



- ▶ WE MISS YOU!.....1
- ▶ QXAS WORKSHOP.....1
- ▶ SULI STUDENTS.....1
- ▶ SOFTWARE DEVELOPMENT2
- ▶ KEY RECENT PUBLICATIONS.....2

Co-ACCESS

Semi-Annual

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

We Miss You!

QXAS Workshop

Co-ACCESS will be organizing a workshop as part of the 2020 SSRL/LCLS Users meeting. The workshop will be held virtually on Monday October 5, 2020. The workshop is entitled “Opportunities in Chemistry & Catalysis Research Using Quick Scanning XAS”, and is jointly organized by Simon R Bare, Adam S Hoffman, and Oliver Mueller. Full details can be found at: <https://conf.slac.stanford.edu/ssrl-lcls-2020/program#Catalysis>.

We look forward to your participation as the invited speakers discuss new scientific opportunities in many areas of chemistry and catalysis using QXAS.

I write this section of the July 2020 Co-ACCESS newsletter at the start of our 17th week of working remotely, and I am sure that we are in a situation similar to you. The coronavirus and its global impact have been devastating to so many. First, I hope that you and your loved ones are all safe and well. Here at Co-ACCESS, we are all well and continue to be as productive as possible given the circumstances. There have been some good things that have resulted from this time of no experiments. It has been a time to analyze data, write manuscripts, and plan for the future – and many Zoom meetings with you all as we endeavor to remain in contact with you. However, if you are like me, it is the monotony of each day that is starting to get old. The overarching reason that we are so dedicated to Co-ACCESS and its success is that we are experimentalists at heart; we greatly enjoy collaborating with you and to enable your science to drive our understanding of catalytic science to the next level. Thus, we are anxious to get back to the beamlines at SSRL, and of course, to being with you at all hours of the day and night as we pore over the data that is collected. We do not know when we’ll be back in that mode of operation again, or what the new normal mode of operation will look like. In the meantime, we ask for your patience, and please reach out to any of us if you have questions or if we can help in any way. There are also several exciting developments taking place, and we look forward to sharing these with you in the coming months. Our first thing to share is that we welcome Hayden and Kenzie as SULI students in our group, and their willingness to work remotely over the summer with us. We are all learning this together. Please take care and stay safe and healthy. We look forward to seeing you all again soon!

SULI Students

This summer Co-ACCESS is mentoring two SULI Students.



Hayden Oliver is a senior at Brigham Young University studying Applied Physics. His undergraduate research is focused on computational alloy discovery. Hayden is interested in metallurgy, chemical battery technologies, and semiconductor development and plans on doing his graduate work in one of these fields. He has a background in software development and has joined Adam to tackle some of the problems of XAS related to data storage, analysis, error-checking, and distribution. He loves to build rockets, climb the Utah mountains with his wife, and hopes to be an astronaut when he grows up.

Kenzie Sanroman currently lives in the Chicago area where she is a rising junior studying chemical engineering at Northwestern University. At her home institution she conducts research on electrocatalysts and the electrochemical production of adipic acid and hydrogen peroxide. She is excited to work on compiling literature references to better help others properly analyze their XAS data and explore the area of QXAS, and of course help make this newsletter! In her spare time, she enjoys hanging out with her dog Pinta, upcycling clothes, and collecting vinyl records.

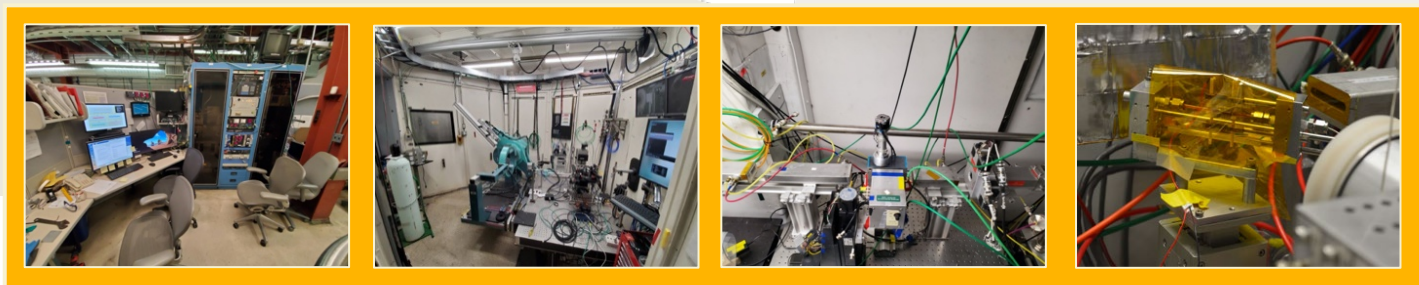


Software Development

Adam has been working on developing a suite of software, for the catalysis and XAS community at large, to aid XAS experimentation from sample preparation to data analysis. To aid in beam time experimental planning he has created a sample mass calculator expanding on those currently available. The new calculator handles catalyst compositions where the materials can be expressed as any combinations of weight fractions and stoichiometric compounds, expanding on the input limitations of the current software. The sample mass calculator also supports dilution inputs, not available in other software, an especially important to catalysis researchers where diluents are commonly used in in-situ reactor packing.

With the help of a SULI intern, Hayden Oliver, Co-ACCESS is developing software to facilitate handling of data generated from the multi-element fluorescence detectors at SSRL. Access to these detectors has allows the single-site/single-atom-alloy catalysis community as well as the electro-/photo-catalysis communities to characterize powders with ultra-low (0.0025 wt%) metal loadings or thin films with limited sample quantity. The new software is designed to import, process, and condense all the multi-element fluorescence data that are generated by SSRL fluorescence detectors into a dataset that can then be imported into conventional XAS analysis software packages.

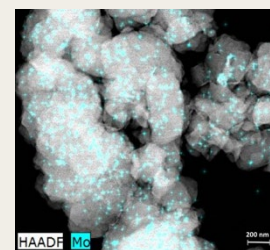
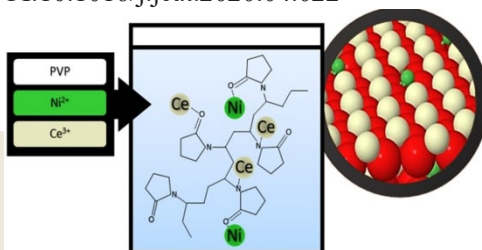
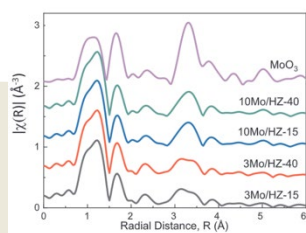
Finally, Hayden and Adam are working on developing software to perform the continuous Cauchy wavelet transform (CCWT) and plot the data. CCWT qualitatively guides EXAFS modeling speeding up the analysis process. This code is currently being wrapped into a friendly user interface by Hayden Oliver, a SULI intern, so that it can be distributed to the user community.



Key Recent Publications

A few recent publications highlighting some of the exciting research conducted in collaboration with Co-ACCESS.

- “Environmentally Benign Synthesis of a PGM-Free Catalyst for Low Temperature CO Oxidation”, C. Riley, G. Canning, A. De La Riva, S. Zhou, E. Peterson, A. Boubnov, A.S. Hoffman, M. Tran, S.R. Bare, S. Lin, H. Guo, A. Datye, *Applied Catalysis B* (2020), **264**, 118547. DOI: 10.1016/j.apcatb.2019.118547.
- “Tunable Catalytic Performance of Palladium Nanoparticles for H₂O₂ Direct Synthesis via Surface-Bonded Ligands”, L. de Lima e Freitas, B. Puértolas, J. Zhang, B. Wang, A.S. Hoffman, S.R. Bare, J. Pérez-Ramírez, W.J. Medlin, E. Nikolla, *ACS Catalysis* (2020), **10**, 5202-5207. DOI: 10.1021/acscatal.0c01517.
- “Effect of Si/Al Ratio of ZSM-5 Support on Structure and Activity of Mo Species in Methane Dehydroaromatization”, M. Rahman, A. Infantes-Molina, A.S. Hoffman, S.R. Bare, K.L. Emerson, S.J. Khatib, *Fuel*, (2020), **278**, 118290; DOI: 10.1016/j.fuel.2020.118290.
- “Unraveling the Individual Influences of Supports and Ionic Liquid Coatings on the Catalytic Properties of Supported Iridium Complexes and Iridium Clusters”, M. Babucci, A.S. Hoffman, L.M. Debeve, S.F. Kurtoglu, S.R. Bare, B.C. Gates, A. Uzun, *J. Catalysis* (2020), accepted. DOI: 10.1016/j.jcat.2020.04.022



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>