

Supplementary information

**Spectroscopic and Electrical Signatures of Acceptor States in
Solution Processed $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$ Solar Cells**

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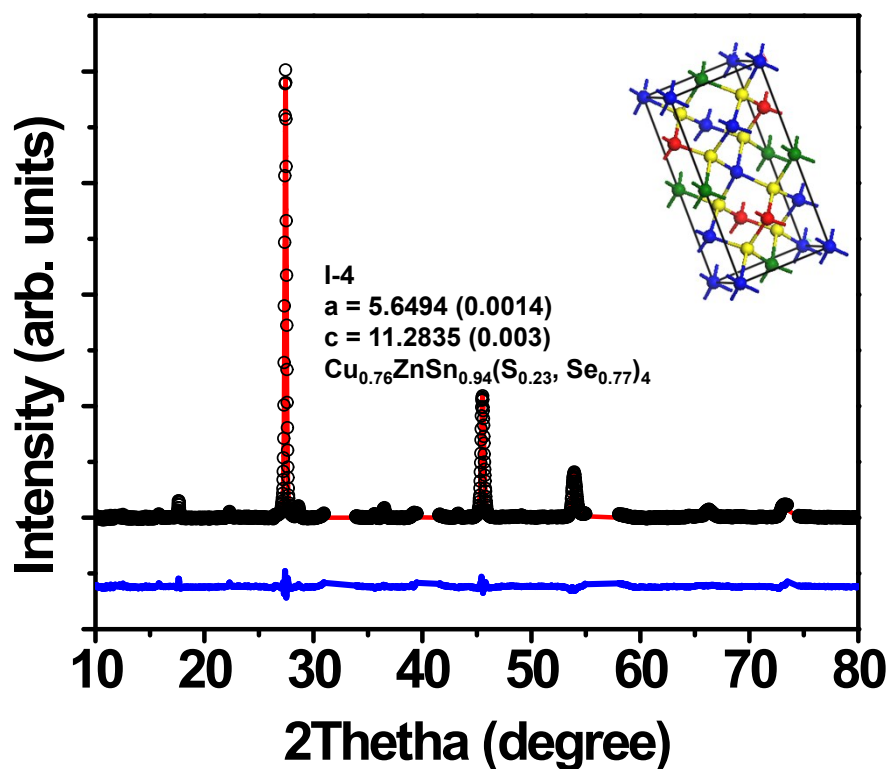


Figure s1: Quantitative Rietveld analysis of CZTSSe X-ray diffraction pattern, Inset shows the schematic of kesterite structure.

Table s1: Structural parameters derived from full profile Rietveld refinement of selective region of CZTSSe peaks in X-diffractogram.

Cu₂ZnSn(S,Se)₄

Symmetry/ Space group	Tetragonal: I-4 (82)	
Quality of fitting	$R_{wp} = 5.23\%$; $R_p = 3.82\%$	
Lattice parameters	a	$5.6494 \pm 0.0014 \text{ \AA}$
	c	$11.2835 \pm 0.0035 \text{ \AA}$

Element	Wyckoff	x	y	z	occupancy
Cu	2a	0	0	0	0.7654
Zn	2d	0	0.5	0.75	1
Sn	2b	0	0	0.5	0.8988
Cu	2c	0	0.5	0.25	0.8363
S	8g	0.2504 ± 0.0032	0.2576 ± 0.0041	0.1283 ± 0.0067	0.2277
Se	8g	0.2504 ± 0.0032	0.2576 ± 0.0041	0.1283 ± 0.0067	0.7723

Table s2: Distribution of key cell parameters measured across 20 CZTSSe devices under simulated AM1.5G spectrum with power density of 100 mW/cm².

	V_{OC} (mV)	J_{SC} (mA/cm²)	FF (%)	Efficiency (%)
Best	396	27.8	52.05	5.71
Mean	370	28.86	44.7	4.86
Std. Dev.	33	4.26	6.8	1.01

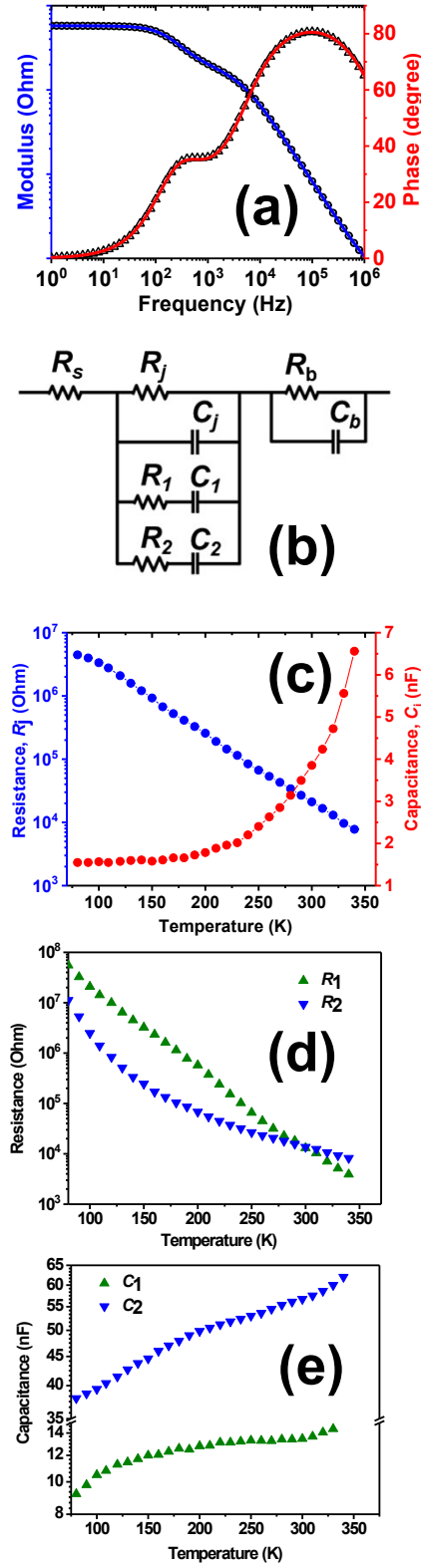


Figure s2: Low-temperature impedance spectroscopy of CZTSSe devices: (a) A typical spectrum with fitting and equivalent circuit used for fitting (b), temperature variation of (c) junction resistance, R_j and capacitance, C_j and of (d) resistances R_1 and R_2 and (e) capacitances C_1 and C_2 related to trap states.

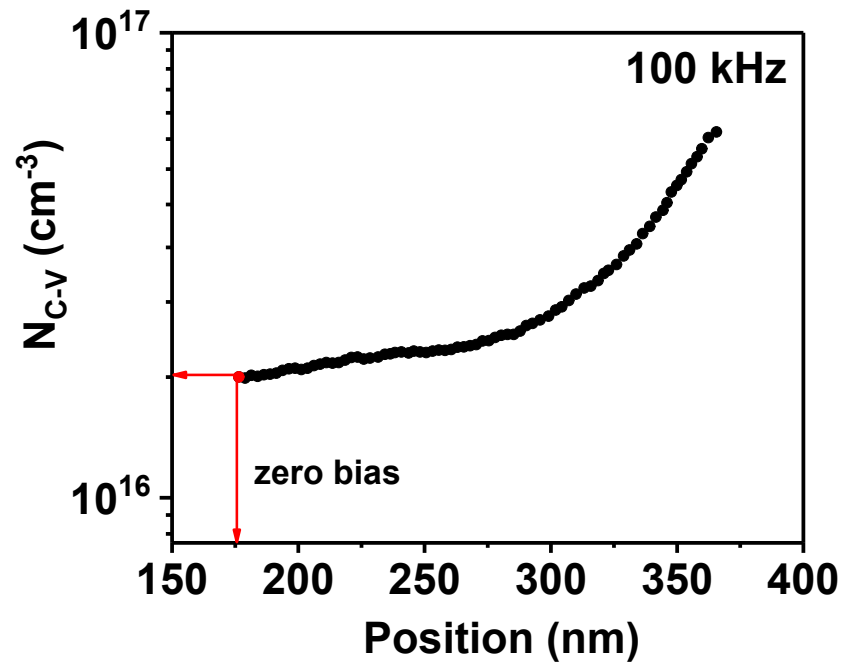


Figure s3: Capacitance-voltage profiling CZTSSe solar cell measured at 100 kHz and between 0 to -1.5 V with AC stimulus of 25 mV