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CDIF-4-XAS: Describing X-Ray Spectroscopy Data for Cross-Domain Use

The CDIF-4-XAS project - Describing X-Ray Spectroscopy Data for Cross-Domain Use, will enable new science by making it easier to access, combine and reuse XAS data across research infrastructures (RIs) and disciplines.
CDIF-4-XAS will enhance the interoperability and reusability of XAS data by applying the Cross-Domain Interoperability Framework (CDIF), a set of guidelines and practices for using domain-agnostic standards to support the interoperability and reusability of FAIR data, especially across domain and institutional boundaries. By embracing FAIR principles, the project aims to streamline the sharing of XAS data, thus enabling more efficient data integration across RIs and scientific domains, including life sciences, chemistry, and environmental sciences.
X-ray Absorption Spectroscopy (XAS) data is vital for many fields, but its specialised formats and metadata conventions hinder cross-domain use. Data sharing between applications, databases, and facilities is inefficient, leading to the loss of essential experimental information. With increasing data volumes and interdisciplinary collaborations, the need for a more interoperable solution becomes urgent.
The CDIF is a set of practical, implementation-level principles designed to improve data management practices within any community and lower the barriers to cross-domain data reuse. CDIF offers standards and methodologies for achieving different levels of interoperability necessary for reusing data across diverse domains. It is built around five core profiles that address the essential functions for implementing cross-domain FAIR principles.
Through CDIF-4-XAS, metadata and provenance for XAS data are standardised, enhancing the integration of XAS datasets into EOSC infrastructures. This promotes data reuse across different research domains, making XAS data more accessible and valuable.
Coordinated by CODATA, and involving a number of PaNOSC partners and key infrastructures, CDIF-4-XAS will unlock new possibilities for research by enabling seamless data combination and analysis across RIs. Researchers in energy, chemistry, and environmental sciences, among others, will benefit from easier access to XAS data. By implementing CDIF for XAS data (XAS-CDIF), the project tackles the interoperability and reusability challenges described above, and can better integrate the XAS data into the emerging EOSC infrastructures for cataloguing, integration and analysis. The benefits will be considerable: existing resources will become more available, and it will become easier and more efficient to use data across RIs and in other domains. Finally, XAS data is a key research product in the domain of energy research, thereby representing key strategic developments towards a sustainable future for the global society. XAS is an important characterization method for materials used in these fields and essential for developing new materials.
The project started in October 2024 and can present now an overview of standards, vocabularies (and ontologies), data formats and practices within the XAS area.

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