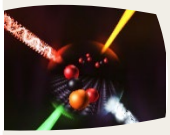




Newsletter 8 |July 2022

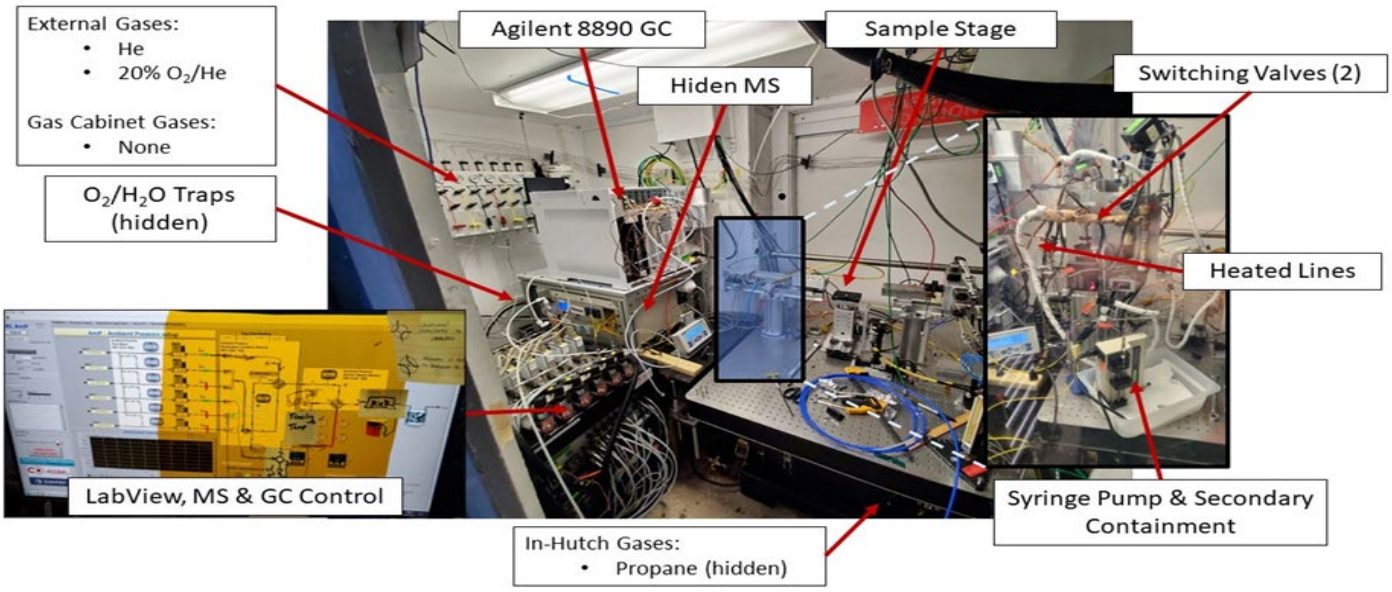
Co-ACCESS Semi-Annual

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

RECENT DEVELOPMENTS

Complex Operando XAS Experiments

Co-ACCESS has recently spearheaded two complex experimental arrangements at beamline 2-2. A group from MIT, with team lead graduate student Ran Zhu, used operando XAS to study a metathesis catalyst and they needed to add known amounts of a vaporized liquid promoter. Moreover, GC analysis was needed to quantify the product yield. Separately a group from UC Santa Barbara, with team lead graduate student Jason Chalmers, used operando XAS to follow the kinetics of the deactivation of their propane dehydrogenation catalyst. This experiment necessitated using both GC and mass spectrometry for the analysis, together with accurate feed composition and residence time in the XAS cell. The figures illustrate the experimental arrangement for the MIT experiments.



Co-ACCESS Office Hours

In June, Co-ACCESS launched its “Office Hours” program. Comparable to how a PI or TA hosts office hours for a course at a college, the program allows collaborators to log into a virtual room and ask any questions they have regarding XAS experimentation and experimental design, data analysis, or anything else Co-ACCESS related that may not require a formal meeting. Office hours will be hosted on SSRL AP Tuesday and then twice a month through the summer down. During the first meeting, two groups attended with questions about how to report data in manuscripts and how to determine the importance of different paths during EXAFS modeling!

Stephen Kristy & Lars Ostervold join Co-ACCESS as SCGSR Fellows

Stephen Kristy is a 3rd-year PhD student in chemical engineering at Oregon State University. His PhD focuses on the design of bimetallic alloy catalysts intended for low temperature oxidation of carbon monoxide in diesel exhaust. As part of the Co-ACCESS team, Stephen plans to perform Quick Scanning Extended X-ray Absorption Fine Structure (QEXAFS) analysis and transmittance Fourier Transform Infrared Spectroscopy (FTIR) with these catalysts during transient temperature experiments under operando conditions. Stephen will use these experiments to elucidate the structural and electrical properties of these catalysts, as well as reagent absorption sites, and relate these properties to the kinetics of CO oxidation. Stephen's goal is to better understand parameters leading to improved low temperature activity for CO oxidation. In completing this work, Stephen will aid in the development of operating procedures and analysis methods required to extract meaningful data from time resolved QEXAFS experiments for future utilization.
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Lars Ostervold is a 5th-year PhD student in chemical engineering at Penn State. His PhD work focuses on applying operando and computational techniques to improve intrinsic electrocatalyst activity by rational design. During his time with the Co-ACCESS group, Lars plans to investigate the electronic and atomic structure of formal Cu3+ materials during the oxygen evolution reaction using EXAFS modeling. Lars will also investigate the effect of cations on the structure of Cu1+ and Cu2+ oxidation states and assist the team in evaluating designs of operando electrochemical cells.

Key Recent Publications

"Catalytic performance and near-surface X-ray characterization of titanium hydride electrodes for the electrochemical nitrate reduction reaction", M. Liu, J. Guo, A.S. Hoffman, J. Stenlid, M. Tang, E. Corson, K. Stone, F. Abild-Pedersen, S.R. Bare, W. Tarpeh, *Journal of the American Chemical Society*, (2022), **144**, 5739–5744. DOI: 0.1021/jacs.2c01274.

"Atomically Dispersed Platinum in Surface and Sub-Surface Sites on MgO have Contrasting Catalytic Properties for CO Oxidation", Y. Chen, R. Rana, Z. Huang, F.D. Vila, T. Sours, J.E. Perez-Aguilar, X. Zhao, J. Hong, A.S. Hoffman, X. Li, C. Shang, T. Blum, J. Zeng, M. Chi, M. Salmeron, C.X. Kronawitter, S.R. Bare, A.R. Kulkarni, B.C. Gates, *J. Phys. Chem Letters*, (2022), **13**, 3896-3903. DOI: 10.1021/acs.jpclett.2c00667.

"Colloidal Platinum-Copper Nanocrystal Alloy Catalysts Surpass Platinum in Low-Temperature Propene Combustion", N. Tahsini, A.-C. Yang, V. Streibel, B. Werghi, E. Goodman, A. Aitbekova, S.R. Bare, Y. Li, F. Abild-Pedersen, M. Cargnello, *Journal of the American Chemical Society*, (2022), **144**, 1612-1621. DOI: 10.1021/jacs.1c10248.

"Fe Coordination Environment, Fe-Incorporated $Ni(OH)_2$ Phase, and Metallic Core are Key Structural Components to Active and Stable Nanoparticle Catalysts for the Oxygen Evolution Reaction", P. Acharya, R. Manso, A.S. Hoffman, S. Bakovic, L. Kékedy-Nagy, S.R. Bare, J. Chen, L. Greenlee, *ACS Catalysis,* (2022), **12**, 1992-2008. DOI: 10.1021/acscatal.1c04881.

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 maximizing the success of your time at SSRL. We look forward to collaborating with you!
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