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Co-ACCESS

Semi-Annual

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

Welcome Back to SSRL

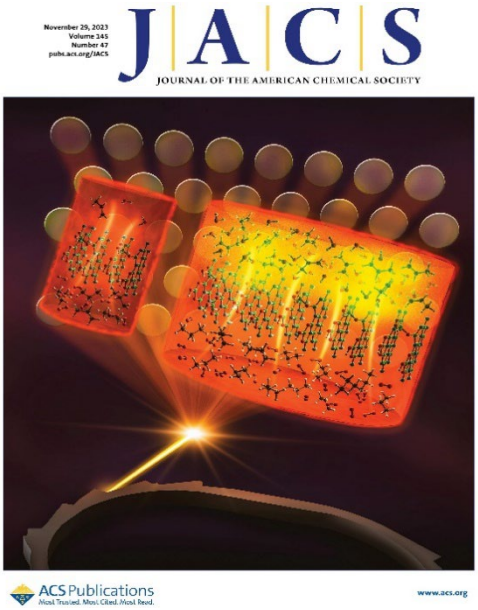
We are delighted to welcome back our collaborators as SSRL resumes operations following an unfortunate extended downtime in 2023. Since the facility's restart in July, the Co-ACCESS team has been actively supporting users returning to the XAS beamlines, conducting *in-situ/operando* experiments. We are thrilled to be working with our collaborators again at the beamlines, collecting the exciting XAS data that all of us have been waiting for! We look forward to the continued collaborations in 2024.

We are thrilled to announce that our 100th publication was recently published. This was a special occasion as the lead author was Melissa Cendejas who is now a postdoctoral associate at SSRL, but the publication stemmed from her time in the Co-ACCESS group as an Office of Science Graduate Student Fellow (SCGSR).

Tracking Active Phase Behavior on Boron Nitride during the Oxidative Dehydrogenation of Propane Using Operando X-ray Raman Spectroscopy

Melissa C. Cendejas, Oscar A. Paredes Mellone, Unni Kurumbail, Zisheng Zhang, Jacob H. Jansen, Faysal Ibrahim, Son Dong, John Vinson, Anastassia N. Alexandrova, Dimosthenis Sokaras, Simon R. Bare, and Ive Hermans

Journal of the American Chemical Society **2023** *145* (47), 25686-25694. DOI: 10.1021/jacs.3c08679



New Website

Co-ACCESS is excited to announce the launch of our new website, featuring a fresh address (https://web.slac.stanford.edu/coaccess/), so please update your bookmark. The website offers a comprehensive update, providing the latest information on our experimental capabilities. Please explore our "Resources" page to access detailed information about the equipment available for *in-situ/operando* XAS experiments. We would also like to highlight our "XAS Theory/Computation" page, which showcases the theoretical support that we offer for XAS data analysis. Lastly, the "Events" page highlights upcoming Co-ACCESS events – conferences we are attending, workshops that we hold, and most importantly, the monthly Co-ACCESS office hours that any of you are welcome to attend and ask any questions related to XAS! Please check out the website, and we encourage you to reach out should you require further information. Your engagement is crucial to the success of Co-ACCESS, and we look forward to connecting with you through our new website.

SULI Student Takes 2nd Place in National Competition!

During the summer of 2023 Sarah Driscoll, an undergraduate student from Vanderbilt University, joined Co-ACCESS for a Science Undergraduate Laboratory Internship (SULI) under mentorship by Adam Hoffman. While here, Sarah's research involved preparing standards to facilitate setup and calibration of the multi-element fluorescence detectors at the XAS beamlines. At the end of here 10-week stay she presented her work at the ORISE Ignite Off! competition, placing second against DOE interns from 5 National Laboratories.

If you know of any undergraduate or graduate students interested in National Laboratory Internships please see details here: https://science.osti.gov/wdts.

Co-ACCESS Office Hours

Do you have a question about XAS, be it analysis, experimental design, or where to get started? Drop in to one of our monthly office hours to chat with members of the Co-ACCESS team. See the Co-ACCESS website for upcoming dates (https://web.slac.stanford.edu/coaccess/events) and send an email to co.access.lab@gmail.com if you would like to be included on the email reminders.

Dr. Rachita Rana

Rachita Rana, a graduate student at UC Davis, and co-mentored by Simon R Bare and Ambarish Kulkarni, recently successfully defended her PhD thesis. She is the developer of QuantEXAFS, which harmonizes the knowledge from DFT calculated structures and EXAFS data. This method has now been applied to a host of different catalytic systems and allows us to visualize structures of the active sites versus a table of bond lengths and coordination numbers. She will soon start a postdoctoral fellowship with Dr. Yuriy Román-Leshkov at MIT. We wish her every success in her future career.

Key Recent Publications

1. "Tracking Active Phase Behavior on Boron Nitride during the Oxidative Dehydrogenation of Propane Using Operando X-Ray Raman Spectroscopy", M. Cendejas, M. Paredes, A. Oscar, U. Kurumbail, Z. Zhang, J. Jansen, F. Ibrahim, S. Dong, J. Vinson, A. Alexandrova, D. Sokaras, Simon R. Bare, I. Hermans, *Journal of the American Chemical Society*, (2023), **145**, 25686-25694. DOI: 10.1021/jacs.3c08679.

2. "Cation Incorporation into Copper Oxide Lattice at Highly Oxidizing Potentials", L. Ostervold, A. Smerigan, M.J. Liu, L. Filardi, F. Vila, J.E. Perez-Aguilar, J. Hong, W.A. Tarpeh, A.S. Hoffman, L. Greenlee, E.L. Clark, M. Janik, S.R. Bare, *ACS Applied Materials & Interfaces*, (2023), **15**, 47025-47036. DOI: 10.1021/acsami.3c10296.

3. "Spectroscopic determination of metal redox and segregation effects during CO and CO/NO oxidation over silica-supported Pd and PdCu catalysts", S.T. Kristy; S. Svadlenak, A.S. Hoffmann; S.R. Bare, K.A Goulas, *Applied Catalysis B: Environmental*, (2023), **342**, 123329. DOI: 10.1016/j.apcatb.2023.123329.

4. "CatMass – Software for calculating optimal sample masses for X-ray absorption spectroscopy experiments involving complex sample compositions". J.E. Perez-Aguilar, A. Caine, S.R. Bare, A.S. Hoffman, *J. Synchrotron Radiation* (2023), **30**, 1023-1029. DOI: 10.1107/S160057752300615X.

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