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Co-ACCESS

Semi-Annual

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

Outreach

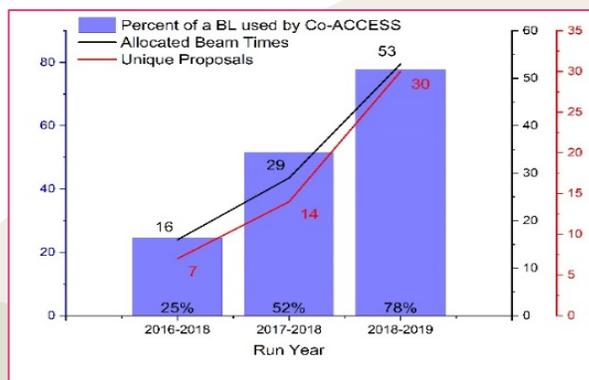
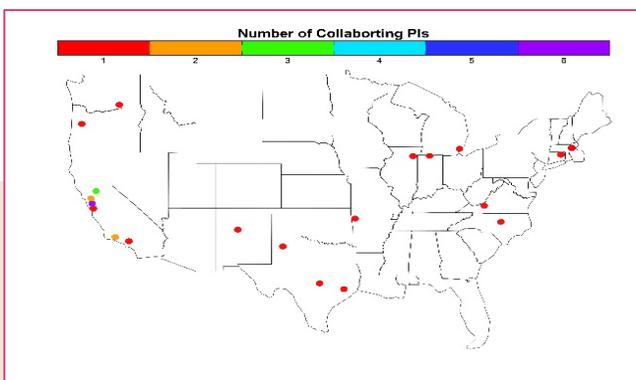
Advancing Catalysis Research with X-ray Absorption Spectroscopy

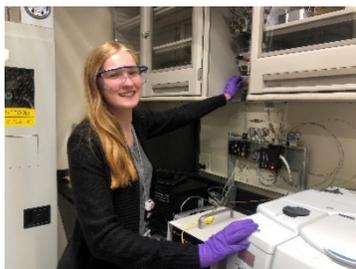


We recently hosted a pre-conference workshop as part of the 2019 North American Catalysis Society meeting in the Hyatt Regency Hotel in Chicago on June 23, 2019. The workshop was limited to 40-50 participants and was vastly oversubscribed. This hands-on mini-course covered important aspects of the application of X-ray absorption spectroscopy (XAS) as applied to the catalyst researcher. The course was designed to enable the researcher to have a firm grasp of how XAS might aid their own research and why they should consider incorporating it into their research program, while educating the participants on the basics of sample preparation and data analysis. The course showcased a live demonstration of an *in-situ* XAS catalysis experiment from beamline 2-2 at SSRL. This was the first time we conducted such a live demonstration with remote control of the beamline so the participants could observe the XAS spectra in real time as we reduced a catalyst!

Growth of Co-ACCESS

There has been significant growth in the number of catalysis users at SSRL over the last two years. We have begun keeping metrics of where these researchers come from, what science they are studying, and the number of proposal and beamtimes that result from the collaborations. While the majority of our collaborators originate from the West coast, as expected, there is a good geographic spread, as illustrated in the map. Regarding the growth in the number of proposals and the resulting beamtime, the figure shows that we have had steady growth in Co-ACCESS associated beam time with the last cycle of the 2018-2019 run supporting 98% of a beam time equivalent.





Jessica Stelzel



Helen Fisher

SULI Students

Co-ACCESS is mentoring two Science Undergraduate laboratory Internship (SULI) students for the summer. Jessica Stelzel is a recent graduate from Georgia Institute of Technology with a B.S. in Materials Science. In September she will be starting a Ph.D. program at Johns Hopkins University. This summer she is working on applying FTIR spectroscopy to characterize supported metallic nanoparticles. She will be comparing DRIFTS and transmission IR methods. Helen Fisher, a rising Physics senior at Cal Poly State University – San Luis Obispo. This summer she is working on several projects related to improving our efficiency of operations, method development, and testing new equipment. We welcome both of them to the group!

Co-ACCESS Equipment

Co-ACCESS has two fully-portable gas manifolds, one for operation at ambient pressure (6 gases), and one for operation at high pressure (3 gases, 80 bar). Each of these is fully automated using LabView control. We also own two mass spectrometers for detection of gas phase reaction products. With these systems we have demonstrated that it now takes less than two hours to have the experiment fully functional at the beamline. A huge improvement on the half-day that was the standard previously.

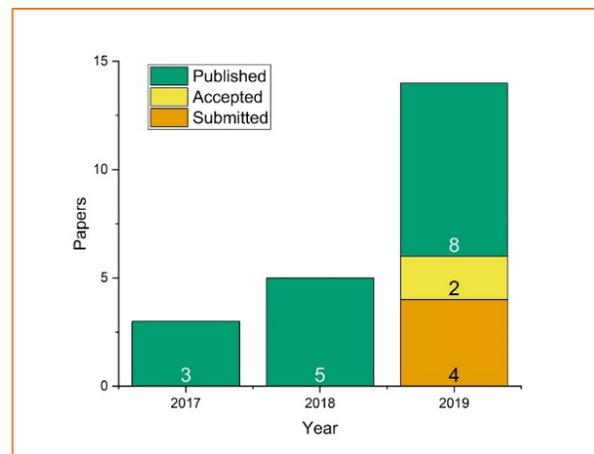
Key Recent Publications

One key metric, of course, is the number and type of publications that result from the beamtime assigned to our collaborators. We highlight a few recent publications here to key you a sense of the breadth of the catalysis research that has been conducted at Co-ACCESS.

Single-atom catalysis: “Structure-function relationships during the dynamic evolution of TiO₂ supported Pt single atom catalysts”, L. DeRita, J. Resasco, S. Dai, A. Boubnov, H.V. Thang, A.S. Hoffman, I. Ro, G.W. Graham, S.R. Bare, G. Pacchioni, X. Pan, P. Christopher, *Nature Materials*, (2019), DOI: 10.1038/s41563-019-0349-9 and “Identification of the Active Complex for CO Oxidation over Single Atom Ir-on-MgAl₂O₄ Catalysts”, Y. Lu, J. Wang, L. Yu, L. Kovarik, X. Zhang, A.S. Hoffman, A. Gallo, S.R. Bare, D. Sokaras, T. Kroll, V. Dagle, H. Xin, A.M. Karim, *Nature Catalysis* **2** 149-156 (2019); DOI: 10.1038/s41929-018-0192-4.

Confinement effects in catalysis: ” Dynamic reorganization and confinement of TiIV active sites controls olefin epoxidation catalysis on two-dimensional zeotypes”, N.A. Grosso-Giordano, A. S. Hoffman, A. Boubnov, D. W. Small, S. R. Bare, S. I. Zones, A. Katz, *Journal of the American Chemical Society*, (2019), **141**, 7090-7106; DOI: 10.1021/jacs.9b02160.

Higher alcohol synthesis from syngas: “Role of Co₂C in ZnO-promoted Co Catalysts for Alcohol Synthesis from Syngas”, J.A. Singh, A.S. Hoffman, J. Schumann, A. Boubnov, A.S. Asundi, S.S. Nathan, J. Nørskov, S.R. Bare, S.F. Bent, *ChemCatChem*, (2019) **11** 799-809; DOI: 10.1002/cctc.201801724.



Alexey Boubnov

Alexey has been a member of Co-ACCESS as a postdoctoral research associate for the last two years and he has been instrumental in our initial growth and success. It is with sadness that we bid him farewell as he begins a new position at Karlsruhe Institute of Technology (KIT). I am sure that all those of you who have had the pleasure of working with him will wish his every success in his future career!

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>