

RefXAS: XAS Reference database under DAPHNE4NFDI

Abhijeet Gaur¹, Sebastian Paripisa², Frank Förste³, Dmitry Doronkin¹, Wolfgang Malzer³, Christopher Schlesiger³, Birgit Kanngießer³, Edmund Welter⁴, Jan-Dierk Grunwaldt¹ and Dirk Lützenkirchen-Hecht²

¹Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany, ²Fk. 4, Physik, Bergische Universität Wuppertal, Wuppertal, Germany

³Technische Universität Berlin, Berlin, Germany, ⁴Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany

E-Mail presenting author: abhijeet.gaur@kit.edu

Abstract: We have established an XAS reference database under DAPHNE4NFDI called RefXAS, where users are provided with well curated XAS reference spectra along with related metadata fields and online processing tools for visualizing the data at the interface. The database interface allows users to easily judge the quality and the usability of each data set by using the formulated quality criteria mentioned for uploaded reference data. The interface of RefXAS database has been tested with different data/file formats so that users would be able to upload the data in different formats as received from experimental facilities which includes synchrotron beamlines as well as laboratory instruments. In the present work, the significance of metadata fields for the reusability as well as reproducibility of results (FAIR data principle) has been discussed. Also, the different features of the database have been presented, i.e., a user-friendly landing page, a full listing of datasets, advanced search capabilities, a streamlined upload process.

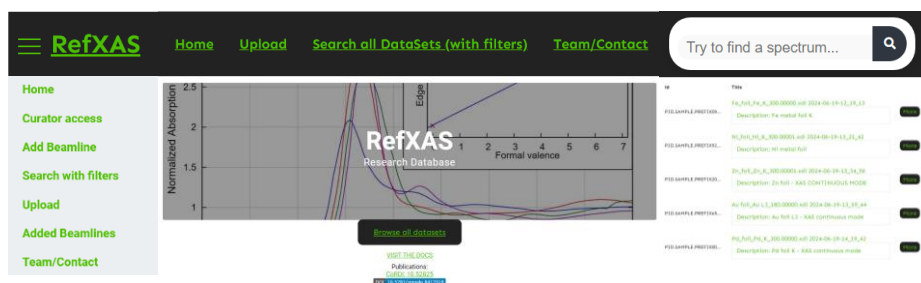


Figure 1: A snapshot of RefXAS database website displaying different features.

[1] A. Gaur, S. Paripisa et al., Proc Conf Res Data Infrastr, 2023, 1,

<http://dx.doi.org/10.52825/cordi.v1i.258>

[2] S. Paripisa, A. Gaur et al., J. Synchrotron Radiat., 2024, accepted for publication.