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RefXAS

XAS reference database under DAPHNE4NFDI

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Abstract

With advancements in the sensitivity of present synchrotron facilities, the upcoming of laboratory-based spectrometers and the refinement of analytical methods, X-ray based techniques have become a standard approach for the structural characterization of intricate solid material systems.

X-ray absorption spectroscopy (XAS) stands out as one of the most effective methodologies utilized for the analysis of various functional materials, particular for non-crystalline materials. Within DAPHNE4NFDI [1], RefXAS [2], [3], [4] serves as a pioneering reference database, which includes a review step, in the field of XAS. It has been developed to enhance scientific research through a sophisticated platform for both submitting and accessing high-quality XAS data. Analysis of XAS data requires comparison with previously measured experimental/simulated reference spectra. Therefore, reference data is essential for data evaluation and, thus, a curated database that offers high-quality reference spectra is required.

In order to achieve that, our system has the ability to execute quality control in the background, i.e. during uploading, predefined quality criteria are checked automatically. Furthermore, RefXAS includes raw and processed data, an intuitive interface for uploading and evaluating the data along with their comprehensive metadata via a dedicated website. Our database supports various data formats from diverse XAS setups, including synchrotron and laboratory instruments, which aids in standardizing data handling within the community while promoting FAIR principles. The classification of the metadata fields for reporting/uploading any data enhances the traceability and usability of data. The currently running and publicly accessible version features a human verification procedure, a user-friendly landing page, a full listing of datasets, advanced search capabilities, a streamlined upload process, and finally, a server-side automatic authentication and (meta-)data storage via MongoDB, PostgreSQL, and (data-) files via relevant APIs.

Recent advancements include the introduction of a standardized download package, improved filtering mechanisms, and the transition to an institutional virtual machine (VM), ensuring long-term accessibility and alignment with FAIR principles. Additionally, automated querying, beam-line registration, and enhanced data visualization have been implemented to improve usability. Future efforts will focus on integrating the NeXus format to enhance interoperability, support machine learning applications (LLM) and making RefXAS data available via ixdb portal [5]. Interlinking with other consortia like NFDI4CAT (catalytic materials), NFDI4Chem (Lablmotion) will allow to connect to other disciplines, which already resulted in first publications using RefXAS [6].

Keywords: X-ray absorption spectroscopy, Database, Metadata

Resources

- RefXAS website. <http://xafsdb.ddns.net/> "Publicly accessible website with running version of reference database for XAS spectra."

Author contributions

Abhijeet Gaur: Investigation, Methodology, Project administration, Visualization; **Sebastian Paripsa:** Data curation, Investigation, Software, Visualization; **Frank Förste:** Data curation, Software; **Dmitry Doronkin:** Methodology; **Wolfgang Malzer:** Methodology; **Christopher Schlesiger:** Investigation, Methodology; **Birgit Kanngießer:** Conceptualization, Funding acquisition, Supervision; **Edmund Welter:** Conceptualization, Investigation; **Dirk Lützenkirchen-Hecht:** Conceptualization, Funding acquisition, Supervision; **Jan-Dierk Grunwaldt:** Conceptualization, Funding acquisition, Methodology, Project administration, Supervision;

Competing interests

The authors declare that they have no competing interests.

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