DAPHNE4NFDI

Data from Photon and Neutron Experiments

J.-D. Grunwaldt (KIT)

B. Murphy (speaker), A. Schneidewind

L. Amelung (coordinator), V. Biniyaminov

28th November 2024

NFDI Consortium

26+1 consortium

DAPHNE 4NFDI

PUNCH 4NFDI

What is „**DA**ta from **PH**oton and **N**eutron **E**xperiments“?

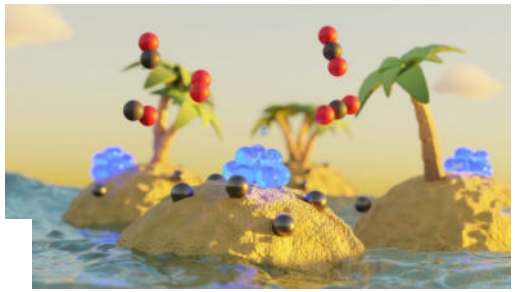
2022/09/01

Back

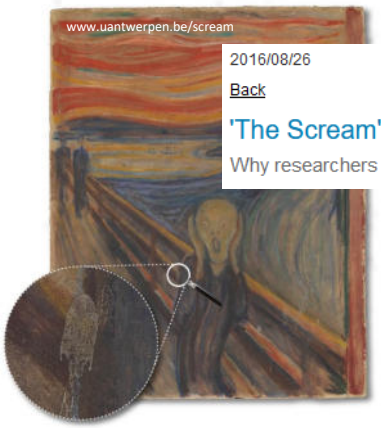
New ant genus named after DESY

Researchers spot previously unknown extinct ant in 20 million-years-old amber

Hereon, Jörg Hammel/Jonas Lauströer



Concept for Efficiency-Enhanced Noble-Metal Catalysts (2024)



2016/08/26

Back

'The Scream' and the secret of the white spots

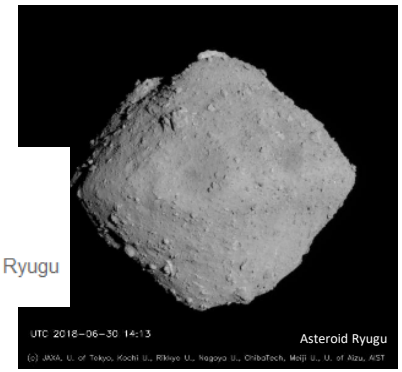
Why researchers look for bird droppings on Edvard Munch's masterpiece with DESY's X-rays

2022/09/23

Back

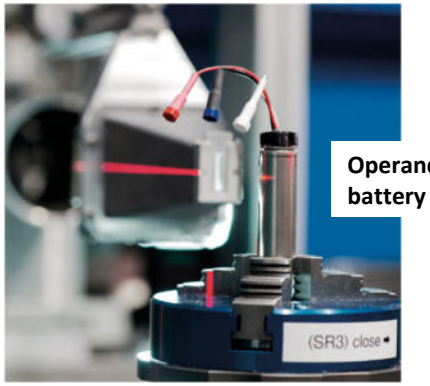
Asteroid dust in the X-ray beam

Large international campaign analyses samples from asteroid Ryugu



https://www.desy.de/information__services/press/press_releases/index_eng.html
https://www.kit.edu/kit/english/pi_2024_057_concept-for-efficiency-enhanced-noble-metal-catalysts.php

What is „**DA**ta from **PH**oton and **N**eutron **E**xperiments“?



Operando experiment on Li-ion battery at MLZ

https://www.sni-portal.de/de/Dateien/neutronenforschung-in-deutschland-fuer-wissenschaft-und-gesellschaft/view

17.08.2023

Organogels: New cleaning agent for artworks

© Bernhard Ludewig/ FRM II

12.06.2023

From Orange to Red: How bacteria protect themselves from sunlight

© Andreas Heddergott, FRM II / TUM

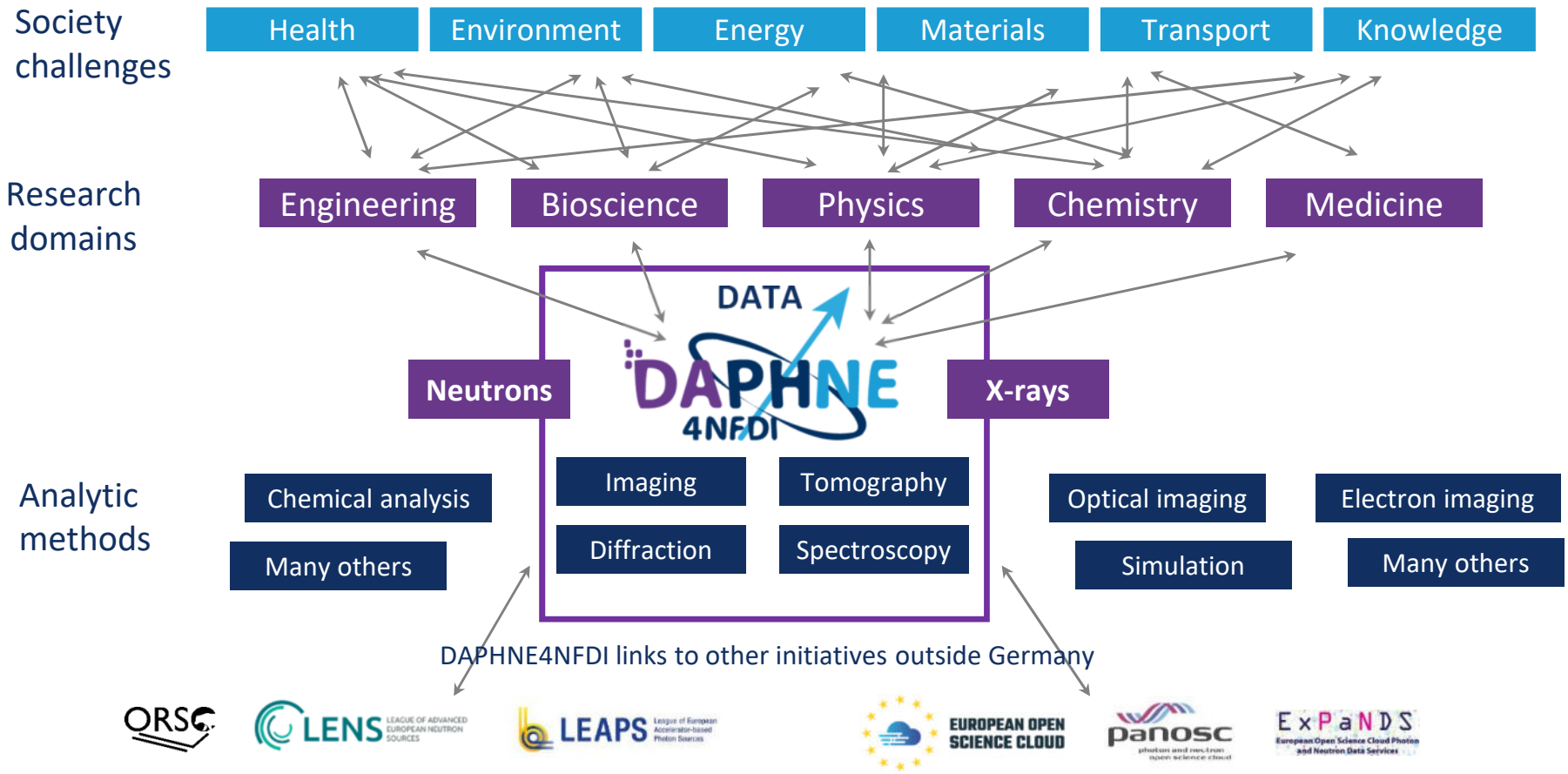
https://mlz-garching.de/englisch/news-und-press.html

14.03.2023

Super methods for superalloys

© Reiner Müller, FRM II/TUM

Our community is widespread



DAPHNE4NFDI aims

to make Scientific data FAIR for the DAPHNE4NFDI community, for the whole NFDI and the scientific community.

These key objectives will be achieved within DAPHNE:

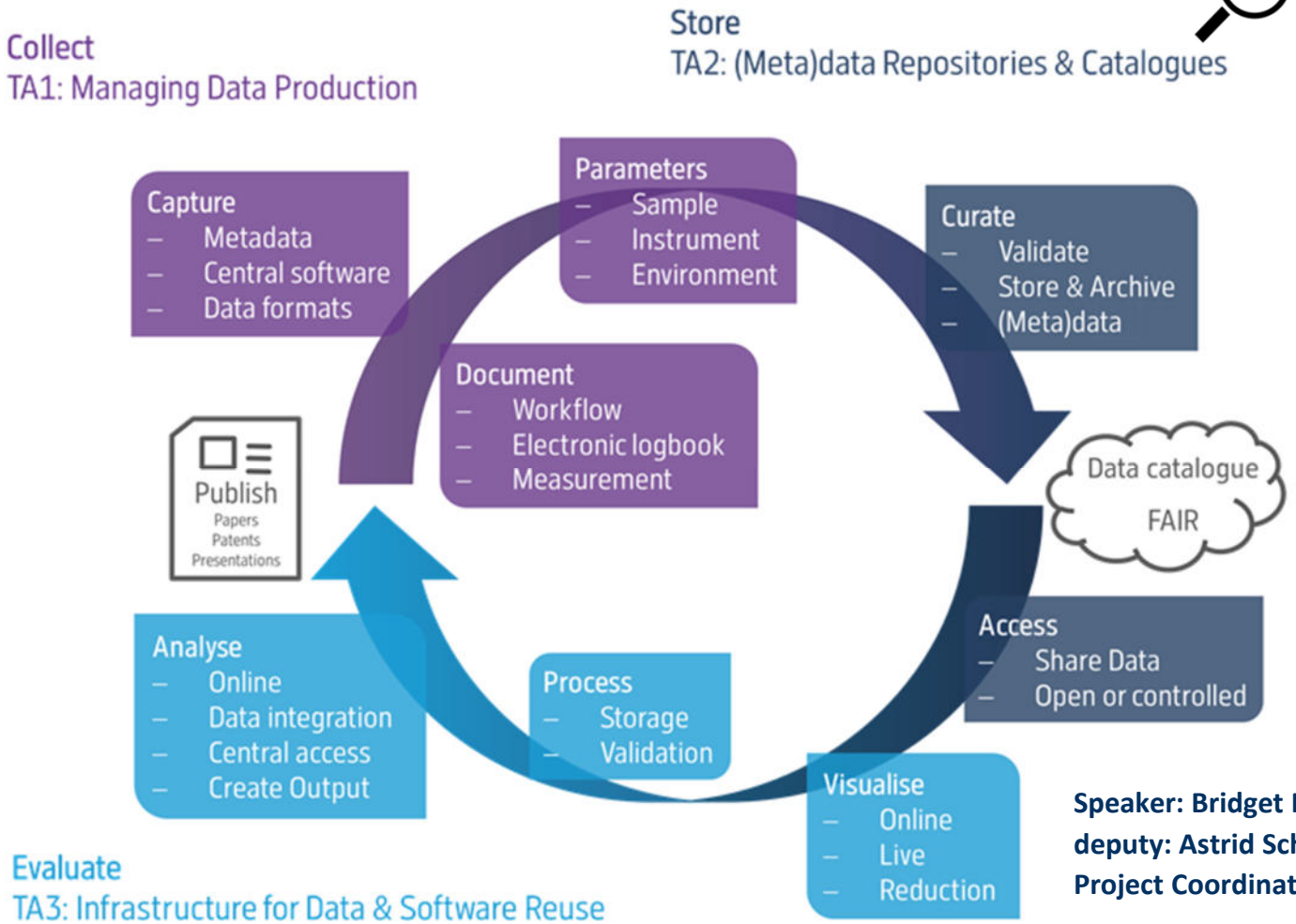
Reuse data by:

1. **Collection** of **(meta)data**
2. **Curated** repository **databases** of data and metadata
3. **Curated** repository of **managed software**
4. **Education** and **training** in research data management
5. **Connection** to other NFDI consortia, national and international organisations

DAPHNE4NFDI

DAPHNE4NFDI - DAta from PHoton and Neutron Experiments

Findable Accessible Interoperable Reusable



Speaker: Bridget Murphy (DESY/CAU Kiel)
deputy: Astrid Schneidewind (JCNS at MLZ, FZ Jülich)
Project Coordinator: Lisa Amelung

Our Use Cases (UCs) serve as flagship projects

Power users advance FAIR data at facilities

Biomaterials
X-ray imaging
LMU - Uni Göttingen

Energy and battery materials, catalysis
Tomography
TUM - MLZ - BAM - hereon - HZB - KIT

Correlated electron systems **Spectroscopy**
KIT - FZJ - MLZ

Soft matter and liquid interfaces
x-ray reflectivity
CAU - Uni Tübingen

Proteins & Food science
Diffraction (small and wide angle) Spectroscopy
FAU - Uni Tübingen - EMBL - CAU

Magnetic structures
Ultrafast / Magnetic x-ray scattering
DESY - Uni Siegen

Dynamics
Correlation spectroscopy - XPCS
Uni Siegen - EuXFEL

Amorphous materials for catalysis
x-ray absorption spectroscopy
KIT - TUB - Uni Wuppertal

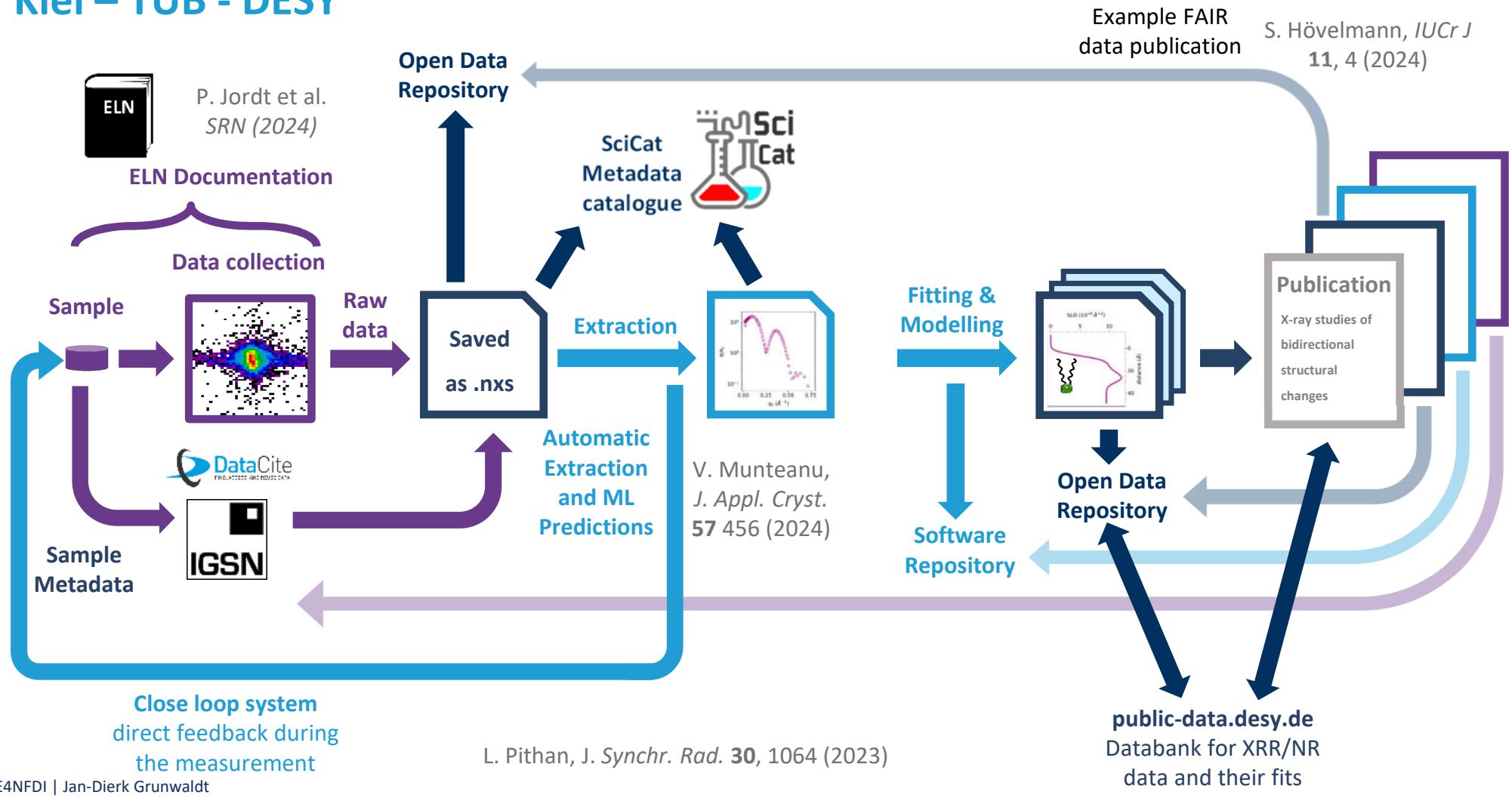
Electrochemistry & Catalysis
High energy x-ray diffraction
HZDR - CAU - DESY

Reusable powder refinement
Neutron TOF diffraction
FZJ - MLZ - ESS - RWTH

Chemical systems
x-ray emission spectra, RIXS etc.
KIT - ESRF - DESY

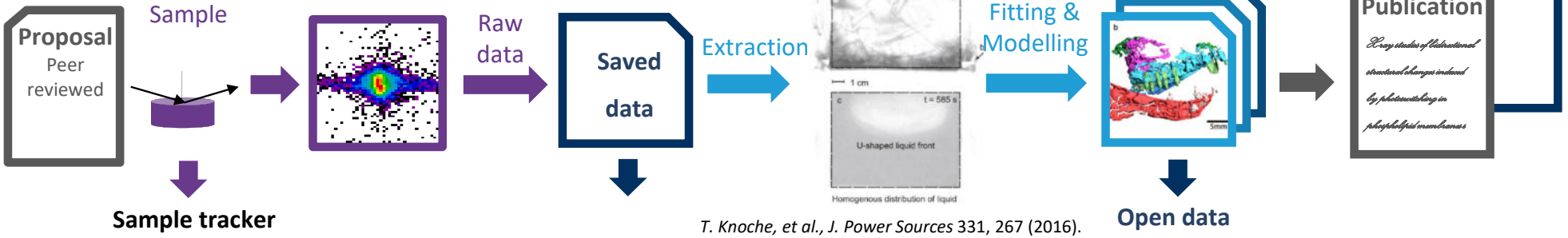
X-ray and Neutron Reflectivity use case

Kiel – TÜB - DESY



Tomography

TUM - MLZ - BAM - HEREON - HZB - KIT



GhOST Garching Online System Tool | NICOS Networked Instrument COntrol System

Antares / Nectar / Medapp
- **Image files +.tif**
- **separate metadata information**

SciCat

Status Server
Hereon@Desy

PO5 P07
Metadata hdf 5
***.tif**

SciCat

Integration into
ICAT database

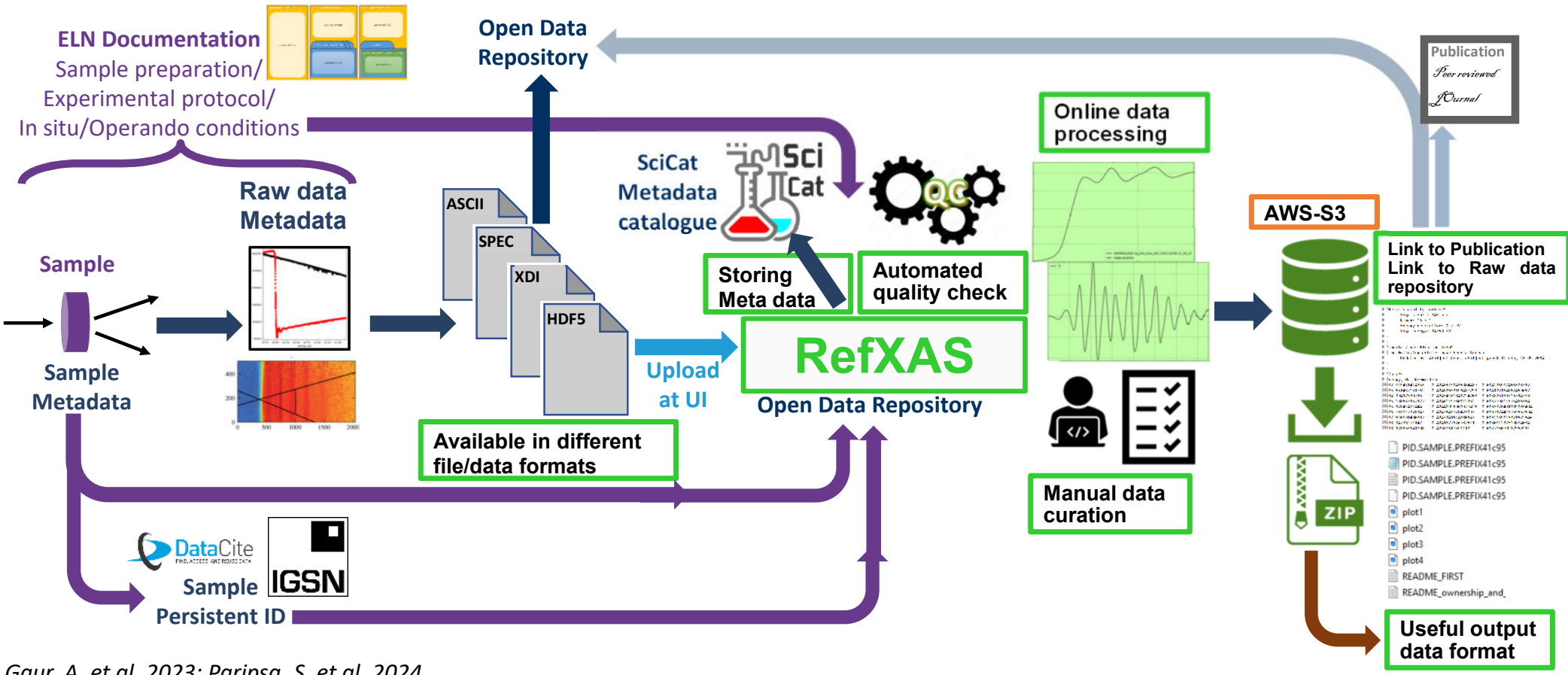
So far
Local storage

ICAT

Courtesy : Wiebke Lohstroh (TUM/MLZ)

FAIR data workflow @RefXAS

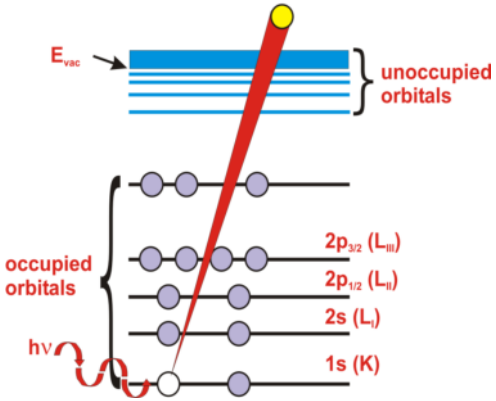
X-ray absorption spectroscopy / amorphous materials and catalysis

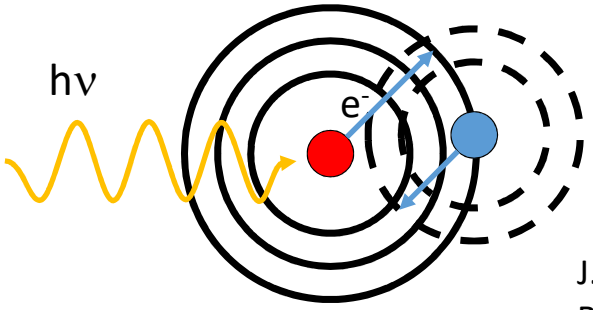


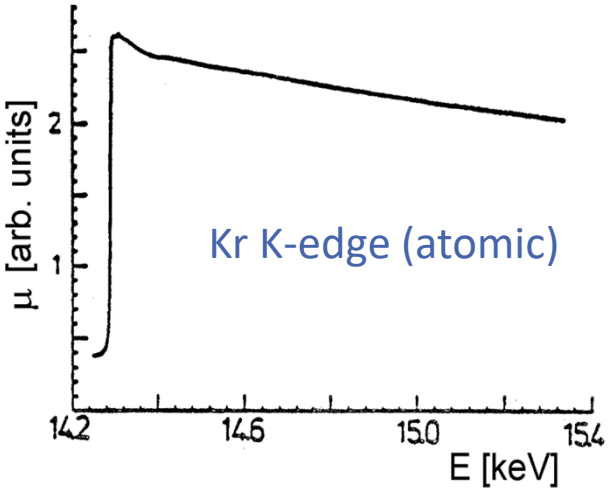
Gaur, A. et al. 2023; Paripsa, S. et al. 2024

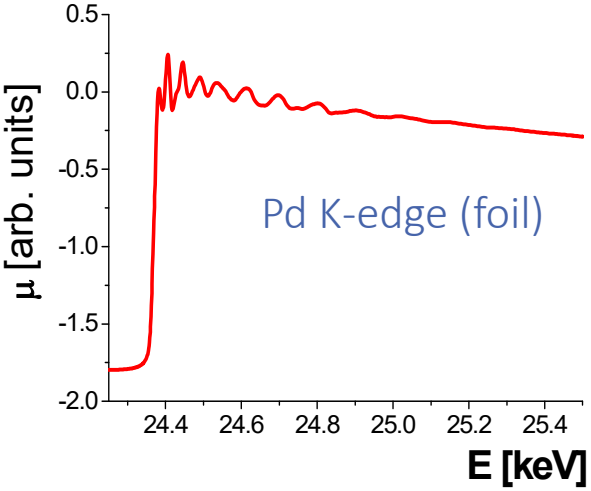
Data Publication: Gashnikova et al., ACS Catal. (2024)

Whether crystalline, liquid or gas: X-ray absorption spectra can be taken!



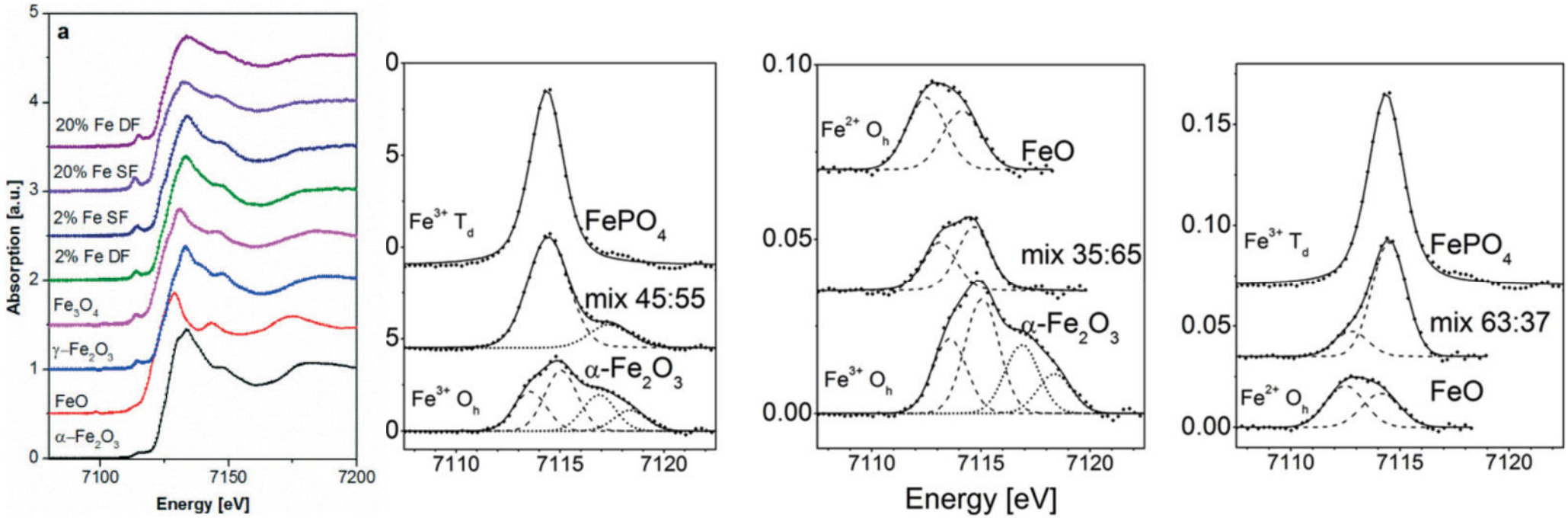






J.-D. Grunwaldt, A. Baiker, Phys. Chem. Chem. Phys. **7**, 3526 (2005).
B. B. Sarma, F. Maurer, D. E. Doronkin and J.-D. Grunwaldt Chem. Rev. 123, 379 (2023)

Another example: iron based samples



M. Tepluchin, D.K. Pham, M. Casapu, L. Mädler, S. Kureti, J.-D. Grunwaldt, Catal. Sci. Technol. **5**, 455 (2015).

A. Boubnov, H. Lichtenberg, S. Mangold, J.-D. Grunwaldt, J. Synchrotron Rad. 22, 410-426 (2015).

FAIR-principles help! Data exchange beyond personal contacts!

RefXAS database under DAPHNE4NFDI

- In the frame of DAPHNE4NFDI, we have set up an X-ray absorption spectroscopy (XAS) **reference database 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.

- To make the data reusable, **defining metadata fields** for the conducted XAS experiments and documentation of this information along with data is essential.

- Based on the mode of measurements, formulation of **quality criteria** is important for initial screening of any uploaded data.

- In this context, examining the usability/interoperability of available XAS **data/file formats** is also crucial.

Classification of Meta data fields

Sample

Sample Info

Sample ID: e.g.: 20210308-PtO2-XAS-
Collection code: e.g.: 20210308-PtO2-XAS-
Physical state: e.g.: Solid
Crystal orientation: e.g.: Miller indices
Temperature in K: e.g.: 298.15
Pressure in bar: e.g.: 1
Sample environment: e.g.: Vacuum chamber
Description: Enter small description
General remarks: Enter general remarks
Sample preparation: Enter technique of sample preparation

Source

Data

Source: SYNCHROTRON
Measurement Mode: Absorption

Instrument

Instrument

Facility: Enter facility
Beamline: P65
Acquistion mode: e.g.: Continuous scan
Crystals: e.g.: DCM
Mirrors: e.g.: Kirkpatrick-Baez (KB)
Detectors: e.g.: Silicon drift detector
Element: As
Edge: K
Max k-range in $Å^{-1}$: Enter max k-range

Source

Data

Source: LABORATORY
Measurement Mode: Transmission

Instrument

Instrument

Mode: Scanning
Geometry: von Hamos
Commercial Instrument Name: e.g.: easyXAFS300+
Institute: Enter LabInstitute name
Source and Anode Material: e.g. side/end window X-ray tube (Mo
Optic: e.g.: HAPG (002) or Si (111)
Diffraction Order for Optic: e.g.: 1
Detector: e.g.: Silicon drift detector
Element: As
Edge: K
Max k-range in $Å^{-1}$: Enter max k-range

Bibliography

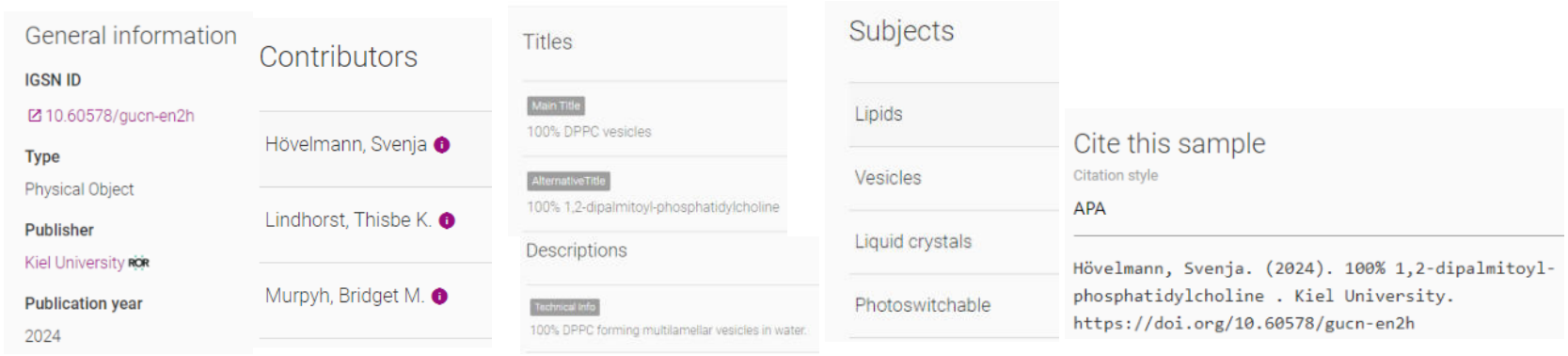
DOI: e.g.: 10.123/456789abcde
Reference: Enter Reference
Institute: Enter institute
Contact person: Enter contact person
Contact email: Enter contact email

Sample

- **Sample ID**
- **Collection code**
- **CAS no. (optional) - *7440-50-8 (Cu)***
- **Physical state - crystalline, powder, thin film, liquid, gas**
- **Structural parameters for crystalline sample**
- **Crystal orientation**
- **Details of sample preparation – Foil, Pellet, Capillary, Powder on tape etc.**
- **Temperature**
- **Pressure**
- **Sample environment - Cell/Microreactor/Batch, gases, solvents, potential**
- **General remarks e.g., sample property (hygroscopic), glove box, heterogeneity**, ..

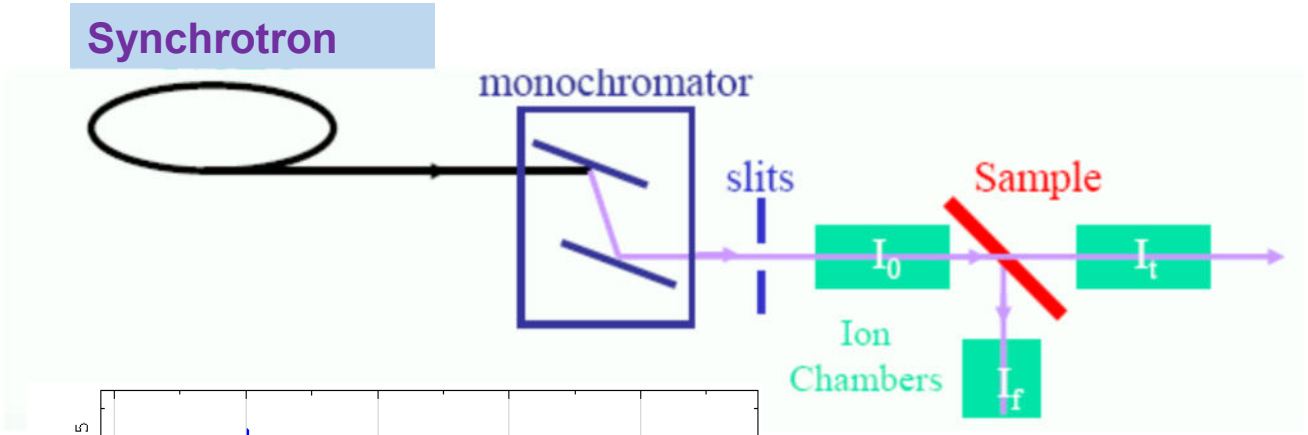
Sample ID

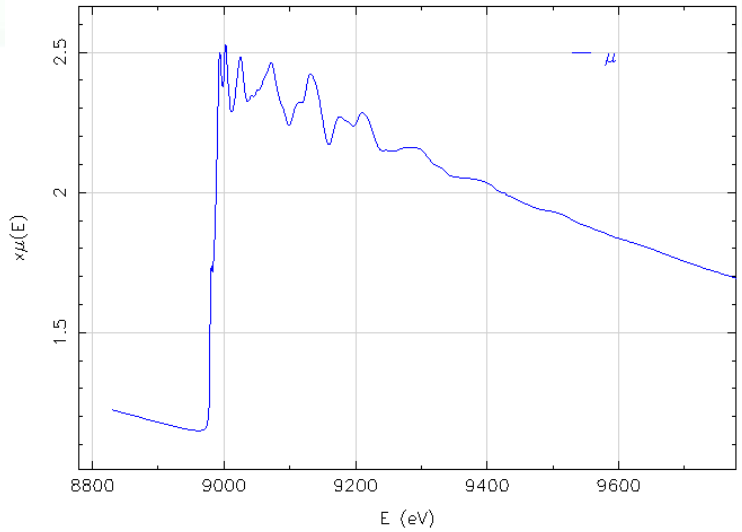
International Generic Sample Numbers (IGSNs): DPPC:1 100:0 (https://doi.org/10.60578/gucn-en2h)

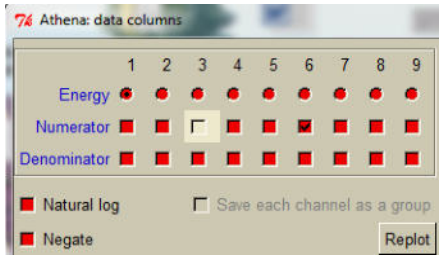


Instrument – Synchrotron facilities

Simple experimental set-up (synchrotron)








```
#This file has been produced by quickread.moulinex (v 2.0.4 - Fe
#E. Fonda, C. La Fontaine - Synchrotron SOLEIL. Covered by GPL l
#Interpolate over grid = 13200, 2, 13370, 0.2, 13570, 1, 13800,
#Average 100 scans - Elapsed time 50.01 s (exposure 25.01 s)
#No smoothing
#Dark =          0       0       0
#offset = 0
#d=3.1356
#Data from HDF File: /nfs/ruche/rock-soleil/com-rock/2016/Projet
#Direction is increasing angle
#Time at start=2016-06-04 20:31:11.415
#Time from start (seconds)=29.8064223634
#Z0=Z+DeltaZ0+offset=8.512908
#Sample temperature (C)=124.4
#Resistor temperature (C)=NaN
#Energy Angle    mux     mus     I0      I1      I2      Directio
13200.00000000  8.61393534      -1.76944436     0.02867609
13202.00000000  8.61262047      -1.77121265     0.02705021
13204.00000000  8.61130601      -1.77263528     0.02713785
13206.00000000  8.60999195      -1.77405739     0.02543318
13208.00000000  8.60867830      -1.77609332     0.02344058
13210.00000000  8.60736505      -1.77723074     0.02377475
13212.00000000  8.60605220      -1.77927786     0.02170750
13214.00000000  8.60473975      -1.78088978     0.01977452
13216.00000000  8.60342770      -1.78230616     0.02123130
13218.00000000  8.60211606      -1.78431520     0.01978865
13220.00000000  8.60080481      -1.78570494     0.01719452
13222.00000000  8.59949397      -1.78760691     0.01669576
13224.00000000  8.59818353      -1.78918626     0.01479195
13226.00000000  8.59687349      -1.79070837     0.01347949
13228.00000000  8.59556385      -1.79263310     0.01466913
13230.00000000  8.59425461      -1.79428165     0.01166506
13232.00000000  8.59294577      -1.79554369     0.01289978
13234.00000000  8.59163733      -1.79739876     0.01100708
13236.00000000  8.59032929      -1.79885575     0.00927669
13238.00000000  8.58902165      -1.80065493     0.00890818
13240.00000000  8.58771441      -1.80281770     0.00767869
13242.00000000  8.58640757      -1.80388107     0.00728518
13244.00000000  8.58510113      -1.80533451     0.00530433
13246.00000000  8.58379509      -1.80728183     0.00549335
13248.00000000  8.58248944      -1.80881568     0.00267667
```

Instrument – Synchrotron facilities

- Facility (Synchrotron)
- Beamline
- Acquisition mode - Transmission
  Total Electron Yield,
  Partial Electron Yield
  Auger Electron Yield
  Fluorescence Yield
- Crystals (Monochromator)
- Mirrors
- Harmonic rejection
- Detectors
- Element
- Edge
- Maximum k range (EXAFS)

Beamline parameters

- Beamline ID
- Scan parameters
- Storage ring
- Source
- Monochromator
- Mirrors
- Filters/Windows
- Detectors

Bibliography

- DOI
- Title
- Author (ORCID)
- Reference
- Funding agency /Grant details
- Beamtime Proposal number

Overview of the defined metadata fields for a beamline.

Beamline metadata field	Description / Example
Facility	
Synchrotron name	identifies the specific synchrotron facility where the research is conducted, with corresponding PID (*The Research Organization Registry (ROR)* 2023)
Beamline	refers to the specific beamline used at the synchrotron, DOI of description if available
Storage ring	
Energy	indicates the energy level of the electron beam in the storage ring. Unit: GeV
Beam emittance	describes the quality of the electron beam. unit: nmrad
Filling mode	refers to the pattern in which electrons are distributed in the storage ring
Mirrors	
Use mirror	Yes, No
Position	before / after monochromator, both
Reflecting surface material	specifies the material composition of the mirror's reflecting surface.
Angle of incidence	refers to the angle at which the synchrotron light strikes the mirror. Unit: mrad
Filters / windows	
Filter	specifies the type and characteristics of the filter used in the beamline.

Detectors	
If IC used gases and pressure (IC: Ionization chamber)	separate fields for I0 and I1 (I0: Ionization chamber before the sample, I1: Ionization chamber after the sample)
If fluorescence detection	type of detection
Scan parameter	
Detection mode	identifies the method used for detecting the synchrotron radiation. e.g. Fluorescence, Transmission, electron yield
Scan mode	refers to the technique employed for scanning the sample with the beam. E.g. Continuous, Steps
Monochromatic flux on sample	indicates the intensity of the monochromatic beam as it interacts with the sample.
Beamsize on sample	specifies the size of the beam when it hits the sample.
Higher harmonic content of beam	actual, measured
Source-type	
Type	undulator (tapered, scanned, …), Wiggler, Bending magnet
Critical energy	indicates the energy at which the intensity of the synchrotron radiation is at its peak. Unit: eV
Maximum k value	refers to the highest wavevector value achievable. Integer (in $Å^{-1}$)
Monochromator	
Type	design and functional type of the monochromator. e.g. DCM (Double crystal monochromator)
Crystals	e.g. Fe2O3 (hematite)DCM, CCM, Polychromator, specify materials and orientation, e.g. Si (111), Ge (220), etc.
Lattice spacing	indicates the spacing between atoms in the monochromator crystals. Used to calculate the energy axis
Temperature of crystals	refers to the operational temperature of the monochromator crystals. Unit: K

S. Paripsa, A. Gaur, F. Förste, D.E. Doronkin, W. Malzer, C. Schlesiger, B. Kanngießer, E. Welter, J.-D. Grunwaldt and D.Lützenkirchen-Hecht(2024). J. Synchrotron Rad. 31 1105-1117

Quality criteria

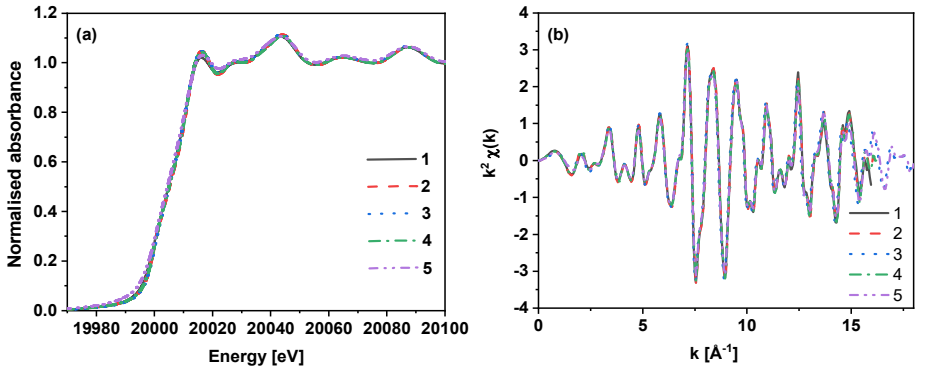
- **Absorption jump/Edge step**
  Directly related to the elemental composition of the sample, the concentration of elements, as well as sample preparation.

- **Energy resolution**
  Generally dependent on the limits of the used beamline/instrument

- **Pre-edge range**
- **Signal to Noise ratio**
  (maximum k-range)
  Depends on both sample and the instrument

- **Amplitude reduction factor**
  (analysed data)

Comparison of Mo foil (distinct) data measured at different beamlines



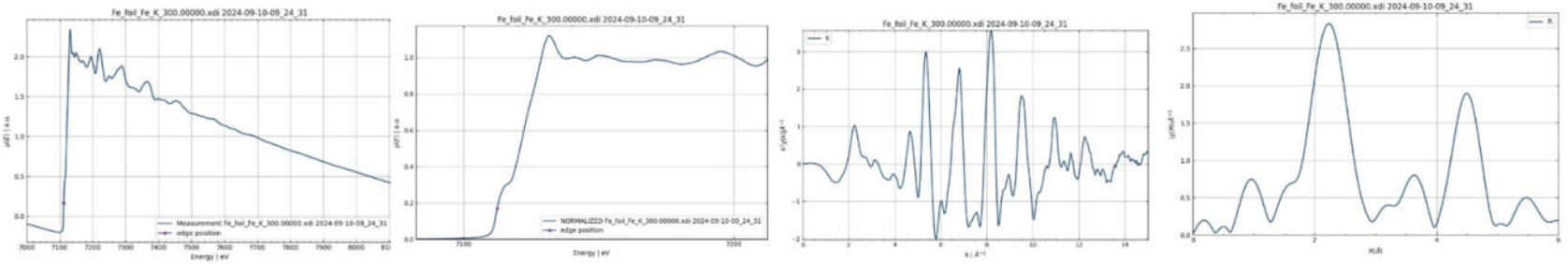
Mo foils (distinct) measured at XAS beamlines from different synchrotron facilities

BL*	N	R (Å)	σ^2 x10^3 (Å^2)	N	R (Å)	σ^2 x10^3 (Å^2)	S_0^2	ΔE	$\mathcal{R}$ *factor*	*k range for FT*
1	8	2.72(0.01)	3.6(0.4)	6	3.14(0.01)	3.6(0.5)	0.97 (0.07)	4.9(0.8)	0.0006	2.2-15.2
2	8	2.72(0.01)	3.7(0.3)	6	3.14(0.01)	3.7(0.4)	0.98 (0.06)	5.2(0.7)	0.0004	2.2-15.2
3	8	2.73(0.01)	4.0(0.2)	6	3.15(0.01)	3.9(0.3)	1.03 (0.05)	5.5(0.5)	0.0004	2.2-18.0
4	8	2.72(0.01)	3.5(0.3)	6	3.14(0.01)	3.6(0.4)	0.94 (0.05)	5.1(0.7)	0.0004	2.2-15.2
5	8	2.72(0.01)	3.8(0.2)	6	3.14(0.01)	3.9(0.3)	0.97 (0.04)	4.8(0.5)	0.0003	2.2-18.0

S. Paripsa, A. Gaur, F. Förste, D.E. Doronkin, W. Malzer, C. Schlesiger, B. Kanngießer, E. Welter, J.-D. Grunwaldt and D.Lützenkirchen-Hecht (2024). J. Synchrotron Rad. 31 1105-1117

Overview - RefXAS

Practical example: http://xafsdb.ddns.net/dataset/details/PID.SAMPLE.PREFIX782d53bc-0b88-4c77-a02a-a9053c0568cd?



Meta data format

Sample Info

Id	Title	Collection code	Physical state	Crystal orient.	Temperature	Pressure	Sample envir...
PID.SAMPLE....	Fe_foil_Fe_K_...		Solid				

Sample

Description: Fe metal foil K

General remarks: Data acquired: 12-05-2020

Sample preparation:

Sample ID:

Instrument

Instrument

Facility	Beamline	Acquisition ...	Crystals	Mirrors	Detectors	Element	Edge	Max k-range
DESY Petra III	P65	XAS CONTIN...	Si 111			Fe	K	16.2

Bibliography

DOI	Owner	Institute	Contact Mail	Reference
	Dmitry Doronkin	KIT	dmitry.doronkin@kit.edu	

Reference

Automated quality check

Scientific metadata*

SOURCE: SYNCHROTRON

MODE: Transmission

RAW:

EDGE STEP (Transmission mode):

VALUE: 2.328
UNIT: a.u.
DOCUMENTATION: Height of the detected edge step.

K-MAX (Maximum usable):

VALUE: 16.2
UNIT: Å⁻¹
DOCUMENTATION: Considered angular wavenumber.

ENERGY RESOLUTION (Point density as calculated from spectral points):

VALUE: 0.7
UNIT: eV
DOCUMENTATION: Energy resolution of the measured spectrum in eV.

EDGE ENERGY:

VALUE: 7112
UNIT: eV

For further explanation, please consult our documentation

Database

Download the file:	File content:
Download this work (ZIP)	Description, metadata (json, yaml, hdf5), data and 4 plots.

Publication

RefXAS – you want to know more?

Abhijeet Gaur

Sebastian Paripsa

Frank Förste

DAPHNE4NFDI

- Florian Maurer
- Daria Gashnikova
- Paolo Dolcet
- Svenja Hoevelmann

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DAPHNE4NFDI…

- Makes DAta from PHoton and Neutron Experiments Findable, Accessible, Interoperable and Reusable

- Engages directly with the user community and links it to IT infrastructure (facilities AND universities)
- Develops user-driven data solutions/infrastructure for the photon and neutron community (use cases)
- Develops new data management and analysis schemes (databases and workflows)
- Deploys metadata capture for re-use with searchable catalogues (whitepaper & public catalogues)
- Develops on-the-fly data analysis and reduction (software)
- Reaches out to scientists and students (dissemination and education)

For more information on our work, please visit our Zenodo community

On behalf of the whole team: Thank you for your attention!

Further interest? Do not miss our Annual Meeting

DAPHNE 4NFDI Annual Meeting 2025

24 – 26 March, Berlin HZB

For more information, please visit the Indico page!

https://events.hifis.net/e/DAPHNE4NFDI_2025