Science with combined scattering and spectroscopy experiments on BM31 at SNBL

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Here we present the science and some technical information on BM31 using combined techniques. The beamline is specifically designed for running fully automated X-ray absorption spectroscopy (XAS), X-ray diffraction (XRD) and X-ray total scattering (XRTS) followed by pair-distribution function (PDF) analysis in a single experiment. The beamline possessing a liquid nitrogen cooled double crystal monochromator with an unfocused crystal pair for spectroscopy from 5-42 keV and a focused crystal (48 keV) for diffraction and total-scattering. The end-station is equipped with16 pre-filled movable ion chambers, fluorescence detectors and movable a Dectris Pilatus 2M CdTe detector. Dedicated sample environments have been developed mimicking large scale (industrially relevant) processes.

The BM31 user community is diverse, serving the needs of groups in Switzerland and Norway through private beamtime. European users have access through public ESRF beamtime. Today a large portion of the experiments are focussed on catalysis and batteries. We will briefly present a case study from each topic.

First we will present [1]. Here the authors use combined *operando* XRD, XAS and PDF to study antiperovskite Li_2FeSeO cathode materials. XAS is used to probe redox activity in Se and Fe quasi-simultaneously, while PDF was used to probe local structure changes including bond-lengths.

Next we will present [2]. Here the authors use *ex situ* XAS and PDF to investigate the role of dehydrated clusters in Zr-MOFs for catalysis of glycerol to glycolic acid. Rapid heat treatment under humid airflow is used to induce O-vacancies in MOFs, giving undercoordinated Zr sites, while also preserving framework connectivity.

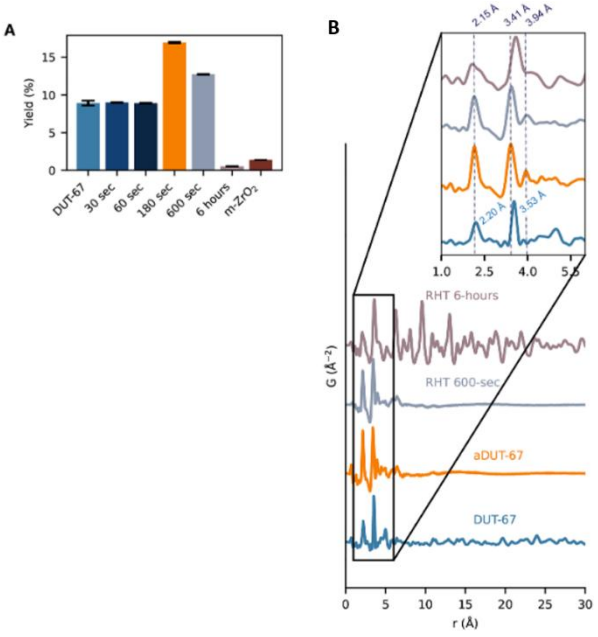


Figure 1. (a) *catalytic activity of MOFs and,* ***(b)*** *PDFs of MOFs with different heat treatment times[2]*

[1] Dai, T., Park, H., Brennhagen, A., Andersen, N. H., Giorgetti, M., Valldor, M., Koposov, A. Y., Chem. Mater. (2025), 37, 9091–9104.
[2] Schertenleib, T., Asgari, M., Mouriño, B., Karve, V. V., Felder, T. M. O., Stoian, D., Bon, V., Hao, J., Ortega-Guerrero, A., Oveisi, E., Agrawal, K. V., Smit, B., Kaskel, S., Billinge, S. J. L., Queen, W. L., Chem. (2025), 11, 102619.