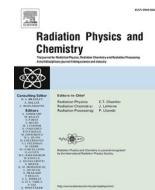




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## XAS databases and repositories – perspective and current status

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## A B S T R A C T

X-ray absorption fine structure (XAFS) methods are widely used, and there is a strong demand to establish well-maintained and reliable XAFS databases. Several XAFS databases have been independently developed based on different requirements of the XAS users' community. These databases mainly consist of XAS data of references or standard samples from dedicated beamlines at synchrotron facilities available to the individuals or group involved in their development. In the present paper, we report the recent activities regarding the development of XAS databases as presented and discussed during Q2XAFS 2023 workshop held at the Australian Synchrotron in Melbourne (Australia). The features of already existing XAS databases are briefly discussed and summarized. The important components and features of two recently developed XAS databases – MDR XAFS database from Japan and RefXAS database under DAPHNE4NFDI from Germany are described. We report on the recent activities and status of these databases. We further discuss the general challenges of developing such databases, including sustainability, metadata structure, sample identification, curation, user feedback and standardization of data formats.

## 1. Introduction

Synchrotron facilities, along with advanced X-ray spectroscopy beamlines, now enable the collection of X-ray absorption spectroscopy data from complex samples both ex-situ and in situ. As the volume and complexity of XAS datasets increase, the XAS community has been actively discussing the critical challenges related to the management, storage, and analysis of XAS data, particularly due to the lack of unified data formats and analysis procedure/tools.

The current status and activities of databases and repositories are discussed here. Several on-line XAFS spectral libraries and databases have been built and developed, but there are still issues and subjects to be solved and improved.

The IXAS XAFS database (Lytle et al., 1995), which has been operated as a service of the IXAS, has a long history and is one of the most famous databases. It is hosted by the Center for Synchrotron Radiation Research and Instrumentation at Illinois Institute of Technology, and is

sometimes called “Lytle database”. Some might feel it an old fashioned, but we should respect the founders and appreciate their devotion.

The IXAS currently manages the IXAS X-ray Absorption Data Library (Newville, 2026). It contains 277 spectra of 20 elements as of Tuesday the 21st January 2025. The spectral data are stored using the XAFS data interchange (XDI) format as discussed during the previous Q2XAFS series and literature (Ravel et al., 2012). The XASLIB database is also one of the first XAS databases made available to general users. The elements are arranged nicely in the form of a periodic table for users making it relatively easy to search the database. For uploading the data, user needs to create a login at the database and then data can be uploaded only in ASCII format along with the metadata fields, e.g., “Sample name”, “Absorbing Element”, “Edge”, “Monochromator d-spacing” etc.

The Canadian Light Source (CLS) also manages their own XAS Database (XASDB) (Spasyuk, 2025), advocating a comprehensive XAS data repository. They hold up their mission: the XASDB aims to facilitate scientific discovery by making XAS data freely available to researchers

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The SSHADE/FAME (Kieffer, 2016) offers XAS data collected at the ESRF BM30B FAME and BM16 FAME-UHD beamlines. They have gathered spectra of standards and characteristic samples provided by the beamlines' users, and 740 spectra are stored based on the current database content statistics. This database created by the French X-ray spectroscopy beamlines at the ESRF also provide detailed sample description and validated quality linked to measured X-ray absorption spectra.

A new Europe based reference XAS database, named RefXAS, has been set-up in Germany (Gaur et al., 2023a; Paripisa et al., 2024, 2025, 2026). Under the DAPHNE4NFDI consortium (Barty et al., 2023), the RefXAS database group which include researchers from Karlsruhe Institute of Technology, Bergische University of Wuppertal and Technical University of Berlin have set up this XAS reference database and developed a data workflow to enable users to submit a raw dataset along with its associated metadata in a structured format. The interface provides users to visualize the uploaded XAS spectrum and pre-processing steps as well as automatized initial quality check of the spectra based on formulated quality criteria which includes metadata as well as scientific quality control. Manual curation has been done for the uploaded spectrum before its final publication to provide users quality checked well curated XAS data sets of reference samples. The database is open access to users for uploading as well as downloading of the data. Currently the database contains 95 XAS reference datasets.

There is another database located in Tsukuba, Japan, which is NIMS MDR XAFS DB (Ishii et al., 2023; Ishii et al., 2026). This database is a collection of XAFS data in the Materials Data Repository (MDR), hosted by the National Institute for Materials Science (NIMS). The XAFS data have been provided by the following six Japanese synchrotron facilities and universities: Japan Synchrotron Radiation Research Institute (JASRI), Ritsumeikan SR Center, Institute for Catalysis at Hokkaido University, Photon Factory at KEK, Aichi Synchrotron Radiation Center and Kyushu Synchrotron Light Research Center. All XAFS spectra are accompanied by metadata common to MDR and XAFS-specific metadata, which are attached to data packages called "works". This database contains more than 210 standard metal foils, as well as 418 oxides, 236 chlorides, and other inorganic materials, and 98 organic materials. The total number of works is 2264, and one of these is the Readme, which is a user guide for the database (as of January 2026).

Another useful initiative is the International XAFS DB Portal by Masashi Ishii which has been created with the aim of making XAFS data from around the world findable (Ishii et al., 2025). Currently, 7 databases are part of this initiative and a total of 4054 spectra (65 absorption elements, 121 absorption edges) are made available at one place from the participating databases (as of January 2026). IXDB's sole purpose is to improve accessibility to each database, and it does not have any spectra. Users must adhere to the data usage license regulations of each database.

## 2. Current status and activities of recently developed XAS databases

### 2.1. NIMS MDR XAFS database

The NIMS MDR XAFS database is located in Tsukuba, Japan (Ishii et al., 2026). The most significant advantage of the MDR XAFS DB is that it integrates data provided from the institutions participating in the project, enabling cross-sectional searches (Ishii et al., 2023). This database has an original materials dictionary MatVoc (NIMS XAFS DB Project Materials) for standardizing material names that differ between institutions, which makes it possible to search for spectra of the same material equally regardless of the institution. In addition, all data are assigned to a DOI (Digital Object Identifier), which allows direct linking

from papers and other documents. Besides this direct approach to individual data, it is also possible to download all recorded data at once using the API (Application Programming Interface). The license for the data was previously Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International (CC BY-NC-SA 4.0), however, from April 2025, some of the data has been changed to Creative Commons Attribution 4.0 International (CC BY 4.0). The permission to use the data commercially is expected to increase the reuse of data by many companies and lead to the revitalization of the XAFS community. Along with promoting the reuse of data, the MDR XAFS DB also emphasizes the importance of clearly indicating the DOI and author when citing data. This is to ensure that the circulation of data is sustainable by bringing benefits to both data providers and users.

One of the challenges of integrating data from multiple institutions is the variation in energy calibration. Currently, the MDR XAFS DB Readme (Ishii et al., 2026) provides the energy calibration rules for each institution. In addition, this Readme-file contains information about the entire database, including data statistics, so we recommend reading it before using the database.

The MDR XAFS DB was renewed in spring 2025. This renewal enables easy access to key metadata characterizing XAFS spectra via API, facilitating data screening. Technical improvements, including faster API response times, have also been achieved.

### 2.2. RefXAS under DAPHNE4NFDI

Within the photon science community, the critical issues of management, storage and analysis of X-ray absorption spectroscopy (XAS) data have been addressed by the development of the RefXAS database (Paripisa et al., 2024) under DAPHNE4NFDI (Barty et al., 2023; Amelung et al., 2025). The main aim or objective for development of the RefXAS database is to provide users with well curated XAS reference spectra along with related metadata fields and online processing tools for visualizing the data. The metadata information as well as the quality criteria are important for making the data reusable. The online availability of processing tools makes it easy for users to understand the steps involved in data analysis. Based on the FAIR data principles (Wilkinson et al., 2016), RefXAS thus provides well curated reference data along with metadata which are ready to use. This also enables knowledge transfer to other scientific fields supports machine-learning activities for XAFS data analysis in the future.

It is important from the database perspective that upload of the data by users should be made easy and automated tools are provided. Currently at RefXAS, during upload of the data, columns Energy (E), Incident intensity ( $I_0$ ) and Transmitted intensity ( $I_t$ ) were selected automatically by the user interface and a preview of the uploaded data has been provided for initial check. Additionally, interactive plots have been implemented to look for any discrepancies in different spectral regions, pre-edge, edge, XANES etc. The header information extraction has been automated for data formats providing this information using the '#' for the metadata. There is an option of uploading a reference data (e.g., metal foil, oxide) along with the sample data given both the datasets are measured at the same beamline/instrument under similar settings. Also, the procedure employed for calibration will always be reported in all cases for clarity.

The current state of the automated data processing and quality assessment system in the RefXAS research database determines certain quality criteria (Gaur et al., 2023b). These include the edge step which is directly proportional to the elemental concentration and thickness of the sample (transmission), and the energy resolution which directly influences the ability to resolve fine spectral features for data interpretation (Paripisa et al., 2024, 2025). Further the useable k-range and the amplitude reduction factor are relevant for better interpretation of the data. Though an automated quality check may provide a nice overview of the data usability, this has been followed by manual curation procedures implemented to verify the data before it was finally published in

the database distributed under the CC BY 4.0 license ([Creative Commons BY, 2024](#)).

The manual curation can be performed at the interface after login into the database as curator. In this way, data included in the RefXAS database has been checked for missing metadata as well as poor quality in cases where automated quality control mechanisms are not sufficient. For the curation as well, most of the steps are automated at the interface. The pre-processed, normalized absorbance,  $\chi(k)$  and  $\chi(R)$  are made available to the curator. Also, the automated check results using the defined quality criteria are given to start with the curation. The curator can download the data (uploaded file) at this point and check for further quality or authenticity of the data.

The database is fully functional with open access to users for data download as well as upload. Structured metadata schema has been formulated according to the need of the user community for data upload. Users are provided with well curated reference spectra along with related metadata fields and online processing tools for visualizing the data. Different XAS data formats, e.g., spec ([spec Software for Diffraction](#)), XAFS data interchange format (XDI) ([Ravel et al., 2016](#)), ascii, txt, from different synchrotron beamlines as well as laboratory XAS facilities can be uploaded at RefXAS. The output data format consists of three columns Energy (E), absorbance  $\mu(E)$  and normalized  $\mu(E)$  along with all the important metadata provided during upload, automated quality check results, any general comment on data by curator and bibliographic details as header information ([Paripisa et al., 2026](#)).

### 3. Discussion and summary

#### 3.1. Sustainability – long term solution

The maintenance and continuous development of research infrastructure, including databases, are essential for any institute or consortium. This necessitates the commitment of dedicated personnel and resources. In addition to local support, sustained backing from the research community and users is crucial for long-term sustainability. Large scale synchrotron radiation facilities or national institutes can provide necessary support to the database developers, i.e., working group of scientists, consortiums, individual projects in such cases.

#### 3.2. Inclusion of metadata and electronic lab notebooks

Reporting relevant metadata fields is essential for describing spectra in the database, as it enhances interpretation, reusability, and reproducibility as well as subsequent use by AI tools. While comprehensive metadata helps, it is in general not necessary to record every technical detail. Distinguishing requirements between raw and processed data aids in choosing suitable metadata fields. Most databases offer processed data collected from the experimental facilities.

In this context, Electronic Laboratory Notebooks (ELNs) ([Jordt et al., 2024](#); [Dolcet et al., 2023](#); [eLabFTW, 2025, 2025](#)) proved to be vital for FAIR data management by recording experiments, data collection, and analysis. Integrating the XAS database with ELNs enables documentation of complementary characterization techniques, such as X-ray diffraction and Raman spectroscopy, and links publications detailing sample properties and preparation to the XAFS data published within the database. This integration also supports tracking Sample IDs ([Hovelmann et al., 2024](#)), facilitating access to synthesis and processing details. ELNs used at the institutes properly document the sample details digitally which make the tasks of ingestion into databases easy by importing that information directly from those ELNs.

#### 3.3. Role of database editors/curators

When data uploaded to a database has been verified by experienced users or domain experts, it enables users to confidently reuse the data without the need for further quality checks. Additionally, the

availability of visualization tools within the database interface allows users to understand various data processing and analysis steps. Accordingly, the role of curators and editors is essential to the development of databases as comprehensive resources. Establishing and consistently reporting quality criteria for both manual and automated curation of XAS data is crucial to ensure that derived results are accurate and reliable. Quality assessment should be an integral part of emerging databases. Rigorous evaluation of the quality of both spectral data and associated metadata supports the accuracy and reliability of information stored, thereby enhancing the database's value for the scientific community.

#### 3.4. Standardization of data/file formats

Reliable data must be reproducible, complete, and free from truncation during pre-processing. The methodology for data collection should be precisely defined, employing optimized equipment and thoroughly documented measurement conditions. Such standards result in structured metadata and well-organized processing information for all measured data. Utilizing standardized formats such as NeXus (neutron, x-ray, and muon science) format ([NeXus, 2024](#); [Konnecke et al., 2015](#)) for XAS data obtained across different facilities can address these needs. Furthermore, conducting round robin tests and sharing outcomes with the community - especially in the context of XAS - promotes transparency and emphasizes the importance of robust scientific practices ([Chantler et al., 2018](#); [Welter, 2026](#)).

One of the earliest reports on XAFS data collection, analysis, and reporting appeared in 2000 by [Sayers \(2000\)](#). Nearly a decade later, standardization efforts resumed at the Q2XAFS workshop (2011) ([Ascone et al., 2012](#)), where challenges in creating unified data formats for sharing were discussed ([Ravel et al., 2012](#); [Ascone et al., 2012](#)). The Q2XAFS workshops aimed to establish standards for XAFS experiments and analyses, including new data formats and deposition practices. XDI format was proposed for single spectra exchange, while the Hierarchical Data Format (HDF5) was recommended for multispectral data ([Ravel et al., 2016](#)). At Q2XAFS 2017 ([Asakura et al., 2018](#)), initial agreements on XAFS data formats and standards were reached.

The outcome of the workshop led to the proposal of conducting a round robin study using well-defined samples across multiple XAFS beamlines and facilities ([Chantler et al., 2018](#)). Recent advances in XAS data formats and quality were discussed at the Q2XAFS workshop held at the Australian Synchrotron, ANSTO, Melbourne (Q2XAFS, 2023) ([Q2XAFS Meetings](#)). XAS community has been discussing a draft proposal for application definition for processed XAS data based on the NeXus standard ([NeXus definitions](#)) to be submitted to NeXus International Advisory Committee. NeXus ([Konnecke et al., 2015](#)) aims to create metadata dictionaries primarily for HDF5 files and outlines a hierarchical format that represents both data and metadata in a tree structure (HDF5). NeXus format has been considered as a preferred option for storing single or multiple XAS datasets, along with metadata and related measurements such as temperature and gas analysis, in a comprehensive, self-describing framework. This format ensures organized metadata and includes all key parameters relevant to data collection.

#### 3.5. User perspective

A database should serve its users, making their feedback and contributions essential. The main goal is to create a collaborative environment where users can not only utilize the available datasets but can also provide feedback to enhance the system based on their needs and interests. However, based on their personal requirements, users' expectation can be different from a database. The requirements of users depend heavily on their role in the research area and their education, i. e., whether the person is a first-time user, e.g., a student having any or very less experience of research data structure or an expert working in

the research area for quite some time and have adequate knowledge about the data structure, analysis and application. Also, there can be different purposes for data search including training, application based, comparison with own data, make use of existing reference data sets to save valuable beamtime, etc. Thus, the database needs to cater to the needs of various types of users, and thus should be developed keeping in mind such diversity existing among users looking for the data due to different purposes as well. The interface of the database should be interactive to provide non-expert users enough support to guide them through different features available. Similarly, for an expert user features like filters and keyword search should make the data search fast and time saving.

### 3.6. Accuracy and precision of XAS measurements

As mentioned in previous section, by creating a collaborative environment for users XAS databases can also promote discussion and awareness about accuracy and precision of XAS measurements. In this context Chantler and co-workers have discussed in detail the various parameters affecting accuracy of XAS measurements (Chantler; Chantlerb; Chantlerc; Chantlerd). The importance of calibrating the energy at or near the sample, especially for intermediate X-ray energy ranges has been reported (Tran et al.). This could help in addressing any issues related to monochromatization, mirrors, mechanical or thermal offsets, drift, or other optical effects that might impact the energy and its bandpass delivered during experiments. Proper energy calibration is a key step to correct systematic errors caused by deviations in encoded photon energies, both in synchrotron and laboratory-based experiments, directly influencing the relative positions of peaks and features within the measured XAFS energy range. Measuring X-ray mass attenuation coefficients with high precision through the X-ray Extended Range Technique (XERT) (Ekanayake et al., 2021; John et al., 2023), as opposed to conventional XAS methods, offers significant advantages - particularly when it is necessary to compare experimental outcomes with established theoretical models. Mass attenuation coefficients are fundamentally associated with the chemical and physical properties of a sample which makes X-ray spectroscopy an important characterization method for numerous systems requiring exact measurements. These precise data can also serve as critical reference points for XAS databases and repositories. Additionally, high-quality spectra of various elements can provide standards to define criteria for the curation of XAS database entries.

## 4. Summary

Several active XAFS databases exist. They have been developed independently and each has its own strong points and purposes. The International XAFS DB Portal is a unique initiative that aims to make XAFS data from around the world findable. The databases need to be maintained to obtain long-term sustainability, and their metadata fields are crucial to utilise spectral data. The scientific community provides experienced experts that are responsible to edit and to curate the databases, and the databases serve their users. Some of the users will be experienced editors and curators of the databases, and this circulation is essentially important to develop the databases with sustainability. In this direction, standardisation of data formats using NeXus with structured metadata schema will be very useful for enhancing the reusability and distribution of XAS data under FAIR data principles.

### CRedit authorship contribution statement

**Abhijeet Gaur:** Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Conceptualization. **Hitoshi Abe:** Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Conceptualization. **Masashi Ishii:** Writing – review & editing, Writing – original draft, Visualization,

Methodology. **Sebastian Paripsa:** Writing – review & editing, Validation, Investigation. **Jan-Dierk Grunwaldt:** Writing – review & editing, Validation, Supervision, Conceptualization. **Dirk Lützenkirchen-Hecht:** Writing – review & editing, Supervision, Methodology, Conceptualization.

### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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### Data availability

No data was used for the research described in the article.

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