DAPHNE4NFDI Annual Meeting, Berlin HZB, 24 - 26 March 2025

Oral/Poster Presentation:

Title: *RefXAS* database under DAPHNE4NFDI: features and status

Authors:

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Abstract:

In the frame of DAPHNE4NFDI, an X-ray absorption spectroscopy (XAS) reference database called RefXAS has been set-up where users are provided with well curated XAS reference spectra along with related metadata fields and online processing tools for visualizing the data. The developed online procedure enables users to submit a raw dataset along with its associated metadata via a dedicated website for inclusion in the database. The published data at the database can be easily linked to the raw data available at other repositories. Quality criteria formulated for the uploaded reference data at the database make users aware of the usability of the data. These quality criteria, which are unique to RefXAS, are further employed for automatic quality check of the uploaded data which is then followed by manual curation at the interface. Different XAS data formats can be uploaded to RefXAS. The output data format consists of all the important metadata provided during upload including quality criteria, curation details and bibliographic details of the data.

DAPHNE Deliverables / Categories:

- 2.2.1 White paper on metadata definition and known metadata

- 2.3.2 Preliminary specification for use cases minimum metadata

- 2.3.3 Prototype implementation of reference database for XAS/EXAFS

- 2.3.4 Provide write access for processing/analysis software to deposit results (with measure 3.2.3)

- 2.3.5 Mechanism for quality assurance developed

- 2.3.8 Deployment of community database

- 2.4.2 Using the XAS/EXAFS reference database (measure 2.3.3) as training set

Topics to be (potentially) discussed/addressed in the course of the meeting:

- Deployment of XAS database at KIT/DESY

- Sample PID, DataCite services

- ELN integration – Integration of Electronic log notebook

Cooperation partners:

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**Publications**

Metadata Fields and Quality Criteria - XAS Reference Database under DAPHNE4NFDI, A. Gaur, S. Paripsa, F. Förste, D. E. Doronkin, W. Malzer, C. Schlesiger, B. Kanngießer, E. Welter, J.-D. Grunwaldt  and D. Lützenkirchen-Hecht, Conf. on Res. Data Infras.  (CoRDI) 1 (2023). doi:/10.52825/CoRDI.v1i.258

RefXAS: an open access database of X-ray absorption spectra, S. Paripsa , A. Gaur , F. Förste, D. E. Doronkin , W. Malzer, C. Schlesiger, B. Kanngießer, E. Welter, J.-D. Grunwaldt  and D. Lützenkirchen-Hecht,  J. Synchrotron Rad., 31, 1105-1117 (2024) doi:10.1107/S1600577524006751

RefXAS: an open access database of X-ray absorption spectra – improvements and outlook, S. Paripsa , A. Gaur , F. Förste, D. E. Doronkin , W. Malzer, C. Schlesiger, B. Kanngießer, E. Welter, J.-D. Grunwaldt  and D. Lützenkirchen-Hecht, SRI 2024, Accepted for publication in Journal of Physics: Conference Series (2025) <https://www.sri2024.eu/proceedings/>

Examples of data publication

<https://doi.org/10.1021/acscatal.4c02077>

<https://doi.org/10.1002/pssa.202400607>

<https://doi.org/10.1002/pssa.202400623>