Poster ID 49

Metadata Fields and Quality Criteria - XAS Reference Database under DAPHNE4NFDI

Abhijeet Gaur[1*], Sebastian Paripsa[3], Frank Förste[4], Dmitry Doronkin[1,2], Wolfgang Malzer[4], Christopher Schlesiger[4], Jan-Dierk Grunwaldt[1,2], Birgit Kanngießer[4], Dirk Lützenkirchen-Hecht[3,], Edmund Welter[5]

[1] Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology (KIT), Engesserstr. 20, Karlsruhe, D-76131 (Germany). [2]Institute of Catalysis Research and Technology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen, D-76344 (Germany), [3]Fk. 4, Physik, Bergische Universität Wuppertal, Gauß-Str. 20, Wuppertal, D-42097 (Germany), [4]Technische Universität Berlin, Hardenbergstr. 36, Berlin, D-10623, [5]Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, Hamburg, D-22607

Aims and Objectives

- **Within the DAPHNE4NFDI consortium, an important pilot project is to develop a reference database in the field of X-ray absorption spectroscopy (XAS) including X-ray emission spectroscopy (XES) and related techniques.**
- **The initial focus was to setup a XANES/EXAFS database of raw and processed data having an interface for the user for data submission as well as an API for data analysis software.**

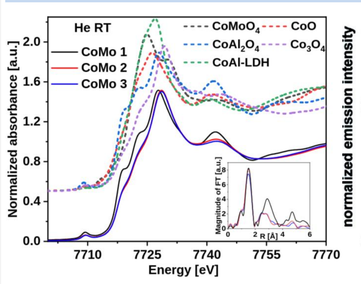
Motivation

In the field of XAS/XES, data is often evaluated by comparison to previously measured or calculated reference spectra.

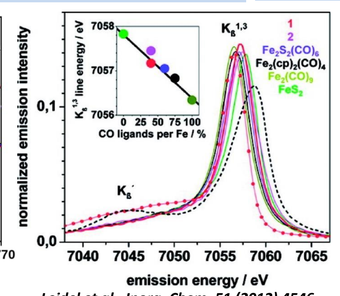
Automation / machine learning also requires repository with high quality reference data & metadata.

This sets high requirements concerning both spectral quality and documentation of the measurements.

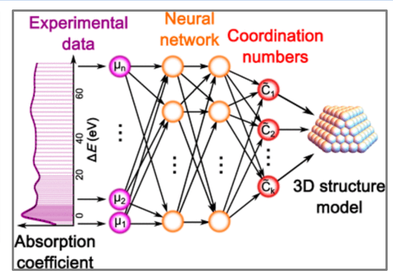
Metadata include important information about the sample, experimental set-up & conditions used, large-scale or Laboratory facility involved, data processing software used etc.



Gaur et al. ACS Catal. 12 (2022) 633



Leidel et al., Inorg. Chem. 51 (2012) 4546



Timoshenko et al. . Phys. Chem. Lett. 8 (2017), 5091

Defined metadata fields for the XAS database

Sample

- Collection mode
- CAS no. (optional)
- Physical state (crystalline, powder, liquid, gas)
- Structural parameters for crystalline sample
- Crystal orientation
- X-ray or neutron diffractogram (if available)
- Temperature. Pressure
- Remarks about sample preparation
- Sample environment, if applicable
- General remarks e.g., sample property

Spectra

- Raw data file
- Absorbance spectrum
- Reference spectrum
- Data/File format

Bibliography

- DOI
- Title/Author
- Reference
- Funding agency/grant details

Instrument

- Facility (synchrotron/lab instrument)
- Beamline
- Acquisition mode
- Crystals
- Mirrors
- Detectors
- Element
- Edge
- Maximum *k* range (EXAFS)

Started with data from selected metal foils

- Ideal samples (thickness and homogeneity)
- Stable and easy to handle
- Availability
- No influence of sample preparation
- Comparing the data from different synchrotron and laboratory facilities will be useful to define meta data and quality criteria (Round Robin)

Ni Cu Au Pt

XAFS database website - features under development

Web-Server

- Current status:

1. Handles multiple formats and Beamlines
2. Automatic extraction of information from file header
3. Preview of raw spectra and Energy-range update
4. Display of Metadata and result of quality control
5. Automatic execution of python scripts on “submit”
   -> Quality control: Dataset check & graphic analysis
   -> Raw & Normalised XAFS | Chi(k) | Chi(R)

Quality Control during data upload

Quality criteria

- edge step [0.5-2.0]
- maximum k-range [15-20 Å^{-1}]
- energy resolution [0.5-2 eV]
- signal to noise ratio
- amplitude reduction factor [0.7 - 1.0]*

*analysed data

Quality criteria: Implementation

- Data pre-processing during upload
- Automated check of quality criteria, noise estimation
- Testing multiple formats used by different experimental facilities

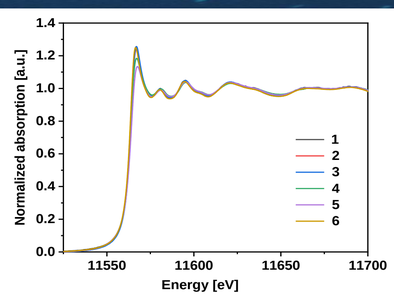
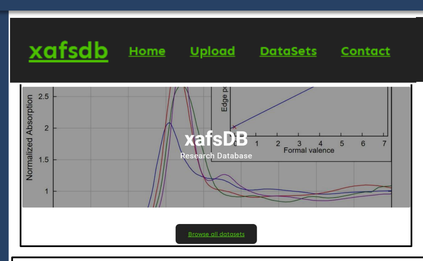
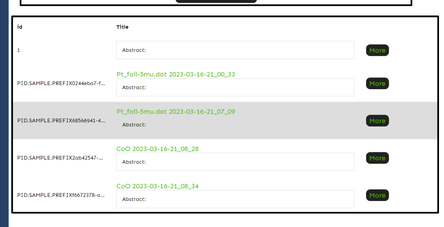
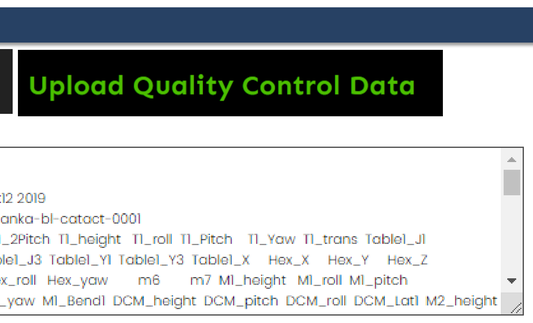


Figure 1. Comparison of Pt foils (distinct) data (Pt L_3-edge) measured at different beamlines.



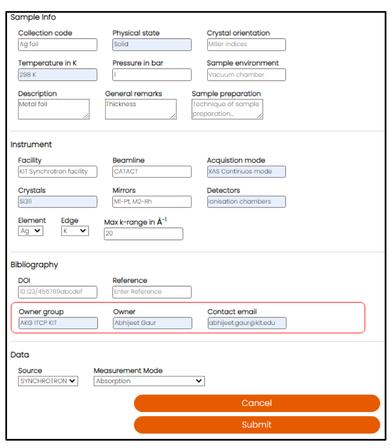


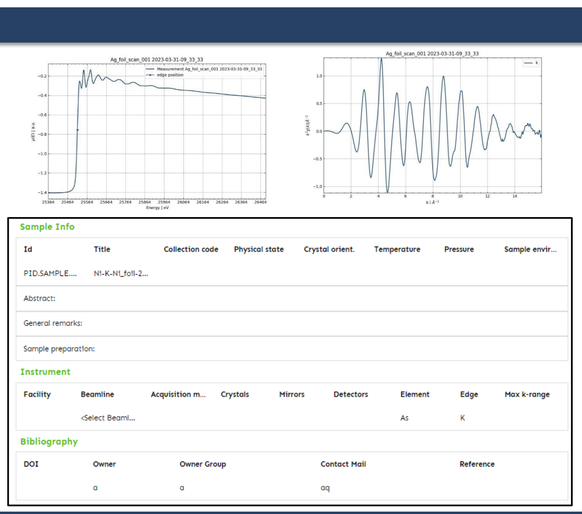


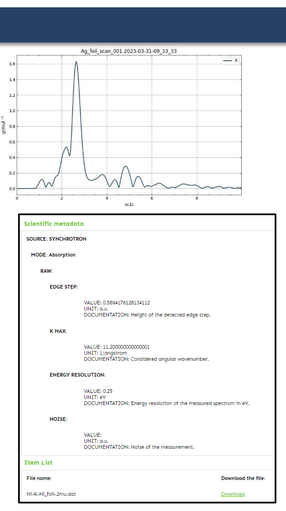
Different data/file formats

```
#Transmission-mode XAS
# E0 (eV) = 8979
# Photon Energy Scan (eV) = -200,-10,20,15k
# Photon Energy Step (eV) = 10,0.3,0.04k
# Time Step (s) = 1,1,1
# Gain = 8, 8
# Points/scan = 440
Energy (eV)     Bragg Angle (deg)     Time Step (s)   I0 (counts)     I1 (counts)     ln(I0/I1)
8.77914E+3      2.06691E+1      1.00000E+0      2.37830E+4      3.16900E+4      -2.87030E-1
8.78907E+3      2.06447E+1      1.00000E+0      2.35040E+4      3.15080E+4      -2.93071E-1
8.79914E+3      2.06200E+1      1.00000E+0      2.32070E+4      3.13250E+4      -2.99963E-1
8.80907E+3      2.05957E+1      1.00000E+0      2.29240E+4      3.11260E+4      -3.05859E-1
```

```
Energies_eV     Nifoil2mu_03_26
7448.445        0.117124223869369
7448.695        0.126539199202244
7448.945        0.127414499400114
7449.195        0.127090148767121
7449.445        0.132294379922562
7449.695        0.138309148202028
7449.945        0.142245318044879
7450.195        0.1400888215512
7450.445        0.135867285616848
7450.695        0.134660130677045
7450.945        0.136135828693538
```







Next steps

- **Improve data submission system – Web interface**
- **Testing with different data/file formats of input files.**
- **Metadata format & Metadata submission on the web interface**
- **Hosting of the database – Long term deployment -> dCache**
- **Defining quality criteria for different modes of XAS – Transmission, Fluorescence, Quick EXAFS**
- **Testing the quality criteria for references, samples**

Contact: abhijeet.gaur@kit.edu, paripsa@uni-wuppertal.de

References

1. K. Asakura *et al.*, J. Synchrotron Rad., 25, pp. 967-971, July, 2018
2. A. Barty *et al.*, Zenodo, DAPHNE4NFDI - Consortium Proposal, June, 2023, doi:https://doi.org/10.5281/zenodo.8040606
3. R. Dimper *et al.*, Synchrotron Radiation News, 32, pp.7-12, May, 2019
4. C. T. Chantler *et al.*, . Synchrotron Rad., 25, pp. 935-943, July, 2018,

Acknowledgement

This work is supported by the consortium DAPHNE4NFDI in the context of the work of the NFDI e.V. The consortium is funded by the DFG - project number 460248799.

Meet us

www.DAPHNE4NFDI.de

1st Conference on Research Data Infrastructure (CoRDI) 2023, 12th - 14th September 2023, Karlsruhe

https://san-wierpa.github.io/xafsdb4daphne/

„Live“-view:

http://xafsdb.ddns.net/