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Co-ACCESS

Semi-Annual

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

Conferences and Outreach

Advancing Catalysis Research with X-ray Absorption Spectroscopy

Over the recent months members from Co-ACCESS participated in numerous conferences. Simon Bare presented an invited talk at the Telluride conference, Theory and Practice of Catalysis, X-ray Absorption Spectroscopy and Catalysis: Past, Present & Future, and he taught at the 5th Anatolian School of Catalysis. Alexey Boubnov presented at talk at 14th European Congress on Catalysis (EuropaCAT), and Adam Hoffman presented a talk at the 19th Annual Meeting of AIChE. Fernando Vila taught at the short course on XAS at Brookhaven National Lab. Recently Adam and Simon participated in the Science Café organized by UC Davis.

science café

A Conversation with Drs. Adam Hoffman & Simon Bare
SLAC National Accelerator Lab & UCD Chemical Engineering

Let There Be Light:
Synchrotrons
Illuminate
Catalyst Science

Wednesday December 11th 5:30 PM
G Street Wunderbar 228 G St, Davis



Hosted by Prof. Jared Shaw
Brought to you by:
UC Davis College of
Letters & Science

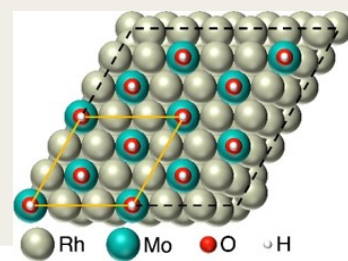
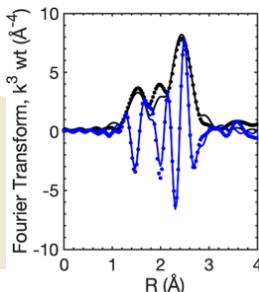
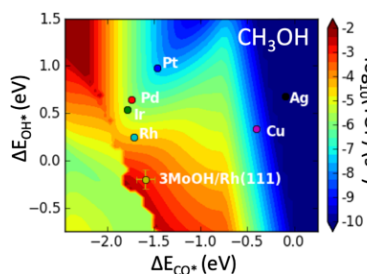


UC DAVIS
DEPARTMENT of CHEMISTRY

Key Recent Publications

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

- “Structure, dynamics, and reactivity for light alkane oxidation of Fe(II) sites situated in the nodes of a Metal-Organic Framework”, M.C. Simons, J.G. Vitillo, M. Babucci, A.S. Hoffman, A. Boubnov, M. Beauvais, Z. Chen, C.J. Cramer, K. Chapman, S.R. Bare, B.C. Gates, C. Lu, L. Gagliardi, A. Bhan, *Journal of the American Chemical Society* (2019), **141**, 18142-18151. DOI: 10.1021/jacs.9b08686.
- “Palladium Oxidation Leads to Methane Combustion Activity: Effects of Particle Size and Alloying with Platinum”, E. Goodman, A. Ye, A. Aitbekova, O. Müller, A. Riscoe, T. Taylor, A.S. Hoffman, A. Boubnov, K.C. Bustillo, M. Nachtegaal, S.R. Bare, M. Cargnello, *Journal of Chemical Physics* (2019), **151**, 154703. DOI: 10.1063/1.5126219
- “Increasing the catalytic stability by optimizing the formation of zeolite-supported Mo carbide species ex situ for methane dehydroaromatization”, M. Rahman, A. Infantes-Molina, A. Boubnov, S.R. Bare, E. Stavitski, A. Sridhar, S.J. Khatib, *J. Catalysis* (2019) **375**, 314-328. DOI: 10.1016/j.jcat.2019.06.002.
- “Understanding Structure-Property Relationships of MoO₃ Promoted Rh Catalysts for Syngas Conversion to Alcohols”, A.S. Asundi, A.S. Hoffman, P. Bothra, A. Boubnov, F.D. Vila, N. Yang, J.A. Singh, L. Zheng, J.A. Raiford, F. Abild-Pedersen, S.R. Bare, S.F. Bent, *Journal of the American Chemical Society* (2019). DOI: 10.1021/jacs.9b07460.



Meet The Team



Simon R. Bare, the lead-PI, received his PhD from the University of Liverpool in 1982, and then held postdoctoral appointments at Cornell University and Lawrence Berkeley National Lab. He then moved to the dark side, and took a position in R&D with The Dow Chemical Company in Midland, MI for 10 years during which time he has his first experience of using synchrotrons for catalyst characterization. This was followed with a move to UOP, a Honeywell Company, for 19 years, and built up a reputation for in-situ and operando characterization of catalysts using primarily x-ray absorption spectroscopy. After spending so much of his time at synchrotrons, he decided he should spend more of his time there, so took a position as a Distinguished Staff Scientist at SSRL at SLAC National Accelerator Lab in 2016.



Adam Hoffman, currently a research associate in Co-ACCESS, joined the SSRL as a postdoctoral research fellow in January 2017. He obtained his PhD at the University of California, Davis under Bruce C. Gates exploring how atomically dispersed metal atoms interact with inert supports using spectroscopic techniques complete his research. In the Co-ACCESS program Adam is heavily involved user support from experimental design, teaching beamline operation, and data analysis. In his free time he is working on the development of time-resolved XAS at SSRL for spectro-kinetic characterization of materials.



Jiyun Hong joined Co-ACCESS as a postdoctoral research fellow in October 2019. She obtained her PhD from Northwestern University under Prof. Lin X. Chen, focusing on using time-resolved X-ray absorption spectroscopy to investigate the excited state dynamics of various transition metal complexes for solar energy applications. Now at Co-ACCESS, she is working on the experimental aspects, facilitating the in-situ X-ray absorption spectroscopy measurements on various catalytic systems at SSRL.



Fernando Vila received his PhD in chemistry from the Univ. of Pittsburgh in 2001. He held Research Associate positions in the Chemistry and Physics Departments at the Univ. of Washington, and transitioned to a Staff Scientist position in 2005. He is a senior member of the FEFF Development Team, where he has pursued a broad range of research interests relating to the interaction between matter and radiation from the infrared to X-rays, and the atomistic aspects of catalysis. He collaborates with both experimentalists and theoreticians to develop and apply theoretical methods for a range of problems in the areas of materials design and nanocatalysis.



Griffin Canning is a graduate student with Abhaya Datye at the University of New Mexico and is visiting the Co-ACCESS group as an SCGSR fellow. His research focuses on understanding alkane transformation catalysts, and the competing roles of various processes in the deactivation of these catalysts. While he is here at Co-ACCESS he will assist with our mission to support catalyst beamline research, as well as work on developing novel multimodal spectroscopic equipment and techniques to further extend our *in situ* capabilities.

X-RAY Spectroscopy Theory

The Co-ACCESS X-ray spectroscopy theory effort is focused on the theoretical support and development that is needed in order to provide a deeper understanding of the experimental X-ray spectroscopic data. The focus is primarily on the structure of the active site(s), and how this site evolves as a function of the reaction conditions. The first results from this research has just been published (J. Am. Chem. Soc. (2019). DOI: 10.1021/jacs.9b07460). Using in situ XAS it was determined that the atomic structure of the catalytic surface under reaction conditions consists of Mo-O species substituted into the surface of the Rh nanoparticles. Critical to this conclusion was comparing the theoretically calculated Mo K-edge XANES, which showed that the spectrum of a Mo-OH entity substituted into a Rh surface is distinctly different to that from bcc Mo metal, and agreed with the experimental data.

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>