Supplementary Information (SI) for Journal of Materials Chemistry A. This journal is © The Royal Society of Chemistry 2025

- 1 Supporting Information
- 2 Growth Behavior and Interface Engineering for Photovoltaic
- 3 Applications of Co-evaporated Sb<sub>2</sub>Se<sub>3</sub> Thin Films on Mo Foil
- 5 Van-Quy Hoang, a,b,‡ Sinae Park, b,‡ Jaebaek Lee, b Dae-Ho Son, b Dae-Kue Hwang, b Quynh Le-Van, a Vo
- 6 Pham Hoang Huy,<sup>b</sup> Se Yun Kim,<sup>d</sup> Kee-Jeong Yang,<sup>b</sup> Jin-Kyu Kang,<sup>b</sup> Shi-Joon Sung,<sup>b,c,★</sup> and Dae-Hwan
- 7 Kim<sup>b,c,★</sup>

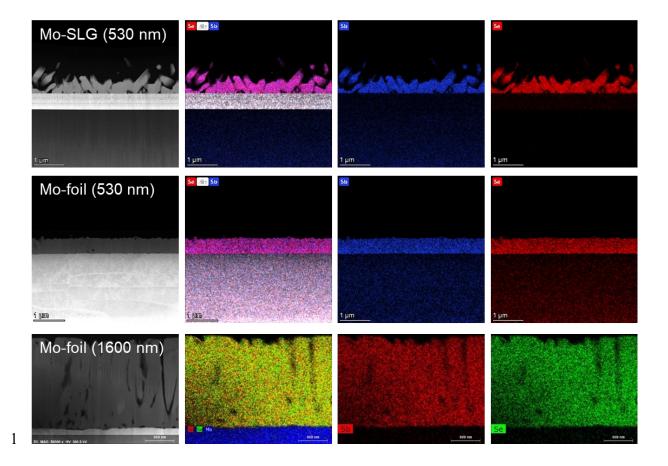
4

14

15

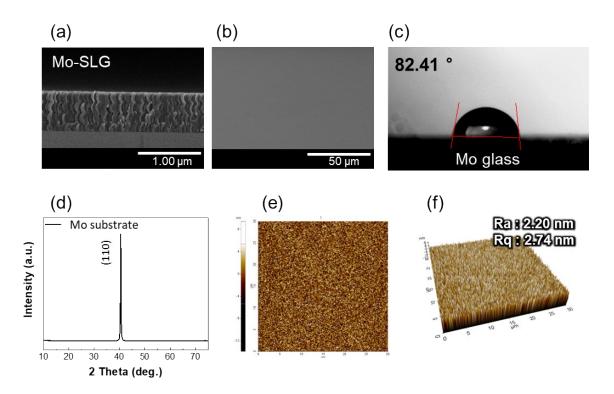
- 8 aCenter for Environmental Intelligence, College of Engineering and Computer Science, VinUniversity,
- 9 Gia Lam district, Hanoi 14000, Vietnam
- 10 bDivision of Energy & Environmental Technology, DGIST, Daegu 42988, Republic of Korea
- 11 °Department of Interdisciplinary Engineering, DGIST, Daegu 42988, Republic of Korea
- 12 dDepartment of Advanced Materials Science & Engineering, Kyungnam University, 51767, Korea
- 13 E-mail: sjsung@dgist.ac.kr, monolith@dgist.ac.kr

- 16 †Electronic supplementary information (ESI) available. See DOI: https://doi.org/xxx
- 17 <sup>‡</sup>These authors contributed equally to this work.
- 19 **Keywords**: Sb<sub>2</sub>Se<sub>3</sub> thin film, flexible photovoltaics, Mo foil, columnar grain growth



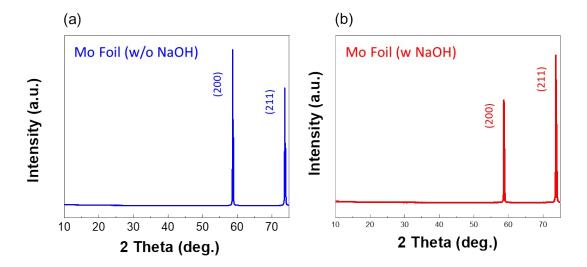
 $2 \quad \textbf{Figure S1}. \ \mathsf{STEM} \ \mathsf{EDS} \ \mathsf{images} \ \mathsf{of} \ \mathsf{Sb}_2\mathsf{Se}_3 \ \mathsf{thin} \ \mathsf{films} \ \mathsf{on} \ \mathsf{Mo} \ \mathsf{or} \ \mathsf{Mo}\text{-foil}. \ \mathsf{For} \ \mathsf{each} \ \mathsf{sample}, \ \mathsf{images} \ \mathsf{from}$ 

- $3\,$  left to right show the cross-sectional STEM image, composite EDX elemental map, and individual
- 4 elemental maps of Sb and Se.



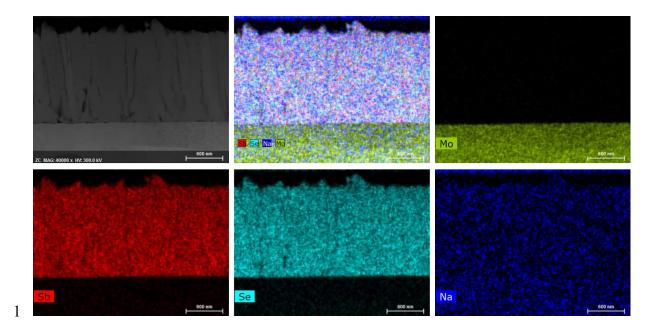
**Figure S2**. (a) Cross-sectional and (b) top-view SEM images of the Mo-SLG substrate, along with (c) 3 the water contact angle measurement of the Mo-coated glass. (d) XRD and (e) AFM topography and

(f) three-dimensional surface profile images, indicating a smooth Mo surface with low roughness.



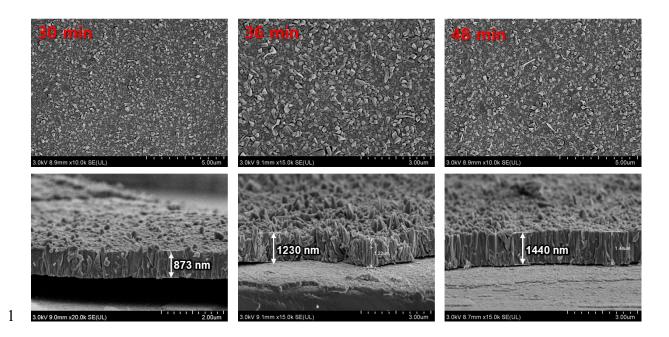
2 Figure S3. XRD data of Mo-foil substrates (a) without NaOH treatment (w/o NaOH) and (b) with NaOH

3 treatment (w NaOH)



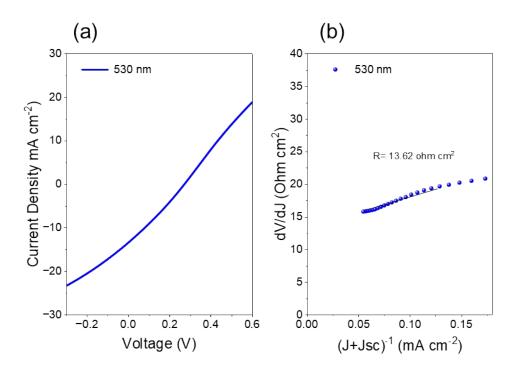
2 Figure S4. TEM-EDS images of 1600 nm-thick Sb<sub>2</sub>Se<sub>3</sub> films on Mo-foil with NaOH treatment showing

- 3 the cross-sectional STEM image, composite EDX elemental map, and individual elemental maps of Mo,
- 4 Sb, Se and Na.

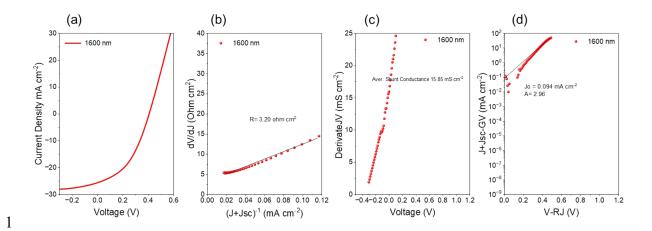


2 Figure S5. Top-view and cross-sectional SEM images of  $Sb_2Se_3$  on  $MoSe_2$  interlayer and NaOH

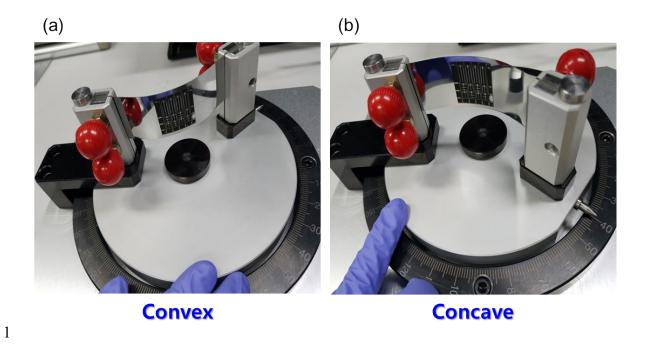
3 treatment with different thickness from 873 nm to 1400 nm.



**Figure S6**. Characteristic behavior of the best-performing devices inclusing (a) *J*–V curves, derivative of dJ/dV for shunt characteristic analysis of 530 nm-thick Sb<sub>2</sub>Se<sub>3</sub> based device.



**Figure S7**. Characteristic behavior of the best-performing devices inclusing (a) *J*–V curves, (b) 3 derivative of dJ/dV for shunt characteristic analysis, (c) derivatives of dV/dJ under forward bias with 4 fitting are used to determine the series resistance and diode ideality factor and (d) In(J + JSC - GV) versus (V - RJ)) curves of 1600 nm-thick Sb<sub>2</sub>Se<sub>3</sub> based device.



**Figure S8**. Experimental setups for convex (stretching) and concave (compressing) bending tests.

 $1 \quad \textbf{Table S1.} \quad \text{Voc, } \textit{J}_{\text{SC}}, \; \text{FF, PCE, } \; \text{R}_{\text{s}} \; \text{and} \; \; \text{R}_{\text{sh}} \; \text{of the flexible Sb}_{2}\text{Se}_{3} \; \text{solar cells without and with NaOH}$ 

## 2 treatment.

Treatment	V <sub>OC</sub>	$J_{ m SC}$	FF	PCE	$R_{\rm s}$	$R_{\rm sh}$
	(V)	(mA/cm <sup>2</sup> )	(%)	(%)	$(\Omega \text{cm}^2)$	$(\Omega \text{cm}^2)$
w/o NaOH	0.349	19.00	44.40	2.94	6.30	100.16
w NaOH	0.341	20.27	46.65	3.23	5.60	110.75