Physik der Molekularen und Biologischen Materie

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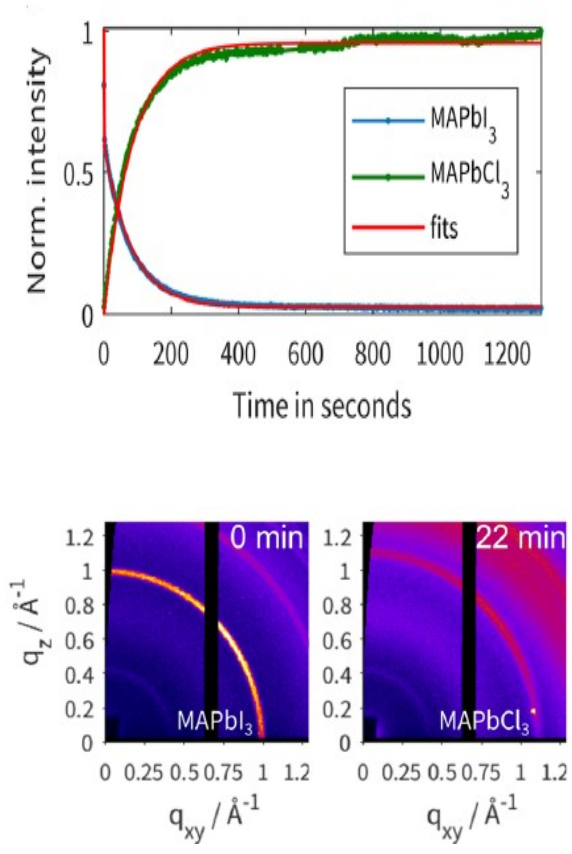
Master and Bachelor Project: Structure analysis of Perovskite Hybrid Solar Cells

Project description:

Organic-inorganic lead halide perovskites are fascinating light absorbers, which have enormous potential for the development of low-cost highly efficient solar cells with efficiencies exceeding 24%. Understanding the kinetic and energetic effects during the film growth is very important since they determine how ions distribute in the structure and how this affects the optoelectronic properties of the perovskite film. X-ray scattering data reduction, background subtraction and model fitting are the main computational methods that are employed to extract the information about the intermediate phases, kinetics and formation rate of perovskite materials.

Within the field of soft-matter physics, our group studies the structural properties and particularly the growth process of organic-inorganic hybrid perovskite thin films [1,2]. In this context, we collect X-ray scattering data using highly specialized synchrotron beamlines, e.g. at the ESRF in Grenoble and at the DESY in Hamburg. Recent progress in 2D-detector technology allows us to follow the growth in real-time and to cover relatively large parts of the reciprocal space with sufficiently high angular resolution. It is crucial for resolving the structure of films completely. In this specific project, you will

- use and improve existing software modules using high-level programming languages (preferably MATLAB or PYTHON),
- perform computer-based modelling of diffraction patterns from manually-defined unit cell to resolve complex 2D/3D perovskite structures,
- analyze large real-time data sets obtained with 2D-detectors using crystallographic methods,
- visualize the results.



a) Integrated Bragg peak intensity of the $MAPbI_3$ (110) and $MAPbCl_3$ (100) during the conversion of $MAPbI_3$ to $MAPbCl_3$, b) GIWAXS images of the beginning and end of the conversion of $MAPbI_3$ to $MAPbCl_3$ [2].

Starting time: *immediately*

Candidates interested in photovoltaics and material science with a solid background in computational methods and programming, are encouraged to apply for this project.

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References and further information:

www.soft-matter.uni-tuebingen.de (see under publications and open positions)

1. N. Arora et al., *Science* **358,** 768–771 (2017)
2. A. Greco et al., Journal of Physical Chemistry Letters **9**, 6750–6754 (2018)