Supporting Information

Transport Limitations and Defect-Mediated Recombination in Lead-Free Double Perovskite Cs_2AgSbI_6: Implications for Solar-Cell Design

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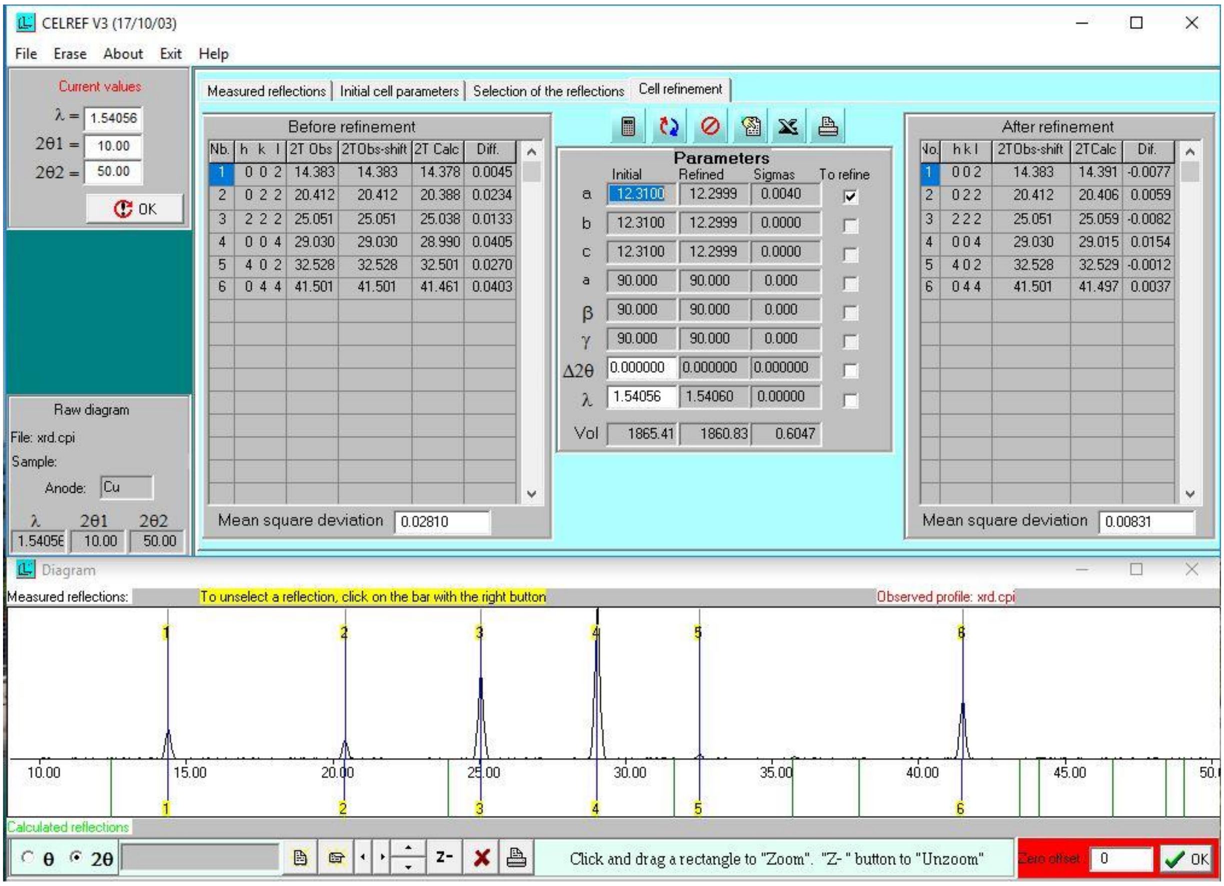
S1. Supplementary Figures



Current values

λ = 1.54056
2θ1 = 10.00
2θ2 = 50.00

Raw diagram

File: xrd.cpi
Sample:
Anode: Cu

λ	2θ1	2θ2
1.5405€	10.00	50.00

Before refinement

Nb.	h k l	2T Obs	2TObs-shift	2T Calc	Diff.
1	0 0 2	14.383	14.383	14.378	0.0045
2	0 2 2	20.412	20.412	20.388	0.0234
3	2 2 2	25.051	25.051	25.038	0.0133
4	0 0 4	29.030	29.030	28.990	0.0405
5	4 0 2	32.528	32.528	32.501	0.0270
6	0 4 4	41.501	41.501	41.461	0.0403

Mean square deviation 0.02810

Parameters

	Initial	Refined	Sigmas	To refine
a	12.3100	12.2999	0.0040	☑
b	12.3100	12.2999	0.0000	☐
c	12.3100	12.2999	0.0000	☐
a	90.000	90.000	0.000	☐
β	90.000	90.000	0.000	☐
γ	90.000	90.000	0.000	☐
Δ2θ	0.000000	0.000000	0.000000	☐
λ	1.54056	1.54060	0.00000	☐
Vol	1865.41	1860.83	0.6047	

After refinement

No.	h k l	2TObs-shift	2TCalc	Dif.
1	0 0 2	14.383	14.391	-0.0077
2	0 2 2	20.412	20.406	0.0059
3	2 2 2	25.051	25.059	-0.0082
4	0 0 4	29.030	29.015	0.0154
5	4 0 2	32.528	32.529	-0.0012
6	0 4 4	41.501	41.497	0.0037

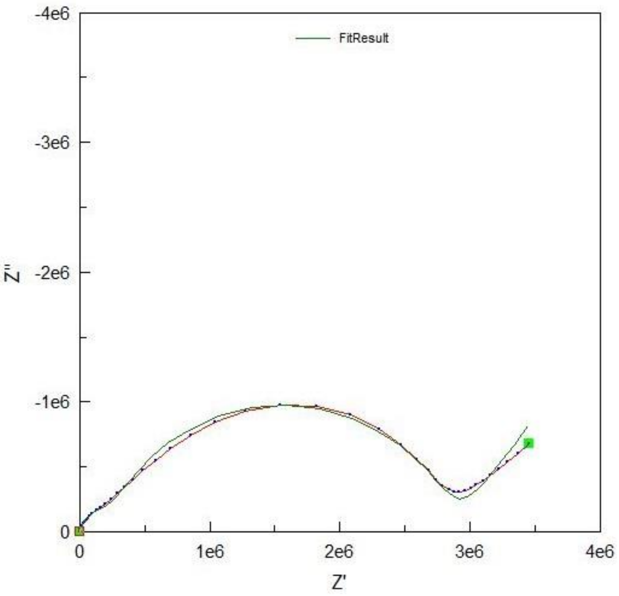
Mean square deviation 0.00831

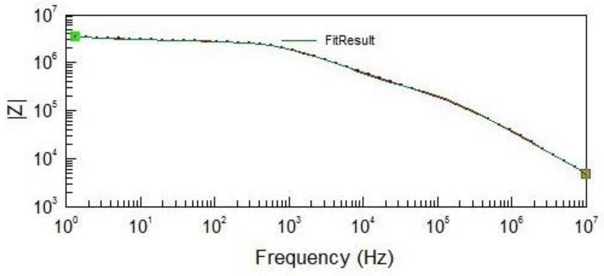
To unselect a reflection, click on the bar with the right button

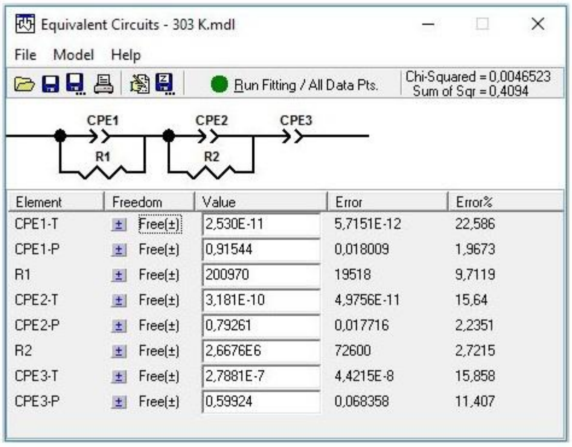
Click and drag a rectangle to "Zoom". "Z- " button to "Unzoom"

Zero offset 0

Figs. S1. CELREF refinement of the room-temperature X-ray diffraction pattern of polycrystalline Cs_2AgSbI_6 assuming a cubic double-perovskite structure.







Chi-Squared = 0,0046523
Sum of Sqr = 0,4094

Element	Freedom	Value	Error	Error%
CPE1-T	Free(±)	2,530E-11	5,7151E-12	22,586
CPE1-P	Free(±)	0,91544	0,018009	1,9673
R1	Free(±)	200970	19518	9,7119
CPE2-T	Free(±)	3,181E-10	4,9756E-11	15,64
CPE2-P	Free(±)	0,79261	0,017716	2,2351
R2	Free(±)	2,6676E6	72600	2,7215
CPE3-T	Free(±)	2,7881E-7	4,4215E-8	15,858
CPE3-P	Free(±)	0,59924	0,068358	11,407

Figs. S2. Representative impedance spectrum of polycrystalline Cs_2AgSbI_6 measured at 303 K under dark conditions together with the corresponding equivalent-circuit fitting.

S2. SCAPS-1D simulation methodology and input parameters

umerical simulations were performed using SCAPS-1D version 3.3.09 (ELIS–UGent). The simulated device architecture corresponds to:

FTO / TiO_2 / Cs_2AgSbI_6 / Spiro-OMeTAD / metal contact

All simulations were carried out at 300 K under AM1.5G illumination (1000 W m^{-2}) unless otherwise stated. The simulations were designed to translate experimentally observed bulk recombination and transport limitations into a device-level framework, rather than to model an optimized photovoltaic device.

S3. Bulk material parameters

Table S1. SCAPS-1D input parameters for Spiro-OMeTAD (HTL)

Parameter	**Symbol**	**Value**	**Unit**
Thickness	d	200	nm
Band gap	E_g	3.0	eV
Electron affinity	χ	2.4	eV
Dielectric constant	ε_r	3.0	–
Electron mobility	μ_n	2×10^{-4}	$cm^2\ V^{-1}\ s^{-1}$
Hole mobility	μ_p	2×10^{-4}	$cm^2\ V^{-1}\ s^{-1}$
Acceptor density	N_A	1×10^{18}	cm^{-3}
Donor density	N_D	0	cm^{-3}

Table S2. SCAPS-1D input parameters for Cs_2AgSbI_6 absorber

Parameter	**Symbol**	**Value**	**Unit**
Thickness	d	600	nm
Band gap	E_g	1.65	eV
Electron affinity	χ	4.0	eV
Dielectric constant	ε_r	10.0	–
Electron mobility	μ_n	1.0	$cm^2\ V^{-1}\ s^{-1}$
Hole mobility	μ_p	0.5	$cm^2\ V^{-1}\ s^{-1}$
Acceptor density	N_A	1×10^{15}	cm^{-3}
Donor density	N_D	0	cm^{-3}

Bulk defect density	N_t	$5\times10^{18} - 1\times10^{20}$	cm^{-3}
Defect type	–	Neutral	–
Defect energy level	E_t	$E_c - 0.10$	eV
Electron lifetime	τ_n	0.01	ns
Hole lifetime	τ_p	0.01	ns

Table S3. SCAPS-1D input parameters for TiO_2 (ETL)

Parameter	**Symbol**	**Value**	**Unit**
Thickness	d	50	nm
Band gap	E_g	3.2	eV
Electron affinity	χ	4.0	eV
Dielectric constant	ε_r	9.0	–
Electron mobility	μ_n	10	$cm^2\ V^{-1}\ s^{-1}$
Hole mobility	μ_p	1×10^{-4}	$cm^2\ V^{-1}\ s^{-1}$
Donor density	N_D	1×10^{18}	cm^{-3}

Table S4. SCAPS-1D input parameters for FTO (TCO)

Parameter	**Symbol**	**Value**	**Unit**
Thickness	d	500	nm
Band gap	E_g	3.5	eV
Electron affinity	χ	4.0	eV
Dielectric constant	ε_r	9.0	–

Electron mobility	μ_n	20	cm^2 V^{-1} s^{-1}
Donor density	N_D	1×10^{20}	cm^{-3}

S3. Interface defect parameters

Table S5. Interface defect states

Interface	**N_t**	**Unit**	**E_t**	**$S_n = S_p$**
Spiro-OMeTAD / Cs_2AgSbI_6	1×10^{14}	cm^{-2}	E_i	1×10^4 cm s^{-1}
Cs_2AgSbI_6 / TiO_2	1×10^{12}	cm^{-2}	E_i	1×10^2 cm s^{-1}

All interface states were assumed neutral with single-level energy distributions.

S4. Contact parameters

Table S6. Electrical contact properties

Contact	**Work function (eV)**	**Electron SRV (cm s^{-1})**	**Hole SRV (cm s^{-1})**
Back contact (metal / Spiro-OMeTAD)	5.1	1×10^5	1×10^7
Front contact (FTO / TiO_2)	4.4	1×10^7	1×10^5

Ohmic contacts were intentionally assumed to isolate bulk and interfacial recombination effects from contact-limited transport.

S5. Numerical and measurement conditions (Action Panel settings)

The current–voltage characteristics were calculated using the following numerical settings:

- Temperature: 300 K
- Illumination spectrum: AM1.5G (1000 W m^{-2})
- Voltage scan range: −0.20 V to +1.20 V
- Voltage step: 0.01 V

- Number of points: 141
- Series resistance: $R_s = 10\ \Omega\cdot\text{cm}^2$
- Shunt resistance: $R_{sh} = 1\times10^{30}\ \Omega\cdot\text{cm}^2$
- Radiative and Auger recombination: neglected
- Recombination mechanism: Shockley–Read–Hall (SRH)

Dark and illuminated conditions were simulated using identical numerical settings, except for the illumination source.

S6. Reproducibility statement

All figures reported in the main manuscript were generated using the parameters summarized above. The Supplementary Information provides full numerical transparency to ensure reproducibility and facilitate comparison with future experimental and simulation studies.