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

Co-ACCESS Operations During COVID-19



These last few months have been a difficult time for so many people. There are so many things that we took for granted and now miss greatly. For those of us at the synchrotron we missed the crazy life of conducting research at such a facility. But from my perspective the part that I miss most is the interaction with the groups of users who come to the beamline to conduct their research: the opportunity to both teach and learn about their research, to inspire and be inspired. We all hope that the situation will change later in 2021.

In the meantime, it was truly exciting to be allowed back into the lab, and to have beamtime starting in mid-October for in-situ/operando catalysis experiments. External users were not allowed on-site and so all the experiments were conducted by Co-ACCESS personnel. In order for these

experiments to be productive and meaningful it required a significant amount of advance planning to ensure the safety of all involved. The user groups mailed their samples and went through the exercise of detailed planning for the experiments. When each group was scheduled, they were present throughout their beamtime via Zoom. The data were transferred to a location where it the user could access and plot it and perform preliminary analysis in real-time. Using this mode of operation, we were able to collect XAS data for 19 user groups in the 7 weeks of beamtime on BL9-3 and 4-3. Towards the end of the allocated beamtime the lab allowed local users (from Stanford University) on site to perform experiments, and the photo above shows Aisulu Aitbekova, a 5th year graduate student in Prof. Matteo Cargnello's group at Stanford, getting ready to load one of her samples.

- Simon R. Bare

Beamline 10-2 Update

Over the past 9 months there has been significant progress towards the conversion the former scattering beamline, BL10-2, into a catalysis-centric beamline. The final design of the SSRL-designed quick-scanning monochromator has been completed and procurement of components has begun. The design of the new mirrors is going through revisions in the design phase. The new hutch table will be installed by May 2021, detectors and motion control systems are being fabricated and tested. In-situ experimentation hardware, gas cabinets, are waiting for install. Conditioning experiments, with the existing optics, are expected to begin during the last cycle of the 2021 run.

VISITING SCGSR STUDENTS



We are privileged to have two visiting DOE Office of Science graduate student research fellows (SCGSR) spending time during with us during their Ph.D. studies. The program provides opportunities for graduate thesis research at a DOE laboratory from 3-12 months, via a competitive application process.

Melissa Cendejas is a fifth year PhD student at the University of Wisconsin. Her PhD work has focused on understanding the active site on boron-based oxidative dehydrogenation catalysts using controlled synthesis techniques and solid state Nuclear Magnetic Resonance Spectroscopy (ssNMR). As a part of the Co-ACCESS team, she will use ambient pressure X-ray Photoelectron Spectroscopy and in-situ X-ray Raman Spectroscopy to investigate the formation and dynamics of active sites on boron-based catalysts.

Taylor Spivey is a third year PhD student at the University of Colorado Boulder. His PhD work has focused on using combined analytical and spectroscopic methods to understand the behavior of model biomass compounds on novel alloy catalysts, focusing on crotonaldehyde electroreduction and furfural electrooxidation. He is also interested in optimizing the design of electrocatalysts structures via colloidal synthesis methods to tune selectivity and activity. As a part of the Co-ACCESS team, he will focus on the design of operando XAS electrochemical cells to gain insight into the electronic structure of adsorbates upon surface hybridization.

In addition to their SCGSR research goals, both, Melissa and Taylor, will assist in Co-ACCESS' on-going projects to gain further experience in catalyst characterization using synchrotron-based methods.

Key Recent Publications

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

“Selective Methanol Carbonylation to Acetic Acid on Heterogeneous Atomically Dispersed $\text{ReO}_4/\text{SiO}_2$ Catalysts, J. Qi, J. Finzel, H. Robotjazi, M. Xu, A.S. Hoffman, S.R. Bare, X. Pan, P. Christopher, Journal of the American Chemical Society (2020), 142, 14178–14189. DOI: 10.1021/jacs.0c05026.

“Understanding Support Effects of ZnO-Promoted Co Catalysts for Syngas Conversion to Alcohols Using Atomic Layer Deposition”, S.S. Nathan, A.S. Asundi, J.A. Singh, A.S. Hoffman, A. Boubnov, J. Hong, S.R. Bare, S.F. Bent ChemCatChem (2020) 12, 1-13. DOI: 10.1002/cctc.202001630.

“Enhanced Alcohol Production over Binary Mo/Co Carbide Catalysts in Syngas Conversion”, A.S. Asundi, A.S. Hoffman, M. Chi, S.S. Nathan, A. Boubnov, J. Hong, S.R. Bare, S.F. Bent, Journal of Catalysis (2020) 391, 466-458. DOI: 10.1016/j.jcat.2020.09.003.

“Electronic Structure of Atomically Dispersed Supported Iridium Catalyst Controls Iridium Aggregation”, S.F. Kurtoğlu, A.S. Hoffman, D. Akgül, M. Babucci, V. Aviyente, B.C. Gates, S.R. Bare, A. Uzun, ACS Catalysis (2020), 10, 12354–12358. DOI: 10.1021/acscatal.0c03909.

*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>*