

Newsletter 9 | December 2022

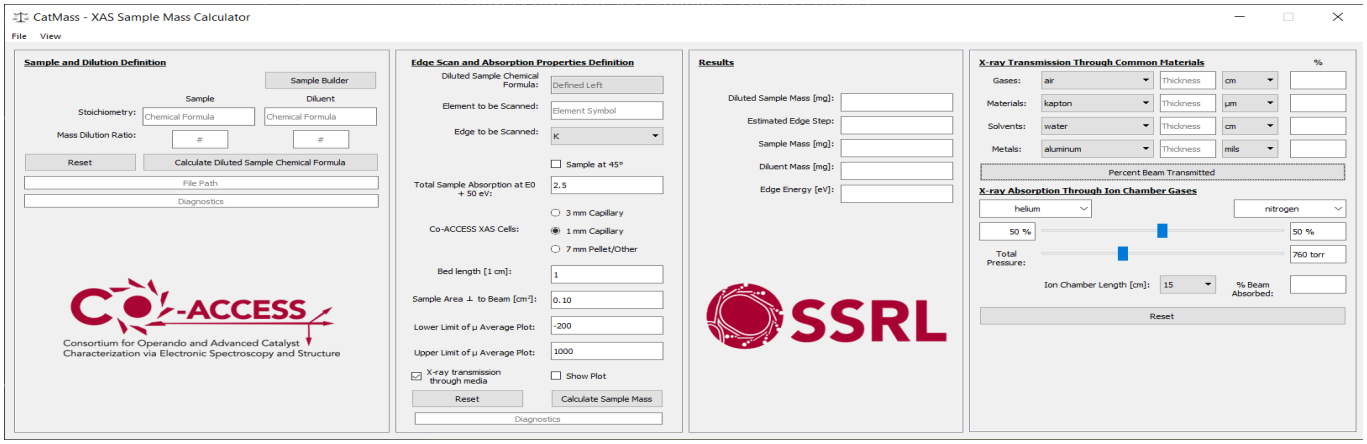
Co-ACCESS Semi-Annual

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

RECENT DEVELOPMENTS

CatMass

We have released an updated, non-python-based version of our X-ray sample mass calculator, CatMass! Over the summer Jorge has taken the bones and functionality from Adam's original release and created an installable program with expanded capabilities. The updated version can now save and open sample calculations, and expands energy ranges and sample geometries to calculate absorption cross sections. The software now allows you to visualize the sample absorption and identify competing edges from other elements in the sample in energy and k-space. Implementing Bruce Ravel's x-ray database absorption from non-sample absorbers such as cell walls and flight paths can also be calculated. You can download the executable (windows only, sorry mac users!) from our Tools for Users section of the Co-ACCESS website: Tools For Users ! | Co-ACCESS | Catalysis at SSRL (stanford.edu). Please reach out to Jorge, jperezag@slac.stanford.edu, if you find any bugs while using it. We plan on releasing a mac-compatible soon.



QuantEXAFS: Picturing Catalytic Sites Using EXAFS

The averaged local coordination environment around an absorbing atom is often probed using EXAFS. Ever wondered how accurately you can identify the true nature of these bonding atoms? Rachita Rana (4th year Ph.D. student at the University of California, Davis in collaboration with Co-ACCESS) has developed a novel python-based workflow (QuantEXAFS) that facilitates automated analysis of EXAFS data. QuantEXAFS, as the name signifies, enables quantitative analysis of EXAFS data using structures derived from quantum chemistry tools such as density functional theory (DFT). QuantEXAFS enables automated one-to-one mapping of 100s of EXAFS spectra with 1000s of DFT-optimized structures. So far, we have analyzed transition metals (TMs) supported on metal oxides and zeolites using QuantEXAFS and identified a representative structure for the majority of sites in the catalysts characterized (published [1,2,3] including Pt/MgO, Pt/ZSM5, etc.). Combining the two independently functioning fields of the experimental EXAFS and computational catalysis communities, QuantEXAFS is instrumental in unifying these two powerful tools and efficiently extracting the local bonding information about catalytic samples.[4] While putting the spotlight on the science question is the key, this method represents a step towards EXAFS analysis with a simple push of a button and adopting FAIR Guiding Principles for collection, analysis and storage of XAS data..

1. *Journal of the American Chemical Society*, (2021), **143**, 20144-20156. DOI: 10.1021/jacs.1c07116.
2. *J. Phys. Chem. Letters*, (2022), **13**, 3896-3903. DOI: 10.1021/acs.jpclett.2c00667.
3. *Journal of the American Chemical Society*, (2022), **144**, 13874–13887. DOI: 10.1021/jacs.2c05386.
4. *ACS Catalysis*, (2022), **12**, 13813−13830. DOI: 10.1021/acscatal.2c03863.

HAPPY HOLIDAYS!

Postdoctoral Associate Opportunities at Co-ACCESS

Co-ACCESS is currently seeking two postdoctoral associates! One position will involve developing and applying time-resolved *in-situ/in-operando* X-ray absorption spectroscopy to the study of a catalytic process of mutual interest. The focus of the project will be in developing the methodology to probe spectro-kinetics of catalytic processes with an emphasis on electrocatalysis and include advanced methods in data processing, data analysis and data modeling. This research will utilize the new upgraded wiggler beamline for quick X-ray absorption spectroscopy (QXAS). The second position will involve using *in-situ/in-operando* synchrotron-based methods, primarily X-ray absorption spectroscopy (XAS), to study all aspects of catalysis and to continue the development of world-class synchrotron catalyst characterization at Co-ACCESS/SSRL. More details can be found on the SLAC website: https://careers.slac.stanford.edu/jobs-slac/ra-and-postdocs

I encourage you to contact me, Simon Bare at srbare@slac.standord.edu or Adam Hoffman at ashoff@slac.stanford.edu if you are interested in learning more

Simon, Adam, Jorge, Jiyun, Fernando and Rachita wish you a happy and safe holiday season!

We are thrilled that we were able to collaborate with you and further your innovative research and it was great to be able to interact with you in person again.

Some interesting end of year facts about Co-ACCESS. Thanks to you all: Co-ACCESS's h-index is 25. Co-ACCESS's 2023 Impact factor (I.F.) is 4.1 (I.F. is defined by the 2 previous years of publications). Co-ACCESS's overall I.F. is 30.

We look forward to your visits in 2023!

Key Recent Publications

"Bridging the Gap between the X-ray Absorption Spectroscopy and the Computational Catalysis Communities in Heterogeneous Catalysis: A Perspective on the Current and Future Research Directions", R. Rana, F.D. Vila, A.R. Kulkarni, S.R. Bare, *ACS Catalysis*, (2022), **12**, 13813−13830. DOI: 10.1021/acscatal.2c03863

"Templated Encapsulation of Pt-based Catalysts Promotes Activity and High-Temperature Stability to 1,100 °C". A. Aitbekova, C. Zhou, M.L. Stone, J. Salvador Lezama-Pacheco, A.-C. Yang, A.S. Hoffman, E.D. Goodman, P. Huber, J.F. Stebbins, K.C. Bustillo, P. Ercius, J. Ciston, S.R. Bare, P.N. Plessow, M. Cargnello, *Nature Materials*, (2022), **21**, 1290-1297. DOI: 10.1038/s41563-022-01376-1.

"Interconversion of Atomically Dispersed Platinum Cations and Platinum Clusters in Zeolite ZSM-5 and Formation of Platinum gem–Dicarbonyls", N. Felvey, J. Guo, R. Rana, Rachita, L. Xu, S.R. Bare, B.C. Gates, A. Katz, A. Kulkarni, R. Runnebaum, C. Kronawitter, *Journal of the American Chemical Society*, (2022), **144**, 13874–13887. DOI: 10.1021/jacs.2c05386.

"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: 10.1021/jacs.2c01274.

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