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Consortium for Operando and Advanced Catalyst

O Newsletter 13 | /January 2025 O

Characterization via Electronic Spectroscopy and Structure

## **Winter Edition**



#### **Co-ACCESS Office Hours:**

Reminder, if you have any questions about XAS data processing or modeling or experimental design, stop in during our monthly office hours. If you would like to be added to the mailing list, please reach out to Adam at <a href="mailto:ashoff@slac.stanford.edu">ashoff@slac.stanford.edu</a>.

### **XAS Bootcamp**

As part of our goal to educate catalysis users on all aspects of XAS, Co-ACCESS hosted an XAS bootcamp at SLAC in August 2024. The bootcamp aimed to introduce new XAS experimentalists to data analysis by covering the basics of data processing and analysis. Over 2.5-days, 11 participants—including PIs, postdocs, and graduate students from several universities—attended a series of lecture sessions led by Co-ACCESS and guest instructors, Prof. Boopesh Mishra (IIT) and Dr. Arun Asundi (SLAC). The lectures provided an in-depth introduction to data processing in Athena and EXAFS modeling in Artemis. Each day, the lectures were followed by hands-on sessions with instructors, offering participants personalized, one-on-one assistance. Participants analyzed their own XAS data and received feedback tailored to their specific research projects. Co-ACCESS hosts periodic bootcamps to educate new experimentalists on all things XAS. Stay tuned for announcements about upcoming bootcamps by subscribing to our mailing list, please reach out if you are interested in attending our next session.



Photo from XAS Bootcamp (August 14-16, 2024)

## Let's Meet Up!

Members of the Co-ACCEESS team will be present at several conferences and meetings this year to give talks and to meet, discuss, and receive feedback from fellow catalysis researchers. We look forward to meeting you in-person at these meetings!

- American Chemical Society National Meeting (San Diego): Adam will be giving a talk on the XAS characterization capabilities to study catalytic CO<sub>x</sub> conversion.
- NAM-29 (Atlanta): Simon and Adam will be co-hosting a Sunday workshop on *in-situ/operando* catalyst characterization at synchrotrons in the USA and will also present during the conference. Also look out for 13 additional Co-ACCESS co-authored contributions during the week!
- Southwest Catalysis Society (SWCS) Symposium (Houston): Simon will present an invited talk.

#### Reflections on my Time with Co-Access/Bare Group

#### **By Melissa Cendejas**

My journey with Co-ACCESS began in grad school when I spent 6 months as a DOE SCGSR fellow. I was immediately hooked by how the team approaches and practices science (I'm particularly fond of the synchronized dance we do when building up or breaking down an experiment). Luckily, Simon had an open postdoc position when I was looking for one and, having already performed the initiation rites into synchrotron life (multiple overnights and a solo beamtime), I rejoined the group as a postdoc in March 2022. My goal was to acquire specific skills to add to my catalysis researcher toolbelt and I am leaving with those skills, and so much more. I've been privileged to work on a variety of interesting projects with wonderful collaborators and I've deepened my fundamental understanding of spectroscopy and the knowledge that can be gained from properly designed experiments and analysis. It is bittersweet to be leaving such a lovely and fun group, but I leave here with new friends and mentors. It's hard to overstate how supportive, encouraging, and curious this team is. I am deeply grateful for my time and experiences here and am excited to apply the knowledge and skills I've learned to the new scientific questions I get to answer as part of the Analytical Science team at Dow. But as synchrotron life is not readily left behind, I look forward to returning as a user at BL 10-2.

#### 10-2 Update: Process Gas Handling

Beamline 10-2 is progressing by leaps and bounds as we look forward to first light in the next few weeks! We are now installing the process control capabilities. The hutch will be outfitted with dedicated ambient and high-pressure flow capabilities, liquid flow control, sample temperature control, and a potentiostat for electrochemical measurements. These will be complemented with a mass spectrometer and GC for product detection and quantification. We received the first major piece of this project, our ambient pressure flow control board - a 14 MFC assembly that will allow more complex flow schemes, and the ability to run two experimental cells at once. Coupled with fixed plumbing, and moisture/O $_2$  traps on select lines we will offer the highest purity feeds possible.



Melissa Cendejas and Adam Hoffman, SSRL 2024

### NSF INTERN Unni Kurumbail

In the Fall of 2024, Unni Kurumbail participated in a 6-month visit to Co-ACCESS through the NSF INTERN program. Unni is currently a 5<sup>th</sup>-year graduate student at the University of Wisconsin – Madison advised by Dr. Ive Hermans. His thesis work mainly focuses on kinetics and mechanism development of boron and vanadium oxide catalysts for the oxidative dehydrogenation of propane. During his time with Co-ACCESS, Unni had the pleasure of participating in Co-ACCESS supported beam times and assisting with reactor development for Co-ACCESS projects. Additionally, Unni has been developing a modified X-ray cell for Beamline 4-3 that will undergo testing in January and enable *operando* X-ray absorption measurements of materials (such as vanadium oxide catalysts) at tender X-ray edges.

# **Key Recent Publications**

"Advanced EXAFS analysis techniques applied to the L-edges of the lanthanide oxides", A. Smerigan, A.S. Hoffman, L. Ostervold, J. Hong, J. Perez-Aguilar, A.C. Caine, L. Greenlee, S.R. Bare, *Journal of Applied Crystallography*, (2024), **57**, 1913-1923. online. DOI: 10.1107/S1600576724010240.

"Selective CO<sub>2</sub> hydrogenation to ethanol over Ru-In catalysts", C. Zhou, A. Aitbekova, M. Stone, E. McShane, B. Werghi, S. Nathan, G. Liccardo, C. Song, J. Ciston, K. Bustillo, A.S, Hoffman, J. Hong, J. Perez-Aguilar, S.R. Bare, M. Cargnello, *Angewandte Chemie Int. Ed.*, (2024), **63**, e202406761. DOI: 10.1002/anie.202406761.

"Quantifying the Site Heterogeneities of Non-Uniform Catalysts Using QuantEXAFS", R. Rana, J. Hong, A.S. Hoffman, B. Werghi, S.R. Bare, A. Kulkarni, *Chemistry Methods*, (2025), **5**, e202400020. DOI:10.1002/cmtd.202400020.

"Dynamic Behavior of Pt Multimetallic Alloys for Active and Stable Propane Dehydrogenation Catalysts", B. Werghi, S. Saini, P-H. Chung, A. Kumar, A. Ebrahim, K. Abels, M. Chi, F. Abild-Pedersen, S.R. Bare, M. Cargnello, *Journal of the American Chemical Society*, (2024), **146**, 30966-30975. DOI: 10.1021/jacs.4c09424.

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