



# Structural and morphological investigations of slot-die coated perovskite layers for photovoltaics

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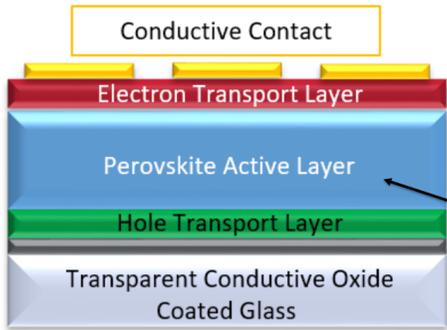
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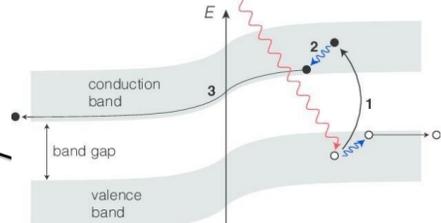
## 1. Perovskite photovoltaics

Light energy is converted into electricity via the **photovoltaic effect**.

**Photon is absorbed by an active layer of solar cell and electron-hole pair is formed and separated producing an electric current.**



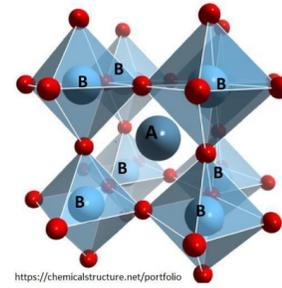
ossila.com



Robert Alicki, David Gelbman, and Alejandro Jenkins. "A thermodynamic cycle for the solar cell". In: *Annals of Physics* 378 (June 2016)

Perovskite structure features:

- + High absorption coefficient
- + Large dielectric constant
- Usually contains lead
- + Tunable bandgap



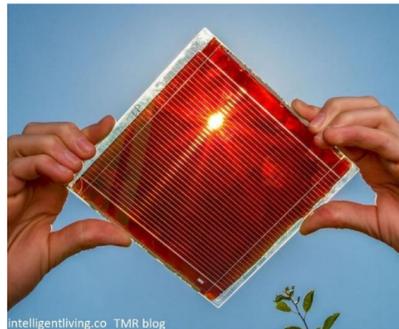
https://chemicalstructure.net/portfolio

Perovskite solar cells features:

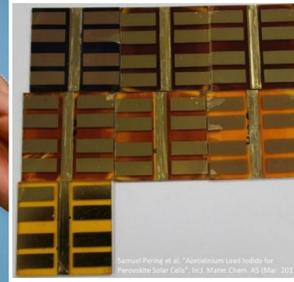
- High achieved efficiency +
- Low-cost scalable production +
- Long-term reliability -
- Flexible substrates available +

Silicon solar cells features:

- High efficiency +
- Existing manufacturing processes +
- Energy demanding production -
- Fixed bandgap -



intelligentliving.co TMR blog

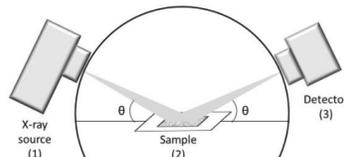


Armin Peberstorf et al. "Perovskite Layer Grows by Solvent Evaporation". *ACS Mater. Lett.* 10 (2017)

## 2. Main studying techniques

XRD:

- To receive a characteristic XRD-pattern
- To compare the changes in the sample content with different additives and printing parameters



Ulrich, D., & Forbes, T. (2019). X-ray Diffraction Techniques. In J. Kenney, H. Veeramani, & D. Alistair (Eds.), *Analytical Geomicrobiology: A Handbook of Instrumental Techniques* (pp. 215-237).

GIWAXS:

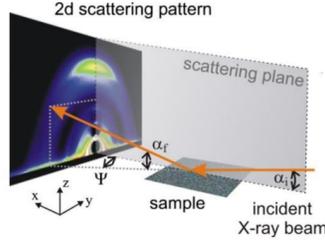
- Surface-sensitive
- Non-destructive
- Large studied area

The method is used for probing the material reciprocal lattice. Parameters used in experiment:

SDD = 170 mm,  $\alpha_i = 0.35-0.45$ , polarization fraction = 0.98

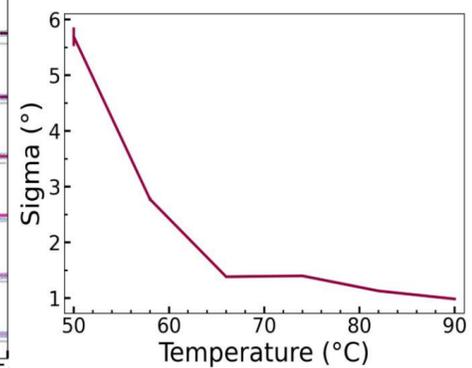
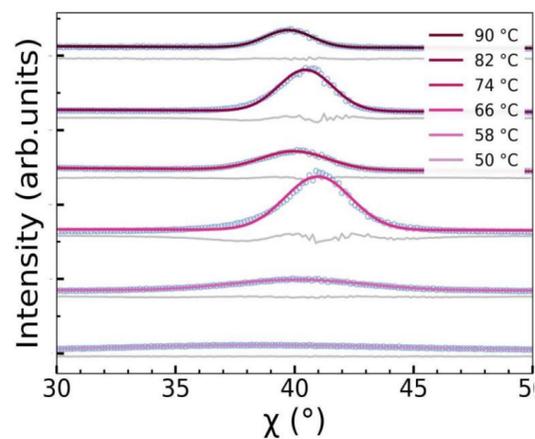
SEM:

- To have an overview of the sample surface and compare it to the results of other experiments



J. Peberstorf et al. "Direct Imaging with single X-ray scattering at the wiggler beamline BW1 of HASYLAB". In: *Review of Scientific Instruments* 81.09 (2010)

## 4. Pbl<sub>2</sub>-(102) reflex analysis



- P3m1 space group
- Face-up orientation
- Orientation rises with temperature
- Peak position does not shift strongly

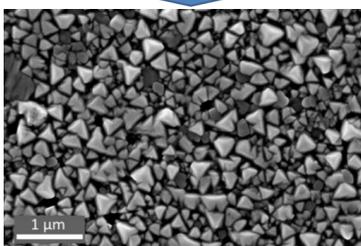
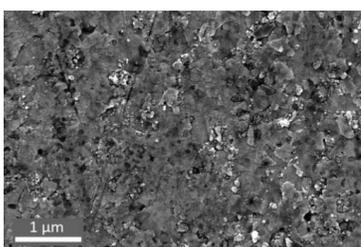
- Other Pbl<sub>2</sub> reflexes demonstrate similar behavior

## 3. Solution engineering and its analysis

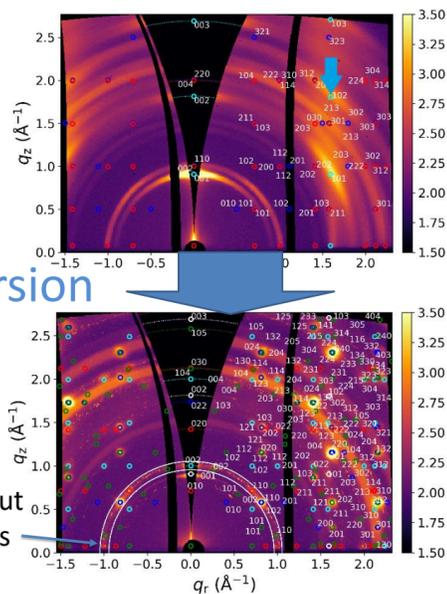
Idea - to try different additives for Pbl<sub>2</sub> layer with two-step method using slot-die coater and estimate its effects on the resulting Pbl<sub>2</sub> and MAPI layer morphology

Probed additives:  
MAI-seeds and DMSO

### MAI-seeded MAPI



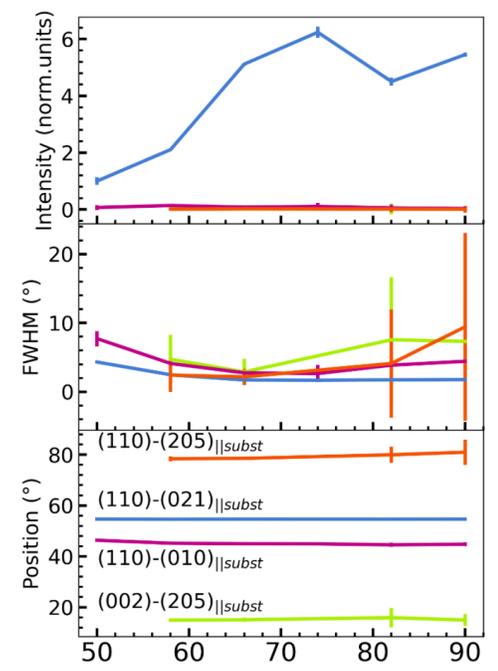
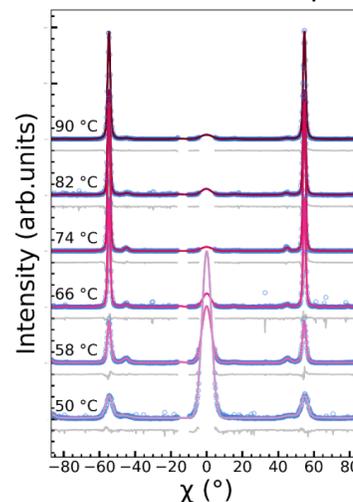
conversion



Tube-cut borders

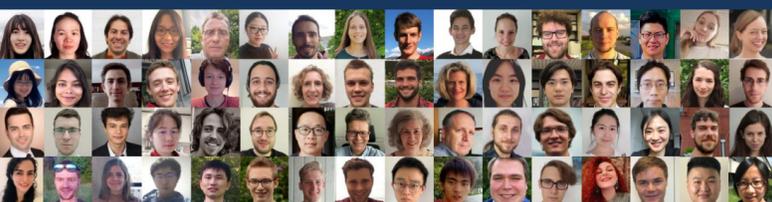
## 5. Analysis of MAPI reflexes around q=1 Å

- Tetragonal phase
- I4cm space group
- 4 different orientations
- Orientation rises with temperature



Overall observed tendencies:

- Higher temperature → narrower peaks → more oriented structure
- Correlation between number of face-up oriented Pbl<sub>2</sub> crystals and corner-up oriented MAPI crystals
- The properties of face-up Pbl<sub>2</sub> are correlated to the corresponding ones of corner-up MAPI crystal



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