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RefXAS: XAS reference database under DAPHNE4NFDI

Abstract: Under the DAPHNE4NFDI consortium, RefXAS has been established as a comprehensive open-access reference database for X-ray absorption spectroscopy (XAS), addressing the need for high-quality reference data with well-documented metadata. The platform provides a structured web interface for data submission, automated metadata handling, and quality control to ensure compliance with predefined standards. Metadata categories such as “Sample,” “Spectra,” “Instrument,” and “Bibliography” facilitate data reusability, enhancing the comparability of experimental and simulated spectra.

Recent advancements include the introduction of a standardised download package, improved filtering mechanisms, and the transition to an institutional VM, ensuring long-term accessibility and alignment with FAIR principles. Additionally, automated querying, beamline registration, and enhanced data visualisation have been implemented to improve usability. Future efforts will focus on integrating the NeXus format to enhance interoperability and support machine learning applications (LLM).

References

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