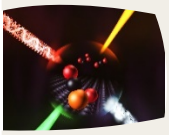
Newsletter 7 | December 2021

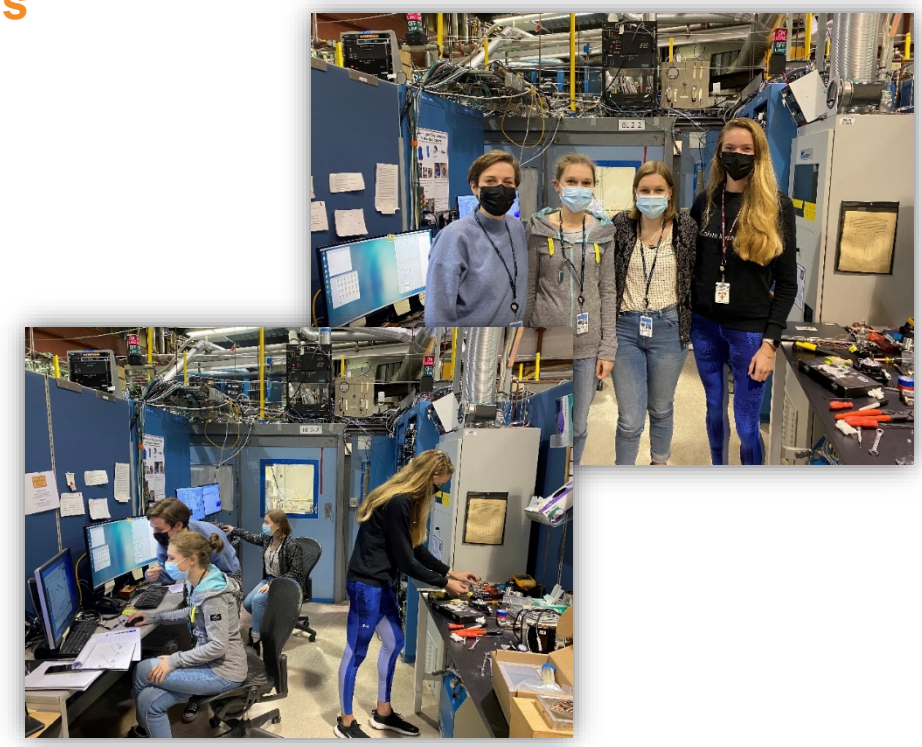


Co-ACCESS Semi-Annual

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

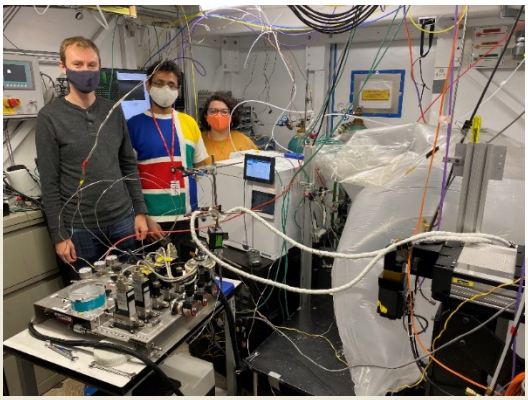
RECENT DEVELOPMENTS

Co-ACCESS Welcomes First International Users Since COVID-19 Restrictions



Co-ACCESS was pleased to host a group of researchers from Utrecht University, The Netherlands in November. They were the first international users to be able to attend in person since the COVID-19 travel restrictions were lifted. This all-female group, Iris ten Have, Nina Genz, Nicolette Maaskant, and Joyce Kromwijk used operando XAS to study a range of catalysts for Fischer-Tropsch synthesis and CO_2 hydrogenation and took full advantage of both the continuous scanning and quick-scanning XAS combined with modulation excitation XAS capability at beamline 2-2.

Expanding Capabilities: Operando X-ray Raman Spectroscopy



A very happy and exhausted team from the Ive Hermans' group (Univ. Wisconsin, Madison) at the end of their recent beamtime at BL 15-2, where they used X-ray Raman spectroscopy to characterize their selective oxidation catalyst at work. This was the first Co-ACCESS collaborative operando catalysis experiment using the new on-line GC and heated transfer lines.

Jorge Perez-Aguilar

Joins Co-ACCESS as a Research Associate

Co-ACCESS is please to welcome Jorge to the Co-ACCESS team. Jorge received his PhD from the University of California, Davis, where he worked on characterizing atomically dispersed Pt and Rh on silica-alumina-phosphates using FTIR, GC, and XAS. He joined Co-ACCESS as a research associate in October 2021.

His work focuses on training and facilitating users in in-situ/operando XAS measurements on catalytic materials, helping the team's effort to broaden the experimental capabilities to accommodate more variety of materials and reaction conditions at various XAS beamlines, including BL10-2.

Jordan Finzel SCGSR Introduction

Jordan Finzel is a 4th year PhD student at the University of California Santa Barbara. His PhD work has centered around the design of alloy catalysts for photocatlytic and thermocatalytic selective oxidation reactions. As a part of the Co-ACCESS team, he plans to combine Extended X-ray Absorption Fine Structure (EXAFS) analysis, High Energy Resolution Fluorescence Detection X-ray Absorption Near Edge Structure (HERFD-XANES), and theoretical XANES calculations to better understand the geometric and electronic structure of alloy catalysts under reactive conditions. He will also aid in the development of combined infrared and X-ray absorption spectroscopy capabilities for the new 10-2 beamline.

Fall *2021 XAS Bootcamp:*

In September 2021, the Co-ACCESS program hosted its Fall XAS bootcamp, which ran for three days in a virtual format. Ten beginner XAS experimentalists from 8 institutions were invited, and we had instructors from SLAC, Stanford University, UC Davis, and the University of Leeds. The student attendees presented their science cases showing how their XAS data could help answer their science questions. Research topics varied from atomically dispersed metals supported on zeolites to single atom alloys and supported nanoparticles, studying fundamental probe reactions to biomass conversion chemistries. During the first two days, mornings consisted of lectures and hands on examples, while the afternoons were spent in breakout groups where attendees worked through their data with instructors. Attendees were able to learn not only from the direct interaction with the instructors, but also through listening to questions and subsequent answers from other attendees. Every morning, the participants would present what they worked on the day before, demonstrating what analysis techniques and steps worked, and what didn't. These summaries showed the growth of skills and understandings from the attendees and helped the instructors to lead discussions on common errors during the XAS analysis process. By the end of the third day, the participants left the bootcamp with the beginnings of a new set of skills to be applied with their budding research endeavors.

Key Recent Publications

"A Theory-guided X-ray Absorption Spectroscopy Approach for Identifying Active Sites in Atomically-Dispersed Transition Metal Catalysts", Y. Chen, R. Rana, T. Sours, F.D. Vila, S. Cao, T. Blum, J. Hong, A.S. Hoffman, C.-Y. Fang, Z. Huang, C. Shang, C. Wang, J. Zeng, M. Chi, C.X. Kronawitter, S.R. Bare, B.C. Gates, A.R. Kulkarni, Journal of the American Chemical Society, (2021), accepted. DOI: 10.1021/jacs.1c07116.

"Monolayer Support Control and Precise Colloidal Nanocrystals Demonstrate Metal-Support Interactions in Heterogeneous Catalysts", E.D. Goodman, A.S. Asundi, A.S. Hoffman, K.C. Bustillo, J.F. Stebbins, S.R. Bare, S.F. Bent, M. Cargnello, Advanced Materials (2021), 2104533. DOI: 10.1002/adma.202104533

"Characterization of Metal-Organic Framework Zr6O8 Node-Supported Atomically Dispersed Iridium Catalyst for Ethylene Hydrogenation by X-ray Absorption Near Edge Structure and Infrared Spectroscopies", M. Babucci, A.S. Hoffman, Simon R. Bare, B.C. Gates, J. Phys. Chem C, (2021) 125, 16995-17007. DOI: 10.1021/acs.jpcc.1c03563.

"Lanthanum Induced Lattice Strain Improves Hydrogen Sulfide Capacities of Copper Oxide Adsorbents", G. Canning, S. Azzam, A.S. Hoffman, A. Boubnov, F. Alshafei, R. Ghosh, B. Ko, A. Datye, S.R. Bare, D. Simonetti, AIChE Journal, (2021), 67, e17484. DOI: 10.1002/aic.17484.

"First Principles Approach to Extracting Chemical Information from X-Ray Absorption Near-Edge Spectra of Ga-Containing Materials", K. Groden, F.D. Vila, L. Li, S.R. Bare, S.L. Scott, J-S. McEwen, J. Phys. Chem C, (2021), accepted. DOI: 10.1021/acs.jpcc.1c07728.

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! simon.bare@slac.stanford.edu
https://www-ssrl.slac.stanford.edu/content/science/chemistry-catalysis