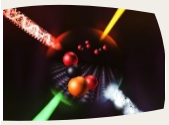



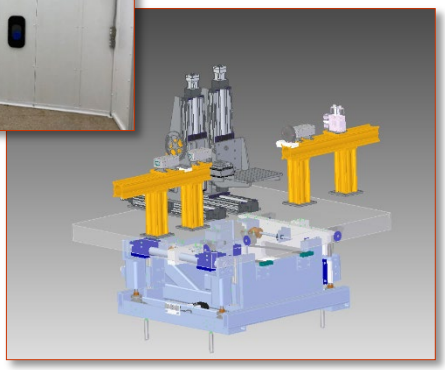

Newsletter 6 | July 2021

Co-ACCESS Semi-Annual

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

DEVELOPMENTS

Beamline 10-2 Update

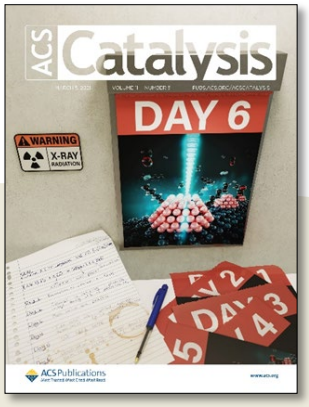


There has been continued progress for the conversion of BL10-2 into a catalysis-centric beamline. The preparation of the BL10-2b hutch for installation of the end station hardware has been completed (see photo, right). The layout of the hutch has been set with a large optical surface for X-ray experiments and a second optical surface for the FTIR and other characterization hardware. The procurement and fabrication of the hutch tables is proceeding on schedule. Procurement of the instrumentation for the XAS experiments is well-underway and we are looking forward to commissioning in the fall. The optics upgrade for the quick scanning monochromator and new mirrors is slated for summer and fall of 2022.

catMass is now Public

Wondering how the addition of a diluent to your sample or changing your support from SiO_2 to CeO_2 affects the adsorption properties and influences your XAS experiment? Adam Hoffman has been working on developing Python codes to aid users in experimental preparation, signal processing, and in workup and analysis of in-situ XAS data collected at the SSRL spectroscopy beamlines. After a year of trials in the Co-ACCESS group the catMass Python package and user interface has now been released on GitHub for all users to access it. This program allows users to calculate the proper sample packing for catalyst samples taking into account the complex naming schemes and use of diluents. This code allows users to determine how easy, or difficult, a sample will be to characterize via XAS giving users a more informed starting position for their experiments. Please see Co-ACCESS website for more information.

ODDS AND ENDS:



XAS Bootcamp planned for Summer 2021

With the Summer down upon us we will be hosting another invitation-only XAS analysis training course. These intense 3-day events allow users to work with their own data as we cover topics from pre-processing in Athena, basic model building in Artemis, to developing complex models and simultaneous fitting to observe trends as samples evolve under process conditions. Look out for more details soon.

Office Hours Starting August 2021

Have a question about the XAS technique, experimental planning, data analysis or something else XAS or Co-ACCESS related? Co-ACCESS will be starting to host bi-weekly office hours where you can log into a public Zoom room to chat with Simon, Adam or Jiyun. Office hours will be held on the first and third Wednesday of the month at 9-10 a.m. Pacific time. For more information, please see the Co-ACCESS website.

Working with Co-ACCESS

SCGSR Student: Melissa Cardejas (she/her) University of Wisconsin-Madison

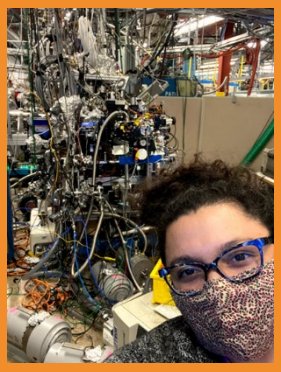


Figure: Pumped to do science at BL13-2 (pun intended).

I was a member of the Co-Access Lab for 6 months in the middle of the pandemic (October 2020 – April 2021) as a DOE Office of Science graduate student research fellow (SCGSR). During my time at SSRL, I used ambient pressure X-ray Photoelectron Spectroscopy (AP-XPS, BL 13-2) and in-situ X-ray Raman Spectroscopy (XRS, BL 15-2) to observe active site formation and dynamics on hexagonal boron nitride catalysts for the oxidative dehydrogenation of light alkanes. This catalytic system – comprised entirely of light elements – has been difficult to investigate in-situ. The experiments performed during my two beamtimes directly show the changes to catalyst composition at a bulk scale (XRS) and at the near-surface (AP-XPS), providing new insights and creating the foundation for future studies.

Aside from my own work, I was also able to participate in experiments the group was running at BL 9-3. Prior to my time at SSRL, I had not done any hard XAS, so the hands-on experience I gained allowed me to learn lots of information in a short amount of time. Working in the Co-Access lab was a dynamic, invigorating, and demanding learning environment, and I was inspired by each of my interactions to understand and enjoy science at the level of the rest of the group. I loved it and am extremely grateful for the opportunity. Working at SSRL during a pandemic made me distinctly aware of the vibrant and supportive community that keeps the place running. Although it was not the same bustling environment because of pandemic restrictions, the strength of the community could be felt, and a lot of cool science got done.

Personnel

Positions Available at Co-ACCESS

Nirmalendu Patra will be completing his postdoctoral fellowship at Co-ACCESS in early September. As such we are actively seeking a new postdoctoral fellow, and a Research Associate. The Postdoctoral Associate will be responsible for developing and applying time-resolved in-situ/in-operando X-ray absorption spectroscopy to the study of a catalytic process of mutual interest.

The Research Associate will work collaboratively with user groups throughout the United States and abroad, assisting in planning experiments, beamtime scheduling, training users, collecting data and providing guidance on the data analysis. Details about these positions can be found at:

https://careers.slac.stanford.edu/sites/careers.slac.stanford.edu/files/RA%20Catalysis%202021.06.17.pdf
and
https://careers.slac.stanford.edu/sites/careers.slac.stanford.edu/files/Postdoctoral%20Position%20at%20SSRL%20for%20Time-resolved%20XAS.pdf

Key Recent Publications and Presentations

"Reduction and Agglomeration of Supported Metal Clusters Induced by High Flux X-ray Absorption Spectroscopy Measurements", M. Albrahim, C. Thompson, D. Leshchev, A. Shrotri, R. Unocic, J. Hong, A.S. Hoffman, M. Meloni, R. Runnebaum, S.R. Bare, E. Stavitski, A. Karim, J. Phys. Chem. C (2021), 125, 11048-11057. DOI: 10.1021/acs.jpcc.1c01823.

"Role of the Oxide Support on the Structural and Chemical Evolution of Fe Catalysts during the Hydrogenation of CO_2", M.L. Luna, J. Timoshenko, D. Kordus, C. Rettenmaier, A.S. Hoffman, S.R. Bare, S. Shaikhutdinov, B. Roldan Cuenya, ACS Catalysis (2021), 11, 6175-6185. DOI: 10.1021/acscatal.1c01549.

"Impurity Control in Catalyst Design: The Role of Sodium in Promoting and Stabilizing Co and Co_2C for Syngas Conversion", A.S. Asundi, A.S. Hoffman, S.S. Nathan, A. Boubnov, S.R. Bare, Stacey F. Bent, ChemCatChem (2021), 13, 1186–1194. DOI: 10.1002/cctc.202001703.

"On the Cobalt Carbide Formation in a Co/TiO_2 Fischer-Tropsch Synthesis Catalyst as Studied by High-Pressure, Long-Term Operando X-Ray Absorption Spectroscopy and Diffraction", I.K. van Ravenhorst, A.S. Hoffman, C. Vogt, A. Boubnov, N. Patra, R. Oord, C. Akatay, F. Meirer, S.R. Bare, B.M. Weckhuysen, ACS Catalysis (2021), 11, 2956-2967. DOI: 10.1021/acscatal.0c04695.

Co-ACCESS Presentations at XAFS2021Virtual While the in-person XAFS2021 conference in Sydney, Australia is postponed to July 2022 due to COVID-19 a virtual event was organized from 11-13 July 2021. The focus of the virtual meeting was on presentations by early career researchers. Both Jiyun Hong and Nirmalendu Patra, Co-ACCESS postdocs, gave oral presentations at the virtual meeting. Jiyun presented a talk on "Evidence of Irreversible Dynamic Changes of Mixed Metal Oxides During Oxygen Evolution Reaction from X-ray Absorption Spectroscopy" from a collaboration with Eranda Nikolla (Wayne State University) , while Nirmalendu gave a talk entitled, "In-situ / operando XAS characterization of ZSM-5 supported Mo catalysts to identify the pathway to the active species for methane dehydroaromatization", presenting results from a collaboration with Sheima Khatib (Texas Tech University).

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