Q2XAFS 2023 | International Workshop on Improving Data Quality and Quantity in XAFS Spectroscopy

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Abstracts – Oral Presentations

ver 11/August 23

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Contribution ID : **51** Type : **Oral presentations**

Comparing the quality of XAFS data collected with different acquisition rates

With the advent of new technology, the traditional step scan XAS spectra collection has been replaced by faster acquisition methods (quick-EXAFS scans, energy dispersive). The better temporal resolution has allowed in-situ and operando experiments, answering the growing needs of the synchrotron scientific community that wants to follow reaction dynamics and capture short living intermediates. However, these new acquisition methods have limitations that could affect the quality of the signal measured such as: different acquisition time per point, homogeneous energy steps for different spectral regions and necessity of an accurate measurement of I0. The aim of this talk is to compare signal quality between different methods with the same total acquisition time and highlight the data acquisition parameters that can still be improved.

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Presenter(s) : GIANOLIO, Diego (Diamond Light Source)

Track Classification : 3. Improving the quality of XAS measurements

Contribution ID : **50** Type : **Oral presentations**

Sharing XAFS data and repositories: where to go?

With the fast development of high throughput data analysis, simulations and Machine Learning, demand for reliable, extensive and curated XAFS data pools is growing.
Those have been established in other fields: policies and interchangeability of datasets has been addressed long ago, thanks to the efforts of large user communities.For XAFS, data sharing across instruments and facilities is mostly left to initiatives at personal or institution level and has not significantly tapped into the contribution of the user communities.
Soon introduction of FAIR- and open- data policies at several facilities will give access to significant amounts of raw datasets.
This poses questions on the suitability of these data sources, not specifically curated for the purpose of sharing, for the integration with modern analysis tools.This contribution presents the challenges identified in the attempt to establish a useful, information-based XAFS library and proposals to progress forward into a community-based shared repository.

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Presenter(s) : CIBIN, Giannantonio (Diamond Light source Ltd)

Track Classification : 1. Sharing and re-using XAS data

Contribution ID : **49** Type : **Oral presentations**

Data quality and standards in x-ray Raman scattering spectroscopy

Inelastic x-ray scattering from core level excitations is known as x-ray Raman scattering (XRS) or non-resonant inelastic x-ray scattering (NIXS) spectroscopy—both acronyms are in use for the same method, effectively meaning x-ray photon energy-loss spectroscopy. XRS provides data similar to soft-x-ray XAS, while being a hard x-ray in – hard x-ray out -method. XRS is an example of spectroscopy with typically a low count rate and non-trivial background, rendering careful data analysis precious for high-quality and quantitatively correct results for both XANES and EXAFS. On the other hand, XRS is free from saturation and self-absorption effects and its energy calibration is precise. These are less used facts that if employed more routinely, could render an open library of XRS data a valuable reference source also for the XAS community.

Primary author(s) : Prof. HUOTARI, Simo (University of Helsinki)

Presenter(s) : Prof. HUOTARI, Simo (University of Helsinki)

Track Classification : 3. Improving the quality of XAS measurements

Contribution ID : **48** Type : **Oral presentations**

Assessing data quality and experimental challenges at medium-energy K-edge absorption (1.5-4 keV) for dilute samples

Our XANES data in a medium energy range (1.5 to 4 keV) were reported in soil-science journals for the speciation of Al, P, S, and Ca in various soil types. Because of low elemental concentrations in the soil samples, the XANES measurements were carried out at the SLRI-BL8 beamline with an incident photon flux of 1E9-1E11 photons/s/100 mA in fluorescent-yield mode using multi-element XRF detectors. The data were assessed in terms of signal-to-noise (SN) ratio and optimized against self-absorption error and long counting times. Good SN ratios between 70 and 260 could be achieved at 1 wt%, 1000 ppm, 500 ppm, and 1 wt% of Al, P, S, and Ca, respectively. Sharp white lines and distinctive fine peaks could be well observed, particularly for phosphate, sulfate, organic calcium, and organic aluminum. Linear combination fit analysis using extensive sets of elemental standards resulted in good fits with R-factor values of 0.005.

Primary author(s) : Prof. PREITZEL, Joerg (TUM School of Life Sciences, Technical University of Munich); Dr KLYSUBUN, Wantana (Synchrotron Light Research Institute)

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Track Classification : 4. Improving the reporting of XAS results

Contribution ID : **47** Type : **Oral presentations**

Best Practices for Data Quality and Documentation for Laboratory XAFS and XES

Improvements over the last decade in x-ray optics, sources, and detectors are driving a rebirth of laboratory-based x-ray absorption fine structure and x-ray emission spectroscopy. We first survey the principles of operation and performance of the most common laboratory spectrometers based on spherically bent crystal analyzers. With that background established, we then focus on general considerations of best practice for data quality, data format, and archiving. This includes a proposed extension of the XDI file format, denoted LABXDI, which includes many new fields to define instrument configurations and has associated recommendations for archiving of raw data. We intend that LABXDI serve as an anchor for intralaboratory reproducibility and for interlaboratory comparison of similar or even nominally identical instruments or comparison between laboratory and synchrotron results.

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Track Classification : 3. Improving the quality of XAS measurements

Contribution ID : **46** Type : **Oral presentations**

Making a comprehensive XAFS data standard actually happen

Following the Q2XAFS meeting in 2011, a paper was published describing four different formats that could be used for encapsulating XAFS data. In the subsequent decade, the only standard based on these formats to see widespread use is the relatively limited XDI standard.

Improving XAFS data transfer standards requires cultural change if technical work is not to sit on the shelf, unused. Cultural decision points involve the interaction between beamline and user; user and software author; and user and journal. One mechanism of influence is the availability of a standard that has been endorsed by a credible body, such as the IUCr or IXS. A practical XAFS data standard development process that is largely format-agnostic, semantically compatible with XDI, and would produce a result acceptable to IUCr COMCIFS is outlined.

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Presenter(s) : HESTER, James (ANSTO)

Track Classification : 1. Sharing and re-using XAS data

Contribution ID : **45** Type : **Oral presentations**

Winds of change at the XAS beamline in Melbourne

We will discuss the evolution of the Australian XAS user community in the context of data quality and quantity. Starting with the beginnings at the Photon Factory in Japan and leading to today at the XAS Beamline in Melbourne, we will examine beamline user statistics and qualitative markers to explain the drivers for user engagement with XAS and how those interplay with data quality/quantity.

Statistics is reflective, and past trends can help explain the present. We see a clear shift in focus, from a strong emphasis on data quality in the early days towards data quantity today, driven by user science and beamline robustness and development. Most recently, this has led to the introduction of energy slew scanning and tools to improve the quality of the XAS measurement experience. Slew scanning data will be presented and discussed, both for the archetypal bulk metallic Cu foil, but also real-life user samples.

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Track Classification : 3. Improving the quality of XAS measurements

Contribution ID : **44** Type : **Oral presentations**

Learning more from X-ray Spectroscopy with Theoretical Methods

X-ray spectroscopies involve transitions from localized core levels to valence levels and beyond furnishing simultaneous geometric and electronic structure description of the system under investigation. Theoretical tools can be used to both interpret the structural and electronic origins of spectral changes which are often convoluted, and to significantly enhance the information content of the experimental data by first calibrating the experimental data through spectral simulation and then using the theoretical tool to predict chemical and physical properties that cannot be directly obtained from the experimental data. In the last two decades several theoretical methods have been developed to interpret x-ray spectra. Some of these have gained significant popularity, such as time dependent density functional theory (TD-DFT), Full potential multiple-scattering (FMS) based theories, Bethe Salpeter Equation (BSE) based approaches and semi empirical methods for Multiplets in x-ray spectra. This presentation will focus on importance of these methods, best practices and outlook.

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Presenter(s) : Dr SARANGI, Ritimukta (SLAC National Accelerator Laboratory)

Track Classification : 4. Improving the reporting of XAS results

Contribution ID : **43** Type : **Oral presentations**

XAFS at extremes: last trends

Pressure is able to produce modifications in electronic structure and crystal packing in matter. As well, together with temperature it causes changes in the physical states of matter and drives chemical reactions.

Diamond anvil cells combined with laser heating are able to produce thermodynamic conditions to study the melting curves of transition metals, investigated also using XAS.

The advent of high-power lasers has provided insights into laboratory high energy density physics. In particular, the properties of warm dense matter is a research area that has garnered significant interest recently.

Recent XAS studies at high P (and high T) in equilibrium conditions will be reviewed. These show that the use of nanocrystalline diamonds lead to a remarkable improvement to data quality allowing a full EXAFS refinement.

Studies on dynamic compression coupled with XAS to probe local and electronic structure in Warm Dense Matter will be reviewed.

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Track Classification : 3. Improving the quality of XAS measurements

Contribution ID : **29** Type : **Oral presentations**

From data collection to reporting in photon-in/photon-out spectroscopies

Photon-in/photon-out core-level spectroscopy has expanded the x-ray spectroscopy toolkit for investigating chemically specific electronic and geometrical structures. By analysing the energy of the emitted photons with high-energy resolution, the range of applications of conventional XAS is increased and some of its shortcomings can be circumvented. High-energy resolution fluorescence detection XAS (HERFD–XAS), non-resonant x-ray emission spectroscopy (XES), and resonant x-ray emission spectroscopy (RXES), have been developed hand in hand with the increasing accessibility of efficient x-ray emission spectrometers that cover a large solid angle of detection. These new instruments have also enabled the exploitation of x-ray Raman scattering (XRS), a bulk-sensitive probe that provides access to low atomic number/low energy absorption edges, thus considered a promising alternative to soft XAS techniques.
In this talk, I will describe the most common instruments dedicated to photon-in/photon-out spectroscopy and discuss how different experiments are conducted, and the parameters that need to be reported.

Primary author(s) : DIAZ-MORENO, Sofia

Presenter(s) : DIAZ-MORENO, Sofia

Track Classification : 4. Improving the reporting of XAS results

Contribution ID : **17** Type : **Oral presentations**

Addressing Rigor and Reproducibility in Heterogeneous Catalysis: XAS

The application of XAS is ubiquitous in catalysis research. Indeed, one of the first papers published by Farrel Lytle was on the application of XAS to study catalyst structure. Today, just about every manuscript in a high impact journal contains XAS data. However, the rigor and reproducibility of XAS data reported in many catalysis publications is inconsistent at best. In this talk I will present the recommendations from a working group on XAS at the recent workshop (July 21-22, 2022) in the USA on Rigor and Reproducibility in Catalysis. This workshop, sponsored by the NSF and US DOE, was to discuss the state of these issues in the field, develop recommendations that can enhance the rigor and reproducibility of data reported in the literature, and to compile collective knowledge about best practices for common methods of study in the field and current knowledge about the availability of benchmark materials. .

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Track Classification : 4. Improving the reporting of XAS results

Contribution ID : **12** Type : **Oral presentations**

Quantity yields quality, using and building XAFS database

XAFS data have been deposited in a couple of XAFS databases for decades. Data-driven approaches to XAFS datasets compel us to reconsider what XAFS database should really be.
A couple of research examples using XAFS database are given. What they wanted to do and what they struggled with are shared. Understanding actual usage of XAFS datasets by non-XAFS experts, what we should examine to build XAFS database as the XAFS community and what we should consider to deposit XAFS spectra as individual researchers will be discussed.
The integrated XAFS database, MDR XAFS DB, is introduced. It is created under NIMS MDR (National Institute for Materials Science, Materials Data Repository). This activity is handled by the Japanese XAFS Society and reported here: M. Ishii, K. Tanabe, A. Matsuda, H. Ofuchi, T. Matsumoto, T. Yaji, Y. Inada, H. Nitani, M. Kimura, and K. Asakura, Sci. Technol. Adv. Mater. Meth. 3, 2197518 (2023).

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Track Classification : 1. Sharing and re-using XAS data

Contribution ID : **6** Type : **Oral presentations**

IUCr, ITC I, IXAS, XERT, Hybrid, Measurement Standards, Reporting Guidelines and Soliloquy on Q2XAFS 2023

Current standards for XAS and XES are improving. Current standards for reporting documentation, publications and supplementary information are improving. If we stand still, the world-wide community will suffer, our data and results will be non-transferable and non-robust, and scientific results and conclusions will be in question. The IUCr formed CXAFS which led to the inaugural Q2XAFS meeting in partnership with IXAS.

The encyclopaedic International Tables for Crystallography Volume I: XAS has 10 Sections, 150 chapters by world experts, circa 1000 pp. The work says a lot about our local, current and international XAS and XES standards.
This talk will: summarise nascent questions for each of us and for each beamline or beamline design crew; raise questions unanswered in XAS theory and analysis; mention ideas which have or have not come up in this meeting, to drive XAS/XES beamlines to their potential of Quality in XAS, significance of results and interpretation.

Primary author(s) : CHANTLER, Christopher Thomas (University of Melbourne)

Presenter(s) : CHANTLER, Christopher Thomas (University of Melbourne)

Track Classification : 4. Improving the reporting of XAS results

Contribution ID : **37** Type : **Oral presentations**

A new protocol for monitoring radiation damage of XAS data, multiple datasets and fitting of XAS measurements with propagated uncertainties.

XAS is a promising technique for determining structural information of biological samples. However, radiation damage (RD) is a key systematic issue. We collected XAS-Eelectro-Chemical measurements of N-truncated amyloid-β. Minimization of RD was achieved using a pulsed flow pattern. A new protocol was developed using XAS data analysis for monitoring RD. Repeated XANES were carefully investigated for monitoring RD. We performed the two-sample t-test to statistically measure the consistency of sample measurements with the minimization of RD. EXAFS analysis of individual scans was performed using eFEFFIT. The individual scans returned the same parameter values confirming no RD.

Multiple-data (MD) refinements in XAFS analysis enables more data points and hence more parameters for a better fit. We developed eFEFFIT package so that, multiple scans can be used for refining. MD were simultaneously fitted to a model after confirming the consistency from eFEFFIT individual refinements. The results confirm the successful development in eFEFFIT.

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Track Classification : 3. Improving the quality of XAS measurements

Contribution ID : **25** Type : **Oral presentations**

Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS) Analysis applied to XAS data: Principles, Strength, Weakness and Strategies to overcome intrinsic limitations.

In the last decade, MCR-ALS is become a powerful method to recover the pure component information (concentration profile and spectral fingerprint) from the spectral mixture XAS data set. According to the Lambert-Beer's law, the method proceeds to a bilinear decomposition of the matrix storing the spectral mixture data D into the concentration profile matrix C and the spectra matrix S, D = C . ST + E, E being the error matrix containing the deviations from ideal bilinearity. Identification of pure species is performed by comparison of their spectra with those of standards or using the commonly used EXAFS extraction and fitting analysis procedure.
In this lecture, a brief description of the MCR-ALS method will be given and examples of its application to Quick-EXAFS data acquired upon monitoring the activation of heterogeneous catalysts will illustrate the strength and weakness of the methodology. Strategies for overcoming some limitations will be discussed.

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Track Classification : 2. Improving the interpretation of XAS data

Contribution ID : **10** Type : **Oral presentations**

Improving the interpretation of XAS data using artificial neural networks

For decades XAS has played a key role in the *operando* studies of functional materials, but the interpretation of experimental data remains challenging. Structural and thermal disorder and co-existence of metal atoms in different local environment result in bond length distributions that are hard to account for in EXAFS fitting. Furthermore, the analysis of contributions of distant coordination shells to EXAFS shows promise for an accurate determination of 3D structural motifs but remains non-trivial. XANES, in turn, is less affected by disorder, but its application for the structural analysis is hindered by the lack of methodology for the extraction of quantitative information. To address these issues and to correlate EXAFS and XANES features with the structural motifs, we introduced supervised machine learning method - artificial neural network -, trained on theoretically simulated XAS spectra. We showcase this method on our recent examples of XAS spectra interpretation in working heterogeneous catalysts.

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Track Classification : 2. Improving the interpretation of XAS data

Contribution ID : **7** Type : **Oral presentations**

A 20-year journey hunting down uncertainties and extracting physical information in Absorption and Fluorescence X-ray Spectroscopy

X-ray Absorption Spectroscopy is widely used to study the nanoscale structure of materials including non-crystalline solids, powders, and solutions. However, existing standards for defining and propagating uncertainty, significance, and hypothesis testing for measurements of nanostructures are in their infancy. The fitting of structural parameters has been based on approximations, which often yield non-physical results. We will highlight areas of possible improvement within the field, theoretically and experimentally. We will describe techniques which may be routinely used for obtaining high-precision absorption and fluorescence spectroscopic data from which nanoscale structural information can be extracted. We will also discuss the propagation of and fitting with uncertainty in combination with energy calibration on the E or k-axis. Key concepts of the X-ray Extended Range and Hybrid Techniques will be described.
Criteria necessary for the provision of portable data (referencing, data deposition) and reliable short-range structure from relative or absolute measurements will be discussed.

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Presenter(s) : TRAN, Chanh (LIMS, School of Molecular Sciences, La Trobe University)

Track Classification : 2. Improving the interpretation of XAS data

Contribution ID : **5** Type : **Oral presentations**

Notes from another world: Precise and accurate X-ray attenuation measurements in the vicinity of the absorption edge

A revolution is underway in the field of XAFS, led by accuracy and precision of measurements. These represent a maturation of the XAFS method, delivering improved acuity and qualified analytical power. Here we report studies of X-ray attenuation that were made in a very different world, now almost 20 years ago. However, that analysis remains one of the most accurate in the literature.

The basis of the approach – the X-ray extended range technique (XERT) – is to perform measurements over a sufficiently broad range of parameter space to enable systematic effects to be characterised and corrected. The presentation demonstrates the XERT with reference to: the roles of repeat, blank and dark measurements; absolute calibration of specimen mass-thickness, and; X-ray bandwidth and roughness. *We will make no reference to the practicality of the measurements for existing XAFS beamlines*; a discussion of this could perhaps be a consequence of the presentation.

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Presenter(s) : Dr DE JONGE, Martin (ANSTO)

Track Classification : 2. Improving the interpretation of XAS data

Contribution ID : **38** Type : **Oral presentations**

Trends in X-ray absorption data sharing, reproducibility, and measurement and interpretation challenges

Databases for sharing X-ray diffraction determined structures are widely used, while those for X-ray absorption are generally small, fragmented, and of limited utility. The need for databases maybe become more acute as synchrotron storge ring facilities require data accessibility and large data sets are required for machine learning algorithms. This talk will explore the challenges databases present for the x-ray absorption community, such as funding and the structure of the data, results and meta-data. As more advanced spectroscopies such as X-ray emission spectroscopy and high energy resolution fluorescence detection (HERFD) become popular, additional consensus on appropriate meta-data are needed. In addition, new analysis methods such as DFT based structures used directly as input to theoretical calculations continue to be developed which could benefit from additional guidance on appropriate data reporting protocols. These challenges for building robust x-ray absorption databases for data sharing and validation will be briefly discussed.

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Presenter(s) : KELLY, Shelly (Argonne National Laboratory)

Track Classification : 1. Sharing and re-using XAS data

Contribution ID : **16** Type : **Oral presentations**

XAS Reference Database under DAPHNE4NFDI

Under the project DAPHNE4NFDI, we have recently set up a XAS reference database including raw and processed data with an interface developed for uploading and evaluating the data. With the defined metadata/data fields and quality criteria a prototype database is running where different features of the database are tested. After going through available options an online data submission for the user is under development. The format/structure of metadata for the uploaded data on the interface is to be finalized. XAS spectra from different beamlines/synchrotron facilities having distinct data/file formats have been tested for uploading at the developed interface. A human verification procedure for the uploaded data will be implemented for checking any anomaly. In this talk, the importance of defined metadata fields and formulation of quality criteria for the data uploaded at the XAS database will be discussed. The developing features of running prototype of the database will be shown.

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Track Classification : 1. Sharing and re-using XAS data

Contribution ID : **14** Type : **Oral presentations**

First experiences and results from an inter-laboratory round robin test of XAFS spectroscopy measurements

Inter laboratory round robin tests are used to compare analytical results from different laboratories. They are important tool in quality control to assess the comparability and reproducibility of analytical results among the participating laboratories and to test the robustness of an analytical method. So far no such test was undertaken in the field of XAFS spectroscopy, although it is certainly of large interest to the user community to test the comparability of results from different beamlines and instruments. After long discussions during the last Q2XAFS workshops a first round robin test was started in 2022. Sets of identical samples, Ti, Cu and Mo foils, were send to facilities worldwide and beamline scientist were asked to measure these samples using their respective standard procedures and best practice. First results and some lessons that were learned during the organisation of the first XAFS round robin test will be presented and discussed.

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Track Classification : 1. Sharing and re-using XAS data

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Silver Sponsors

Contribution ID : **33** Type : **Poster presentations**

Measuring the Complex Atomic Fine Structure on an Absolute Scale

Precision measurements of x-ray absorption fine structure have been critical to the development of our understanding and applications of fine structure analysis. However, the application of XAFS to weakly absorbing samples is limited due to the high penetrating power of X-rays. XAFS uses the imaginary component of the complex atomic form factor to describe X-ray interactions with matter. However, the real component of this factor is several orders of magnitude more sensitive. We have developed a method of measuring the complex refractive index of a thin foil using holographic spectroscopy and have found that in order to further understand and characterize the complex interactions between light and matter, an absolute scale measurement is required. Through advancements in sample design and beam characterization, we have devised such a method and demonstrated it in an experiment using a copper thin film, the results of which will be presented.

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Presenter(s) : DI PASQUALE, Paul (La Trobe University)

Track Classification : 5. Other XAS topics

Contribution ID : **32** Type : **Poster presentations**

A Novel Approach to Unravel the Complex Atomic Fine Structure Across the Copper and Iron K-edges

X-ray Absorption Spectroscopy (XAS) is a routinely used technique in probing short-range structures of materials. However, current applications to low-absorbing samples such as ultra-thin films and nano-devices have been limited. This is not expected for the phase component of the fine structure as it is generally orders of magnitude larger than the absorption component in the X-ray regime.

In this presentation, we introduce a novel technique that allows for the precise simultaneous measurement of both the absorption and phase components of the Complex Atomic Fine Structure (CAFS). The approach combines spectroscopy (X-ray Extended Range Technique) and X-ray imaging (Fourier Transform Holography with Extended Reference). Measured at the Australian Synchrotron, the CAFS spectra across the K-edges of copper and iron on a relative scale will be discussed. The results provide a critical experimental benchmark for further theoretical development and demonstrate the potential to delve into the phase equivalent of XAS.

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Track Classification : 5. Other XAS topics

Contribution ID : **27** Type : **Poster presentations**

Quati at SIRIUS, the XAS beamline dedicated to dynamic studies

The development of innovative materials requires an in-depth understanding of their structure related to their macroscopic properties. For that, operando time-resolved XAS studies under complex conditions are required. At the Brazilian synchrotron light source SIRIUS [1], the new beamline Quati has focused its design to probe functional materials under realistic conditions.
Based on a 3.2 T superbend, the beamline will provide a high photon flux of 10E10-10E11 ph/s from 4.5 to 35 keV with an in-house designed monochromator: HD-DCM [2]. Besides, a moveable experimental table provides an adaptable spot size from 10's µm to 6 mm (flexibility on beam size and flux density).
Integrated experimental controls, pipelines of data acquisition/treatment/analysis are integer parts of the beamline's developments to ensure the quality of XAS studies.

1 L. Liu, et al., J. Synchrotron Rad., 2014, 21, 904.
2 G. S. De Albuquerque, et al., Proc. ICALEPCS2021, 2021, 619.

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Presenter(s) : ROCHET, Amélie (CNPEM - Sirius)

Track Classification : 5. Other XAS topics

Contribution ID : **23** Type : **Poster presentations**

The joys and tears of industrial research

Increasing the utilization of synchrotron radiation facilities by industrial users is one of the declarative goals of most facilities worldwide. In particular, X-ray absorption spectroscopy, is a unique technique with high potential to attract industrial users. This is due to a wide variety of chemical and structural information that can be obtained, (semi) quantitative character, relatively easy sample preparation and the possibility to perform *in-situ* and *operando* experiments, as well as measurements in ambient conditions. However, XAS results are not straightforward to interpret, often require lenghty characterization of numerous reference compounds, strongly increasing costs for customers, and are still considered as relatively novel and complex. Results from pilot industrial experiments, conducted within the framework of the Sylinda project at the SOLARIS National Synchrotron Radiation Centre will be presented as a case study, highlighting the challenges and opportunities of industrial research and the need of standardisation and automation of XAS measurements.

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Track Classification : 5. Other XAS topics

Contribution ID : **8** Type : **Poster presentations**

Insight into SO2 Resistance of MnFeOx Catalysts for NH3-Selective Catalytic Reduction (SCR) Reaction: A Comprehensive X-ray Absorption Fine Structure (XAFS) and Density Function Theory (DFT) Study

This study introduces a strategy to improve SO2 resistance in MnFeOx, a promising NH3-SCR catalyst, using a simple surface pre-treatment method. The SO2 poisoning mechanism and improved SO2 resistance of the modified catalyst are investigated using a combination of experimental characterizations, including X-ray photoelectron spectroscopy (XPS) and XAFS, and DFT calculations. The result confirmed that SO2 decreased the activity of the active metal in the MnFeOx catalyst, while the MnSO4 coating layer on the modified catalyst hindered the adsorption of SO2, thereby protecting the active sites within the catalysts. Through the utilization of EXAFS fitting, a rational structure of the catalyst was constructed for the DFT calculations, which provide insights into the influence of SO2 exposure on the active sites of the catalyst. Our research provides a fundamental understanding of SO2 poisoning and catalyst deactivation, propelling the development of robust SCR catalysts with superior SO2 tolerance.

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Track Classification : 5. Other XAS topics

Contribution ID : **34** Type : **Poster presentations**

Assessing Data Quality from Quick-Scanning X-ray Absorption Spectroscopy in Fluorescence Mode

Time-resolved X-ray absorption spectroscopy (XAS) provides the ability to monitor in-situ/operando reactions. Although this method has been extensively used for transmission measurements, its application in fluorescence mode encounters challenges, mainly due to constraints in signal collection and detector technology.

Recent research indicates that extended X-ray absorption fine-structure data of diluted samples can be rapidly collected in quick-scanning fluorescence mode. It is of interest to compare the data quality of these diluted samples, featuring an edge step of approximately 0.01. The findings demonstrate that even with a dilute sample, satisfactory data can be obtained via the fluorescence method. The quality of the quick scanning XANES data is comparable to that of step scanning, and in EXAFS it can still provide a level of data quality that is relatively comparable.

Therefore, the quick-scanning fluorescence mode holds considerable potential for in-situ experiments, particularly when studying samples for which transmission measurements are not feasible.

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Presenter(s) : HSU, Liang-Ching

Track Classification : 3. Improving the quality of XAS measurements

Contribution ID : **24** Type : **Poster presentations**

Data acquisition at the MEX beamlines

XAS measurements can only be as good as permitted by the underlying data acquisition system. The data acquisition system of the MEX beamlines was designed to improve on the system extant at the XAS beamline, whilst being sufficiently flexible to cover all operation modes demanded at MEX, from low-energy XAFS at MEX2 to high-speed multi-element mapping at the MEX1 microprobe. A fundamental design decision was the abandonment of a centralised data acquisition system built around the Struck multichannel scaler in favour of a distributed system built around the d-tAcq ACQ1002/ACQ430 8-channel, simultaneous sampling, 128 kHz voltage digitiser, employing the philosophy of oversampling and averaging.

The poster will present a performance comparison of the V2F-scaler and d-tAcq systems, as well as numerous examples of the performance and features of the data acquisition system at the MEX beamlines.

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Presenter(s) : WYKES, Jeremy (Australian Synchrotron)

Track Classification : 3. Improving the quality of XAS measurements

Contribution ID : **22** Type : **Poster presentations**

An interlaboratory round robin test of XAFS results

In inter laboratory round robin tests the same or similar samples are analysed in different laboratories and the results compared to test the comparability and repeatability of analytical procedures. While round robin test are a standard instrument of quality assurance in analytical chemistry and related fields no such test was undertaken so far for XAFS spectroscopy. The poster will present first results and experiences from a round robin test on a set of metal foils that were send to many XAFS beamlines around the world.

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Track Classification : 3. Improving the quality of XAS measurements

Contribution ID : **15** Type : **Poster presentations**

In-situ PTRF-XAFS application for Pt-based model catalyst structure investigation toward ORR

Core@shell structure of Pt-based catalysts (M@Pt, M=Pd, Au, etc.) has been proved to possess an outstanding catalytic property in fuel cell systems. A model catalyst system of PtML/PdML/Au (111) is introduced in this research to identify whether the Pt catalytic activity is determined by charge transfer between metals or d-band center variation caused by Pt-Pt bond distance change. The polarization dependent total reflection fluorescence XAFS (PTRF-XAFS) can provide 3D structure information from different polarization directions. However, the solution layer present on the surface has deteriorated the XAFS signal due to the absorption and scattering of X-rays. To overcome these problems, we developed a novel apparatus for in-situ Pt structure investigation, and we successfully obtained the Pt monolayer XAFS spectrum. This apparatus is suitable for diluted sample systems, and in-situ interface structure studies.

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Track Classification : 3. Improving the quality of XAS measurements

Contribution ID : **4** Type : **Poster presentations**

The ROCK-IT project

The ROCK-IT project (remote, operando controlled, knowledge-driven, IT-based), will provide solutions to improve the efficiency of catalysis research, tailor-made, yet composed of generic building blocks portable enough to be applicable to a wide range of measurements. The building blocks include standardized and interchangeable data formats, standardized metadata collection, interfaces to electronic lab books, sample tracking and handling, machine learning based experiment control and data evaluation, and automation of experiments under remote control. Here, standardization and automation are prerequisites for making the solutions developed available to a broad user base and industry via remote-access modes, providing a consistent "look & feel" at different sources, and thus removing barriers to access and thereby potentially accelerating innovation cycles. The core partners of ROCK-IT are Deutsches Elektronen-Synchrotron DESY, Helmholtz-Zentrum Berlin HZB, Helmholtz-Zentrum Dresden-Rossendorf HZDR, and Karlsruher Institut für Technology KIT.

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Track Classification : 3. Improving the quality of XAS measurements

Contribution ID : **28** Type : **Poster presentations**

Solving complex problems from deep Earth: Diamond micro inclusions characterizations by using a spectroscopic multi-technique approach

Our knowledge of the Earth´s interior has been obtained through studies of natural rock samples found close to the surface. The possibilities that open facilities like SIRIUS [1] with beamlines like CARNAUBA [2] and EMA [3] give experimentalists new opportunities to measure significantly smaller samples down to the nanoscale. Therefore, we could move our research from the rock scale to the small impurities inside the rock (micro inclusions). We present the results of a super-deep diamond that gives an intriguing problem from a characterization point of view. This mineral inclusion reveals essential information from the inner mantle process. It is also a puzzle to be solved with several techniques and theoretical simulations to progress our knowledge of this kind of new science offered by the 4th generation of light sources.

[1] L. Liu, et al., https://doi.org/10.18429/JACoW-IPAC2022-TUPOMS002.

[2] H.C.N. Tolentino, et al., https://doi.org/10.1016/j.elspec.2023.147340.

[3] R.D. dos Reis, et al., https://doi.org/10.1088/1742-6596/1609/1/012015.

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Track Classification : 2. Improving the interpretation of XAS data

Contribution ID : **26** Type : **Poster presentations**

Understanding excited state absorption (ESA) in Ce-doped UV laser crystals and the confounding Ce L3-edge XANES spectra

Solid-state UV lasers based on cerium-doped crystals can offer high-resolution pump-probe spectroscopies and lithography due to their short-wavelength emissions. Past studies have extensively employed optical spectroscopy to probe their optical and lasing properties. From these studies, the existence of excited state absorption (ESA) on various host crystals has been found to significantly reduce their lasing performances. We performed Ce L3-edge XANES analysis to investigate the structural origin of ESA in Ce-doped LiCaAlF6 and LiSrAlF6 crystals. Both crystals exhibited multiple peaks associated with Ce3+ and Ce4+ oxidation states. However, interpreting these peaks should be done with circumspection because our Ce K-edge XANES analysis strongly indicated a singular Ce3+ state. Our DFT and FDMNES simulations assign the dominant Ce L3-edge peak to a trigonally-coordinated Ce3+ ion, whereas ESA and the two peaks associated with the Ce4+ states are due to the strong coupling (covalency) between Ce and neighboring F and Al atoms.

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Track Classification : 2. Improving the interpretation of XAS data

Contribution ID : **36** Type : **Poster presentations**

XAS Reference Database under DAPHNE4NFDI

Within DAPHNE4NFDI, we developed the prototype of a reference database in the field of XAS including a method to submit a raw dataset along with its associated metadata via a dedicated website. The implementation involves uploading metadata to the Scientific Catalogue and (data-)files via object storage. We provide automated query capabilities through a web server, including checks of predefined quality criteria and an automatic graphical analysis (absorbance, normalized absorbance, Chi(k), and Chi(R)), based on a user-selected energy range. The website features a landing page, a comprehensive list of all datasets, the search functionality, and an upload functionality including a "verify and edit" mask, which leads to a server-sided automatic authentication process, the storing of metadata/data in mongoDB and PostgreSQL, and (data-)files via API. We seek to discuss the status of development, as well as evolving features of our current prototype.

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Track Classification : 1. Sharing and re-using XAS data

Contribution ID : **31** Type : **Poster presentations**

Investigating radiolytic stability of metal (IV) phosphonate sorbents designed for nuclear waste treatment using x-ray absorption spectroscopy

Nuclear power is an intrinsically clean source of energy. However, improvements in nuclear waste treatment are required. The minor actinide (MA) elements in nuclear waste are problematic due to their radiotoxicity and long half-lives. In this study, three metal(IV) phosphonate coordination polymers—zirconium(IV) bistriazolylpyridine (ZrBTPhos), zirconium(IV) aminotris methylphosphonic acid (ZrATMP), and titanium(IV) aminotris methylphosphonic acid (TiATMP)—designed for MA sorption from nuclear waste were synthesised. To be suitable for nuclear waste treatment, these materials must be highly resistant to radiation. The sorbents were irradiated with high energy electrons from a linear accelerator at doses up to 2 MGy to determine their radiolytic stability. XAS on the Zr K- and L3-edge; Ti K-edge; and P K-edge was then used to compare the as-synthesised and irradiated sorbents. This analysis demonstrated excellent radiolytic stability for all three sorbents, with the best stability observed for ZrBTPhos. Additionally, the data suggests that Zr may impart improved stability.

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Track Classification : 5. Other XAS topics

Contribution ID : **19** Type : **Poster presentations**

An Attempt to Integrate the Open Databases in Japan

In the last Q2XAFS, we proposed international collaborations to make an open database system where data were directly and automatically uploaded from the beamlines.[1] Since then we Japanese XAFS Society members have tried to construct the open databases connecting to each SR facility. The open databases are now integrated into the one database (https://mdr.nims.go.jp/collections/qz20st57x) in the MDR (Material Data Repository) project of NIMS (National Institute for Materials Science) under the FAIRS (Findable, Accessible, Interoperable, Reusable) principle.[2] We also discussed the unified metadata in detail. We share the problems for the integration processes of the databases in Japan for future extension to the collaborations for the worldwide database.
[1] K. Asakura, H. Abe, and M. Kimura, J.Synchron. Rad. 25, 967-971 (2018).
[2] M. Ishii, K. Tanabe, A. Matsuda, H. Ofuchi, T. Matsumoto, T. Yaji, Y. Inada, H. Nitani, M. Kimura, and K. Asakura, STAM, 3, 2197518 (2023).

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Track Classification : 1. Sharing and re-using XAS data

Contribution ID : **21** Type : **Poster presentations**

Strategies to correct motion artefacts in XANES mapping of Mn speciation in leaf tissue

Plant fungal diseases are major threats affecting global production of essential crops (e.g., wheat). Nutritional immunity is a defence mechanism used by organisms involving active restriction or accumulation to toxic levels of metals. Increased understanding of nutritional immunity could identify strategies to manipulate these pathways, providing increased disease resistance / tolerance.

Plant cells maintain balanced levels of metals (e.g., Mn, Zn, Cu), with biological function closely related to chemical speciation. Synchrotron-XFM recently revealed significant accumulation of Mn in fungal lesions on leaves during wheat disease. XANES spectroscopic mapping has subsequently been used to characterise changes in Mn speciation, during accumulation.

Challenges were encountered for interpretation of XAS data due to spectral artefacts induced by leaf motion during XANES mapping, in addition to the issue of photo-damage in hydrated biological specimens. This poster presents the data processing pipeline to correct XANES spectra for sample motion artefacts, and the photo-damage reduction strategy.

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Track Classification : 2. Improving the interpretation of XAS data

Contribution ID : **20** Type : **Poster presentations**

Measurements of Satellites in Manganese through Extended-Range High-Energy-Resolution Fluorescence Detection to Elucidate the Nature of the Many-body Reduction Factor

The discovery of a new physical process in manganese metal is reported, by applying our new technique of XR-HERFD (Extended Range High Energy Resolution Fluorescence Detection), developed from the popular high resolution RIXS (Resonant Inelastic X-ray Scattering) and HERFD approaches [1].
This is a first success of XR-HERFD and highlights a method for identification and characterisation of many-body processes which can shed light on the XAFS spectra and how to interpret them, and hence how to measure the dynamical nanostructure observable with these technologies. This particularly applies to the interpretation and determination of S02, which has previously only been represented as a constant reduction factor. Here, we prove the energy dependence of S02 with measurement of these satellite structures in manganese.

[1] Tran, N. T. T., Sier, D., Kirk, T., Tran, C. Q., Mosselmans, J. F. W., Diaz-Moreno, S., Chantler, C. T., (2023) J. Synch. Rad., 30(3), 605-612. https://doi.org/10.1107/S1600577523002539

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Track Classification : 2. Improving the interpretation of XAS data

Contribution ID : **18** Type : **Poster presentations**

Level up your XAS - Recognising and avoiding common XAS data phenomena

X-ray absorption spectroscopy (XAS) plays a critical role in the characterization of energy materials, including thinfilm electrocatalysts and battery materials. XAS is well-suited for this purpose because it is element-specific and can target distinct chemical environments within a material, even in a mixed or complicated matrix. Even so, some key energy materials are far from "ideal" XAS samples. This means that both sample preparation and experimental conditions need to be considered when collecting and interpreting data to ensure that conclusions are correct.This poster examines instances where the sample matrix can distort XAS data.

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Track Classification : 2. Improving the interpretation of XAS data

Contribution ID : **13** Type : **Poster presentations**

Exploring limitations of using X-ray absorption spectroscopy on celadon glazes

Celadon glazes are high temperature ceramic glazes introduced with iron (Fe) to produce a wide range of colors. The oxidation states and coordination structures of Fe have been probed in various studies using Mössbauer spectroscopy and X-ray absorption spectroscopy (XAS) since these properties affect the resulting appearance. We performed XAS on celadon glaze surfaces and observed discrepancies with previous Mössbauer spectroscopy results. Multiple subsequent XAS measurements did not reveal Fe photo-ionization by longer X-ray irradiation and ruled this out as an issue in XAS of celadon glazes. However, depth-resolved XAS of glaze cross-sections revealed Fe surface oxidation caused by the glaze firing process [1]. The possibility of surface oxidation in celadon glazes limits the interpretation of fluorescence XAS spectra taken from glaze surfaces since it poses uncertainty of misrepresenting the glaze interior properties.

[1] A.P. Rillera et al., Journal of the European Ceramic Society, 43, (2023), 5706-5711.

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Track Classification : 2. Improving the interpretation of XAS data

Contribution ID : **30** Type : **Poster presentations**

Commissioning of the new Medium Energy XAS Beamlines at the Australian Synchrotron

Two new beamlines for X-ray Absorption Spectroscopy have been installed and commissioned at the Australian Synchrotron, and are open for user experiments. The beamlines share a common bend mangnet source and are designated MEX1 (3.3 - 13.6 keV) and MEX2 (1.7 - 3.3 keV)

In this presentation we focus on the commissioning and optimization process of MEX1 and MEX2, highlighting key beamline performance that impact the quality of obtained XAS data.

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Track Classification : 5. Other XAS topics