Session Program

5–6 Jan 2026

Symposium for Data-Driven Approaches in X-ray Absorption Spectroscopy (DataXAS)

Flash Presentations

ETH Zurich, Siemens Auditorium
Campus Hönggerberg

Monday 5 January

15:50

Flash Presentations

Session | **Location:** ETH Zurich, Siemens Auditorium, Campus Hönggerberg

15:50–15:53

INSIGHTS INTO MOF SYNTHESIS WITH COMBINED IN SITU APPROACH: RAMAN SCATTERING, X-RAY ABSORPTION, X-RAY DIFFRACTION

Speaker
Olena Zavorotynska

15:53–15:56

Quantitative EXAFS Thermometry with Universal Machine Learning Interatomic Potentials

Speaker
Dr Pjotrs Žguns

15:56–15:59

A Data-Driven Workflow for Preprocessing, Anomaly Detection, and Simulation-Guided EXAFS Analysis of Cu in Steel

Speaker
Duc-Chau Nguyen

15:59–16:02

Similarity Metric for Automated FDMNES Parameter Optimization for XANES Simulations

Speakers
Dr Hester Blommaert, Dr Mohamed Redhouane BOUDJEHEM

16:02–16:05

Intelligent Analysis Pipeline for X-ray Absorption Spectroscopy: Near Real-Time Processing and Adaptive Experimentation

Speaker
Diana Rueda

16:05–16:08

EXAFS study of thermoelectric Bi$_{2-x}$Sb$_x$Te$_3$ using the reverse Monte Carlo method

Speaker
Inga Pudza

16:08–16:11

Combined MCR-ALS and MEXAS-PSD to unravel the electrochemical behavior of a Co3Mn-based LDH

Speaker
Dr Anthony Beauvois

16:11–16:14 **Interpreting Non-Redox Responses in Modulation-Excitation XAS**

Speaker
Mr Servaas Lips

16:14–16:17

Advanced Operando XAS Methodologies for Active-Site Identification and Quantification in Materials with Complex Speciation

Speakers
Marie-Gabrielle Ameres, Gabriela-Teodora Dutca

16:17–16:20

Fast elemental composition analysis of X-ray fluorescence spectroscopy with Neural Network

Speaker
Francesco La Porta

16:20–16:23

First-principle simulated Fe4 L-edge XAS reveals redox-sensitive spectral shifts upon Li doping.

Speaker
Nanchen Dongfang

16:26–16:29

Machine learning application for automatic structural information extraction from experimental operando data for Ni and Mn based cathodes materials

Speaker
Oleg Usoltsev

16:29–16:32

A TDDFT-based Method for the Calculation of Resonant Inelastic X-Ray Scattering in Condensed Phases

Speaker
Beliz Gökmen

16:32–16:35

Cation-Site Disordered Cu3PdN Nanoparticles for Hydrogen Evolution Electrocatalysis

Speaker
Jagadesh Kopula Kesavan

16:35–16:38

Spectroscopic insights into the electronic structure of non-critical rare earth containing permanent magnets

Speaker
Benedikt Eggert

16:38–16:41

A Bayesian Framework for Feature Extraction in Noisy Operando X-ray Absorption Spectroscopy

Speakers
Mr Tommaso Rodani, Matteo Biagetti

16:41–16:44

Real-Time TDDFT Simulations of Core-Level Spectroscopies in the Condensed Phase

Speaker
Michael Coates

16:44–16:47

Data-Driven Analysis of Nuclear Resonance Vibrational Spectra with Machine-Learning Potentials

Speaker
Alexey Rulev

16:50–16:53

Linking Structure and Electrochemistry in Pt Supported on Mesoporous N-Doped Carbon (MPNC) Fuel-Cell Catalysts: A Complete X-ray Picture from XAS to XRS

Speaker
Dr S. Esmael Balaghi

16:53–16:56 **In-house X-ray absorption spectroscopy instrumentation at MPI CEC**

Speaker
Yves Kayser

17:00