Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary Information

Structural, optical, and electronic studies of wide-bandgap lead halide perovskites

Riccardo Comin, Grant Walters, Emmanuel Thibau, Oleksandr Voznyy, Zheng-Hong Lu, Edward H. Sargent

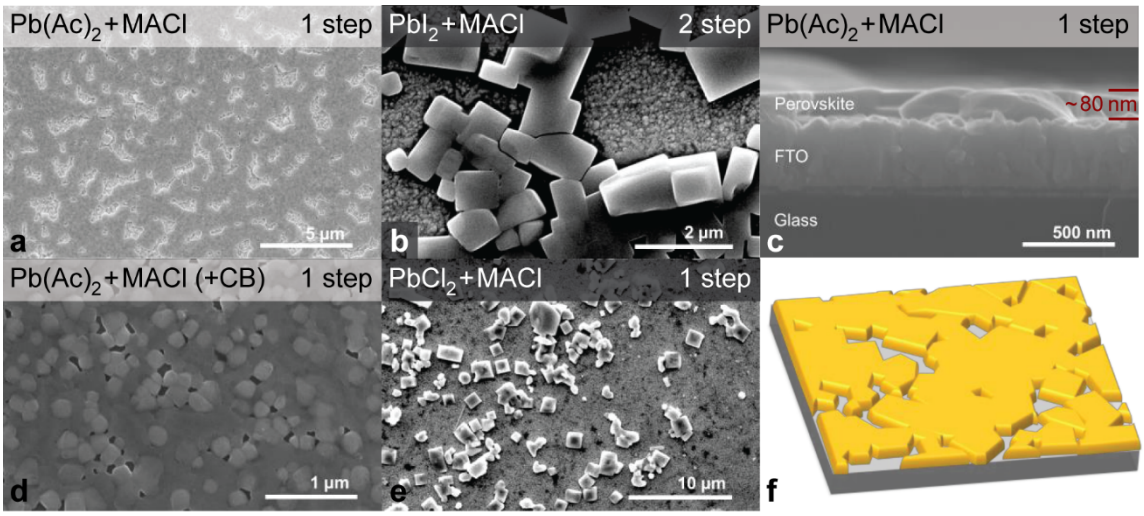

Figure S1. a),b),d),e) SEM images of $MAPbCl_3$ films on FTO prepared using different synthetic routes. Labels indicate the precursors used and whether a single spin-coating deposition or a two-step sequential spin- and dip-coating preparation was used. In d) chlorobenzene (CB) was used to demonstrate antisolvent-induced rapid crystallization during the spin-coating process. c) SEM cross-sectional view of an ~ 80 nm $MAPbCl_3$ film on FTO prepared according to the procedure used for a). f) Three-dimensional rendering of a portion of the film shown in a).

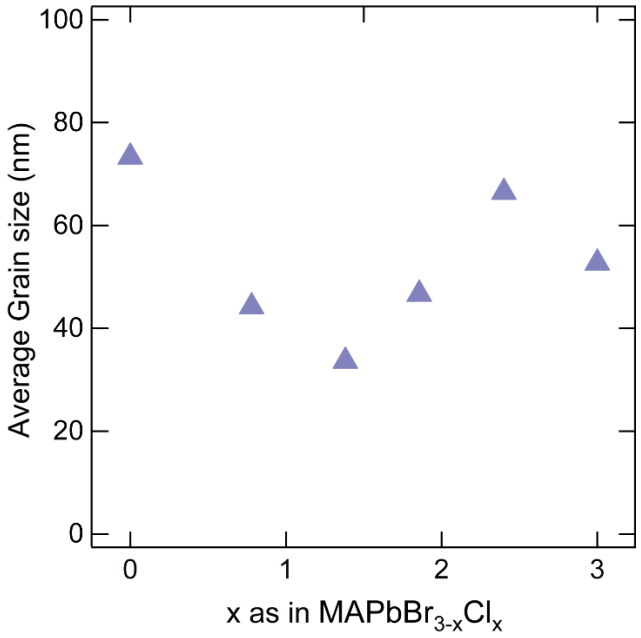

Figure S2. Average grain size of $MAPbBr_{3-x}Cl_x$ films as determined from the analysis of XRD peak broadening. These values are representative of the shortest average grain dimension, and are consistent with the average grain height as determined from SEM (Figure S1).

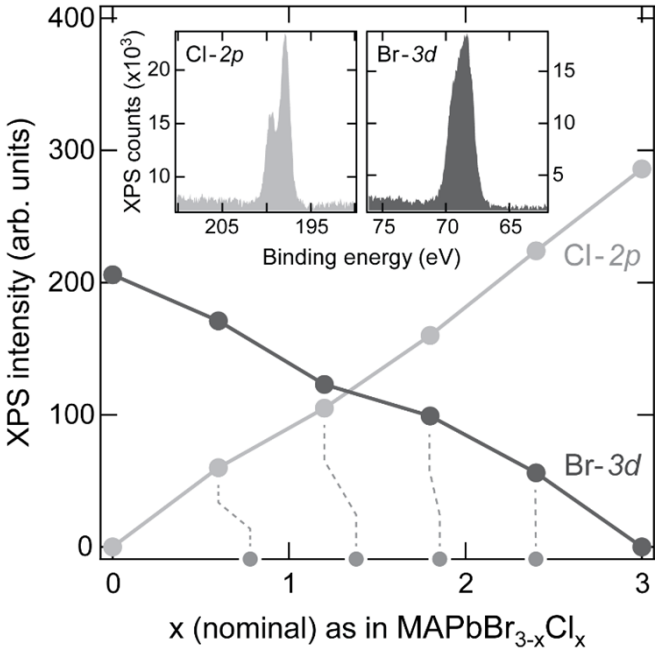

Figure S3. Plot of the Br and Cl XPS intensity (integrated area of the core-level peaks shown in the insets) as a function of nominal Br:Cl concentration (determined from the ratio of precursor molar mass). The Br:Cl ratio of XPS intensities, here used as a measure of the relative halide concentration, is represented by grey markers on the horizontal axis, with dashed lines highlighting the deviation from the nominal value.

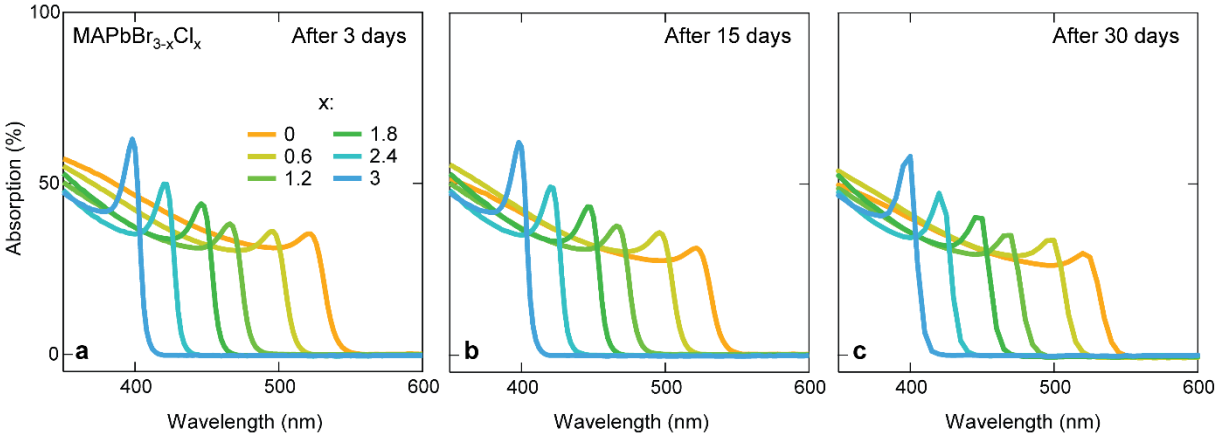

Figure S4. Optical absorption of $MAPbBr_{3-x}Cl_x$ films measured over time after a) 3 days, b) 15 days, and c) 30 days from the day of fabrication.

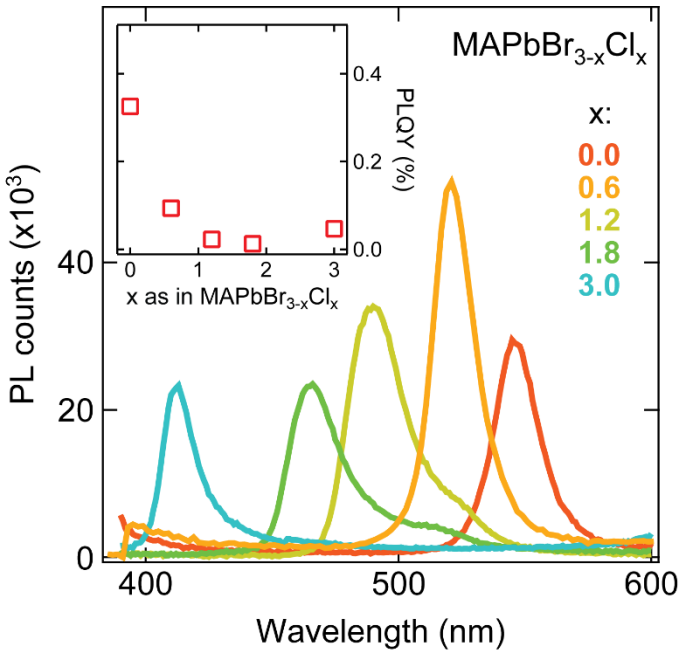

Figure S5. Raw photoluminescence spectra of $MAPbBr_{3-x}Cl_x$ films. Inset: corresponding photoluminescence quantum efficiency (PLQY), expressed in percentage of emitted over absorbed photons.

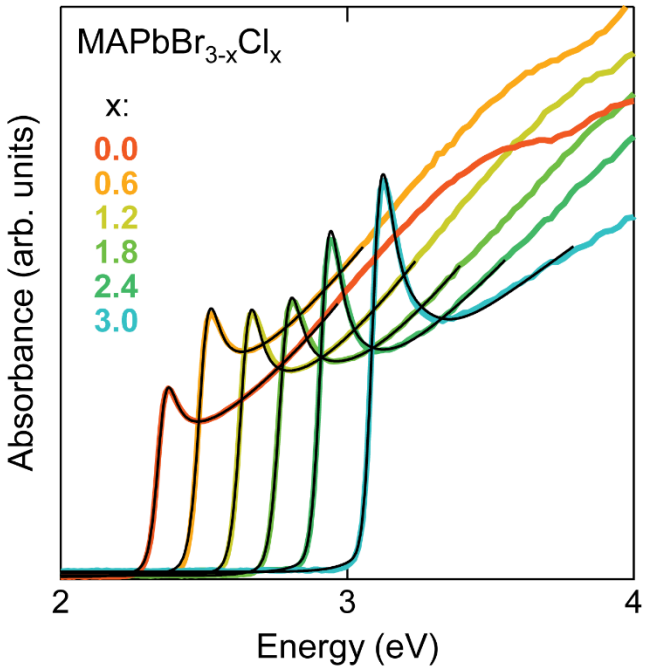

Figure S6. Optical absorption of $MAPbBr_{3-x}Cl_x$ films (colored traces) and corresponding fit (black thin lines) combining the excitonic contribution (Equation 1) and the particle-hole continuum (Equation 2).

Table S1. Near-gap electronic parameters in $MAPbBr_{3-x}Cl_x$

x	Bandgap (eV)	Exciton binding energy (meV)	Valence band maximum (eV)	Conduction band minimum (eV)	Work function (eV)
0	2.392 +/- 0.001	21 +/- 1	6.73	4.34	4.89
0.6	2.547 +/- 0.002	29 +/- 2	5.77	3.23	4.68
1.2	2.694 +/- 0.001	36 +/- 1	6.83	4.14	4.77
1.8	2.842 +/- 0.001	41 +/- 1	6.72	3.88	5.05
2.4	2.983 +/- 0.004	44 +/- 4	6.78	3.80	5.35
3	3.177 +/- 0.006	52 +/- 6	6.57	3.40	4.61