

Supporting Information

Defect-Level Trap optimization in $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$ Photovoltaic Materials via Sb^{3+} -Doping for over 13% Efficient Solar Cell

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Table S1 Parameters of CZTSSe, CdS, and ITO layers.

Layer properties	CZTSSe	CdS	ITO
thickness (nm)	1700	30	500
E_g (eV)	1.14	2.4	3.65
χ (eV)	4.05	4.27	4.8
N_C (cm^{-3})	2.2×10^{18}	2.3×10^{18}	5.2×10^{18}
N_V (cm^{-3})	1.8×10^{19}	1.8×10^{19}	1.0×10^{18}
v_e (cm/s)	1.0×10^7	2.6×10^7	2.0×10^7
v_h (cm/s)	1.0×10^7	1.3×10^7	1.0×10^7
μ_e (cm^2/Vs)	20	340	10
μ_h (cm^2/Vs)	25	10	10
Doping (cm^{-3})	1×10^{15} (a)	1×10^{15} (d)	1×10^{20} (d)

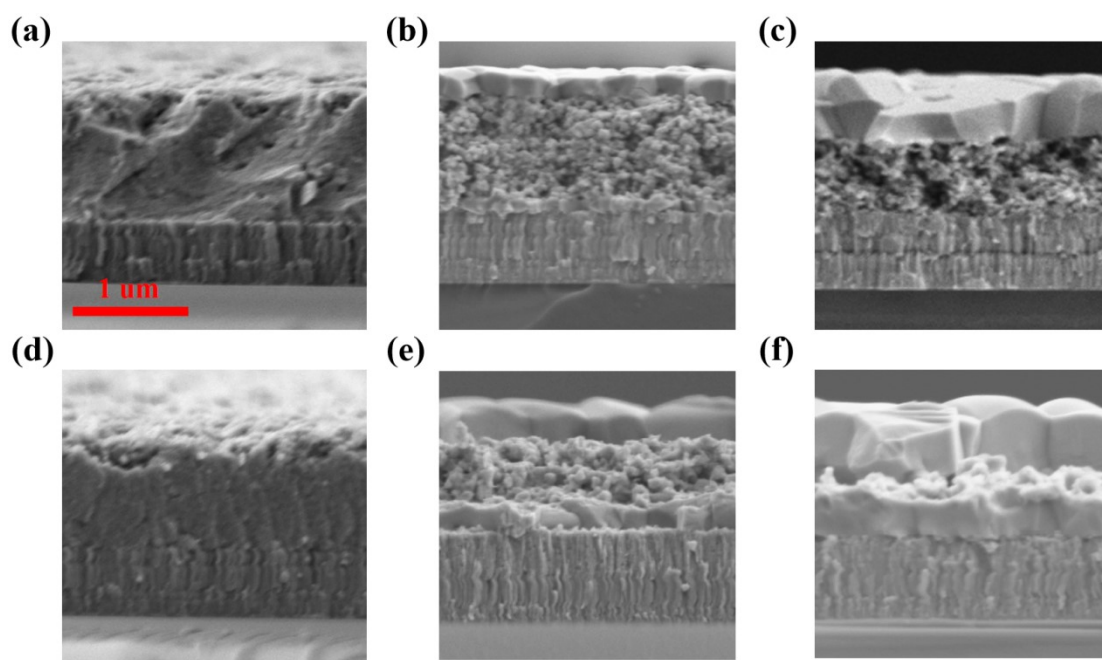


Figure S1 Cross-section SEM images of (a-c) Reference and (d-f) Sb-doped thin film during different selenization times (0, 100 and 900 seconds).

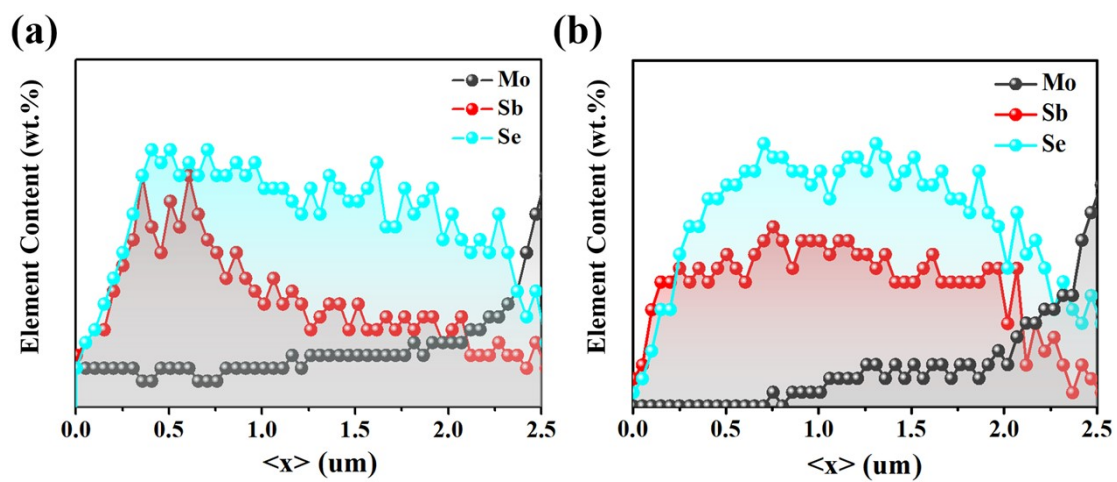


Figure S2 The element distribution of the thin films prepared by (a) one-step and (b) two-step methods was scanned by EDS line scans.

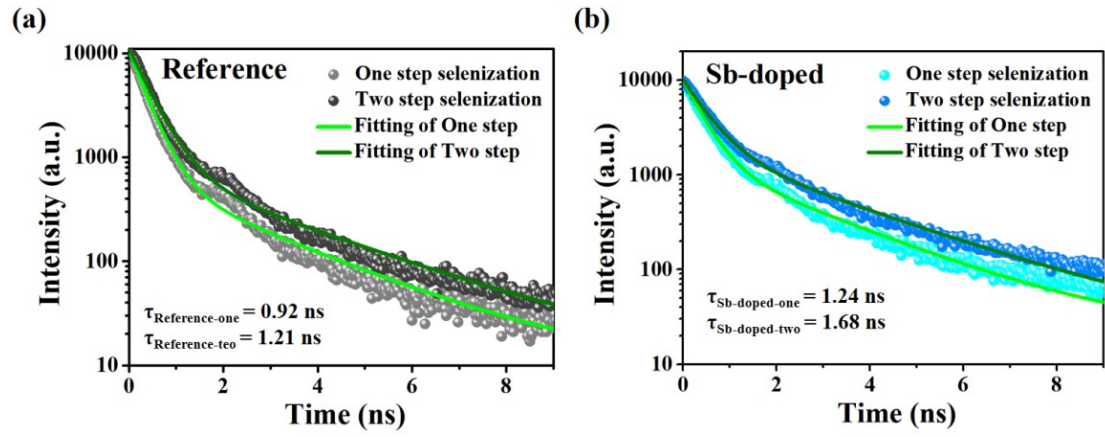


Figure S3 The TRPL decay curves of (a) Reference and (b) Sb-doped thin films during one-step and two-step selenization.

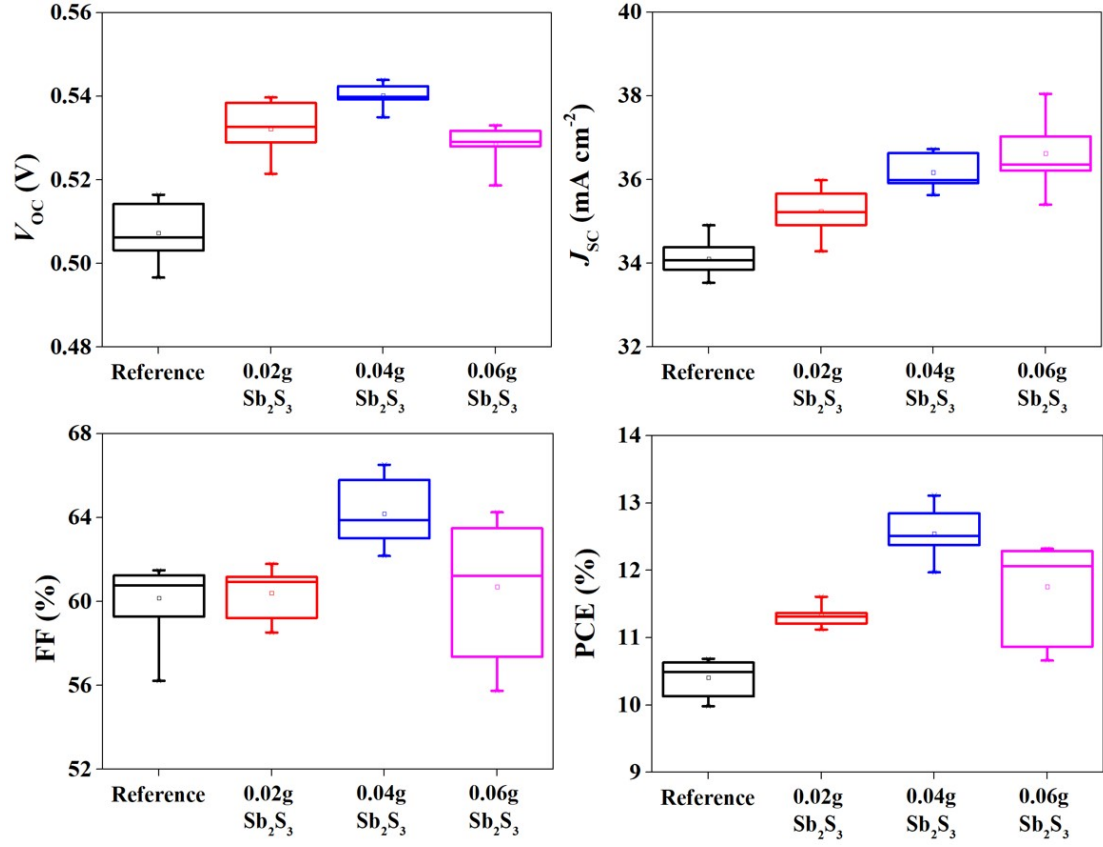


Figure S4 Statistical photovoltaic performance data for the CZTSSe-based devices, including V_{OC} , J_{SC} , FF, and PCE.

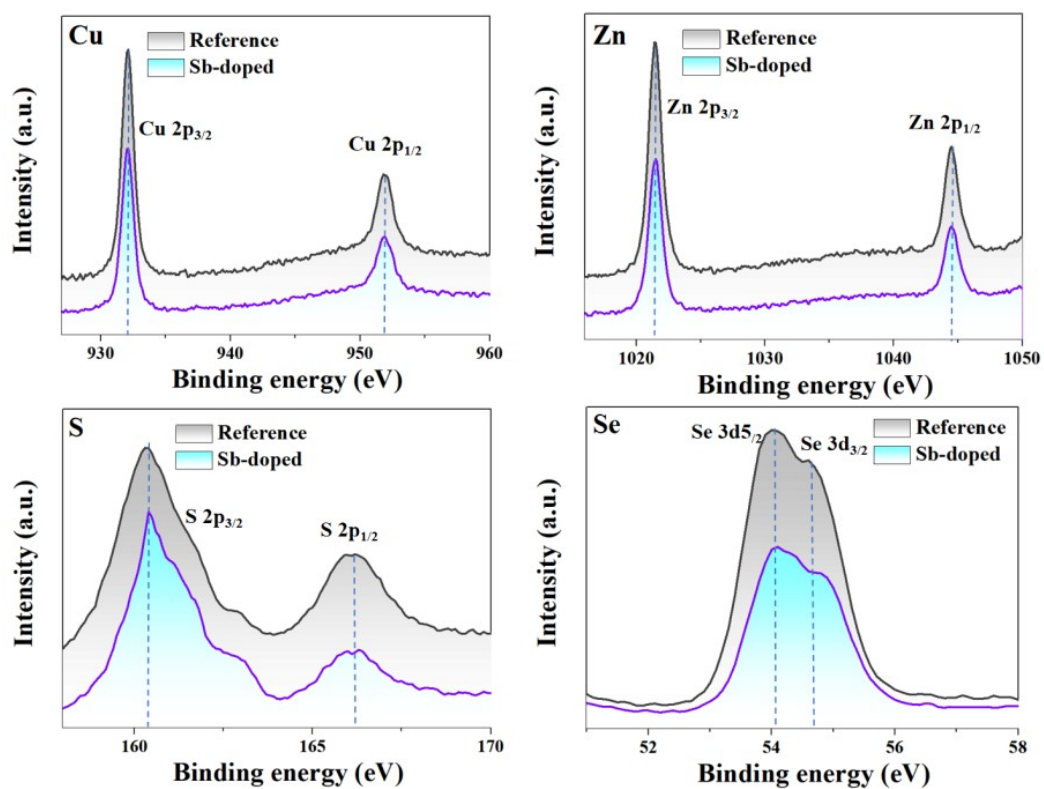


Figure S5 XPS spectra of Cu 2p, Zn 2p, S 2p and Se 3d peaks with the reference and Sb-doped films.

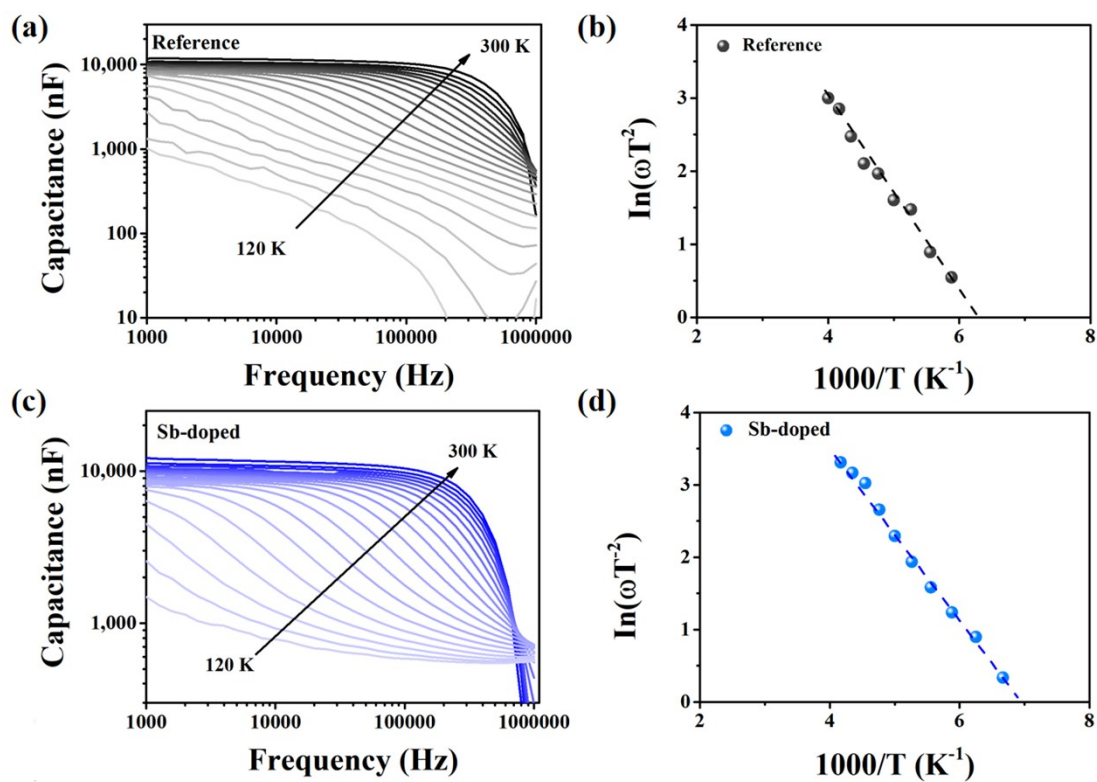


Figure S6 The AS spectra and Arrhenius plot with the (a-b) Reference and (c-d) Sb-doped films.

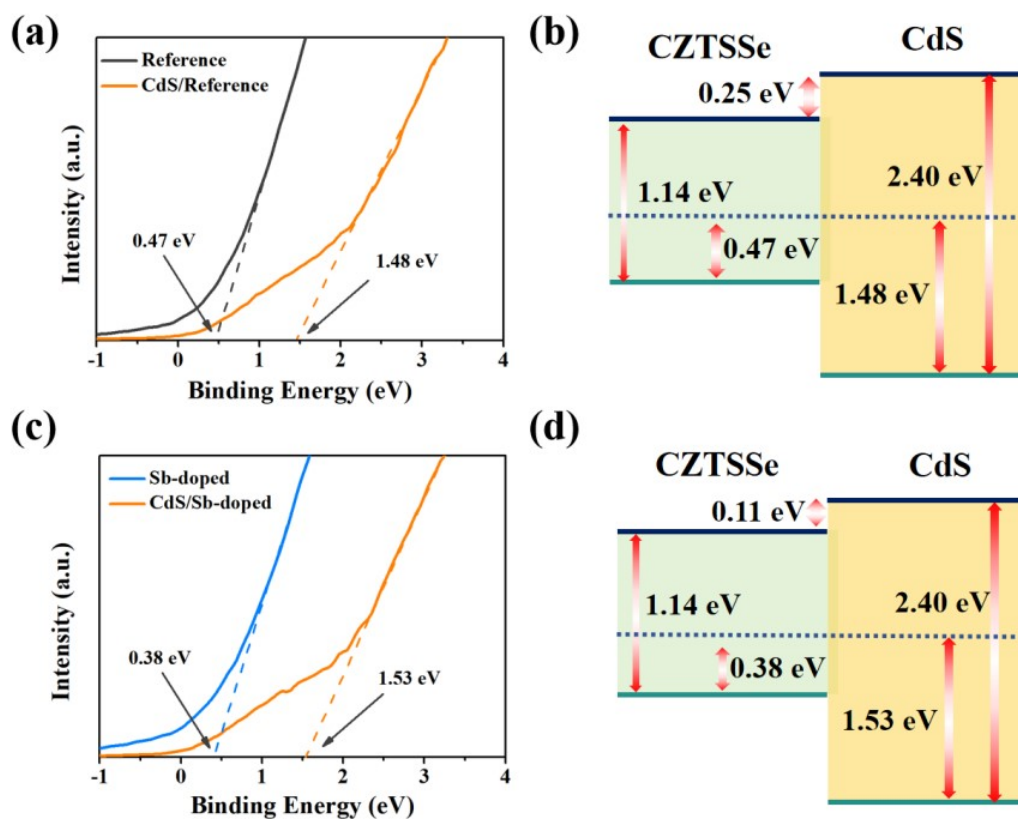


Figure S7 The magnified UPS spectra region and energy band diagram with (a-b) reference and (c-d) Sb-doped samples.

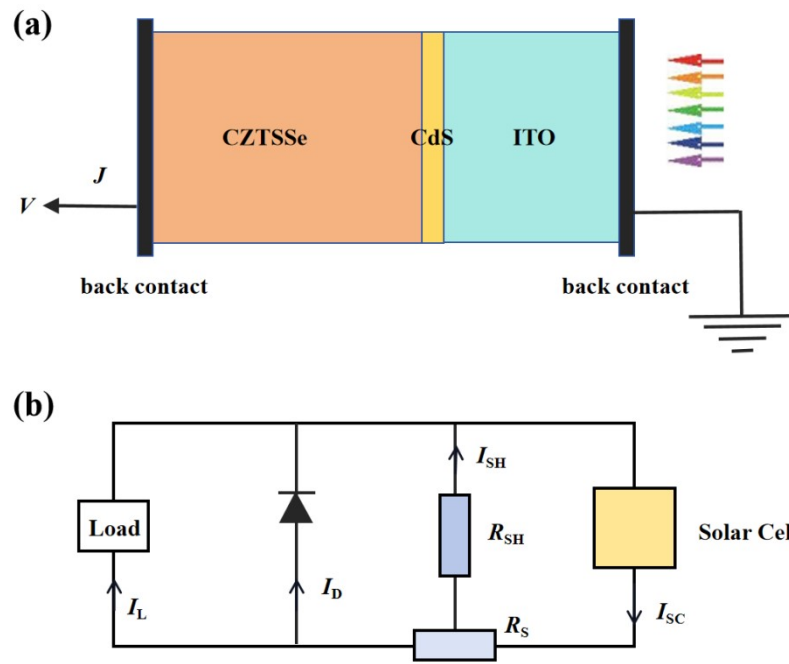


Figure S8 (a) Schematic view of illumination position in the simulation model device,
(c) Equivalent electrical network of a solar cell under illumination.

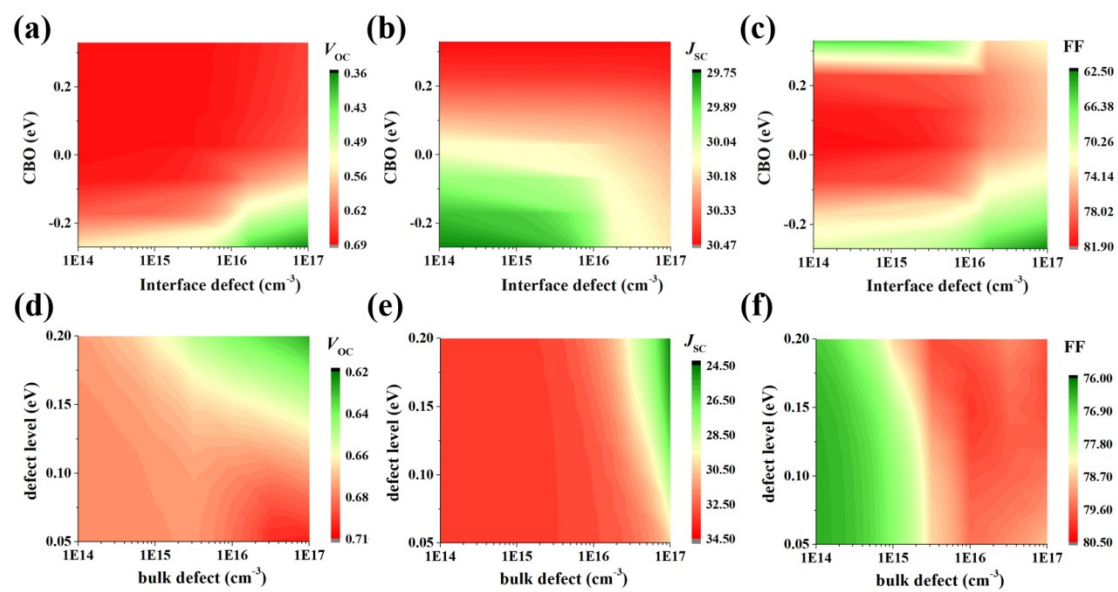


Figure S9 Device performance versus (a-c) CBO, interface defect and (d-f) bulk defect for simulated CZTSSe devices.

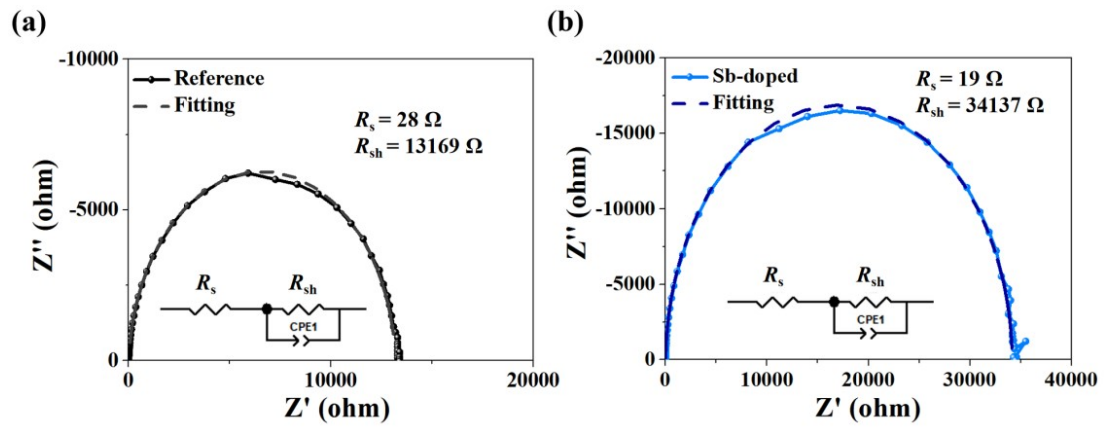


Figure S10 Device equivalent circuit diagram and the EIS plots with the (a) Reference and (b) Sb-doped films.