

SUPPORTING INFORMATION

Supporting Information for

High thermoelectric performance based on CsSnI₃ thin films with improved stability

Weidong Tang,^a Tianjun Liu^a and Oliver Fenwick^{a}*

*^a School of Engineering and Materials Science, Queen Mary University of
London, Mile End Road, London E1 4NS, United Kingdom;*

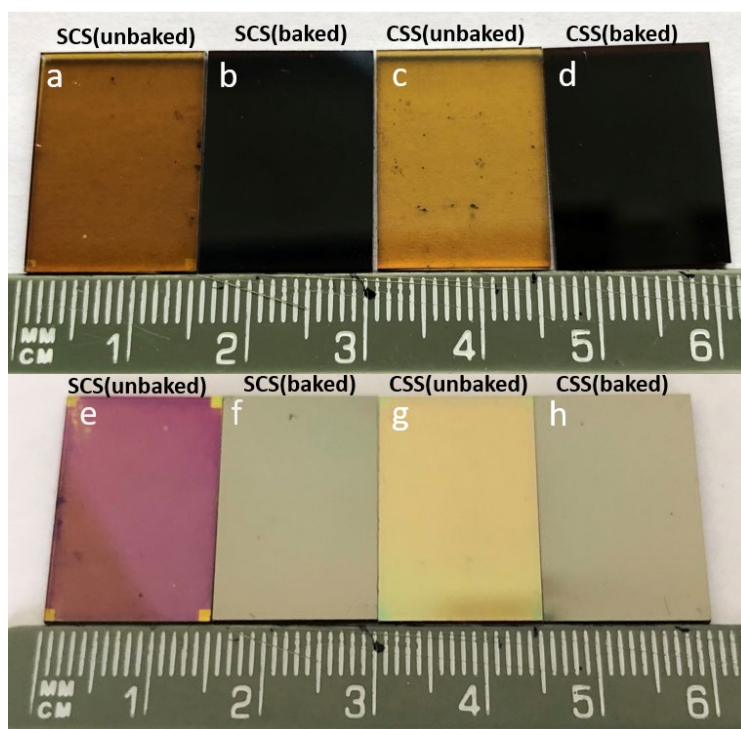


Figure S1. Optical images of the two types CsSnI_3 thin films before and after annealing steps. (a-d) Back-lit films and (e-h) front-lit films.

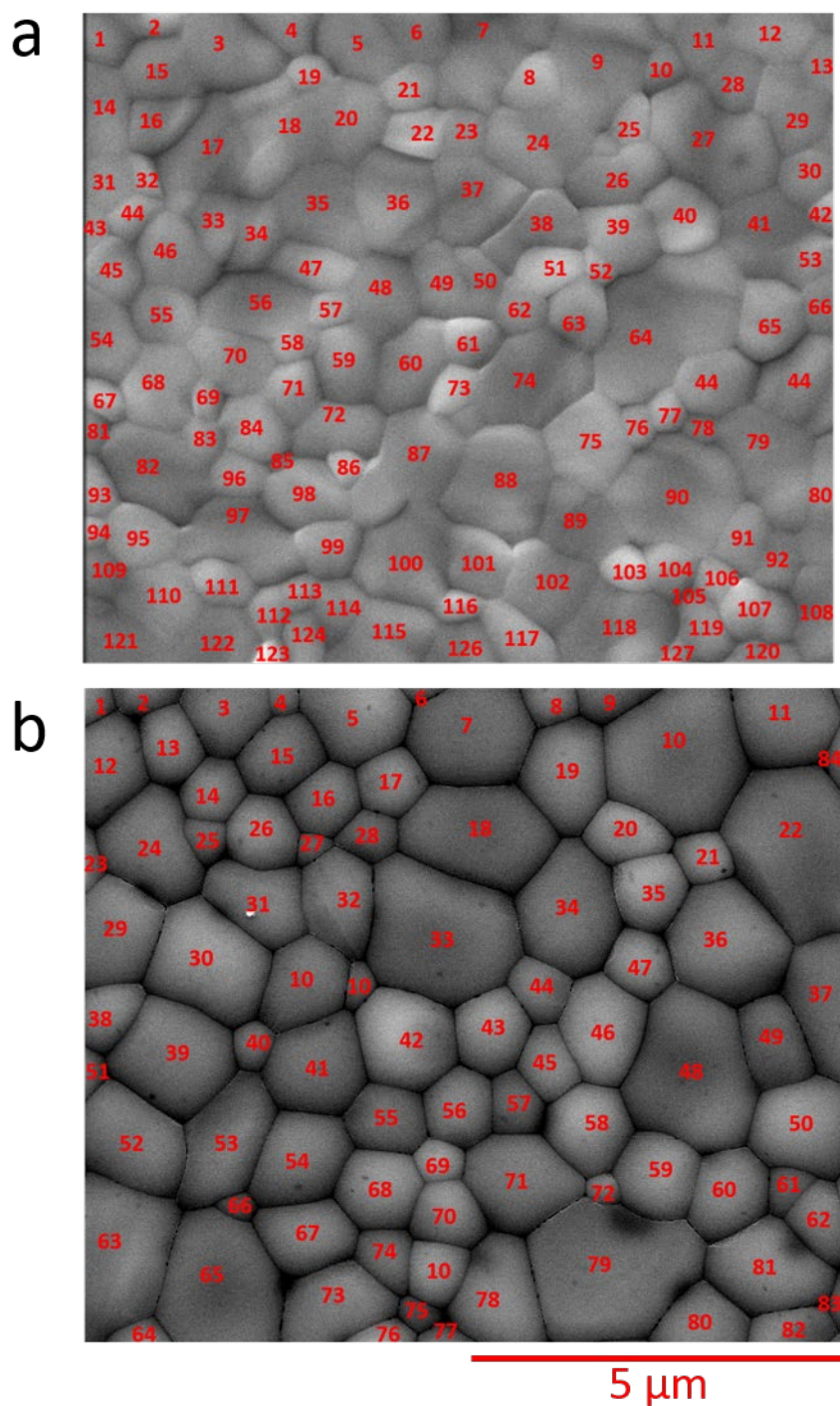


Figure S2. Grain counts and average grain size calculation of CsSnI_3 thin films **(a)** CSS and **(b)** SCS.

$$\text{The average grain size} = \frac{\text{total area}}{\text{total number}}$$

$$\text{The average grain size of SCS} = 1.06 \mu\text{m}^2$$

$$\text{The average grain size of CSS} = 0.71 \mu\text{m}^2$$

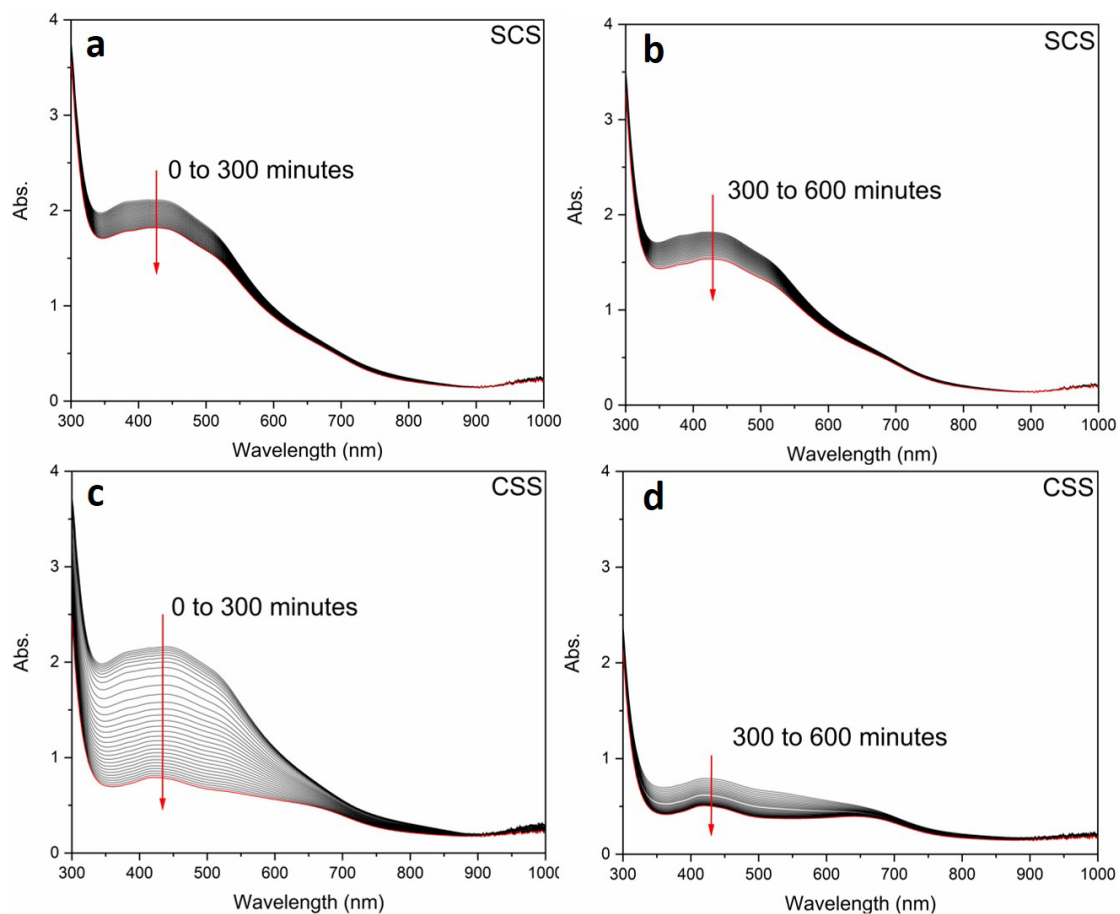


Figure S3. UV-vis absorption spectra of the two types CsSnI_3 thin films. Time dependent UV-vis absorption spectra of SCS CsSnI_3 thin films **(a)** from 0 to 300 minutes and **(b)** from 300 to 600 minutes. Time dependent UV-vis absorption spectra of CSS CsSnI_3 thin films **(c)** from 0 to 300 minutes and **(d)** from 300 to 600 minutes.

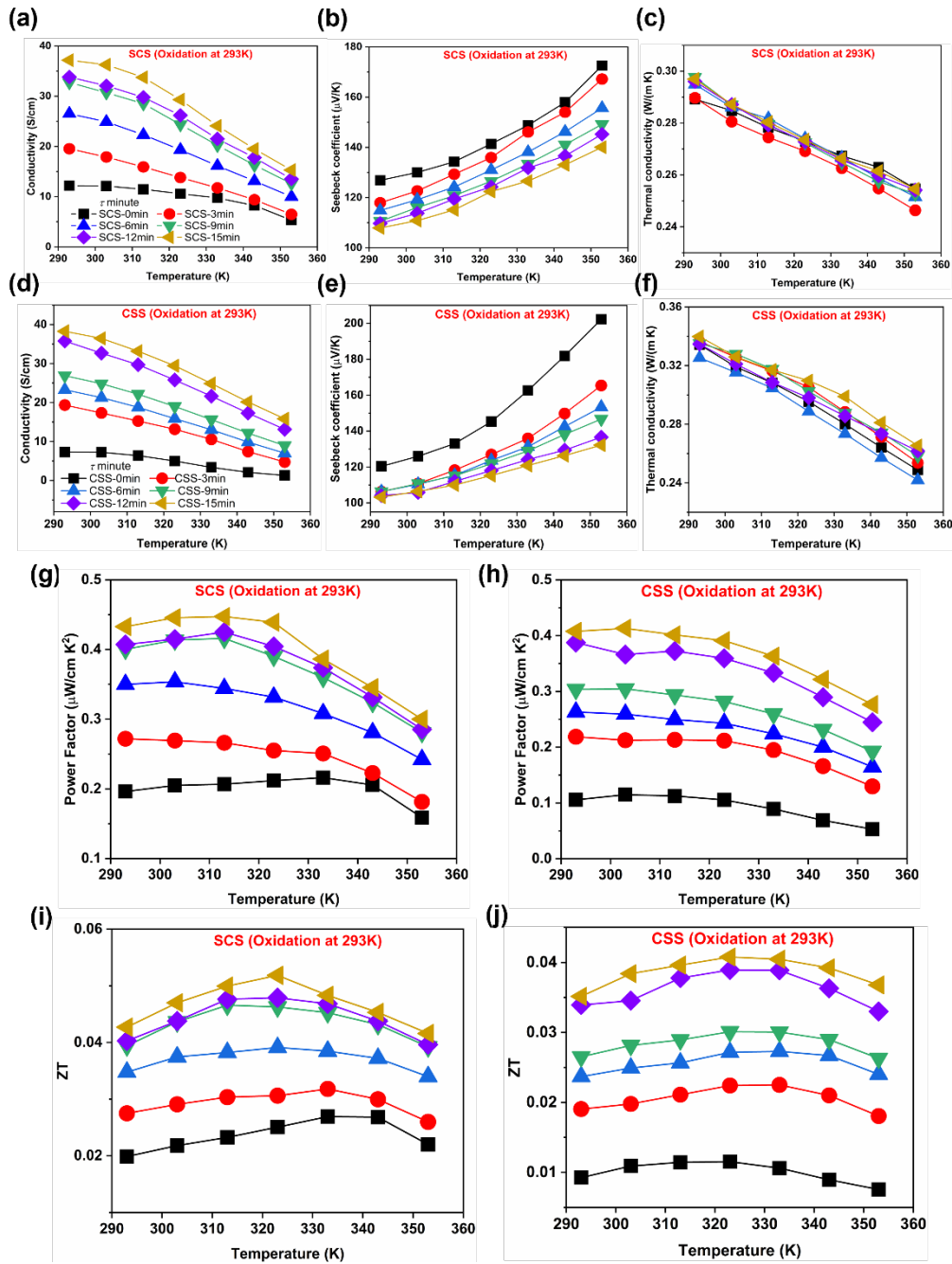


Figure S4. Thermoelectric properties of the two types CsSnI_3 thin films oxidised at 20 °C. Temperature dependent electrical conductivity, σ (a), Seebeck coefficient, S (b), thermal conductivity, κ_{total} (c), power factor, PF (g) and figure-of-merit, zT (i), of SCS CsSnI_3 thin films with air exposure at 20 °C. Temperature dependent electrical conductivity, σ (d), Seebeck coefficient, S (e), thermal conductivity, κ_{total} (f), power factor, PF (h) and figure-of-merit, zT (j) of CSS CsSnI_3 thin films with air exposure at 20 °C.

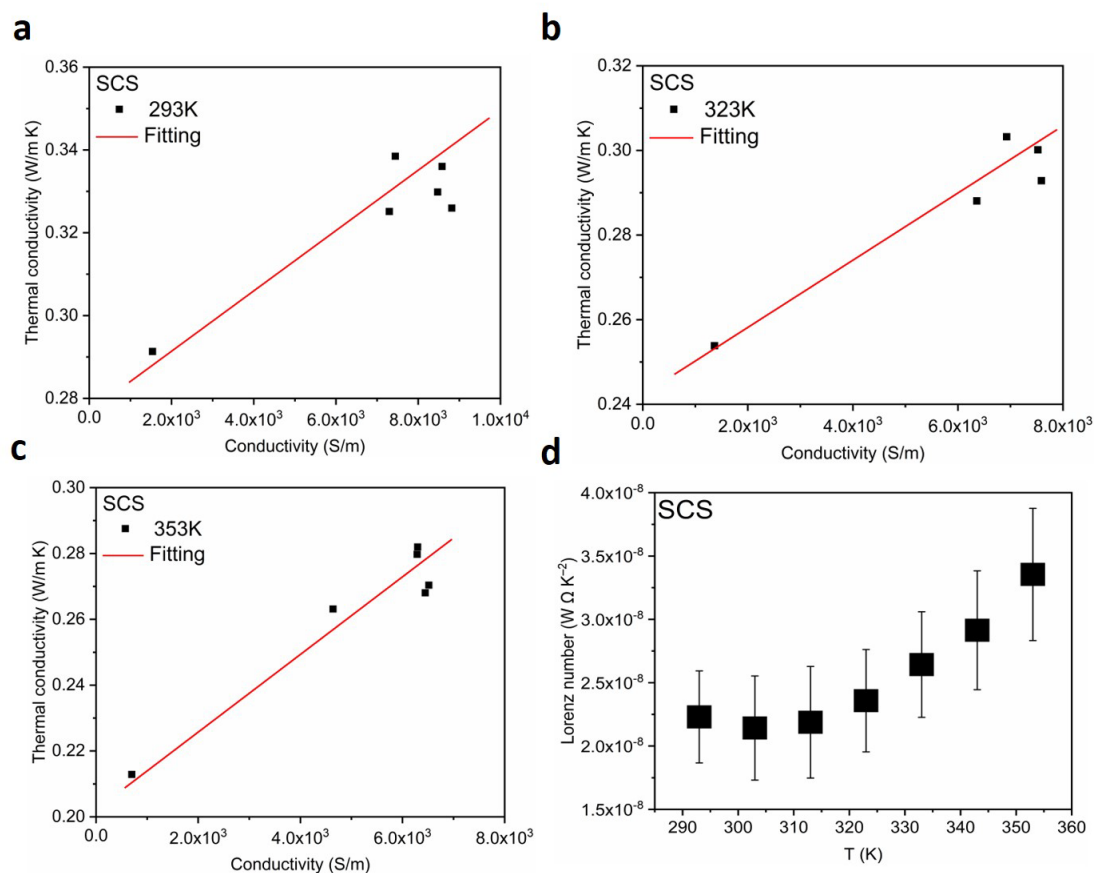


Figure S5. The relationship between thermal conductivity (total) and electrical conductivity of SCS CsSnI_3 thin films. **(a-c)** The total thermal conductivity as a function of electrical conductivity with linear fitting at 293 K, 323 K and 353 K. **(d)** Temperature dependence of Lorenz number from 293 K to 353 K.

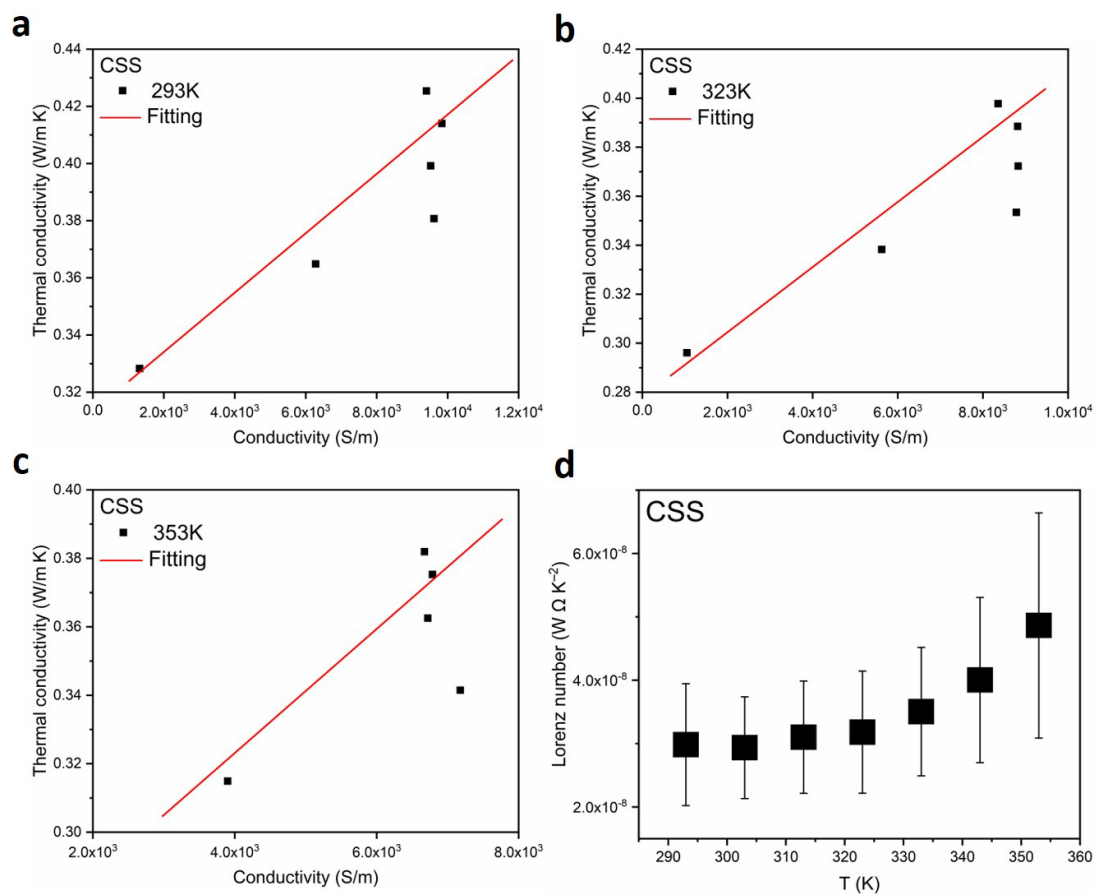


Figure S6. The relationship between thermal conductivity (total) and electrical conductivity of CSS CsSnI_3 thin films. **(a-c)** The total thermal conductivity as a function of electrical conductivity with linear fitting at 293 K, 323 K and 353 K. **(d)** Temperature dependence of Lorenz number from 293 K to 353 K.

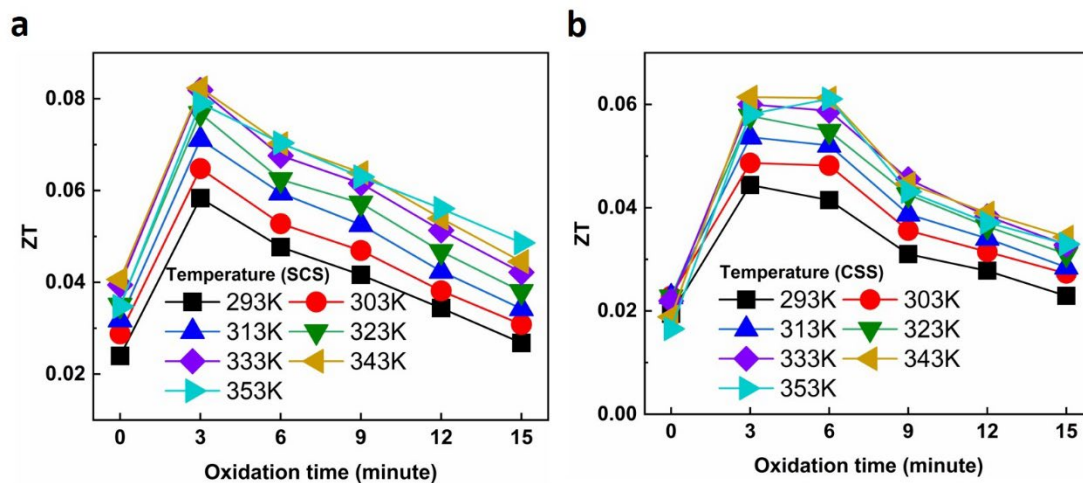


Figure S7. The Figure of merit, zT , stability measurement of CsSnI_3 thin films oxidised at 80°C . (a) zT of a SCS film and (b) zT of a CSS film.

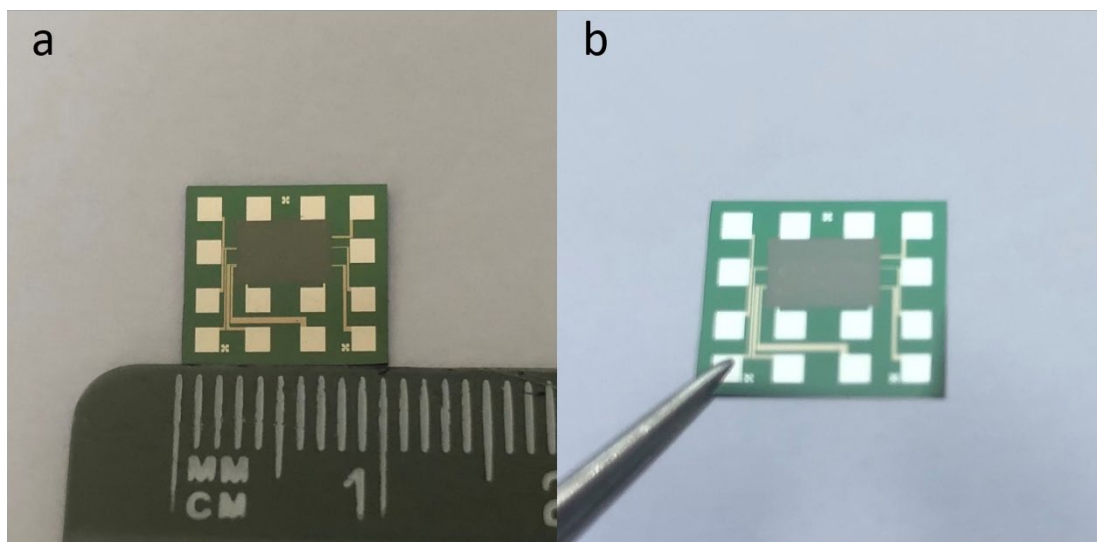


Figure S8. Images of thermoelectrical property measurement chips with deposited CsSnI_3 thin films.

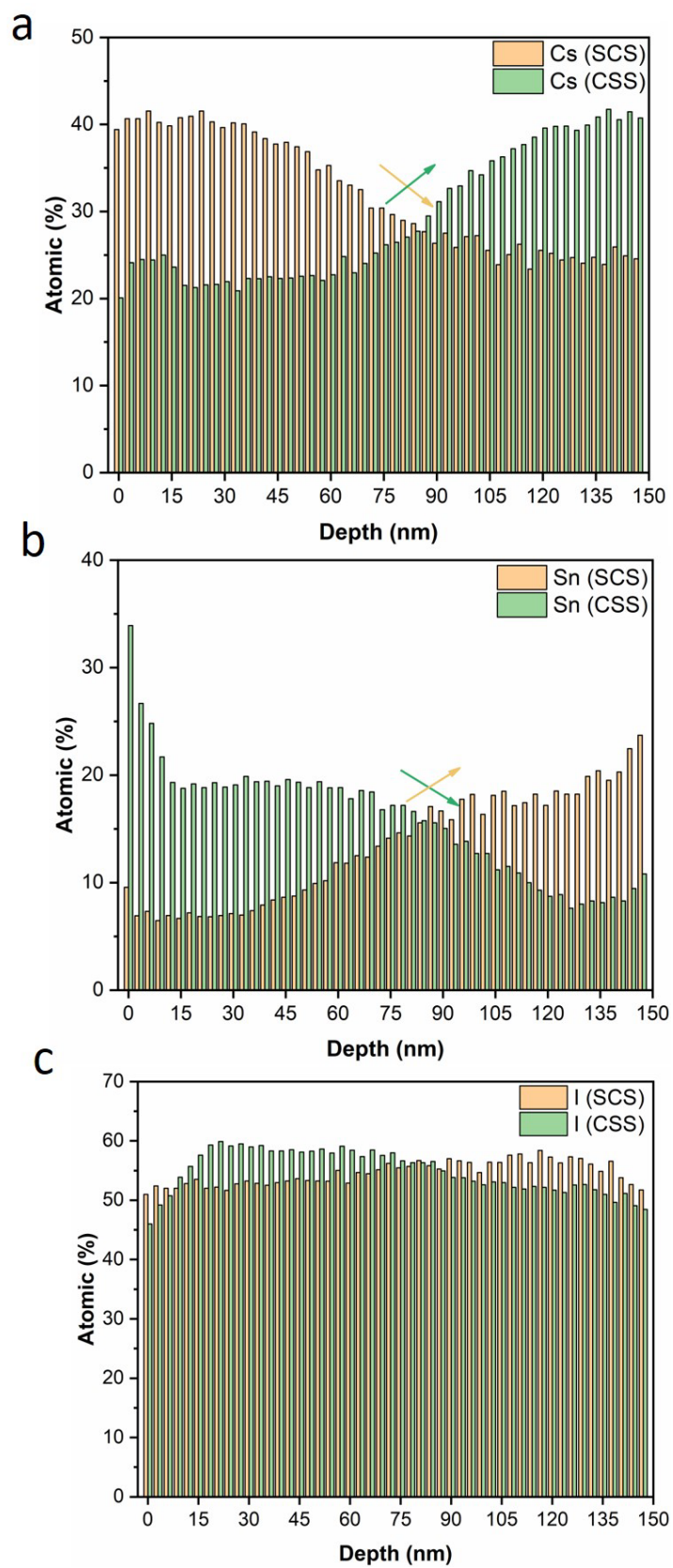


Figure S9. XPS depth profile of elemental concentration for CsSnI_3 thin films (from 0 to 150 nm). (a) Cesium (b) Tin (c) Iodide.

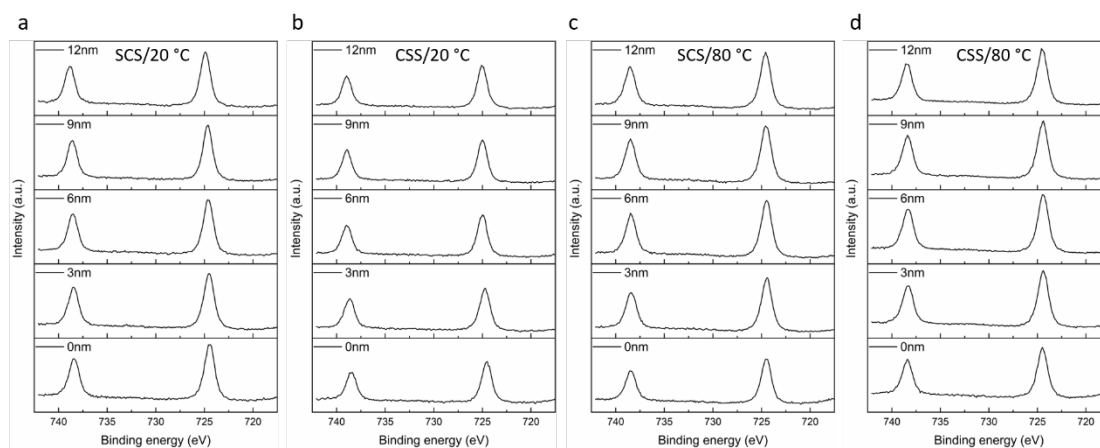


Figure S10. XPS depth profile of Cs 3d (Caesium) for CsSnI_3 thin films (from 0 to 12 nm). (a) SCS film oxidised at 20 °C (b) CSS film oxidised at 20 °C (c) SCS oxidised at 80 °C (d) CSS oxidised at 80 °C.

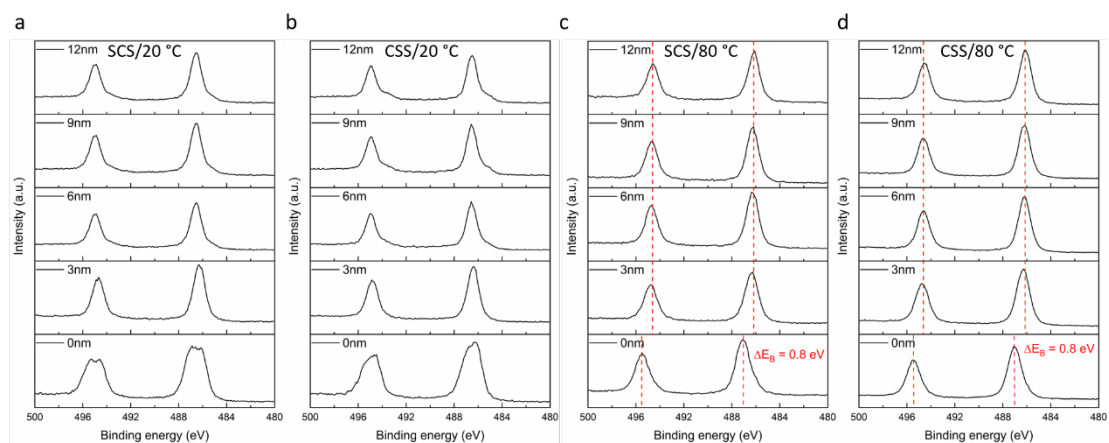


Figure S11. XPS depth profile of Sn 3d (Tin) for CsSnI₃ thin films (from 0 to 12 nm).
(a) SCS film oxidised at 20 °C **(b)** CSS film oxidised at 20 °C **(c)** SCS oxidised at 80 °C **(d)** CSS oxidised at 80 °C.

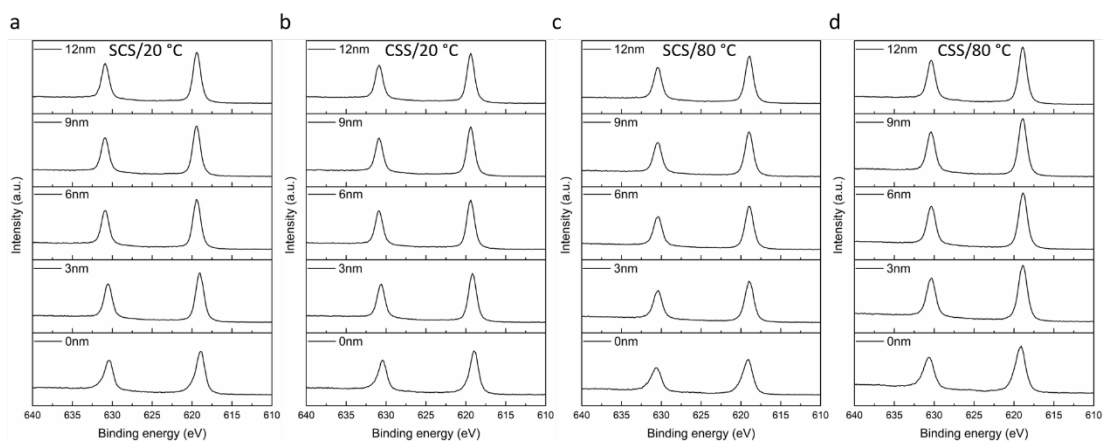


Figure S12. XPS depth profile of I 3d (Iodide) for CsSnI₃ thin films (from 0 to 12 nm).
(a) SCS film oxidised at 20 °C **(b)** CSS film oxidised at 20 °C **(c)** SCS oxidised at 80 °C **(d)** CSS oxidised at 80 °C.

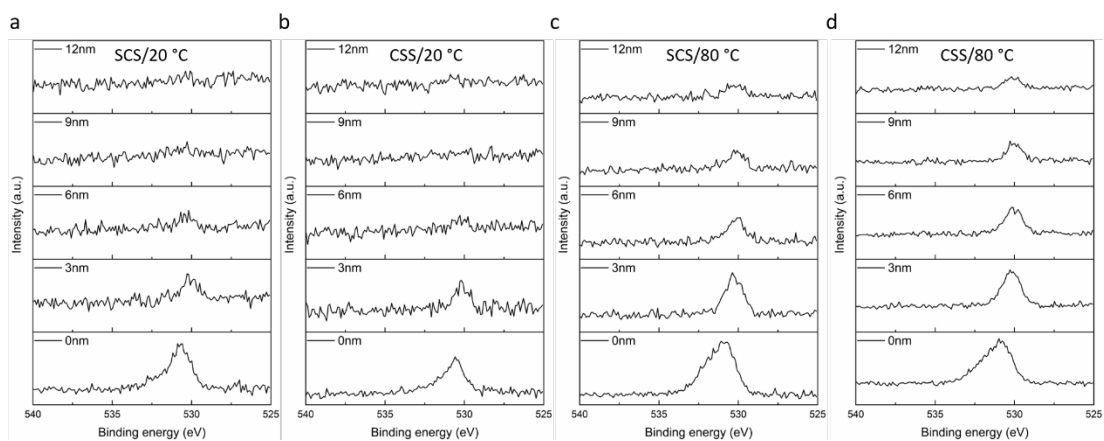


Figure S13. XPS depth profile of O 1s (Oxygen) for CsSnI₃ thin films (from 0 to 12 nm). (a) SCS film oxidised at 20 °C (b) CSS film oxidised at 20 °C (c) SCS oxidised at 80 °C (d) CSS oxidised at 80 °C.

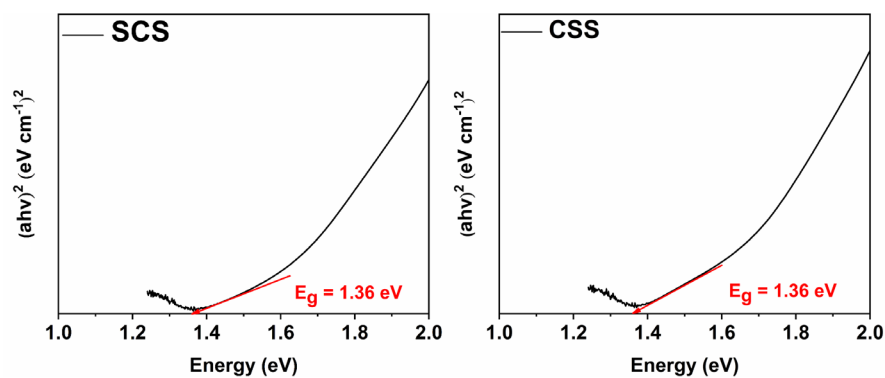


Figure S14 Tauc plots of the absorption spectra of SCS and CSS CsSnI_3 thin films, confirming a band gap of 1.36 eV in both cases.

Table S1: Auger peaks of reference Sn metal (Sn^0) and our CsSnI_3 thin films.

Sample (ev)	$\text{M}_5\text{N}_{4,5}\text{N}_{4,5}$					$\text{M}_4\text{N}_{4,5}\text{N}_{4,5}$	
	peak a	peak b				peak c	peak d
	$^1\text{S}_0$	$^1\text{G}_4$	$^3\text{P}_2$	$^3\text{F}_{2,3}$	$^3\text{F}_4$	$^1\text{G}_4^1\text{D}_2$	$^3\text{F}_{2,3}$
Barlow* Ref. ¹	421.3	425.6	426.8	427.9	428.7	434.1	436.3
Pessa Ref. ²	422.9	425.6		427.6		434.1	
SCS-20(0nm)	422.5	426.4				432.7	436.1
SCS-20(3nm)	421.5	427.2				433.1	435.3
SCS-20(6nm)	421.2	427.8					435.3
SCS-20(9nm)	421.3	428					435.6
SCS-20(12nm)	421.1	428					435.5
CSS-20(0nm)	422.8	426.7				432.7	435.6
CSS-20(3nm)	421.2	427.7				433.4	435.8
CSS-20(6nm)	421.3	428.1					435.5
CSS-20(9nm)	421.3	428.3					435.6
CSS-20(12nm)	421.6	428.2					435.6
SCS-80(0nm)	422.5	425.5				432	434.7
SCS-80(3nm)	421.3	426.4				433.4	435.6
SCS-80(6nm)	421.7	426.8				433.7	435.9
SCS-80(9nm)	421.8	427.2					435
SCS-80(12nm)	421.6	428					435.6
CSS-80(0nm)	423.1	425.5				432.4	435.5
CSS-80(3nm)	421.3	426.5				433.6	436.2
CSS-80(6nm)	421.5	426.9				433.9	435.8
CSS-80(9nm)	421.6	427.2					435
CSS-80(12nm)	421.8	427.7					435.4

Table S2: Experimental binding, Auger kinetic energy values and Auger parameter for SCS and CSS films compare to references.

Sample	E_b 3d _{5/2} (ev)	* ΔE_b 3d _{5/2} (oxide-metal) (ev)	E_k M ₅ N ₄₅ N ₄₅ (ev)	* ΔE_k (oxide-metal) (ev)	α' (ev)	Ref.
Sn-metal	483.8		431.6		915.4	³
Sn-metal	484.9		430		914.9	⁴
SnO	486.4	2.6	426.2	5.4	912.6	⁴
SnO ₂	487.1	3.3	424.1	7.5	911.2	⁴
SCS-20(0nm)	486.6	2.8	426.4	5.2	913.0	This work
SCS-20(3nm)	486.4	2.6	427.2	4.4	913.6	This work
SCS-20(6nm)	486.6	2.8	427.8	3.8	914.4	This work
SCS-20(9nm)	486.6	2.8	428.0	3.6	914.6	This work
SCS-20(12nm)	486.6	2.8	428.0	3.6	914.6	This work
CSS-20(0nm)	486.4	2.6	426.7	4.9	913.1	This work
CSS-20(3nm)	486.5	2.7	427.7	3.9	914.2	This work
CSS-20(6nm)	486.6	2.8	428.1	3.5	914.7	This work
CSS-20(9nm)	486.6	2.8	428.3	3.3	914.9	This work
CSS-20(12nm)	486.6	2.8	428.2	3.4	914.8	This work
SCS-80(0nm)	487.1	3.3	425.5	6.1	912.6	This work
SCS-80(3nm)	486.3	2.5	426.4	5.2	912.7	This work
SCS-80(6nm)	486.4	2.6	426.8	4.8	913.2	This work
SCS-80(9nm)	486.2	2.4	427.2	4.4	913.4	This work
SCS-80(12nm)	486.3	2.5	428.0	3.6	914.3	This work
CSS-80(0nm)	487.1	3.3	425.5	6.1	912.6	This work
CSS-80(3nm)	486.3	2.5	426.5	5.1	912.8	This work
CSS-80(6nm)	486.2	2.4	426.9	4.7	913.1	This work
CSS-80(9nm)	486.2	2.4	427.2	4.4	913.4	This work
CSS-80(12nm)	486.1	2.3	427.5	3.9	913.8	This work

Supporting References

1. S. Barlow, P. Bayat-Mokhtari and T. E. Gallon, *Journal of Physics C: Solid State Physics*, 1979, **12**, 5577-5584.
2. M. Pessa, S. Aksela and M. Karras, *Physics Letters A*, 1970, **31**, 382-383.
3. A. F. Lee and R. M. Lambert, *Physical Review B*, 1998, **58**, 4156-4165.
4. L. Kövér, Z. Kovács, R. Sanjinés, G. Moretti, I. Cserny, G. Margaritondo, J. Pálinkás and H. Adachi, *Surface and Interface Analysis*, 1995, **23**, 461-466.