

Session Program

5-6 Jan 2026



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

Bridging Simulations and Experiments with Machine Learning

ETH Zurich, Siemens Auditorium
Campus Höggerberg

Tuesday 6 January

13:30

Bridging Simulations and Experiments with Machine Learning

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

13:30–14:10

Machine learning potentials applied to MD-EXAFS

Speaker

Dr Alexei Kuzmin

14:10–14:50

Combining Reverse Monte Carlo Analysis of X-ray Scattering and Extended X-ray absorption Spectroscopy

Speaker

Prof. Markus Winterer

14:50–15:30

Coffee Break

15:30–16:10

X-ray absorption spectral shapes

Speaker

Prof. Frank de Groot

16:10–16:50

DFT-assisted XANES simulations

Speaker

Dr Grigory Smolentsev

16:50