

Integrating large-scale deposition and wide energy range spectroscopy at EMIL

Regan G Wilks^{*1,2}, Klaus Lips^{2,3,6}, Simone Raoux^{2,3,5}, David E. Starr¹, Florian Ruske¹, Franz Schäfers⁴, Stefan Hendel^{2,4}, Mihaela Gorgoi^{2,3}, Michael Hävecker⁷, and Marcus Bär^{1,2}

¹*Renewable Energy, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany*

²*Energy Materials In-situ Laboratory Berlin, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany*

³*Energy Materials, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany*

⁴*Research at Large-Scale Facilities, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany*

⁵*Department of Physics, Humboldt-Universität zu Berlin, Berlin, Germany*

⁶*Department of Physics, Freien Universität Berlin, Berlin, Germany*

⁷*Heterogeneous Reactions, Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr, Germany*

*regan.wilks@helmholtz-berlin.de

The Energy Materials In-situ Laboratory Berlin (EMIL) at BESSY II is a joint flagship initiative of the Fritz-Haber-Institute of the Max-Planck Society and the Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), created with the goal of setting up a dedicated infrastructure to study energy conversion and catalyst candidate materials in-system, in-situ, and operando. The HZB focuses on energy conversion materials research by bringing world-class expertise in fabrication and characterization under the same roof. In this user facility, a multi spectroscopic endstation is connected via UHV transfer system to state-of-the-art deposition tools. The automated transfer system can handle large samples, up to 6" round wafers, or 10 cm x 10 cm on glass, making it uniquely capable of studying materials on an industry scale as well as samples deposited using combinatorial synthesis. The multi-chamber system is designed to accommodate the highest degree of flexibility so that it can be easily expanded. The most complex deposition tool is currently a cluster, combining ALD, PECVD (x2), and PVD, which is dedicated to the deposition of thin film solar cell structures. An 8-source magnetron sputter tool for synthesis of thermoelectric materials is also in operation. Two simpler sample preparation chambers, one that is a dedicated chamber for thermal evaporation of organic materials and another containing an electron-beam evaporator, an atomic hydrogen source, and an ion sputter gun are also available to general users. A N₂ glove box can be used for sample mounting and is directly connected to a UHV load lock for clean introduction and removal of samples.

The beamline will use two undulators and three monochromators to deliver photons across the continuous energy range from 80 eV – 10 keV to 10 μm-scale spot sizes and variable polarization. The light from the undulators can be focused at any of 5 different endstations, each with specific capabilities. The Sissy-I interaction point is connected via UHV to the deposition chambers described above; in this endstation a Scienta EW4000 photoelectron analyzer will allow high transmission as well as “one shot” depth profiling of materials. Fluorescence detection via Bruker SDD can be used for absorption spectroscopy. A high-transmission, moderate resolution spectrometer for soft x-ray emission spectroscopy (XES) is under construction, and will operate in the energy range from 45 eV – 1 keV. The Sissy-II interaction point is a free position for “roll-up” stations, including for *in situ* and *operando* spectroscopy using XES.

The combination of dedicated deposition and spectroscopic tools with the wide energy range provided by the “two color” beamline, together with the anticipated “cross-fertilization” and synergy effects between research fields is expected to be crucial for an insight-driven development of energy conversion materials (e.g., as needed for next-generation photovoltaics, thermoelectrics, batteries, etc.) required for rapid and disruptive advancements.