Electronic supplementary information (ESI)

Chemical insight into the hydrothermal deposition of $Sb_2(S,Se)_3$ towards delicate microstructure engineering

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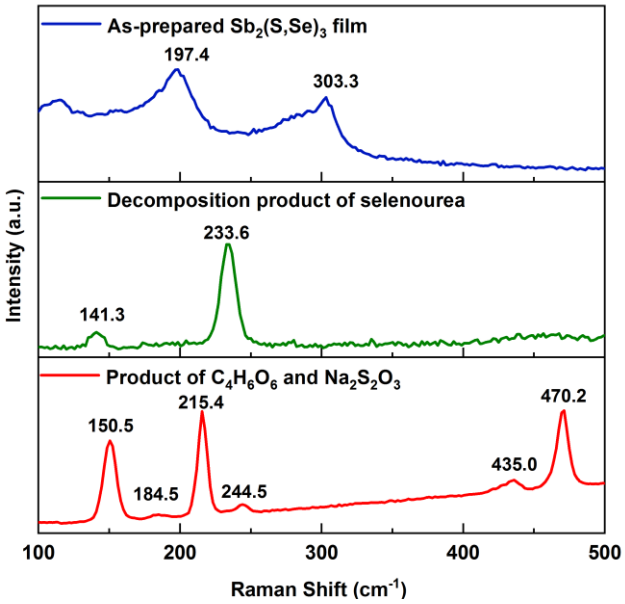

Fig. S1 Raman spectra of the product of $C_4H_6O_6$ and $Na_2S_2O_3$, the decomposition product of selenourea and the as-prepared $Sb_2(S,Se)_3$ film.

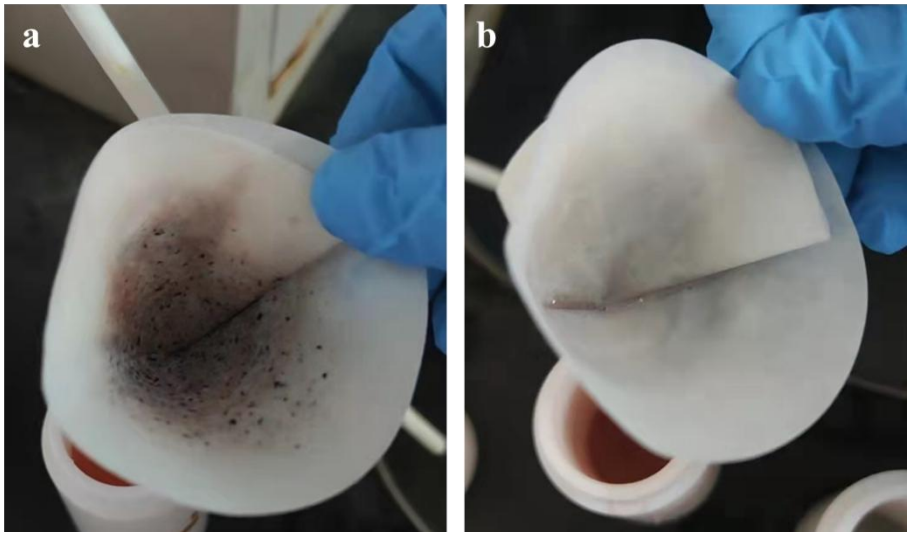

Fig. S2 (a) The hydrothermal reaction with selenourea alone will get elemental Se. (b) Almost no elemental Se was formed when we used elemental S, selenourea and water to repeat the hydrothermal reaction.

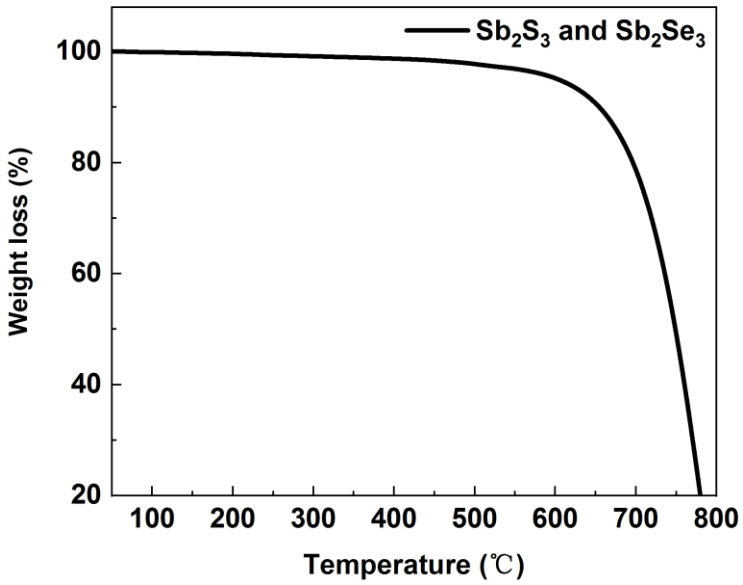

Fig. S3 Thermogravimetric curve of Sb_2S_3 and Sb_2Se_3 mixture.

Table S1 EDS data of as-prepared and annealed $Sb_2(S,Se)_3$ films (atomic ratio (%)).

Sample	Sb	Se	S	Cd	Se/(S+Se)	(S+Se-Cd):Sb
As-prepared film	35.88	24.10	36.42	3.60	42.34	1.59:1
Annealed film	38.18	22.76	34.68	4.38	42.89	1.39:1

Table S2 Defect state, energy level (E_T), cross-section (σ), defect density (N_T) of the detected defects in as-prepared $Sb_2(S,Se)_3$ devices.

Trap	E_T (eV)	σ (cm^2)	N_T (cm^{-3})
E1	E_C-0.548	1.18×10^{-17}	2.10×10^{14}
E2	E_C-0.762	1.91×10^{-15}	1.84×10^{14}

Table S3 EDS data of as-prepared and annealed $Sb_2(S,Se)_3$ films with zeolite additive (atomic ratio (%)).

Sample	Sb	Se	S	Cd	Se/(S+Se)	(S+Se-Cd):Sb
As-prepared film	34.89	24.89	36.33	3.89	43.41	1.64:1
Annealed film	36.30	24.58	34.39	4.73	45.33	1.49:1

Table S4 Defect state, energy level (E_T), cross-section (σ), defect density (N_T) of the detected defects in as-prepared $Sb_2(S,Se)_3$ devices with zeolite additive.

Trap	E_T (eV)	σ (cm^2)	N_T (cm^{-3})
H1	E_V+0.541	6.86×10^{-18}	3.85×10^{13}

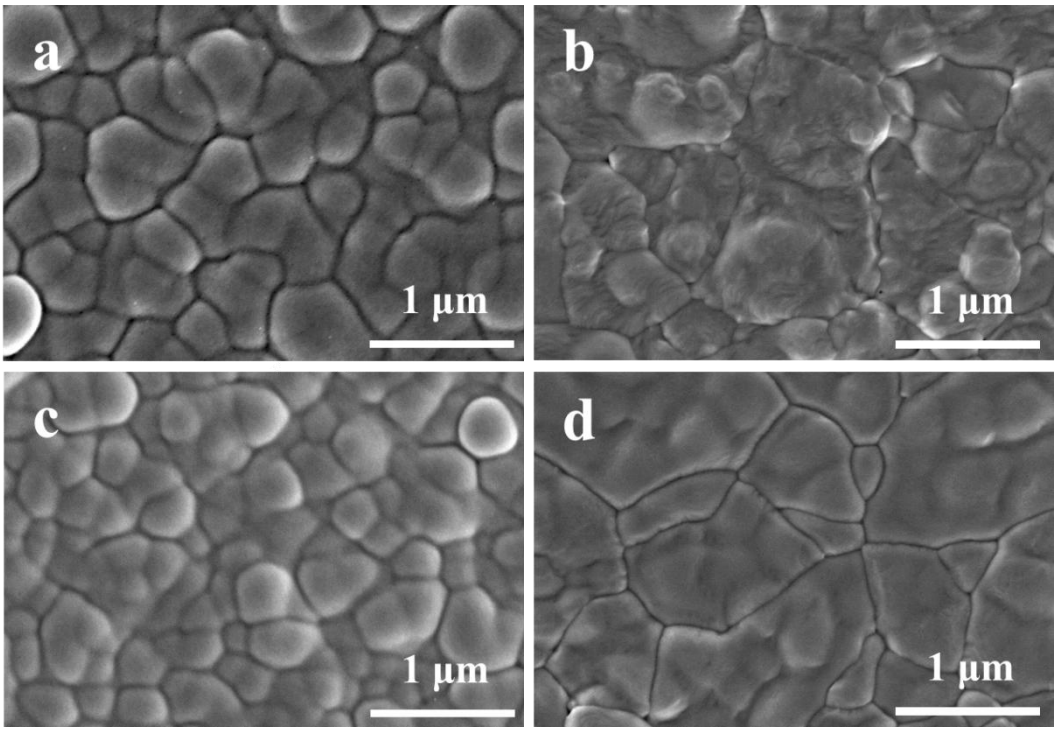

Fig. S4 Surface SEM images of as-prepared (a) and annealed (b) $Sb_2(S,Se)_3$ W/O on the CdS/FTO/glass substrates. Surface SEM images of as-prepared (c) and annealed (d) $Sb_2(S,Se)_3$ W/ on the CdS/FTO/glass substrates.

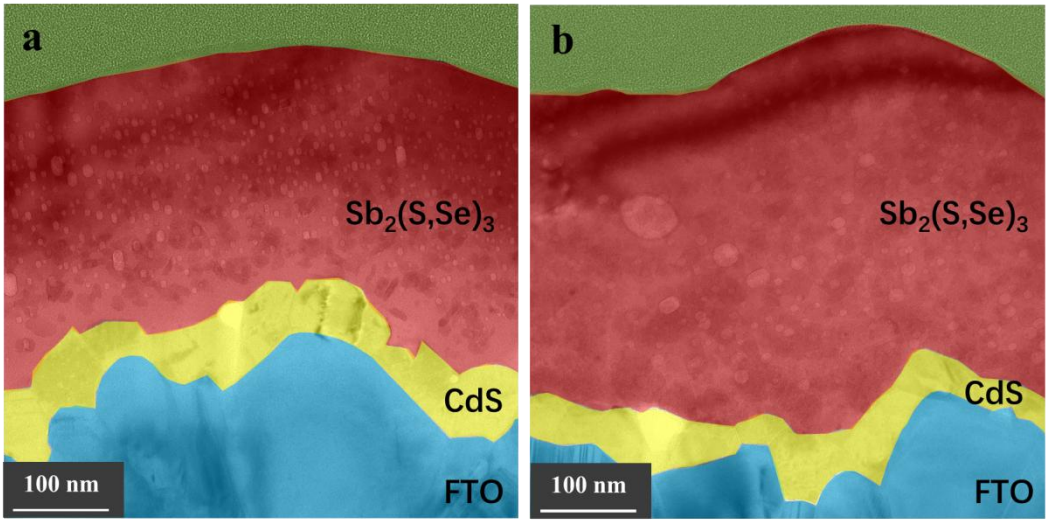

Fig. S5 Cross-sectional HRTEM images of $Sb_2(S,Se)_3$/CdS heterojunction W/O (a) and W/ (b).

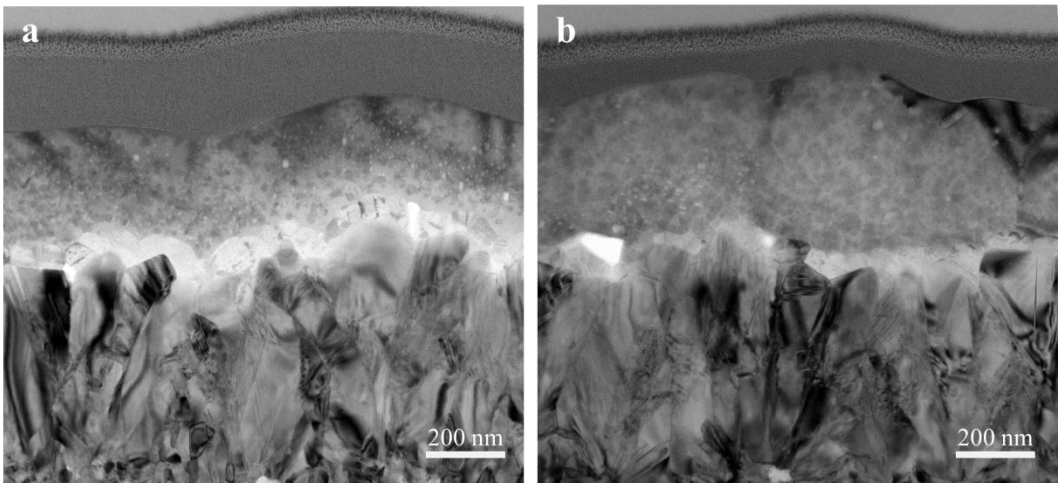

Fig. S6 Cross-sectional TEM images of $Sb_2(S,Se)_3$/CdS heterojunction W/O (a) and W/ (b).

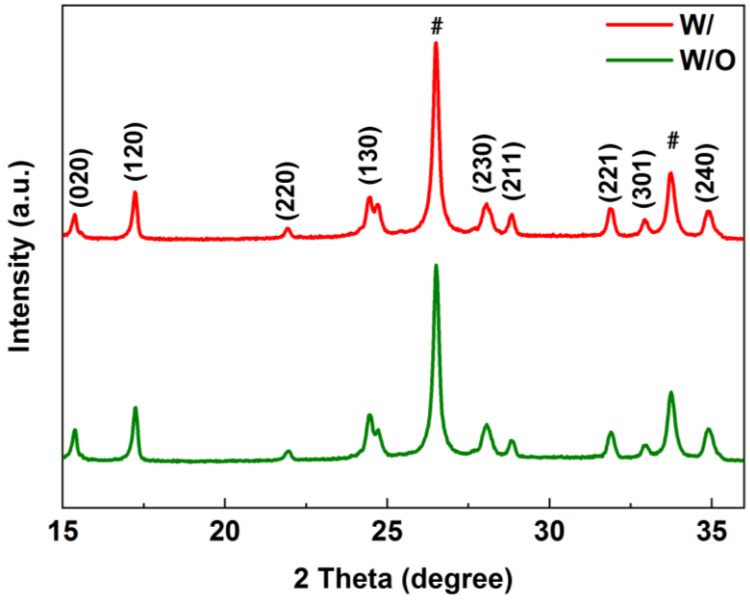

Fig. S7 X-ray diffraction spectra of $Sb_2(S,Se)_3$ W/O and W/.

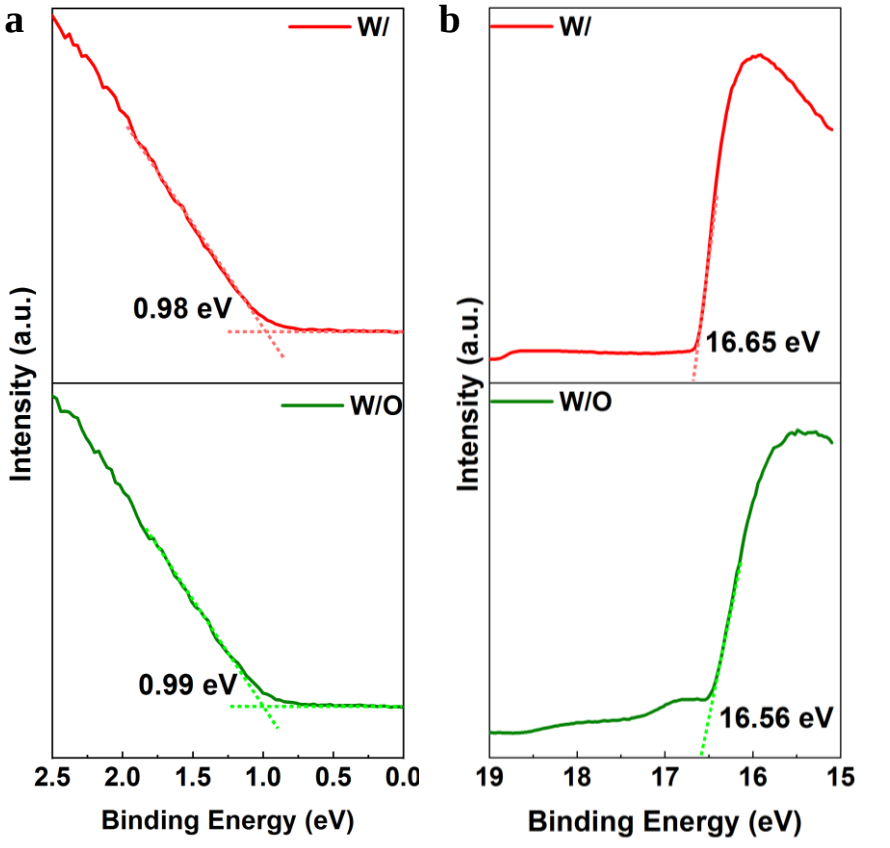

Fig. S8 Magnified UPS spectra of samples W/O (a) and W/ (b).

Table S5 The energy level parameters of $Sb_2(S,Se)_3$ W/O and W/ films.

$Sb_2(S,Se)_3$	**Band gap** [eV]	**Fermi level** [eV]	**VBM** [eV]	**CBM** [eV]
W/O	1.45	-4.64	-5.63	-4.18
W/	1.43	-4.55	-5.53	-4.10

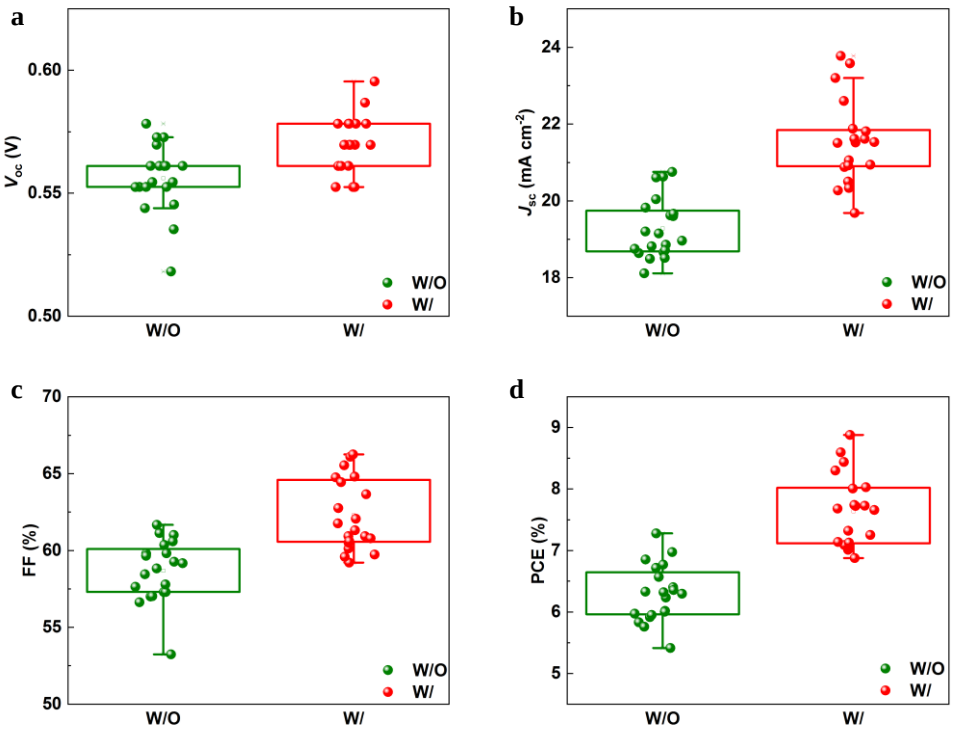

Fig. S9 Statistical distribution of photovoltaic parameters for the $Sb_2(S,Se)_3$-W/O and $Sb_2(S,Se)_3$-W/ devices: (a) distribution of V_{oc}, (b) distribution of J_{sc}, (c) distribution of FF and (d) distribution of PCE, respectively.

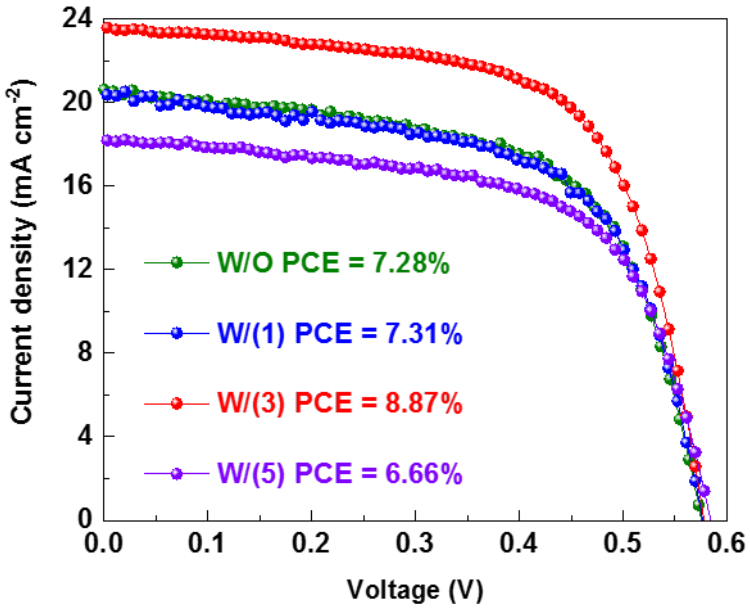

Fig. S10 *J-V* characteristics of $Sb_2(S,Se)_3$ devices using different numbers of zeolite particles under standard AM 1.5G illumination.