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# 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

$$D = \frac{K\lambda}{\beta_{hkl} \cos\theta} \qquad \text{(A)}$$

Where D is the crystallite sizes, λ is the wavelength of the X-ray radiation (0.15406 nm), K is the shape factor (0.9), θ is the diffraction angle (in radians), and β 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

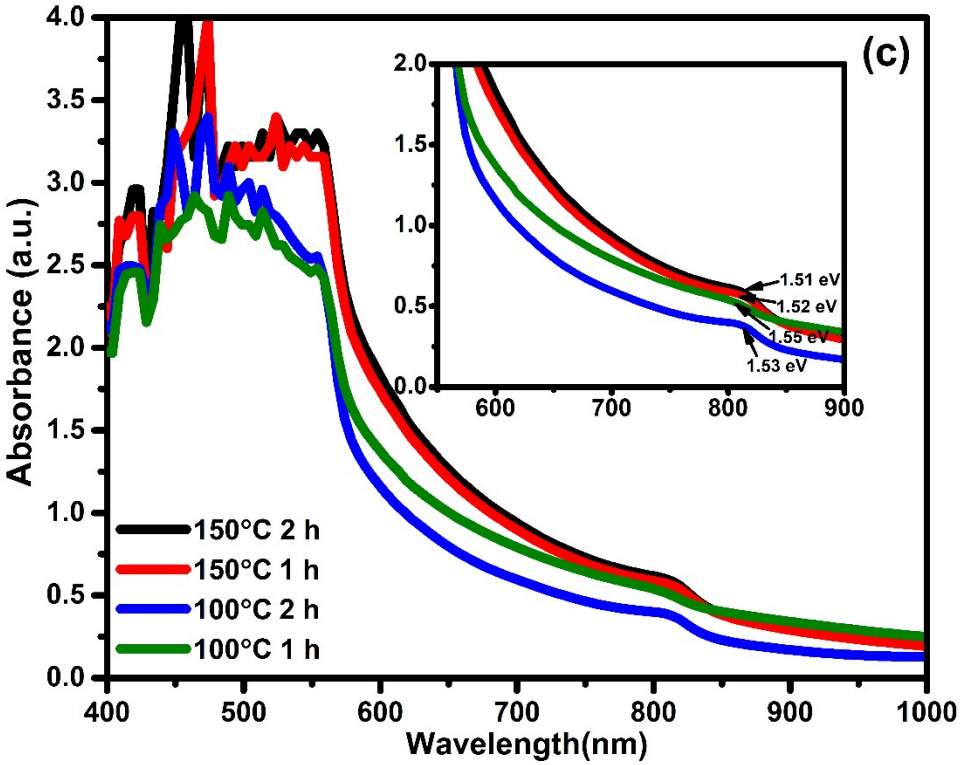


**Figure S1.** Absorption spectra of $MAPbI_3$ perovskite annealing at 100 °C and 150 °C for 1 and 2 hours.

# XPS survey spectra with elemental concentration

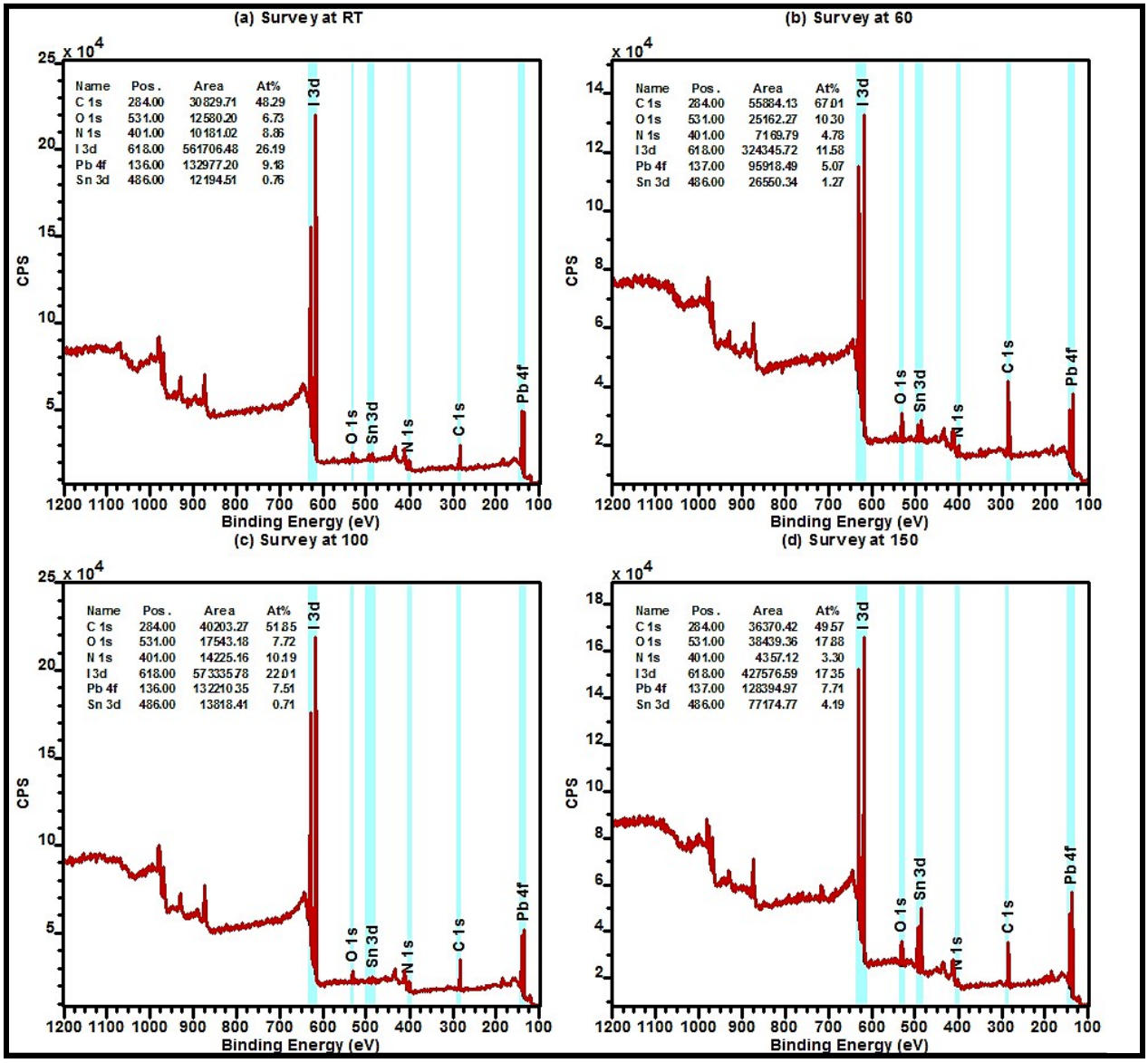


**Figure S2.** a) XPS survey spectra of $MAPbI_3$ at RT, 60 °C, 100 °C, and 150 °C under atmospheric conditions.

**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.

$$C_A = \frac{I_A / S_A}{\sum_i \left( I_i / S_i \right)} \qquad \text{(B)}$$

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.

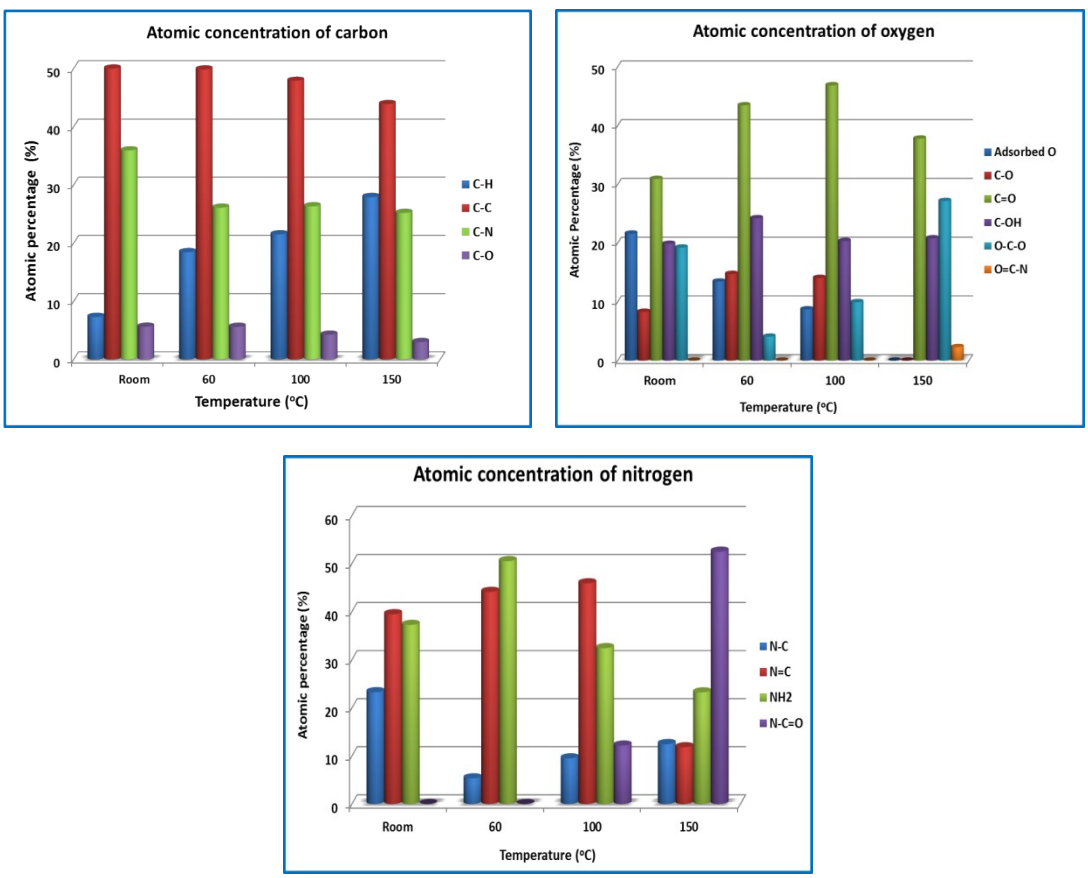


**Figure S3.** The atomic percentage of chemical components in the C 1s, O 1s and N 1s elements at RT, 60 °C, 100 °C, and 150 °C in air.

## Reference

(1) T. Ungár, J. Gubicza, G. Ribárik and A. Borbély. Crystallite size distribution and dislocation structure determined by diffraction profile analysis: principles and practical application to cubic and hexagonal crystals. *J. Appl. Crystallogr.* **2001**, 34, 298-310.