WORKSHOP #6

Multi-modal Operando Characterization Methods to Comprehend Catalytic Reaction Dynamics under Reactive Environments

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In addressing the demands of catalyst design and development, operando characterizations focusing on the dynamics of catalytic reactions have emerged as crucial areas of exploration. These approaches prove potent in pinpointing active sites, unraveling reaction mechanisms, and delineating degradation pathways. The recent advancements in environmental transmission electron microscopy (TEM) have enabled the direct monitoring of atomic-scale reaction dynamics during catalytic processes across the surface and interface, with the temperature-, pressure- and time-resolved imaging capability. Moreover, the incorporation of the closed-cell technique has extended the gas pressure range from approximately 1 mbar to around 1 bar, effectively surpassing the pressure constraints inherent in Environmental Transmission Electron Microscopy (ETEM). This expansion establishes a direct and seamless linkage between reaction dynamics and performance, as measured by real catalytic reactors. Despite the considerable progress in integrating chemical measurements with TEM image capability, employing techniques like X-ray Energy Dispersive Spectroscopy (EDS) and Electron Energy Loss Spectroscopy (EELS), persistent concerns persist regarding measurement spatial limitations and electron beam effects within the field. The electron beam's influence, causing knock-on damage, irradiation, and heating effects, has impacted the reliability of captured results. Consequently, control and comparison experiments stand as widely employed methods to mitigate potential electron beam effects. However, these strategies represent an absolute necessity to surmount this challenge due to the specific requirements inherent in characterizations.

An effective approach to overcome these challenges involves utilizing a combination of diverse tools, especially average techniques like Ambient-Pressure X-ray Photoelectron Spectroscopy (AP-XPS), in-situ X-ray Diffraction (XRD), and X-ray Absorption Spectroscopy (XAS). These tools yield crucial insights into chemical state changes, phase transitions, and the evolution of coordination conditions across a wide spatial and temporal range. Notably, they offer general information that aids in interpreting localized observations made in TEMs, presenting a holistic strategy to address characterization challenges in studying catalytic reaction dynamics. The multi-modal characterization, encompassing pressure, temperature, gas composition, resolution, and chemical mapping, provides a comprehensive exploration of reaction dynamics.

Start Time (ET)	Title	Speaker (Affiliation)
9:30 am	Welcome	
9:40 am	The role of operando X-ray absorption spectroscopy in probing catalyst dynamics	Simon R Bare (SLAC National Accelerator Laboratory)
10:10 am	Exploring the Reactivity of Metal-Oxide Interfaces using Near Ambient Pressure XPS	Michael White (Brookhaven National Laboratory)
10:40 am	Correlative electron microscopy for chemo-mechanical studies	Yang Yang (Pennsylvania State University)
11:10 am	Untangling structure-function relationships for reconstructing Rh/TiO2 catalysts under CO2 hydrogenation conditions	Emily Schroeder (University of California, Santa Barbara)

11:40 am	Highly Active Oxygen Atom on Reconstructed Cu_2O Surface Oxidizes CO at Low Temperatures	Ashley Head (Brookhaven National Laboratory)
12:10 pm	Break	
2:00 pm	Resolving Phase Evolution in Complex Systems using Multi-modal data.	Deyu Lu (Brookhaven National Laboratory)
2:30 pm	In situ microscopy and spectroscopy study on dynamics of nanostructure in catalysis for sustainable energy	Gengnan Li (Argonne National Laboratory)
3:00 pm	Break	
3:30 pm	Investigating Interfacial Interactions in Catalysts under CO2 Hydrogenation Environments: Insights from Multi-modal In-situ Characterizations	Kaixi Deng (Argonne National Laboratory)
4:00 pm	Insights into Interfacial Dislocation Nucleation and Motion Dynamics in NiO/Ni: An In-Situ Atomic-Scale Visualization Study	Linna Qiao (Binghamton University)
4:15 pm -5:00 pm	Discussion and Closeout	