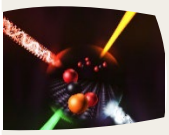



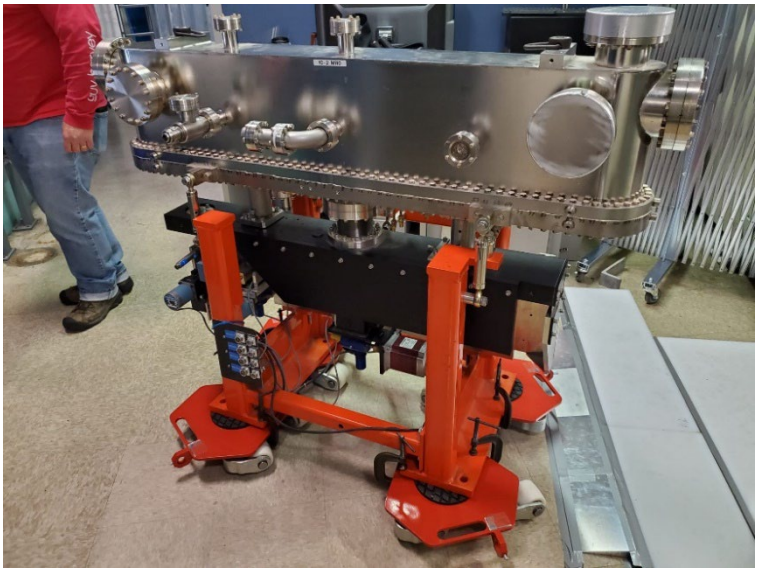

Newsletter 10 | July 2023

Co-ACCESS Semi-Annual

Consortium for Operando and Advanced Catalyst Characterization via Electronic Spectroscopy and Structure

Beamline 10-2 QXAS Development

Significant progress continues to be made in the retrofitting of beamline 10-2 for QXAS experiments. The experimental end station is nearing completion, we are finalizing the flow scheme for the permanent gas handling system, and we await the delivery of the multi-element detector. Installation of the additional exhaust to support our gas cabinets has started, and we are optimizing the user space. We have taken advantage of the unscheduled downtime of SSRL to make progress on the optics upgrade. The vacuum shop and beamline development teams have removed the original mirror and monochromator leaving a blank canvas for the first round of hardware installation during the summer down. We plan on starting to commission the harmonic rejection/collimating mirror and the quick-scanning monochromator at the start of the 2024 run, with installation and commissioning of our focusing mirror in November-February. While it is hard to predict how the commissioning process will go, we are hoping to see the first user experiments late 2024!



10-2 M_0 removal. This mirror will be repackaged with a stiffer base and will be reinstalled at the new 10-2 M_1 mirror creating a focused beam in the front hutch.

Co-Access Team at NAM28

The Co-ACCESS team had a fantastic time attending the 28th North American Catalysis Society Meeting in Providence, Rhode Island. Adam taught at a successful Sunday workshop with Zili Wu (ORNL) and Frédéric A. Perras (Ames National Lab), which was attended by a group of 40 participants. Adam delivered a comprehensive introduction to *operando* catalysis experiments using X-ray absorption spectroscopy and showcased *operando* XAS research that Co-ACCESS has conducted. In the following week, Simon presented a poster on the topic of "Identifying the Active Site in Catalysis: What is the Future for X-ray Absorption Spectroscopy?" to discuss the current state of catalysis research using XAS and its future. Jorge (presented by Adam) also presented a poster titled "Software Developments and Simulating Flow Systems for X-ray Absorption Spectroscopy Characterization of Catalysts at SSRL" to introduce ***CatMass*** and ***CatXAS***, software developed for users, and to discuss gas impurities in the flow system used for XAS experiments. Jiyun gave an oral presentation titled "Revealing Structural Complexity in Catalyst via Advanced X-ray Absorption Spectroscopy Data Analysis" to discuss XAS data analysis strategy that can provide insights into catalyst structures. Aside from attending remarkable lectures and presentations by fellow researchers, we were especially excited to reconnect with our collaborators in person and establish new connections that sparked engaging conversations for potential future collaborations. In total there were 23 presentations/posters connected to Co-ACCESS. We look forward to seeing all of you again at NAM29 in Atlanta in 2024!

Postdoctoral Associate Opportunity at Co-ACCESS

Co-ACCESS is currently seeking a motivated postdoctoral associate to develop and apply time-resolved *in-situ/in-operando* X-ray absorption spectroscopy to the study of a catalytic process of mutual interest. The focus of the project will be in developing the methodology to probe spectro-kinetics of catalytic processes with an emphasis on electrocatalysis and include advanced methods in data processing, data analysis and data modeling. This research will utilize the new upgraded wiggler beamline for quick X-ray absorption spectroscopy (QXAS).

I encourage you to contact me,
Simon Bare at srbare@slac.standord.edu or
Adam Hoffman at ashoff@slac.stanford.edu if you are interested in learning more.

Unexpected Downtime

We acknowledge that the unexpected outage at SSRL has had significant impact on the Co-ACCESS user community, and we sincerely appreciate your patience as the facility works diligently to restart operations. We are as anxious as you to welcome you back to SSRL for *in-situ/operando* catalysis experiments. Please reach out to us if you have questions. On a positive note it has given us an opportunity to make progress on beamline 10-2, to develop new hardware, data processing capabilities, and catch up on analyzing and interpreting data already collected.

Interns at Co-ACCESS

Rachita Rana is a 4th year Ph.D. student in chemical engineering at University of California, Davis. Her Ph.D. work focuses on developing automated theory-driven EXAFS analysis tool (QuantEXAFS). She uses DFT-based techniques to study the thermodynamic stability, reaction barriers, and activity of atomically dispersed catalysts for different reactions. During her time with the Co-ACCESS group, Rachita plans to experimentally investigate the scope of using atomically dispersed catalysts and nanoparticles (with the Cargnello lab) for more industrially relevant reactions like epoxidation. She also plans to conduct *operando* XAS studies to understand the dynamic evolution of catalytic sites.

Sarah Driscoll is an undergraduate at Vanderbilt University where she is studying chemical engineering and climate studies. This summer she is a SULI student working with the Co-ACCESS group. Her summer research involves synthesizing standards with known absorption characteristics to aid in the setup of solid-state fluorescence detectors at the SSRL XAS beamlines which will greatly improve detector setup times and beamtime efficienty.

Rachita Rana Sarah Driscoll

Key Recent Publications

"X-ray Absorption Spectro-Kinetics Observations of Ethylene-for-CO Ligand Exchanges on Zeolite-supported Single-site Rh Catalysts", A.S. Hoffman, O. Müller, J. Hong, G. A. Canning, C.-Yu Fang, J. E. Perez-Aguilar, B. C. Gates, S. R. Bare, *J. Phys. Chem Letters*, (2023), **14**, 4591–459. DOI: 10.1021/acs.jpclett.3c00349.

"Rigorous Oxidation State Assignments for Supported Ga-Containing Catalysts Using Theory-Informed X-Ray Absorption Spectroscopy Signatures from Well-Defined Ga(I) and Ga(III) Compounds", L. Li, J. Chalmers, S.R. Bare, S.L. Scott, F.D. Vila, *ACS Catalysis* (2023), **13**, 6549-6561. DOI: 10.1021/acscatal.3c01021

"Limits of Detection for X-ray Absorption Spectroscopy of Heterogenous Single Atom Catalysts", J. Finzel, K. Sanroman, A.S. Hoffman, J. Resasco, P. Christopher, S.R. Bare, *ACS Catalysis* (2023), **13**, 6462-6473. DOI: 10.1021/acscatal.3c01116.

"Dynamic Tracking of NiFe Smart Catalysts using In Situ X-Ray Absorption Spectroscopy for the Dry Methane Reforming Reaction", S. Shah, J. Hong, L. Cruz, S. Wasantwisut, S.R. Bare, K.L. Gilliard-AbdulAziz, *ACS Catalysis*, (2023), **13**, 3990-4002. DOI: 10.1021/acscatal.2c05572.

We invite any catalysis researcher to contact us prior to submitting a proposal to SSRL, or prior to their upcoming experiment. We can advise you at the appropriate level with the expressed aim of trying to maximize the success of your time at SSRL. We look forward to collaborating with you!
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https://www-ssrl.slac.stanford.edu/content/science/chemistry-catalysis