Supporting information

Phase transition kinetics and surface binding states of methylammonium lead iodide perovskite

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Scherer Formula for Crystalline Size Calculation

The average crystalline size can be estimated by the Scherrer’s formula, given by

\[ D = \frac{K\lambda}{\beta_{\text{hkl}} \cos \theta} \]  \hspace{1cm} (A)

Where \( D \) is the crystallite sizes, \( \lambda \) is the wavelength of the X-ray radiation (0.15406 nm), \( K \) is the shape factor (0.9), \( \theta \) is the diffraction angle (in radians), and \( \beta \) is the full width at half maximum (FWHM) of the selected diffraction peak (in radians).
Optical Spectra of MAPbI$_3$ perovskite at 100 °C and 150 °C for 1 and 2 hours

Figure S1. Absorption spectra of MAPbI$_3$ perovskite annealing at 100 °C and 150 °C for 1 and 2 hours.
Figure S2. a) XPS survey spectra of MAPbI$_3$ at RT, 60 °C, 100 °C, and 150 °C under atmospheric conditions.
Estimation of atomic percentage of C 1s, O 1s, and N 1s using AM-RSFs method

For facile quantification, the relative intensities of the spectral peaks were obtained by integrating peak areas from curve-fitting that directly lead to relative amount of corresponding atoms in the sample from equation D.

\[
C_A = \frac{I_A/S_A}{\sum_i (I_i/S_i)}
\]  

Here, \(C_A\) is the concentration of atomic species \(A\), \(I_A\) is the measured intensity of the spectral line attributed to \(A\) and \(S_A\) is the sensitivity factor of the spectrometer to \(A\). \(I_i\) is the total peak area of the components found in the element \((i)\) and \(S_i\) represents the RSF of the element \(i\).

**Figure S3.** The atomic percentage of chemical components in the C 1s, O 1s and N 1s elements at RT, 60 °C, 100 °C, and 150 °C in air.
Reference