISO/IEC 17025:2017.
- 本中心所出具的量值均可溯源至国家计量基准或国际单位制(SI)。  
All data issued by this laboratory are traceable to national primary standards and/or International System of Units (SI).
- 校准地点、环境条件:  
Place and environmental conditions of the calibration:  
地点: 本院二基地1-402 温度: (25±2) °C 相对湿度: (50±5) %  
Place: 二基地1-402 Temperature: °C Humidity: %
- 本次校准的技术依据:  
Reference documents for the calibration:  
JJF1622-2017 太阳能电池校准规范; 光电性能 C.S. for Solar Cells; Photoelectric Properties
- 本次校准所使用的主要计量标准器具:  
Major standards of measurement used in the calibration:  
设备名称/型号规格/测量范围 编号 证书号/有效期/溯源单位 计量特性  
Name of Equipment Model/Type/Range Serial No. Certificate No./Date Data Metrological Characteristic

MET 稳态太阳能模拟器 1000W (full) spectrum solar simulator /SIX2000/ (300-1300)nm	374	NY1202300606 /2024-01-02 /本中心	光源功率; 光谱辐照度不均匀性; 光谱辐照度不稳定性; 光谱
标准源表 /标准源表 /4230/ (0-60V), (0-33A)	8051271	080202300681 /2023-03-06 /本中心	电压: $U_{10}$ =0.1%, 电流: $I_{10}$ =0.1%, $U_{10}$ =0.1%, $I_{10}$ =0.1% (4-2)
太阳能电池 /303-551/(1-1000)μm	JN0153	NY1202300212 /2024-05-03 /本中心	灵敏度: $k_{20}$ =2.1% (4-2)

注: 1. 本证书校准结果只与受控源仪器有关。The results relate only to the items calibrated.  
2. 本证书的有效性依赖于本中心所获得的证书。This certificate shall not be reproduced except in full, without the authority of our Laboratory. “日期”、“证书编号”、“设备名称”、“出厂编号”以及“设备编号”为强制信息。若客户对上述内容有任何疑问, 请及时联系我们。The information Client and Contact Information are provided by client, and the Manufacturer, Model/Type, Serial No. and Equipment No. are marked on the items. Client shall submit any objection within 30 working days after receiving the certificate for the information above.  
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## 校准结果

RESULTS OF CALIBRATION

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二、外观检查: 符合要求  
Apparent Inspection Pass

三、测试条件: 温度: (25±2) °C; 辐照度: 1000W/m<sup>2</sup>  
Test conditions: Temperature: (25±2) °C; Irradiance: 1000W/m<sup>2</sup>

三、电流-电压曲线:  
The IV curve:

四、光电性能参数:  
Results of photoelectric properties:

短路电流	开路电压	填充因子	最大功率	最佳工作电压	最佳工作电流	转换效率
$I_{sc}$	$V_{oc}$	FF	$P_m$	$V_{opt}$	$I_{opt}$	$\eta$
Short circuit current density	Open circuit voltage	Fill factor	Maximum power	Optimum working voltage	Optimum working current	Efficiency
mA/cm <sup>2</sup>	V	%	mW	V	mA	%
23.777	1.622	0.672	65.9	0.717	1.318	8.526

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## 校准结果

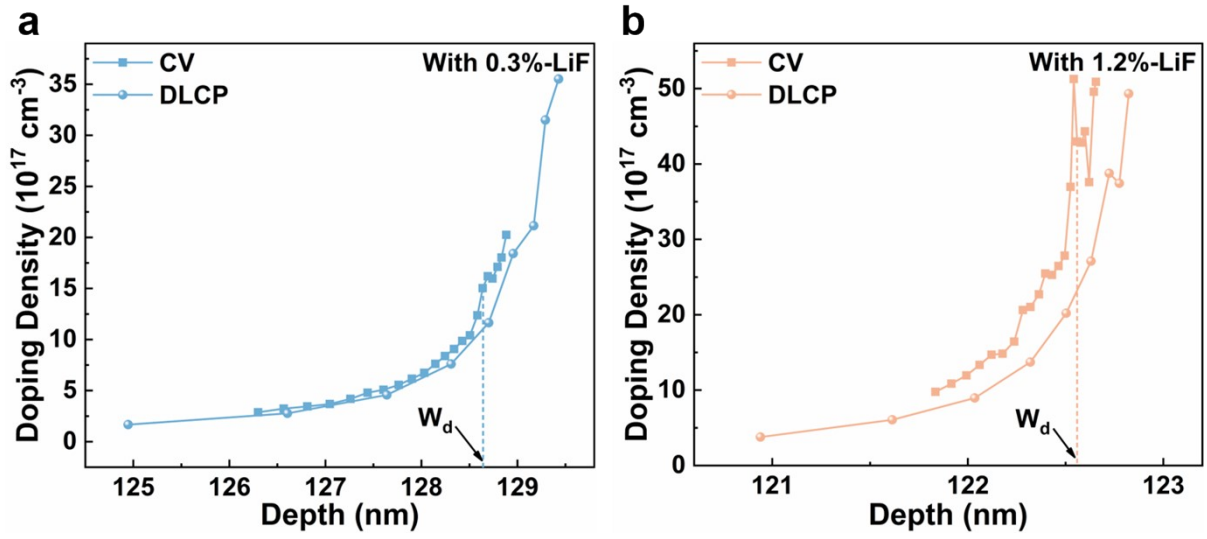
RESULTS OF CALIBRATION

证书编号: NY1202300558 原始记录号: NY1202300558 第 4 页, 共 4 页  
Certificate No. Record No. Page of

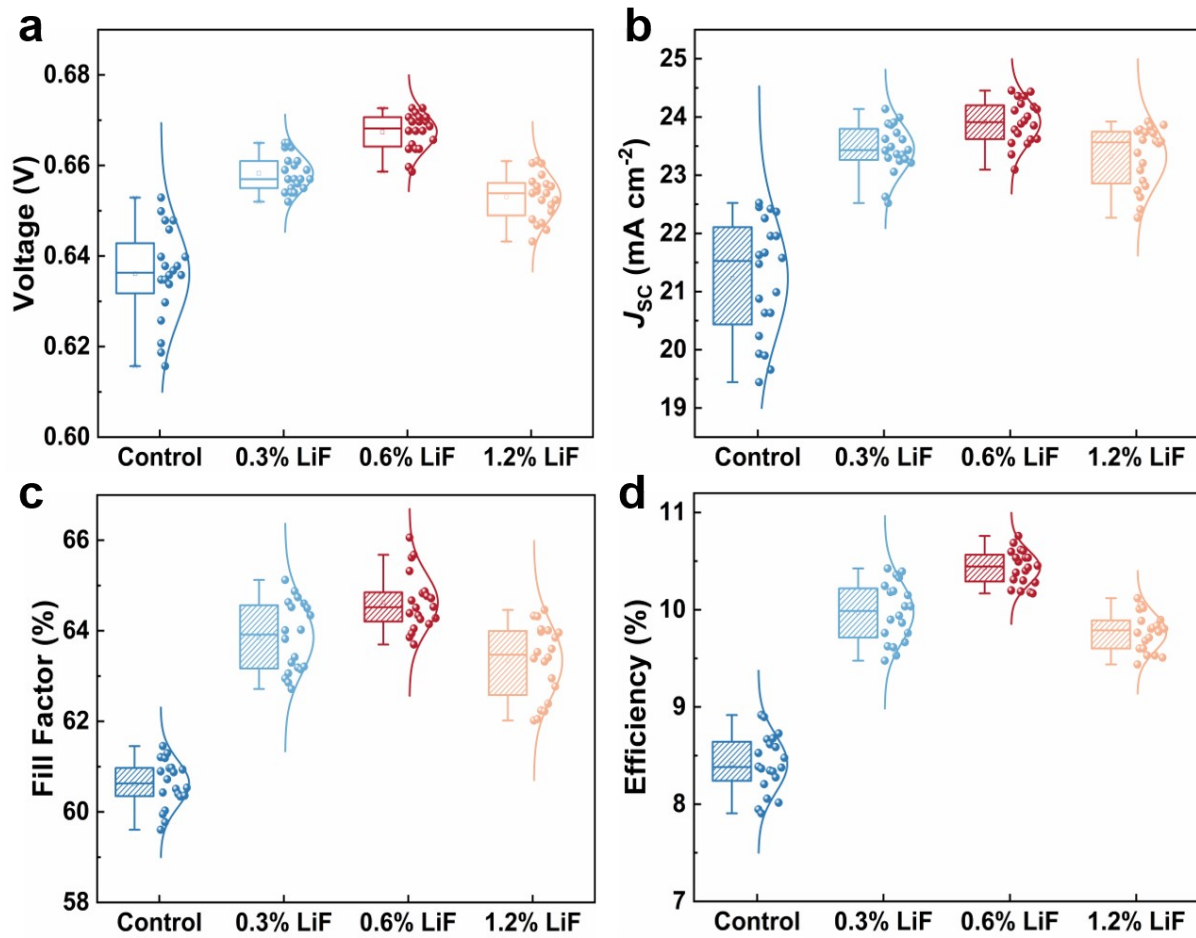
说明:  
Note:

- 电池有效面积数据为 0.0684cm<sup>2</sup> (有效面积经金属掩膜校准面积)。  
The effective area data of the cell is 0.0684cm<sup>2</sup> (Effective area calibrated by a metal aperture mask).
- 本次测量结果的扩展不确定度为: 开路电压  $U_{10}$ :  $U_{10}$ =1.2%, 短路电流  $I_{10}$ :  $I_{10}$ =2.7%, 最大功率  $P_m$ :  $P_m$ =1.0%, (4-2)。  
The expanded uncertainty of measuring results:  $U_{10}$ :  $U_{10}$ =1.2%,  $I_{10}$ :  $I_{10}$ =2.7%,  $P_m$ :  $P_m$ =1.0%, (4-2).
- 本证书中给出的扩展不确定度依据 JJF 1059.1-2012《测量不确定度评定与表示》评定, 由合成标准不确定度乘以包含概率为 95% 时对应的包含因子得到。  
The expanded uncertainty given in this certificate is evaluated according to JJF 1059.1-2012 "Evaluation and Expression of Uncertainty in Measurement" which is obtained by multiplying the combined standard uncertainty by the coverage factor k corresponding to the coverage probability of about 95%.
- 由于仪器使用时间的长短及使用部位的使用情况, 使用者, 仪器本身量值溯源来源决定的, 因此, 送检单位可根据实际使用情况自主决定复校时间间隔, 更换量源材料, 维修或对仪器性能有怀疑时, 应及时校准。Since the calibration interval is determined by the use of the instrument, operation of the user, the quality of the instrument itself and other factors, the re-calibration date can be decided by the user according to the actual situation. In case of replacement of important parts, maintenance or doubt on the performance of the instrument, it shall be calibrated in time.

**Fig. S11** Certification reports of our champion cell were received from the South China National Center of Metrology (SCM).

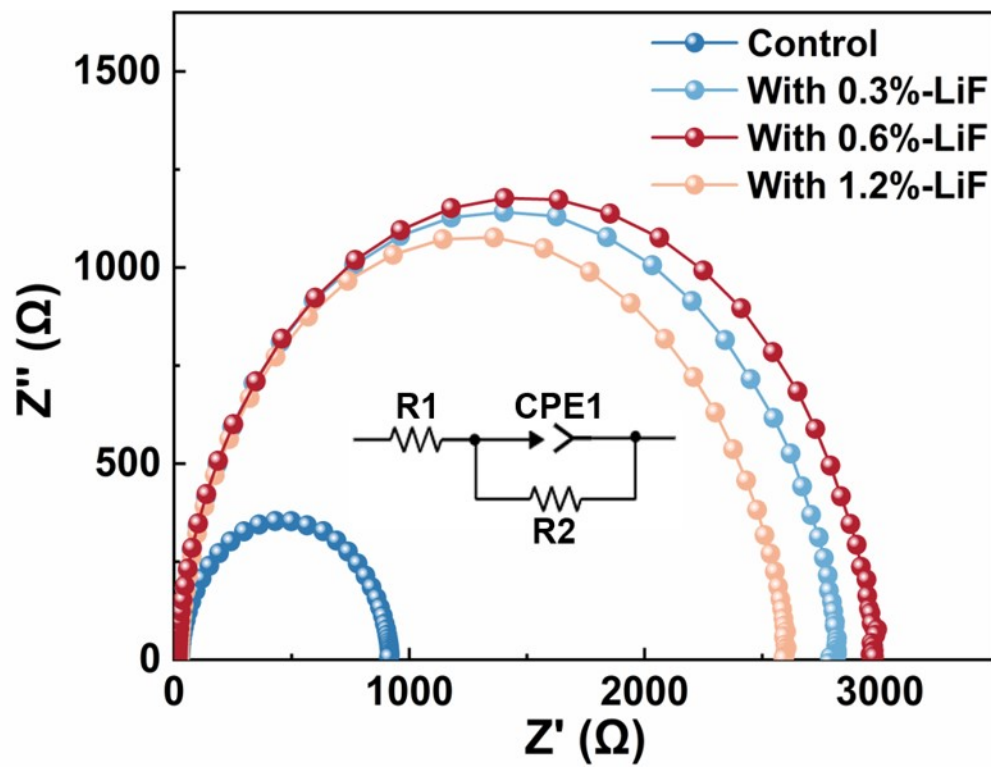


**Fig. S12** (a, b) C-V and DLCP profiling for the 0.3% and 1.2% LiF incorporated devices, respectively.

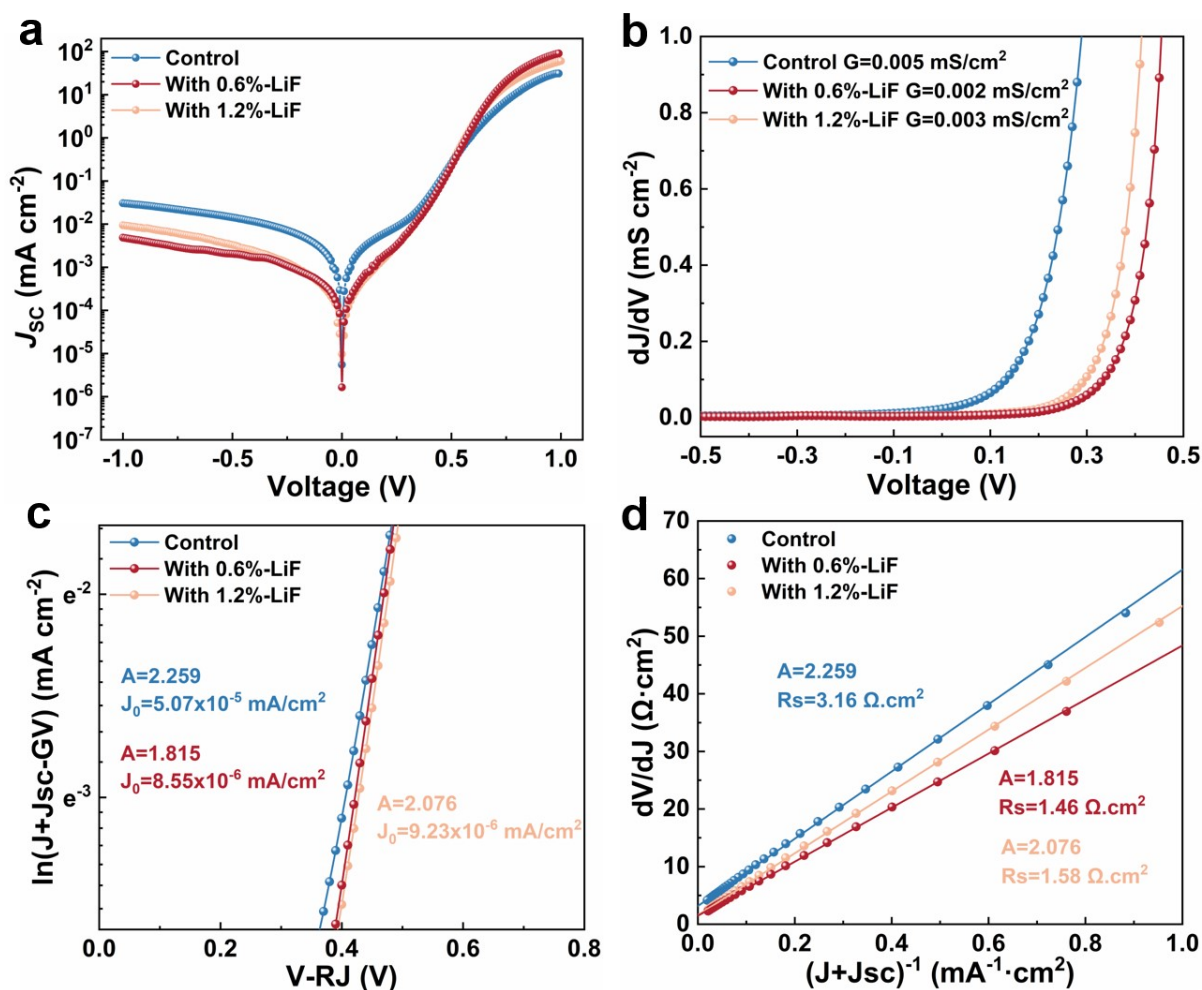


**Fig. S13** Photovoltaic parameters statistics. Statistical box plots of (a)  $V_{OC}$ , (b)  $J_{SC}$ , (c) Fill Factor and (d) Efficiency for the control, 0.3%, 0.6% and 1.2% LiF incorporated devices, respectively.





**Fig. S14** Electrical impedance spectra (EIS) for the control and LiF incorporated devices.



**Fig. S15** Device Dark  $J$ - $V$  Characteristics. (a) Dark  $J$ - $V$  curves of the control and LiF-incorporated devices. (b) Characterization of shunt conductance  $G$ . (c)  $\ln(J+J_{sc}-GV)$  with the fit used to determine  $A$  and  $J_0$ . (d)  $dV/dJ$  with the fit used to determine  $R_s$  and  $A$ .

**Table S1.** Hall tests of the control and LiF incorporated CdS films.

Sample	Resistivity ( $\Omega$ cm)	Conductivity ( $1/\Omega$ cm)	Mobility ( $\text{cm}^2/\text{Vs}$ )	Carrier Concentration ( $1/\text{cm}^3$ )	Hall Coefficient ( $\text{cm}^3/\text{C}$ )
Control	$1.17 \times 10^4$	$8.53 \times 10^{-5}$	$1.96 \times 10^1$	$-2.72 \times 10^{13}$	$-2.30 \times 10^5$
With LiF	$1.13 \times 10^4$	$8.81 \times 10^{-5}$	$8.73 \times 10^0$	$-6.30 \times 10^{13}$	$-9.91 \times 10^4$

**Table S2.** Biexponential fitting results of decay kinetics curves.

<b>Sample</b>	<b>A<sub>1</sub> (%)</b>	<b>τ<sub>1</sub> (ps)</b>	<b>A<sub>2</sub> (%)</b>	<b>τ<sub>2</sub> (ps)</b>	<b>A<sub>3</sub> (%)</b>	<b>τ<sub>3</sub> (ps)</b>	<b>τ<sub>av</sub> (ps)</b>
Control	34.19	7.525	34.87	428.14	30.94	2955.51	2954.50
With LiF	23.16	9.056	32.79	435.58	44.05	3792.61	3524.12

**Table S3.** Interfacial defects of the control, 0.3%, 0.6% and 1.2% LiF incorporated devices, respectively.

<b>Sample</b>	<b><math>N_{CV}</math> (1/cm<sup>3</sup>)</b>	<b><math>W_d</math>(nm)</b>	<b><math>N_{DLCP}</math> (1/cm<sup>3</sup>)</b>	<b><math>N_{IT}</math> (1/cm<sup>3</sup>)</b>
Control	$6.34 \times 10^{18}$	116.36	$3.55 \times 10^{18}$	$2.79 \times 10^{18}$
With 0.3% LiF	$1.50 \times 10^{18}$	128.64	$1.16 \times 10^{18}$	$3.39 \times 10^{17}$
With 0.6% LiF	$1.33 \times 10^{18}$	145.09	$1.09 \times 10^{18}$	$2.40 \times 10^{17}$
With 1.2% LiF	$4.30 \times 10^{18}$	122.56	$2.02 \times 10^{18}$	$2.28 \times 10^{18}$