Supplementary Information: Cl Alloying Improves Thermal Stability and Increases Luminescence in Iodine-Rich Inorganic Perovskites

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Table S1 Material specifications. Vendor, purity, and weighing precision per chemical across all samples that were used for experiments.

Chemical	Purity (%)	Precision (% wt)
CsI	$\geq$99.999	$\leq$0.84% wt
PbI_2	$\geq$99.999	$\leq$0.93% wt
$PbBr_2$	$\geq$99.999	$\leq$2.36% wt
$PbCl_2$	$\geq$99.999	$\leq$4.5% wt
FAAc	$\geq$99	$\leq$4.9% wt
DMF	$\geq$99.8	$\leq 1\mu$L
DMSO	$\geq$99.9	$\leq 1\mu$L
MeOAc	$\geq$99.5	$\leq 1\mu$L

Table S2 Resulting de Wolff figure of merit, lattice constants, and volume of $CsPb(I_{0.80}Br_{0.20-x}Cl_x)_3$ films from DICVOL14 peak indexing.

Cl %	FoM	Lattice Constant a (Å)	Lattice Constant b (Å)	Lattice Constant c (Å)	Lattice Volume (Å³)
0	17.1	8.500±0.023	8.535±0.008	12.106±0.005	878.30±2.57
1	15.6	8.490±0.018	8.525±0.012	12.076±0.011	874.01±2.40
5	13.3	8.506±0.012	8.419±0.040	12.030±0.009	861.55±4.28
10	12.4	8.662±0.072	8.543±0.015	12.208±0.008	903.38±7.69

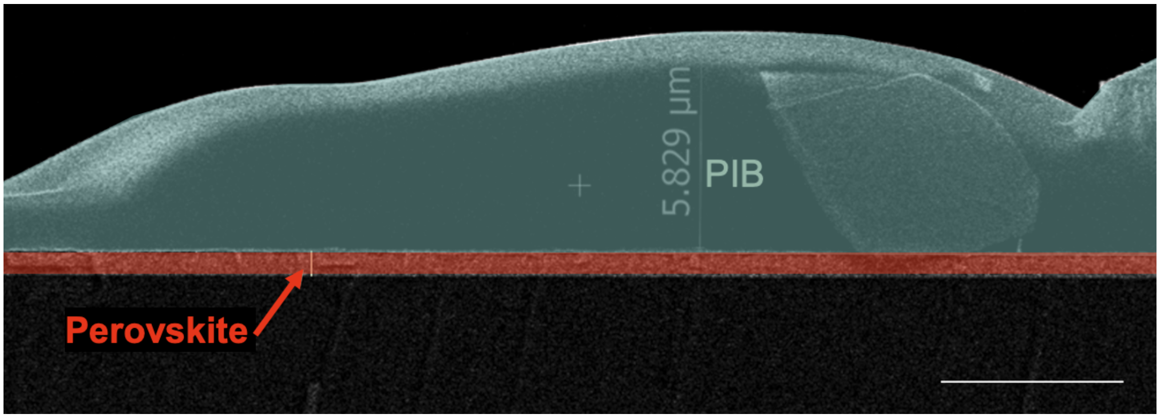

Figure S1 False color cross sectional SEM image with 5 μm scale bar of a $CsPbI_{0.80}Br_{0.2}$ film using an in-lens back scattered electron detector and 4000x magnification, showing an approximate perovskite thickness of 550nm. A thick layer of PIB (blue) was coated on top of the perovskite (red) to protect the perovskite layer during sample transfers for characterization to minimize exposure to the humid ambient environment.

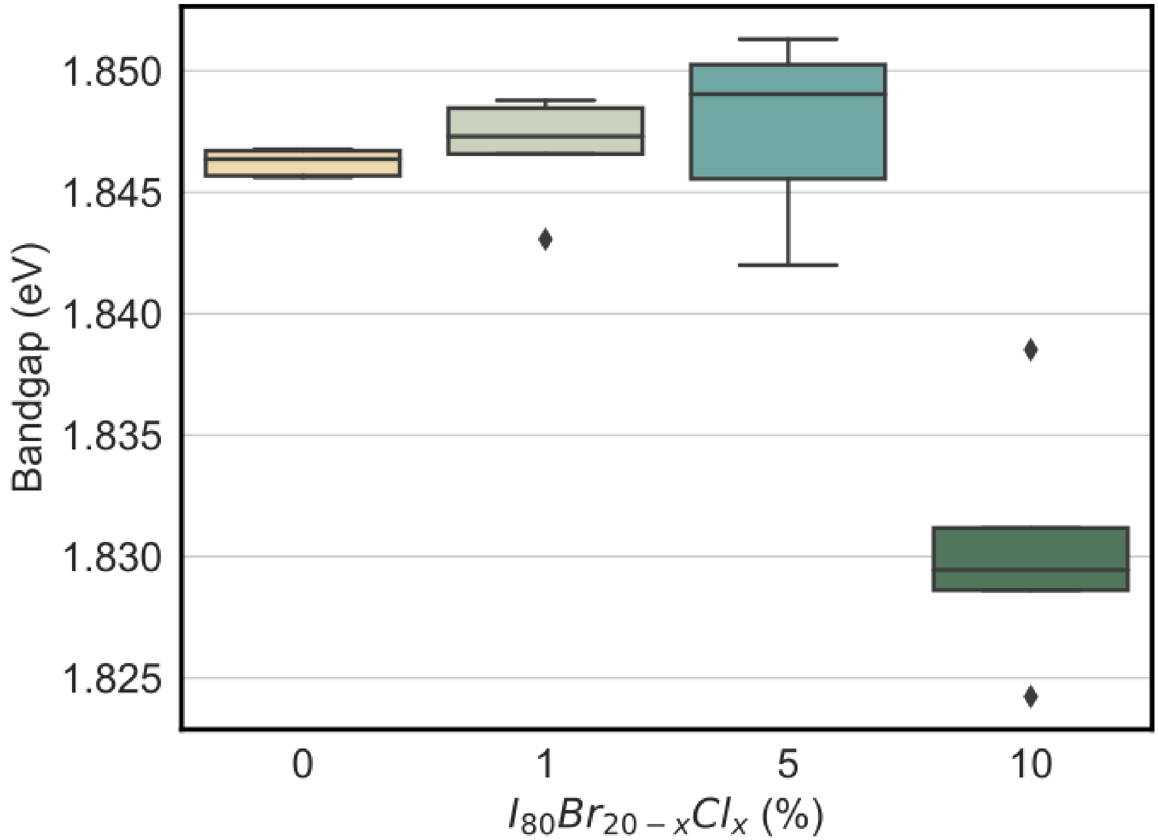

Figure S2 Box plots of estimated bandgap from direct Tauc plot analysis for each Cl loading ($CsPb(I_{0.80}Br_{0.20-x}Cl_x)_3$) film with 5 repeats per condition.

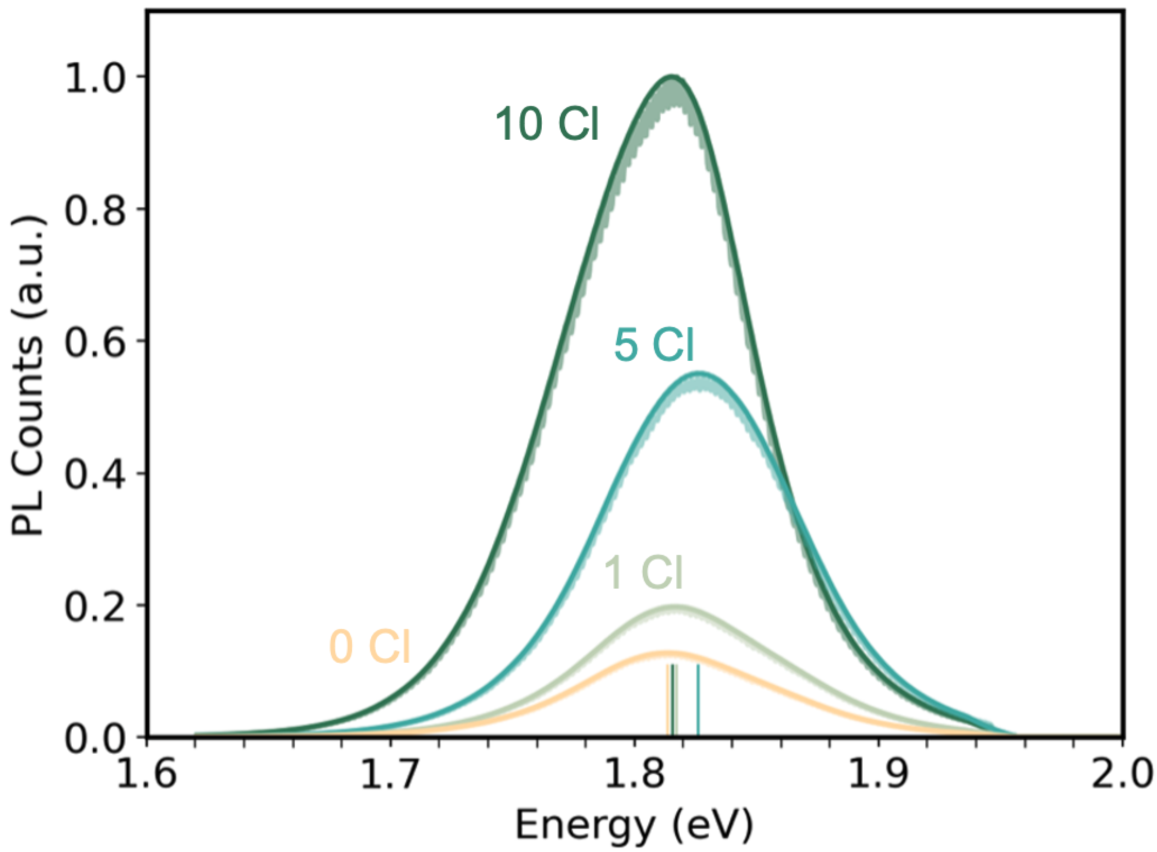

Figure S3 As-measured PL spectra (lighter color) and smoothed curve (darker) using a 1st order Savitzky-Golay filter with a filter-window size of 0.015eV to remove interference from the thin glass encapsulating layer on $CsPb(I_{0.80}Br_{0.20-x}Cl_x)_3$ films.

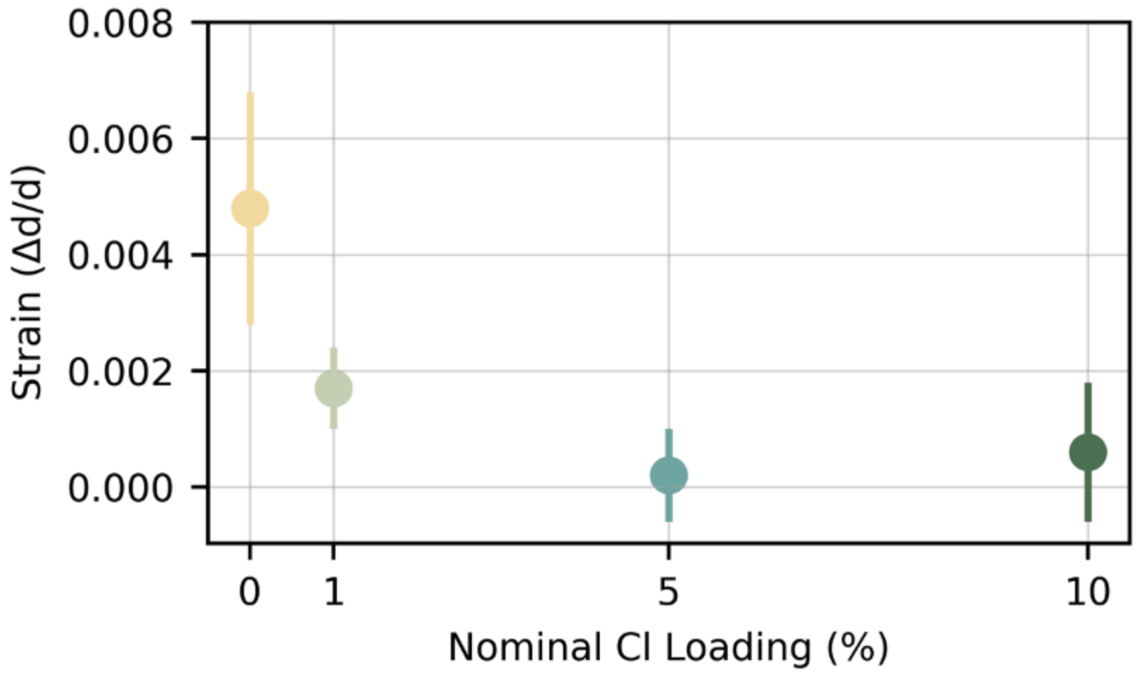

Figure S4 Williamson-Hall analysis of $CsPb(I_{0.80}Br_{0.20-x}Cl_x)_3$ films showing calculated strain in film.

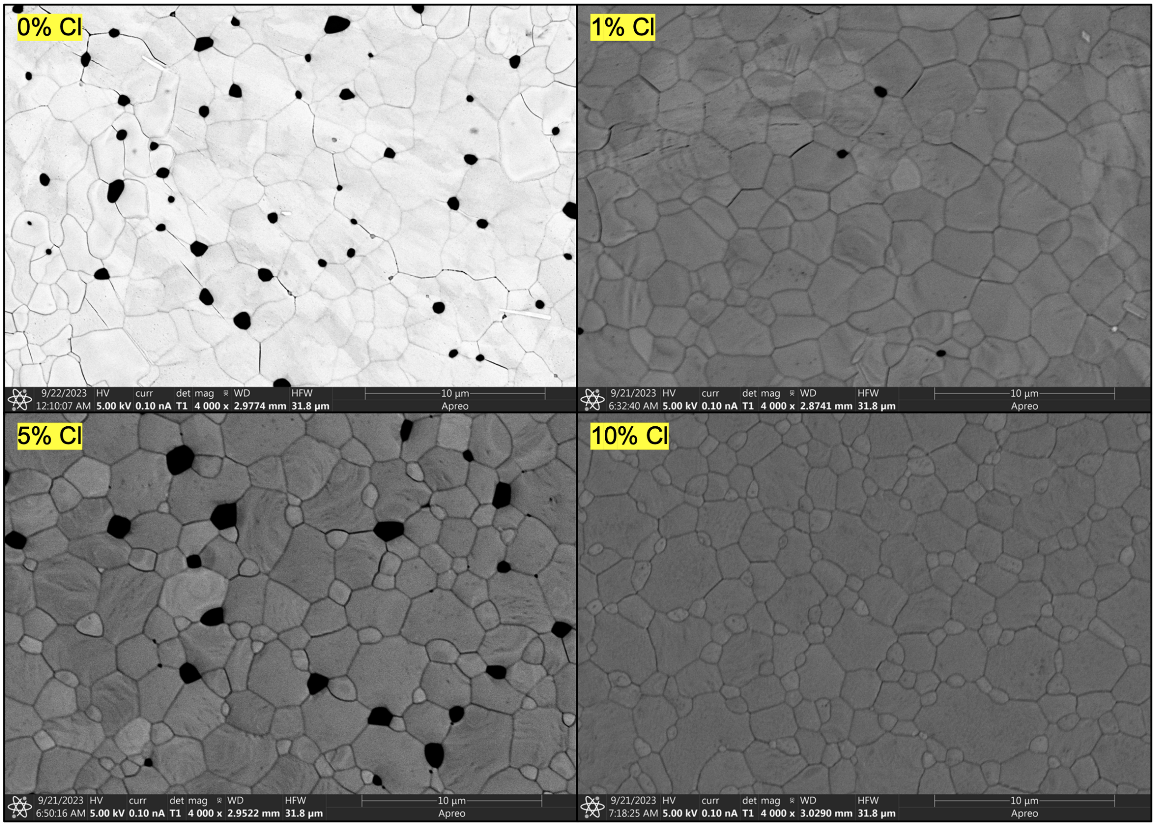

Figure S5 As-measured SEM images of $CsPb(I_{0.80}Br_{0.20-x}Cl_x)_3$ films. Inset text contains Cl condition label.

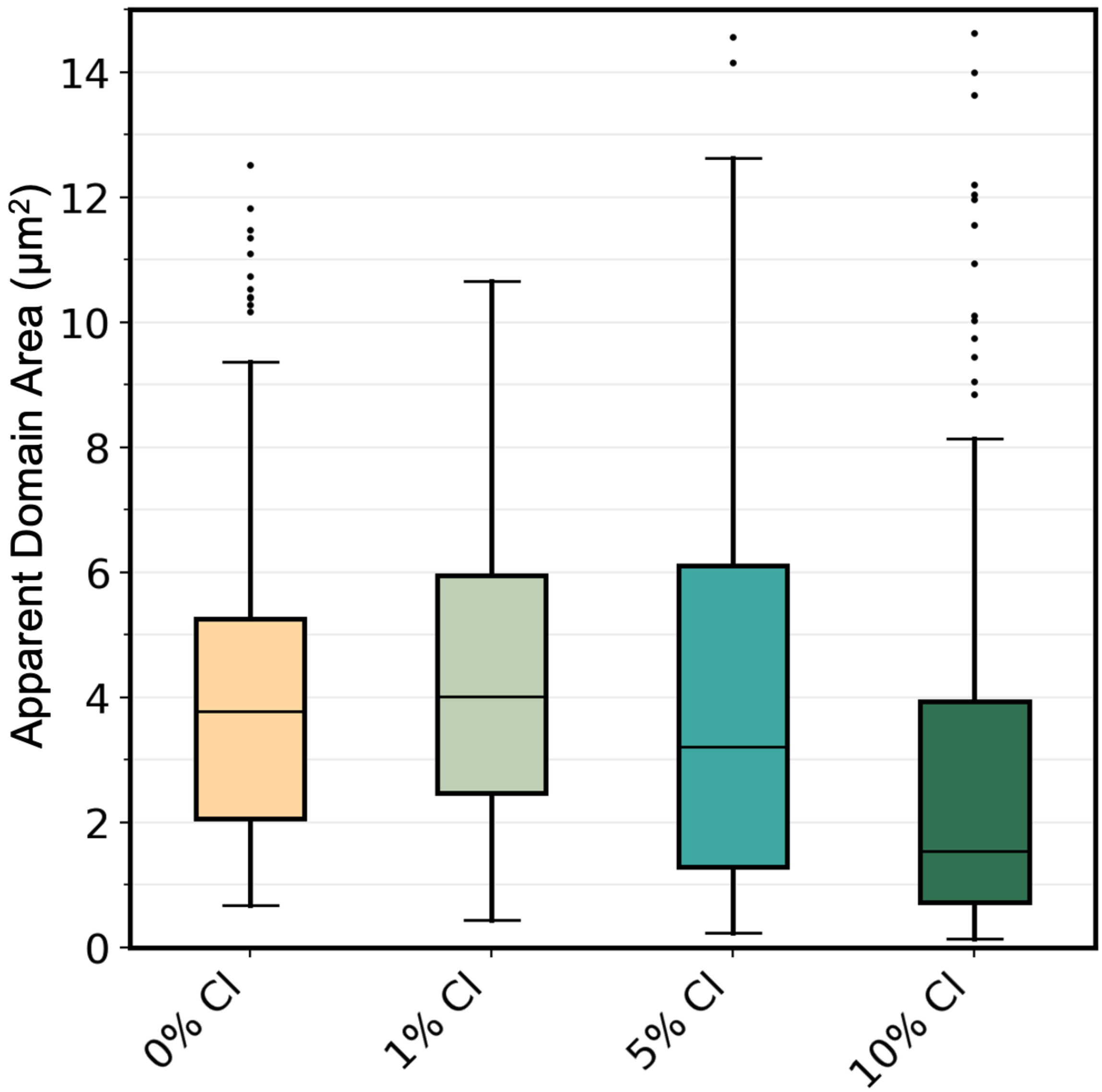

Figure S6 Box plots representing the apparent grain size analysis from SEM images of $CsPb(I_{0.80}Br_{0.20-x}Cl_x)_3$ films.

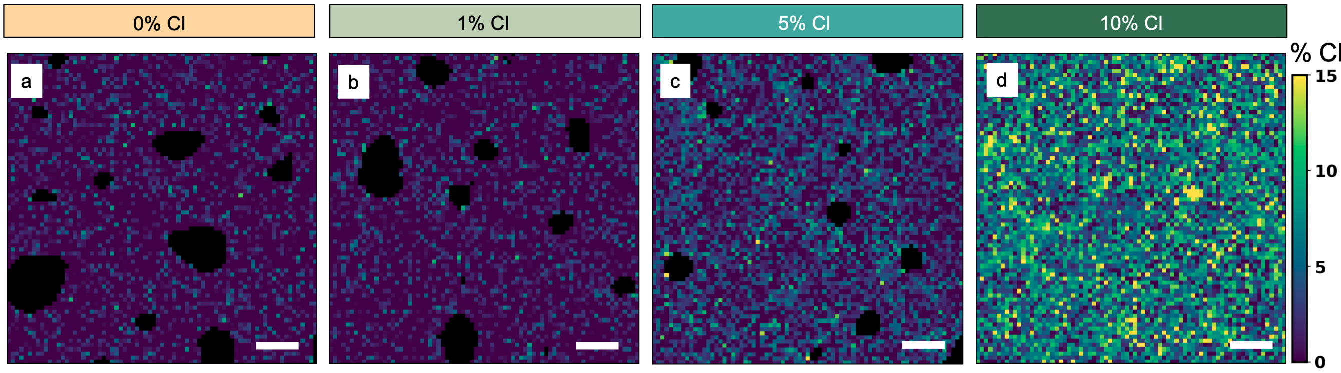

Figure S7 (a-d) Background subtracted nXRF maps of $CsPb(I_{0.80}Br_{0.20-x}Cl_x)_3$ with nominal Cl varied from 0% to 10%. Scale bar 2 μm. Colorbar shows measured Cl% in the film.

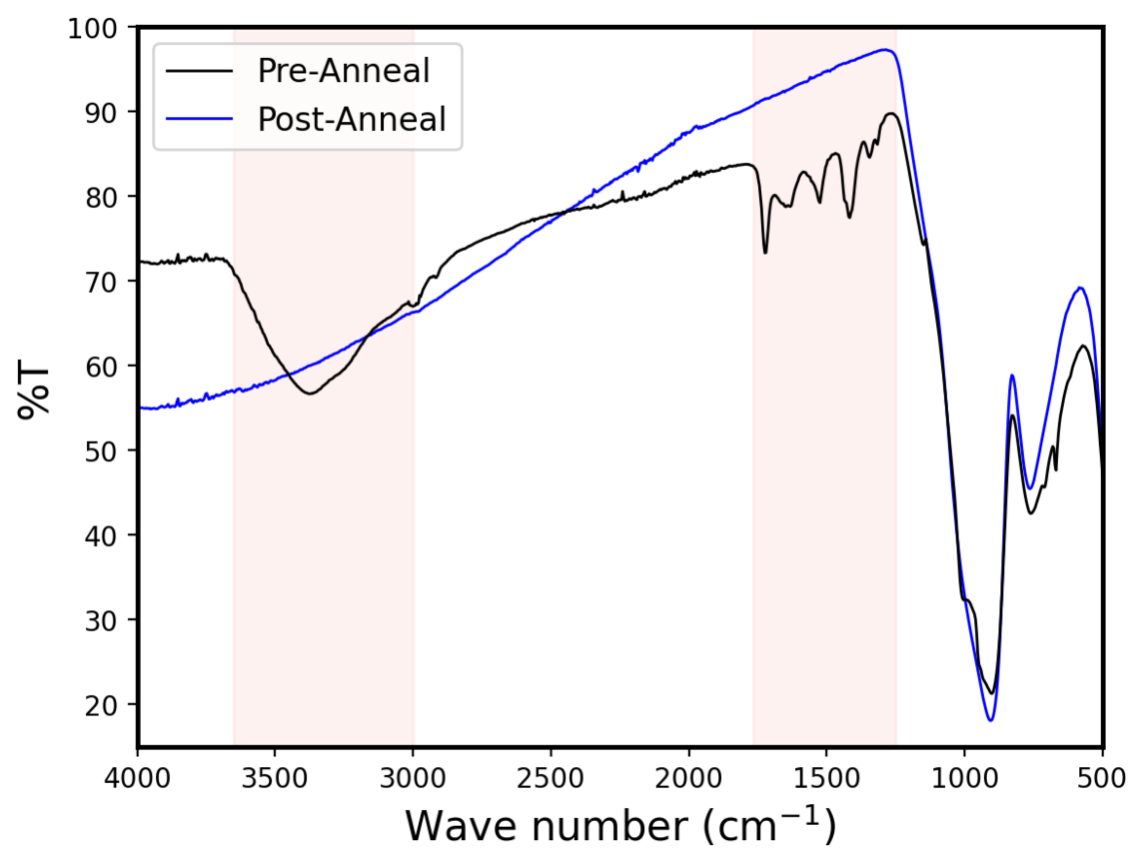

Figure S8 Pre- and post-anneal FTIR-ATR spectra of $CsPb(I_{0.80}Br_{0.15}Cl_5)_3$ films. Highlighted areas represent the characteristic signal from FAAc.[1]

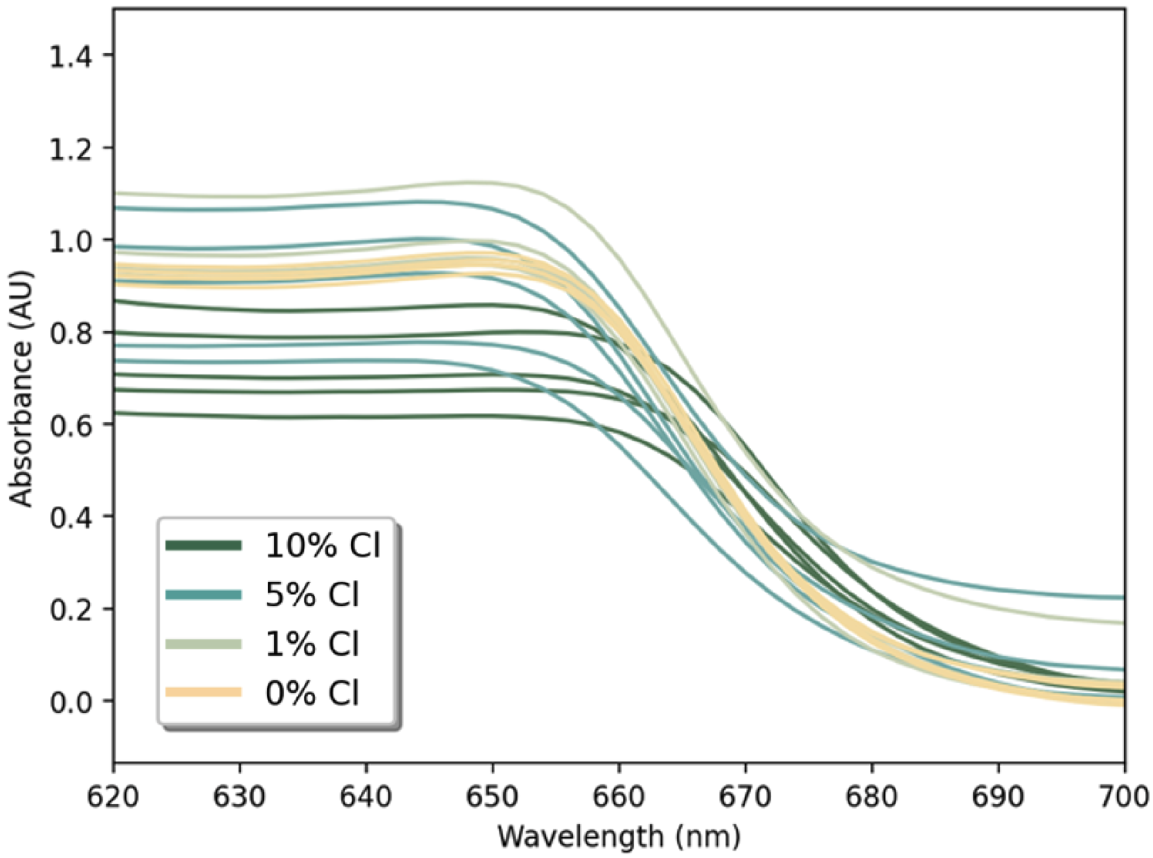

Figure S9 UV-vis absorbance spectra for each Cl loading ($CsPb(I_{0.80}Br_{0.20-x}Cl_x)_3$) film with 5 repeats per condition.

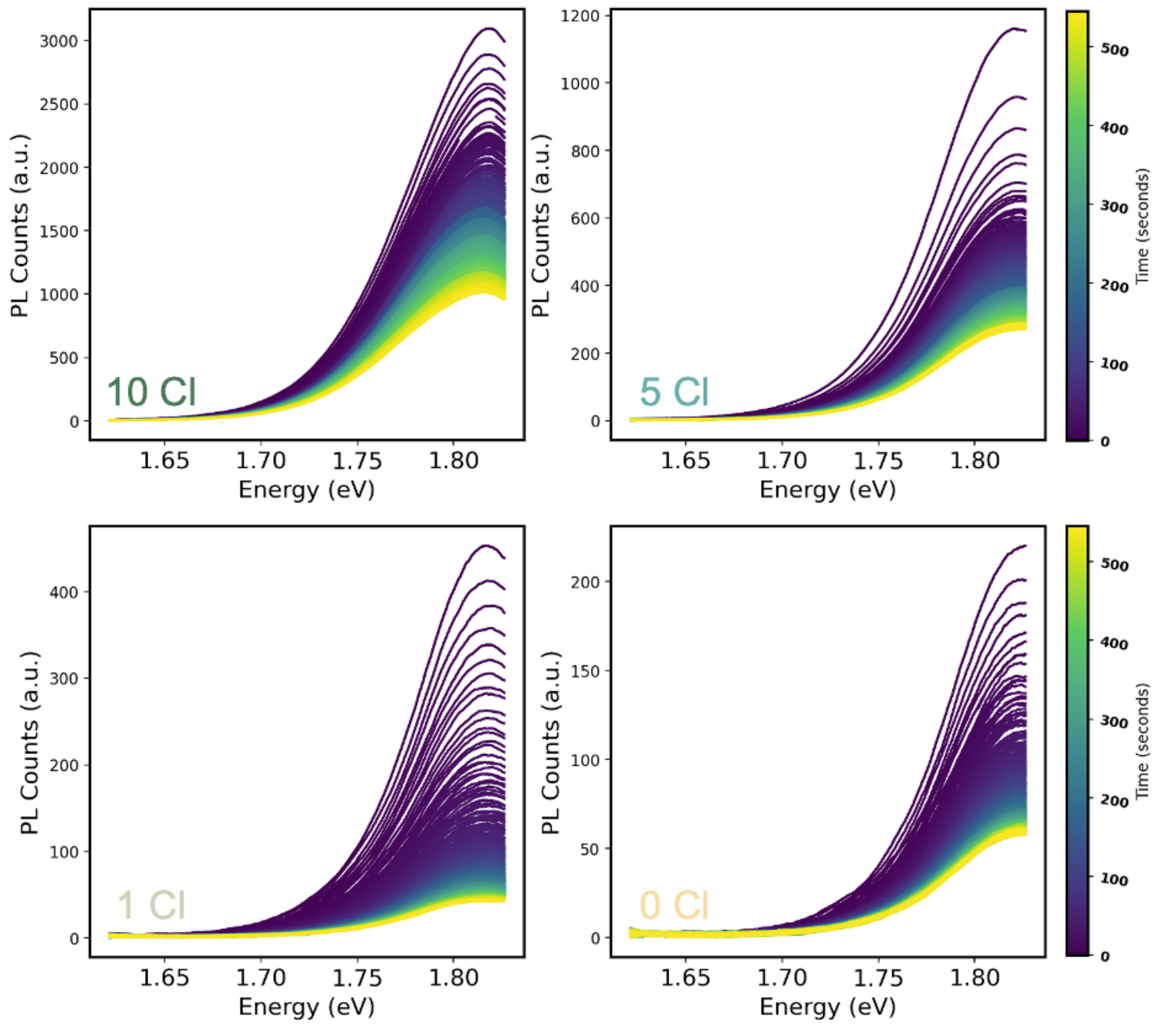

Figure S10 Smoothed PL spectra of all Cl loading conditions ($CsPb(I_{0.80}Br_{0.20-x}Cl_x)_3$) films collected from a single point (6μm) over 545s.

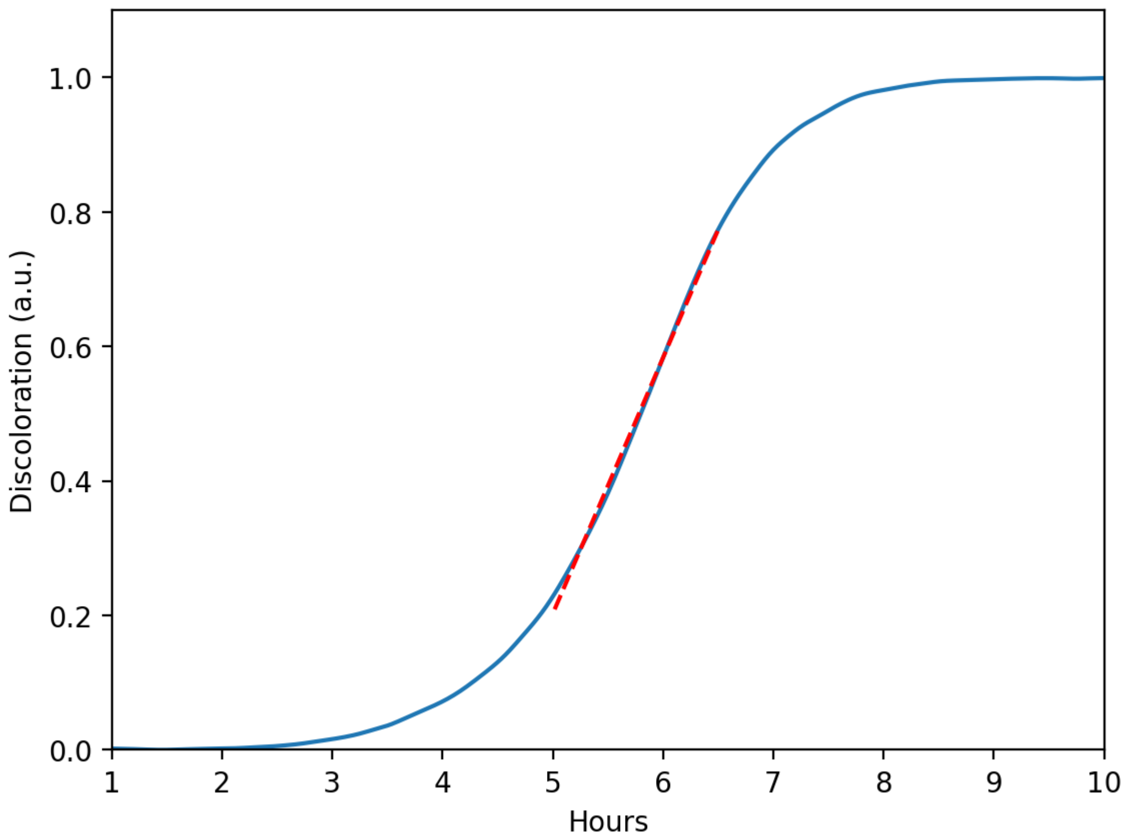

Figure S11 Example onset of discoloration fit of a $CsPb(I_{0.80}Br_{0.1}Cl_{0.1})_3$ film at 85°C. Onset of discoloration is determined by fitting the linear portion of the discoloration curve and using the x-axis intercept as the onset value.

References

[1] National Institute of Advanced Industrial Science and Technology (AIST), *SDBS-3590: formamidine acetate - Collection of Spectral data*, Spectral Database for Organic Compounds, 1999, `https://sdbs.db.aist.go.jp/sdbs/cgi-bin/landingpage?sdbsno=3590`, Accessed on January 3, 2024.