



	Experiment title: Layered Hybrid Perovskites with Enhanced Functionalities for Photovoltaics	Experiment number: A01-2-1290
Beamline:	Date of experiment: from: <i>January 20</i> to: <i>January 23, 2023</i>	Date of report: <i>August 25, 2023</i>
Shifts:	Local contact(s): Dmitry Chernyshov	
Names and affiliations of applicants (* indicates experimentalists): <ul style="list-style-type: none"> ▪ *Masaud Almalki, EPFL, Switzerland (instead of Ghewa AlSabeih, EPFL, Switzerland) ▪ *Weifan Luo, Adolphe Merkle Institute, Fribourg, Switzerland ▪ *Lena Merten, University of Tuebingen, Germany ▪ *Paul Zimmermann, University of Tuebingen, Germany ▪ Alexander Hinderhofer, University of Tuebingen, Germany (coordination) ▪ Jovana V. Milić, Adolphe Merkle Institute, Fribourg, Switzerland (coordination) 		

Report

The aim of this experiment was to obtain a detailed structural overview of the series of new layered hybrid perovskite materials with enhanced functionalities. In the course of the experiments, we investigated material structures, their orientation relative to the substrates, and changes of their properties in response to light.

In terms of methodology, we analyzed the materials by grazing incidence X-ray scattering before and after UV irradiation for more information on their structure and orientation. The focus was on perovskite compositions that typically form well-defined 2D phases ($n = 1$), whereas other higher compositions ($n = 2$) were also assessed. In addition, we complemented the analysis with the optoelectronic characterization of these systems in thin films and photovoltaic devices for a better understanding of their properties and operational stabilities. We used two different substrates, namely microscopic glass slides and indium-doped tin oxide (ITO) conductive glass substrates. Light irradiation was performed using broad white-light irradiation and UV irradiation at 350 nm. Finally, GIWAXS measurements were performed with continuous scanning in reciprocal space (between 0–2.5 Å⁻¹ both in q_{xy} and q_z), and the variation of the angle of incidence provided depth-dependent information on the crystal quality, along with lattice parameters and domain orientation of hybrid 2D superstructures.

In summary, the combined results from X-ray scattering measurements and further optoelectronic characterization enabled unraveling of the factors for operating these materials in perovskite photovoltaics. Further analysis is ongoing to correlate some of the structural changes upon irradiation to the changes in optoelectronic characteristics, photovoltaic performances, and operational stabilities. We are also in the process of preparing two manuscripts incorporating the results of these experiments. Finally, the results of the experiments enabled us to advance the design of layered hybrid perovskite materials in our future research.

The results are available through the ESRF data portal via doi:10.15151/ESRF-ES-1021690577.