## **Supporting Information**

## Unveiling the Influence of Absorber Thickness on Efficient Sb<sub>2</sub>(S, Se)<sub>3</sub> Solar Cells Through Controlled Chemical Bath Deposition

Jun Zhao<sup>1#</sup>, Xuerui Li<sup>1#</sup>, Junhui Lin<sup>1,2\*</sup>, Xiaofang Zhao<sup>2\*</sup>, Muhammad Ishaq<sup>1</sup>, Shuo Chen<sup>1</sup>, Zhuanghao Zheng<sup>1</sup>, Zhenghua Su<sup>1</sup>, Xianghua Zhang<sup>3</sup>, Guang-Xing Liang<sup>1</sup>

<sup>1.</sup> Shenzhen Key Laboratory of Advanced Thin Films and Applications, Key Laboratory of Optoelectronic Devices and Systems of Ministry of Education and Guangdong Province, College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, Guangdong, P. R. China.

<sup>2.</sup> International School of Microelectronics, Dongguan University of Technology, Dongguan 523000, Guangdong, P. R. China

<sup>3.</sup> Institut des Sciences Chimiques de Rennes, UMR 6226, Rennes, F-35000, France

<sup>#</sup> Jun Zhao and Xuerui Li contributed equally.

\* Corresponding author. E-mail: <u>13669872773@163.com</u> (Prof. Lin)

zhaoxf@dgut.edu.cn (Prof. Zhao)

Table S1. Prepared materials for each layers of solar cells.

| Each layers of solar cells                          | Prepared materials   |
|---|--|
| CdS   | Thiourea, NH <sub>3</sub> OH aqueous solution, and   |
|   | Cadmium Sulfate  |
| $Sb_2(S,Se)_3$                                      | $C_4H_4KO_7Sb\cdot 0.5H_2O$ , $Na_2S_2O_3\cdot 5H_2O$ , and  |
|   | Selenourea (CH <sub>4</sub> N <sub>2</sub> Se)   |
| Spiro-OMeTAD  | Spiro-OMeTAD, Chlorobenzene, and 4-  |
|   | tert-butylpyridine lithium bis   |
| Sb <sub>2</sub> (S,Se) <sub>3</sub><br>Spiro-OMeTAD | C <sub>4</sub> H <sub>4</sub> KO <sub>7</sub> Sb·0.5H <sub>2</sub> O, Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> ·5H <sub>2</sub> O, and<br>Selenourea (CH <sub>4</sub> N <sub>2</sub> Se)<br>Spiro-OMeTAD, Chlorobenzene, and 4-<br>tert-butylpyridine lithium bis |

## Supplementary note 1. Background of DLTS measurements

The deep-level transient spectroscopy (DLTS) was used to analyze the deep defects in the  $Sb_2(S,Se)_3$  absorber layer of 2H and 4H solar cells. Fig. 6(b) shows the arrhenius plots obtained from defect peaks in DLTS signal. The active energy ( $E_A$ ,  $E_C-E_T$  or  $E_T-E_V$ ) and capture cross section ( $\sigma$ ) of electron and hole defects are calculated from the Arrhenius plots according to the following equations.

$$\ln(\tau_{e} \upsilon_{ih,n} N_{c}) = \frac{E_{c} - E_{T}}{k_{B} T} - \ln(X_{n} \sigma_{n})$$
(1)

$$\ln(\tau_e \upsilon_{h,p} N_v) = \frac{E_T - E_v}{k_B T} - \ln(X_p \sigma_p)$$
<sup>(2)</sup>

There,  $\tau_{e}$ ,  $N_{C}$ ,  $N_{V}$ ,  $E_{C}$ ,  $E_{V}$  and  $E_{T}$  are the emission time constant, conduction band state density, valence band state density, conduction band, valence band, and trap energy level, respectively.  $X_{n}$  and  $X_{p}$  are the entropy factor of hole and electron,  $\sigma_{n}$  and  $\sigma_{p}$  are the electron and hole defects capture cross-section, respectively. T and  $k_{B}$  are the temperature and Boltzmann constant,

respectively.  $v_{th,n}$  and  $v_{th,p}$  are the thermal velocities associated with electron and hole defects. The  $v_{th,n}$  and  $N_C$  can be obtained by following equations.

$$v th, n = \sqrt{\frac{3kT}{m_n^*}}$$
 (3)  $N_c = 2(\frac{2\pi m_n^* kT}{h^2})^{\frac{3}{2}}$ 

(4)

Where  $m_n^*$  is the effective mass for electrons, with similar equations for  $v_{th,p}$  and  $N_V$ . The activation energy of electron ( $E_C$ - $E_T$ ) and hole ( $E_T$ - $E_C$ ) traps were obtained from the slopes of equations (2) and (3) through linear regression.  $\sigma_n$  and  $\sigma_p$  values can be extracted from the intersection with y-axis. Defect concentration ( $N_T$ ) can be obtained from following equations.

$$N_{T} = 2N_{s} \frac{\Delta C}{C_{R}}$$

$$N_{s} = \frac{2C^{2}}{q \varepsilon A^{2}} (V + V_{d})$$
(5)
(6)

Where  $N_{\rm T}$  and  $N_{\rm S}$  are the trap density and the shallow dopant concentration, respectively.  $C_{\rm R}$  is the capacitance under reverse bias, and  $\Delta C$  is the amplitude of capacitance transient. V and  $V_{\rm d}$  are the applied voltage and diffusion voltage, respectively."