WORKSHOP # 7 - Thursday, April 23, 2026

High Energy Resolution Spectroscopy for Operando Studies

Organizers: Jorge Moncada (NSLS-II), Dali Yang (NSLS-II), Akhil Tayal (NSLS-II), Dominik Wierzbicki (NSLS-II), Evan Jahrman (NIST)

Many catalytic, electrochemical, and environmental processes involve materials that change their electronic and chemical state under operating conditions. Capturing these changes requires sophisticated spectroscopic techniques capable of probing active sites while reactions are taking place for non-ambiguous identification. X-ray Emission Spectroscopy (XES), High-Energy Resolution Fluorescence Detected X-ray Absorption Near Edge Spectroscopy (HERFD-XANES), and Resonant Inelastic X-ray Spectroscopy (RIXS) provide element-specific sensitivity to oxidation state, spin state, ligand environment, and metal-ligand interactions beyond what is accessible with conventional XAS. This workshop will focus on the application of high energy-resolution XAS and XES in operando studies of catalysis, battery systems, and environmentally relevant materials. Similarly, research where theoretical simulations are used for the analysis of complex XES/HERFD datasets will be shown. Discussions will highlight how the mentioned methods are used to follow active-site evolution, identify reaction intermediates, resolve redox chemical state heterogeneity, and track degradation processes under industrially relevant operating conditions. The workshop will showcase relevant science cases where the use of advanced spectroscopic techniques is crucial, facilitating breakthroughs in different scientific areas.

By sharing case studies and best practices, the workshop will clarify how these techniques enable mechanistic understanding that is difficult or impossible to obtain with conventional approaches. Likewise, this workshop will also identify how conventional theoretical methods and AI/ML tools could potentially be used to get real-time assessment of the data and how they can help to push forward rational design of more efficient and durable materials.

Start Time (ET)	Title	Speaker (Affiliation)
8:30	Breakfast	
8:50	Welcome and Introduction	
9:00	Tender X-ray photon-in-photon-out spectroscopy (keynote talk)	**Pieter Glatzel (ESRF)**
9:30	Metal-Centered X-ray Absorption and Emission Spectroscopy of Iron Corroles: Implications for Ligand Non-Innocence	**Meiyuan Guo (Uppsala University)**
10:00	*Break*	
10:30	Improving the sensitivity of X-ray techniques by the experimental design	**Davide Ferri (Paul Scherrer Institute)**
11:00	A NIST Testbed for High Energy Resolution Soft X-ray Emission Measurements of Catalysts	**Evan Jahrman (NIST)**

11:30	What Computational X-ray Spectroscopy Can Tell Us About Materials Properties	**John Vinson (NIST)**
12:00 – 2:00 pm	*Lunch Break (travel to/from SUSC to Berkner Hall)*	
2:00	Spectroscopic Characterization of Reactive Transition Metal Sites in Porous Materials	**Jonas Börgel (NYU)**
2:30	High resolution X-ray emission spectroscopy for clean energy applications	**Yulia Pushkar (Purdue University)**
3:00	Linking Local Structure and Electronic State Evolution in f-Element Materials via EXAFS and High-Resolution X-ray Spectroscopy	**Arjen van Veelen (LANL)**
3:30	*Break*	
4:00	Talk 9	**Jerry Seidler (University of Washington)**
4:30	Discussion and Wrap-Up Session	
5:15	SST-1, QAS, ISS, and TES Beamlines Tour	
6:15	Adjourn	