

Integrated XAFS databases for Data-Driven Advances in Material Science

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23th September, 2024



Outline

- Demand on XAFS database
- XAFS database at SPring-8
- Discussions toward Integrated XAFS databases
- **MDR XAFS DB**
- Summary

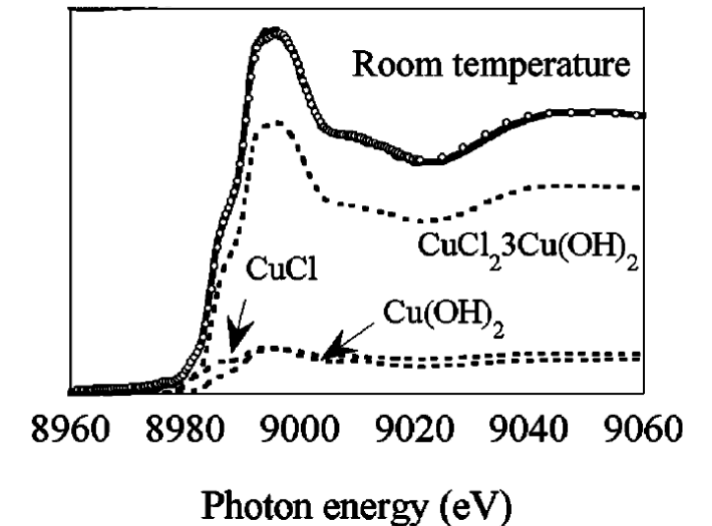
Demand on XAFS database

- XAFS spectral data of standard sample is usually used to analyze unknown target (Fingerprinting , LCF etc.)

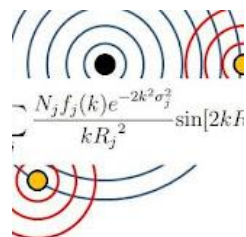
➔ XAFS database reduces the time and cost needed to measure reference sample by yourself

- Data-Driven analysis (AI, Machine Learning) will give us structure directly from the spectral database

X-ray Absorption Fine Structure (XAFS)



[†] M. Takaoka et al., Environ. Sci. Technol. 39, 5878 (2005)



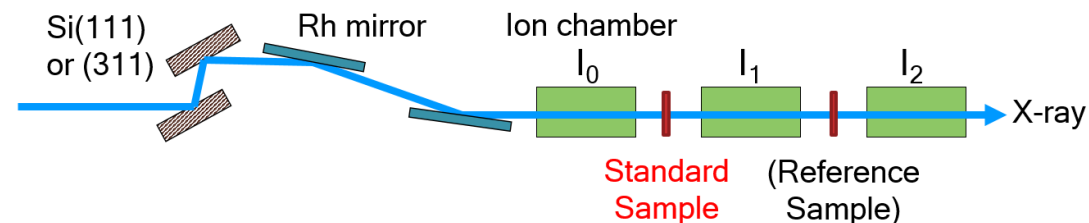
Global XAFS Journal Club on  YouTube

<https://tinyurl.com/XASvideos>

Activities on Data format, Machine learning...

XAFS database at SPring-8

- Measured by JASRI staff at BL14B2
 - Transmission mode
 - Quick scan (Energy: 3~70 keV)
 - Sample: commercial reagents
 - Available for Product info. (lot no. etc.)

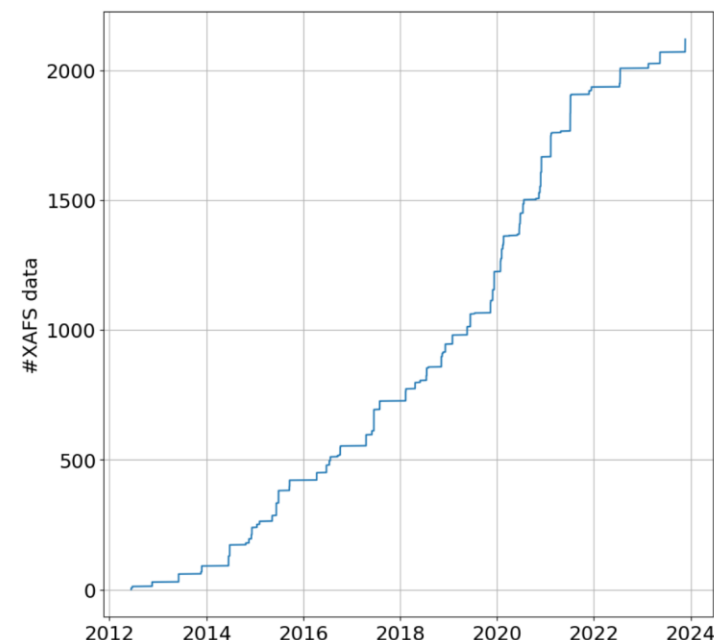


- Database service

- Experimental Data Transfer System, BENTEN
- Largest XAFS dataset among Japan SR facilities
- HAXPES (Hard X-ray Photoelectron Spectroscopy) database for standard samples at BL46XU is also available

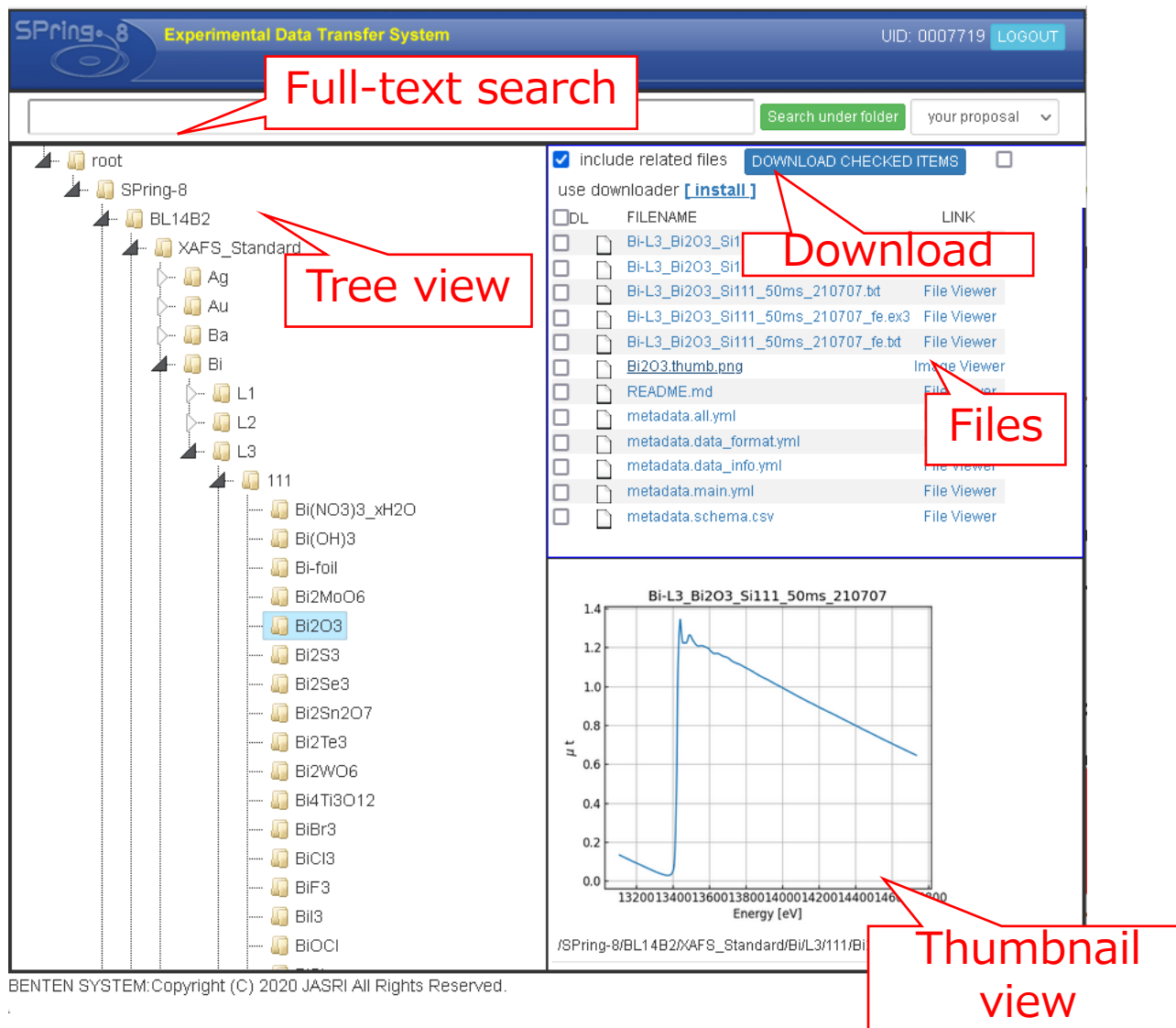
Ref.

- H. Ofuchi et al., Radiation Physics and Chemistry, Vol. 218, 2024, 111581
- <https://support.spring8.or.jp/BL/bl14b2/xafs/standardDB/index-e.html>



Data Access Web portal, BENTEN

<https://benten.spring8.or.jp/>



Full-text search

Tree view

Download

Files

Thumbnail view

BENTEN SYSTEM: Copyright (C) 2020 JASRI All Rights Reserved.

- Authentication
 - E-mail address registration
 - Text data
 - Raw: PF9801
 - Processed: Athena, Rex2000
- + Metadata with YAML

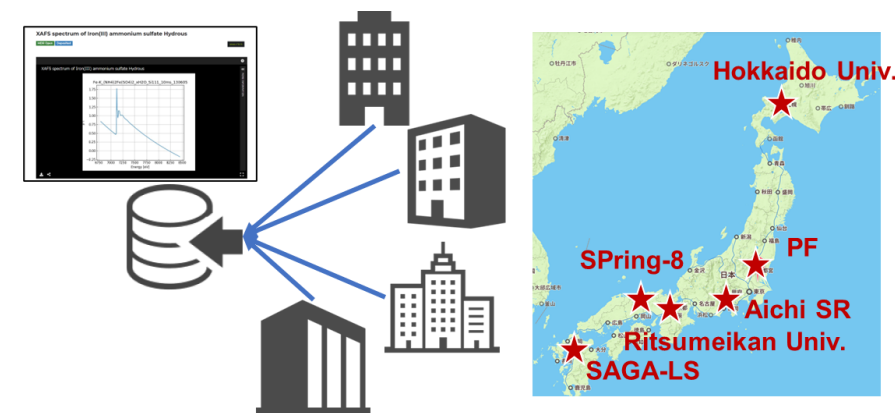
H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	L	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	A															
		L	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
		A	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

... K Edge,
 ... K&L Edge,
 ... L Edge,
 ... unavailable

	Statistics(2024.09)
Element	41
Sample	813
Dataset	2,119

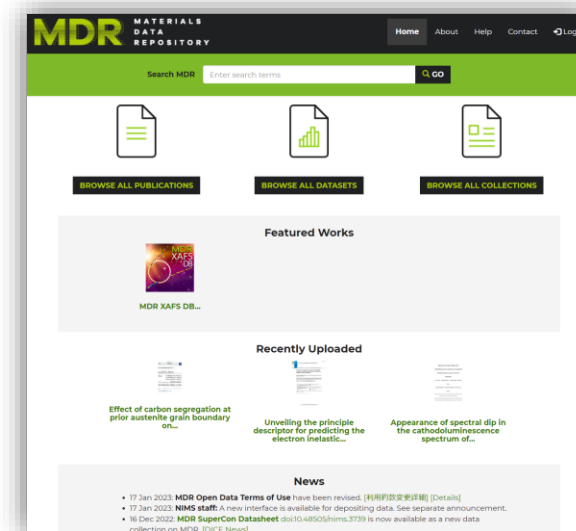
Discussions toward Integrated XAFS databases

- Individual XAFS databases at Japan
 - SPring-8, KEK PF, Ritsumeikan SR, ...
 - **How to establish cross-facility search?**

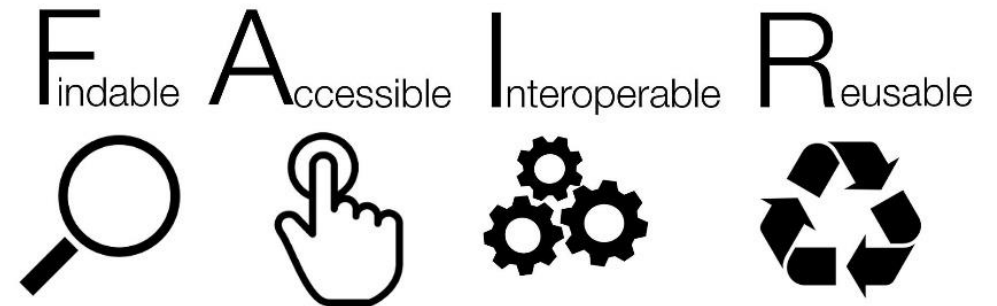


- Discussions in Japanese XAFS Society
 - Use of NIMS MDR (Materials Data Repository)
 - DOI to each dataset, Flexible search, API
 - How to establish data sharing culture ? (incentive)
 - Data registration Process (DOI)
 - Common Metadata format
 - Data License
 - Collaboration with IXAS (International XAS community)
 - etc.

<https://mdr.nims.go.jp/>



- History
- Basic functions
 - Search, Download, API
- Machine readable XAFS metadata
 - Designed for Reusable
- MatVoc Dictionary
- Cross-Search of International XAFS databases



MDR XAFS DB History: From Individual Data to Global stage

- **NIMS-JASRI Joint Research**
 - June 2018 – : Development of Data-sharing platform Integrating material data and experimental repositories for Data utilization
- **XAFS Database Meetings (XAFS DB Workshop etc.)**
 - 1st (Sep. 2018), 2nd(Mar. 2019), ..., 18th (Sep. 2024)
- **XAFS Database project using MDR**
 - K.Asakura et al., Presented at 23rd XAFS Discussion Conference (2020)
- **July 2021: MDR XAFS DB public release**
 - <https://doi.org/10.48505/nims.1447>
 - **Realization of Cross-Facility database**
 - 2022: Ritsumeikan SR, Hokkaido Univ., KEK PF
 - 2023: Aichi SR, SAGA-LS
- **May 2024: Realization of International Cross-Search**
 - Japan-US-Europe XAFS DB portal
 - <https://ixdb.jxafs.org/>

MDR XAFS DB



Integration of XAFS data from 6 institutions*

➔ Seamless cross-search across institutions

	#Spectra	Remarks
SPring-8	1,757	Hard X-ray
KEK PF	136	
Hokkaido Univ.	199	Collection from User
Ritsumeikan SR	75	Soft X-ray
Aichi SR	72	
SAGA-LS	24	
Total	2,263	

#Element = 56, #K edge = 50, #L edge = 24

* Data registration for two new institutions in progress

<https://doi.org/10.48505/nims.1447>

The screenshot shows the MDR XAFS DB website interface. At the top, there is a navigation bar with 'Home', 'About', 'Help', 'Contact', and 'Login'. Below this is a search bar with the text 'Search MDR' and 'Enter search terms'. The main content area is divided into several sections. On the left, there is a 'Limit your search' sidebar with filters for 'Type of work', 'Collection', and 'Keyword'. The 'Collection' filter is set to 'MDR XAFS DB' with 58 results. The 'Keyword' filter is set to 'Cu K-edge' with 58 results. The main content area shows the search results for 'XAFS spectrum of Copper nitride'. It includes a plot of Intensity (arb. units) versus Energy [eV] from 450 to 480 eV. The plot shows a sharp peak at approximately 460 eV and several smaller peaks at higher energies. To the right of the plot is a 'Description/Abstract' section with the text: 'This dataset consists of X-ray absorption fine structure (XAFS) spectra at Cu K-edge of Copper nitride measured at SPring-8 BL14B2, and i...'. Below the abstract is a list of keywords: 'BL14B2, Copper nitride, Cu K-edge, Cu3N, Nitride, and i...'. The interface also includes a 'Filtering by' section at the top right with 'KEYWORD > CU K-EDGE' and 'COLLECTION > MDR XAFS DB'. There are also navigation links for 'Previous', 'Next', and 'Start Over'.

MDR XAFS DB: Homepage



<https://doi.org/10.48505/nims.1447>

The screenshot shows the homepage of the MDR XAFS DB. At the top, there is a search bar with the text "Search MDR" and "Enter search terms". Below the search bar, there is a navigation menu with "Home" selected. The main heading is "MDR XAFS DB" with two buttons: "User Collection" and "MDR Open". A small icon for "MDR XAFS DB" is shown, followed by the text "2168 Items · Created by: ISHII, Masashi · Last Updated: 27/09/2022". A paragraph describes the collection: "This collection of data has been compiled at the National Institute for Materials Science (NIMS) with the cooperation of related organizations for the purpose of wide use of X-ray Absorption Fine Structure (XAFS) spectra." Another paragraph states: "The data published in this collection are publicly known data, and the data providers have guaranteed that the publication of the data does not violate the Copyright Law, the Personal Information Protection Law, or any other laws and regulations by submitting the 'Application for Data Publication in the Materials Data Repository (MDR)'." A list of data providers as of July 2022 is provided: Japan Synchrotron Radiation Research Institute, Ritsumeikan SR Center, Hokkaido University, Institute for Catalysis, and Photon Factory, KEK. A final paragraph explains that the data can be used to determine the electronic state and local structure of materials, and refers to a README for file formats and other details.

Collection Details

Total items	2264
Size	unknown
Resource type	Dataset
Creator	ISHII, Masashi
Contributor	MATSUDA, Asahiko TANABE, Kosuke NAGAO, Hiroko YOSHIKAWA, Hideki
Keyword	spectroscopy x-ray absorption local structure
License	Creative Commons BY-NC-SA Attribution-NonCommercial-ShareAlike 4.0 International
Publisher	National Institute for Materials Science
Date Created	2021-07-21
Language	English
Identifier	https://doi.org/10.48505/nims.1447



Open Access

XAFS Spectral list (2,263 spectra)

MDR MATERIALS DATA REPOSITORY Home About Help Contact Login

Search MDR Enter search terms **GO**

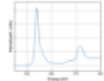
Limit your search

- Type of work **Dataset** 2,264
- Collection **MDR XAFS DB** 2,264
- Keyword
- Publisher
- Resource type
- Visibility
- Rights Statement Sim
- Data origin
- Characterization methods
- Material/Specimen
- Date updated
- Author

Filtering by: **TYPE OF WORK > DATASET** **COLLECTION > MDR XAFS DB** Start Over

« Previous | 1 - 10 of 2,264 | Next » **SORT BY RELEVANCE** 10 PER PAGE

XAFS spectrum of Nickel(II) oxide

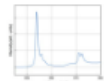


Description/Abstract:

Keyword:

Resource Type:
Data origin:
Date Uploaded:

XAFS spectrum of Nickel(II) oxide

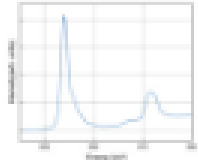


Description/Abstract:

Keyword:

Resource Type:
Data origin:
Date Uploaded:

XAFS spectrum of Nickel(II) oxide

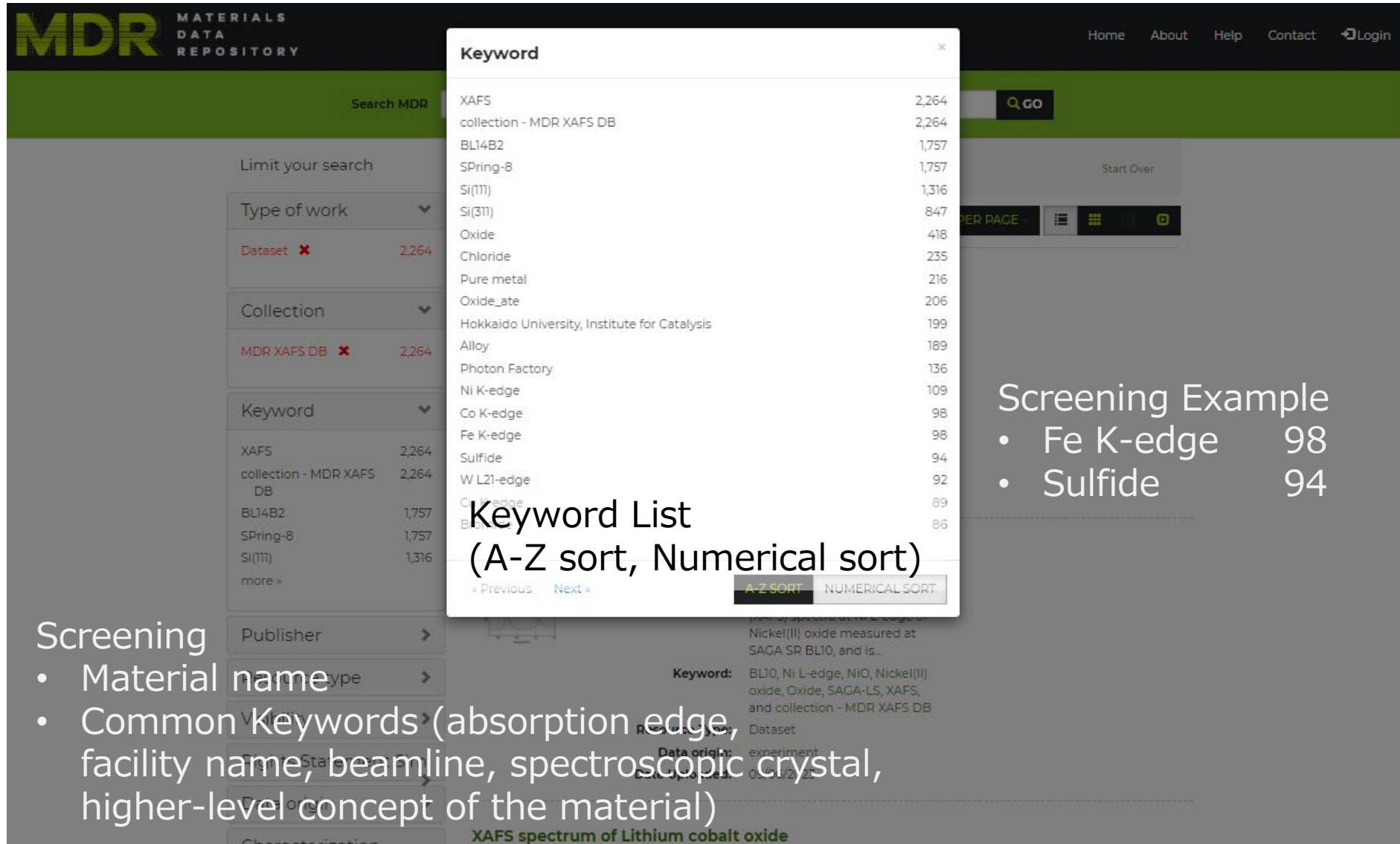


Description/Abstract: This dataset consists of X-ray absorption fine structure (XAFS) spectra at Ni L-edge of Nickel(II) oxide measured at SAGA SR BL12, and is...

Keyword: BL12, Ni L-edge, NiO, Nickel(II) oxide, Oxide, SAGA-LS, XAFS, and collection - MDR XAFS DB

Resource Type: Dataset
Data origin: experiment
Date Uploaded: 09/06/2023

Screening: Rapid access to the target spectra



The screenshot shows the MDR Materials Data Repository website. A search bar at the top right contains the text "Q GO". A "Keyword" dropdown menu is open, displaying a list of keywords and their corresponding counts. The list is sorted by numerical value in descending order. The keywords include XAFS (2,264), collection - MDR XAFS DB (2,264), BL14B2 (1,757), SPring-8 (1,757), Si(111) (1,316), Si(311) (847), Oxide (418), Chloride (235), Pure metal (216), Oxide_ate (206), Hokkaido University, Institute for Catalysis (199), Alloy (189), Photon Factory (136), Ni K-edge (109), Co K-edge (98), Fe K-edge (98), Sulfide (94), W L21-edge (92), and Cl K-edge (89). Below the list are buttons for "A-Z SORT" and "NUMERICAL SORT", with "NUMERICAL SORT" being the active selection. The background shows search filters for "Type of work", "Collection", and "Keyword". The "Keyword" filter is currently set to "XAFS" with a count of 2,264. Other filters include "Dataset" (2,264), "Collection" (MDR_XAFS_DB, 2,264), and "Publisher".

Keyword List (A-Z sort, Numerical sort)

Keyword	Count
XAFS	2,264
collection - MDR XAFS DB	2,264
BL14B2	1,757
SPring-8	1,757
Si(111)	1,316
Si(311)	847
Oxide	418
Chloride	235
Pure metal	216
Oxide_ate	206
Hokkaido University, Institute for Catalysis	199
Alloy	189
Photon Factory	136
Ni K-edge	109
Co K-edge	98
Fe K-edge	98
Sulfide	94
W L21-edge	92
Cl K-edge	89

Screening Example

- Fe K-edge 98
- Sulfide 94

Screening

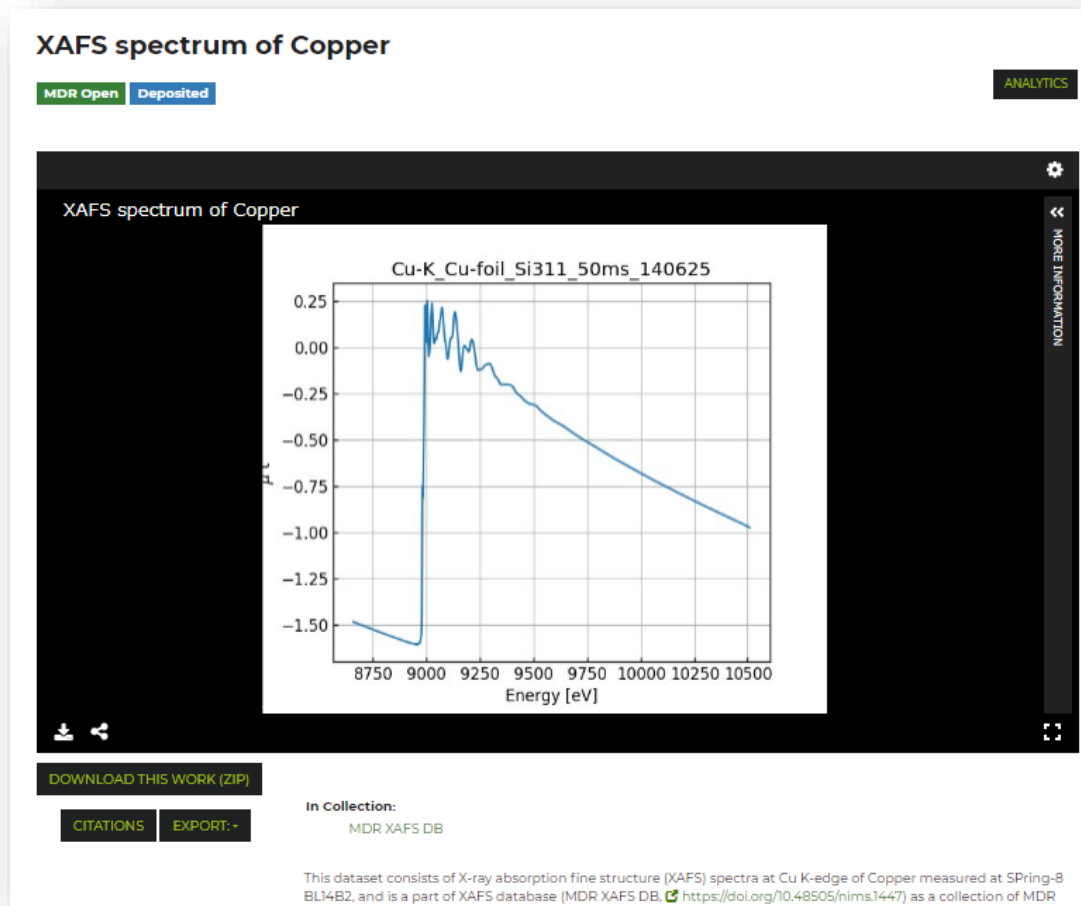
- Material name
- Common Keywords (absorption edge, facility name, beamline, spectroscopic crystal, higher-level concept of the material)

XAFS spectrum of Lithium cobalt oxide

Dataset View, DOI Landing page



Data details with thumbnails



- Assign DOI to all spectral data
- Access spectra from anywhere via DOI

Common Metadata

Description

DOI
<https://doi.org/10.48505/nims.1812>

Creator
Name: Industrial Application and Partnership Division
Role: contact person

Keyword
BL14B2
Copper
Cu K-edge
Cu-foil
Pure metal
SPring-8
Si(311)
XAFS
collection - MDR XAFS DB

Resource type
Dataset

Data origin
experiments

Material/Specimen
Copper

Rights statement
Creative Commons BY-NC-SA Attribution-NonCommercial-ShareAlike 4.0 International

Identifier
Identifier - Persistent: urn:DATA_IDENTIFIER.dpfc.nims.go.jp:916b6019-1076-4fca-a367-06c6996ba9f;
Identifier - Local: RDEtag-67392508

Metadata for SR, XAFS

Preview: primary.tsv

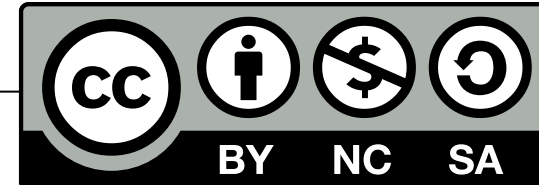
Show 10 entries Search:

key	value
@data_info@identifier@pid	spring8.845c32f7-3915-410e-a830-c5e0cf83758a
@data_info@identifier@proposal_number	201450000
@data_info@identifier@register_name	/SPring-8/BL14B2/XAFS_Standard/Cu/K/311/Cu-foil
@data_info@date@create_time	2020-01-15 19:10:54
@data_info@date@update_time	2021-03-19 17:17:55
@data_info@access_rights	open
@data_info@contact_name@affiliation@organization	JASRI Industrial Application and Partnership Division
@data_info@contact_name@name	organization
@data_info@contact_name@role	JASRI
@data_info@data_depositor@affiliation@organization	JASRI

Showing 1 to 10 of 102 entries

Previous 1 2 3 4 5 ... 11 Next

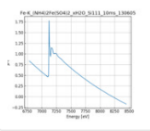




All Data available for download with CC BY-NC-SA



- Credit must be given
- **For non-commercial use only**
- Modification allowed, but must be shared with under the same license

@data_info@contact_name@role organization
@data_info@data_depositor@affiliation@organizationJASRI

Showing 1 to 10 of 102 entries

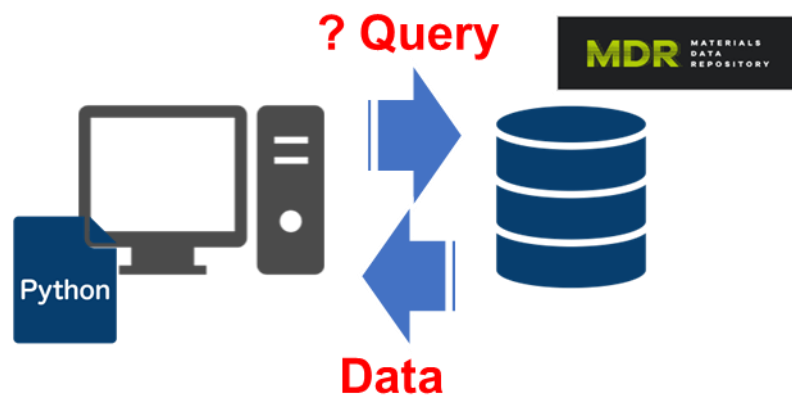
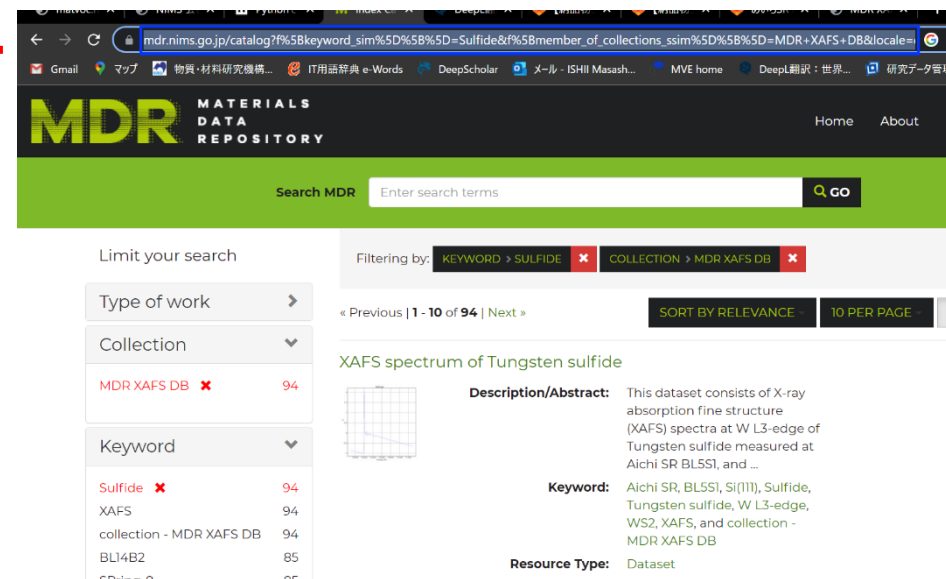
Thumbnail	Title	Date Uploaded	Size	Visibility	Actions
	(NH4)2Fe(SO4)2_xH2O.thumb.png		37.3 KB	MDR Open	SELECT AN ACTION ▾
	Fe-K_(NH4)2Fe(SO4)2_xH2O_Si111_10ms_130605.dat		230 KB	MDR Open	SELECT AN ACTION ▾ Download
	Fe-K_(NH4)2Fe(SO4)2_xH2O_Si111_10ms_130605.ex3		14.4 KB	MDR Open	SELECT AN ACTION ▾
	Fe-K_(NH4)2Fe(SO4)2_xH2O_Si111_10ms_130605.txt		14 KB	MDR Open	SELECT AN ACTION ▾
	metadata.all.json		6.57 KB	MDR Open	SELECT AN ACTION ▾

Under discussion for Update
CC BY-NC-SA → CC BY
Changes needed
as use of SR in industry
are progressing ?

Example of Application with API

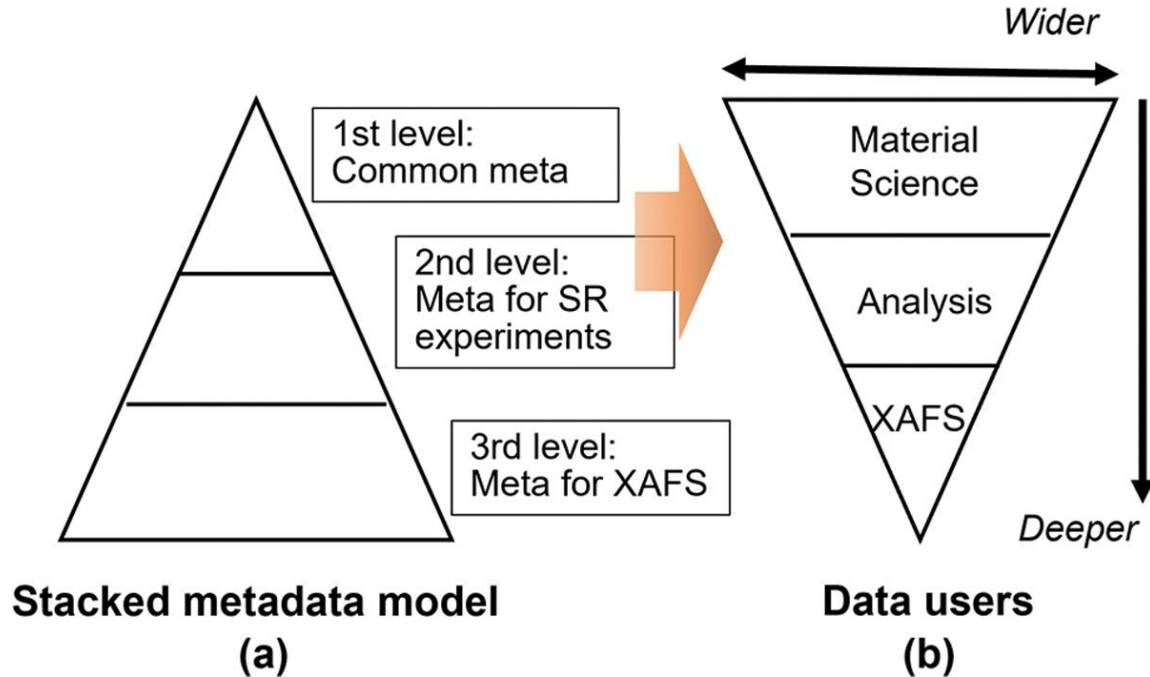
Batch Download GUI for XAFS DB

Seamless connection from GUI → API



- After Screening XAFS data, GUI URL can be used as API query parameter

Metadata initiatives



- Hierarchical structure
- Common Metadata
 - Material dictionary etc.
 - Designed by NIMS MDR
- XAFS metadata
 - Specialized
 - Designed by XAFS community

- 2022-2023: Created common metadata for synchrotron experiments at the Data Structuring Advisory Committee of the Japanese Society of Synchrotron Radiation Research (JSRR)
- Feb. 2023: Published the common XAFS metadata approved by the Japanese XAFS Society
 - Adopted by Aichi SR and SAGA-LS, and published in the MDR XAFS DB

Machine readable XAFS Metadata

```

91 instrument:
92   arrangement: 4WS0//M0//4WS1//DCM//M1//4WS2//M2//4WS3
93   monochromator:
94     name: DCM
95     distance: 14510
96     distance_unit: mm
97     type: DCM
98     scan_mode: Quick XAFS
99   detail:
100     crystal_material: Si
101     crystal_plane: (311)
102     crystal_d: 1.63748
103     crystal_d_unit: Å
104   mirrors:
105     name: M0
106     distance: 12508
107     distance_unit: mm
108     role: collimation
109     type: single
110     coating: Pt
111     shape: bend
112     name: M1
113     distance: 16000
114     distance_unit: mm
115     role: focusing
116     type: single
117     coating: Pt
  
```

YAML Ain't Markup Language

YAML
JSON

Key name	Option	Data type	Description (ja)	Description	Example
@data_info@data_depositor@organization	required	string	データ登録者の組織	organization of data depositor	Kyushu Synchrotron Light Research Center
@data_info@data_depositor@affiliation	optional	string	データ登録者の所属	affiliation of data depositor	Beamline Group
@data_info@data_depositor@name	required	string	データ登録者の名前	name of data depositor	Kyushu Synchrotron Light Research Center
@data_info@data_depositor@role	optional	string	データ登録者の役割	role of data depositor	Beamline staff
@data_info@contact_name@organization	required	string	データ責任者の組織	organization of data depositor	Kyushu Synchrotron Light Research Center
@data_info@contact_name@affiliation	optional	string	データ責任者の所属	affiliation of data depositor	Beamline Group
@data_info@contact_name@name	required	string	データ責任者(所属名でもよい)	contact name (person or affiliation)	Kyushu Synchrotron Light Resea
@data_info@contact_name@role	optional	string	データ責任者の役割	role of data contact name	Beamline staff
@data_info@access_rights	optional	string	アクセス権限	access rights	open
@data_info@license	optional	string	ライセンス	license	
@data_info@deposit_time@create_time	required	date	データ登録の生成日時	create time of data deposite	2017.12
@data_info@deposit_time@update_time	optional	date	データ登録の更新日時	update time of data deposite	2017.12
@data_info@title	required	text	データセットの題名(英語)	title of work (english)	NEXAFS spectrum of h-BN
@data_info@title_ja	optional	text	データセットの題名(日本語)	title of work (japanses)	h-BNのNEXAFSスペクトル

Metadata items > 254 items

Category	#Items
data_info	27
facility	12
files	14
instrument	45
measurement	101
sample	33
reference	22

User input
> 134 items

Metadata Schema Definition

- <https://raw.githubusercontent.com/xafs-db/xafs-schema/main/release/20230203/xafs-schema.json>

- Filled for used items (~100 for SPring-8)
- Only a few are frequently used (Sample name, Absorption edge,...)

Frequently used metadata

➔ **Converted to Dictionary**

Standardization of Chemicals name

- e.g. “Zinc oxide” :
Equivalent expression of following terms
 - *Zinc white*
 - *philosopher's wool*
 - *flowers of zinc*
 - *Chinese white*
 - *calamine*
 - *ZnO*
 - *1314-13-2*

- ID (URI) + Representative name
 - (wd: Q1800, Zinc oxide)
- Search index was implemented



NIMS XAFS DB Project Materials Dictionary > Chemicals > Inorganic materials > Oxide > Zinc oxide

Q1800: Zinc oxide

Vocabulary ID <http://matvoc.nims.go.jp/entity/Q1800>

Language	Label	Description	Alias
English	Zinc oxide	BENTEN-registered chemicals, ZnO	ZnO, Zinc white, Zinc oxide (Zn O), Zinc oxide, philosopher's wool, flowers of zinc, Chinese white, calamine, 1314-13-2
Japanese	酸化亜鉛	BENTEN登録済み化学物質、ZnO	ZnO

Open Access

MatVoc

Semantic Relatives

▼ Parents

- ▶ [Q735: Oxide](#)

DICE Links

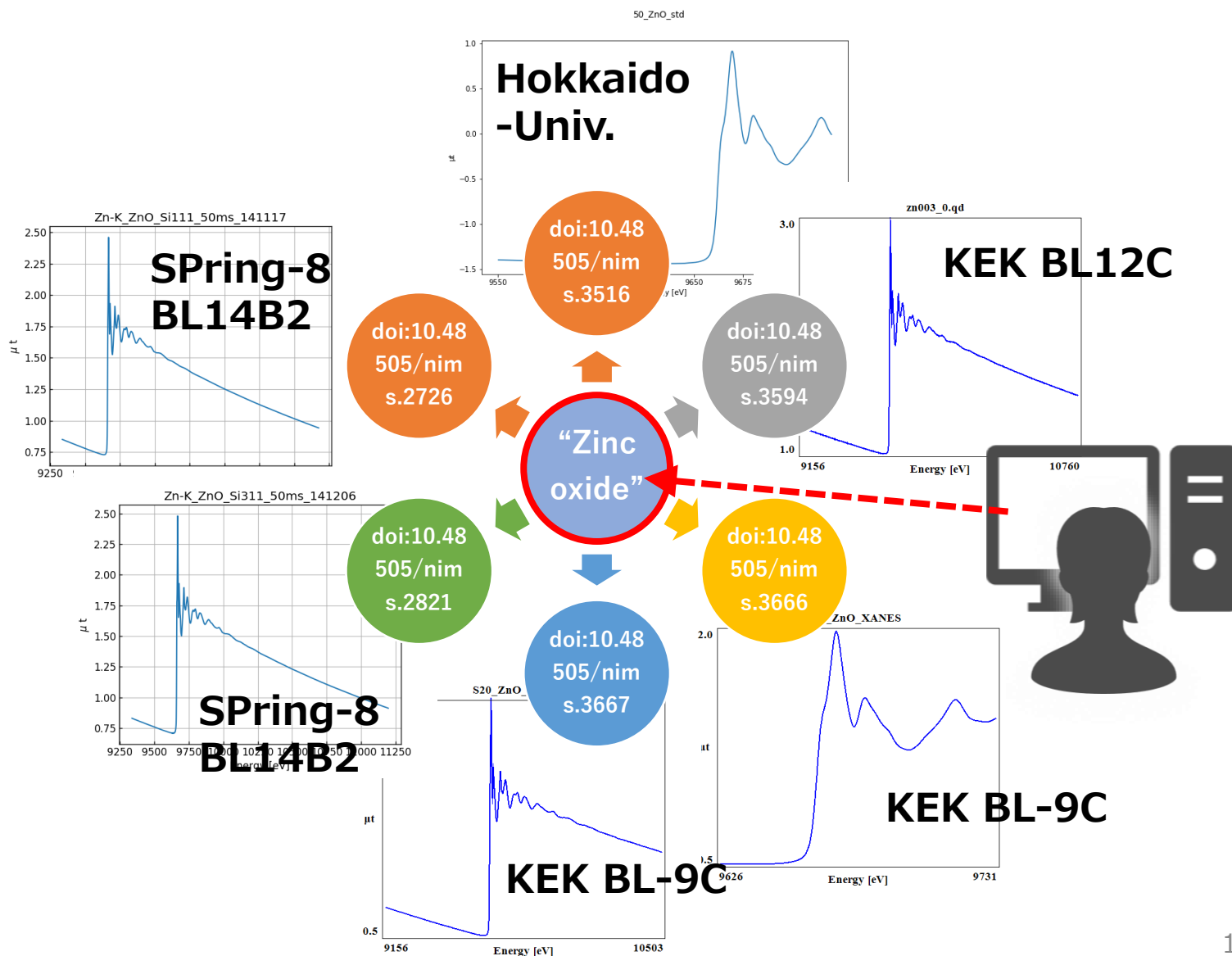
[AtomWork Zn+O](#) , [MDR Zinc+oxide](#)

<https://matvoc.nims.go.jp/explore/en/results/Q713>

Metadata : Key+Value

- Key management → Reproducibility, Reliability (Academic)
- **Value management → Cross-search (Machine understandable)**

Cross-search example in MDR XAFS DB



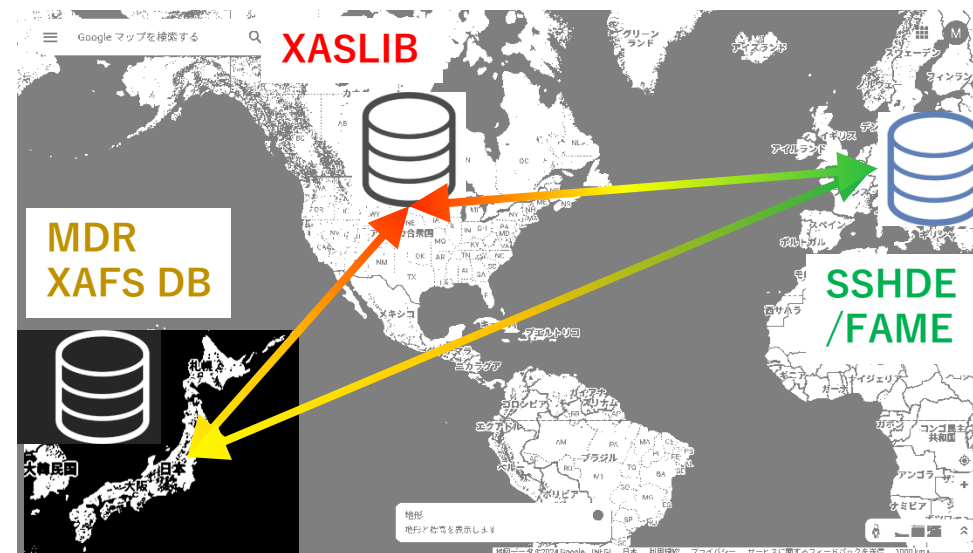
International Dictionary sharing

Expansion of
XAFS Materials Vocabulary,
MatVoc (value management)

➔ **Cross-search of
Japan-US-Europe
XAFS databases**

International Cross-Search (May 2024)

Category	Value
Number of Items	1,481
Item Names (Japanese/English)	2,958
Synonyms (Japanese/English)	9,103
Chemical Formulas	748
Chemical Substance Classification	4 Levels



Target Databases

Japan : MDR XAFS DB 2,263 spectra
US : XASLIB 277 spectra
EU: SSHADE/FAME 516 spectra

* LISA XAS Database 48 spectra
added on 13th Sep. 2024

International XAFS DB Portal, IXDB



① Top page

e.g. Search for material name with
“銅”(Copper)

Search International DBs in Japanese !

International XAFS DB Portal

Absorption edge search

Absorption element :

Edge :

Search

Material name search

Material name containing:

(Chemical formula, customary name, etc.)

Search

<https://ixdb.jxafs.org/>

② Display a list of **Material names**

containing “銅”

Note. **Material names** ≠ **Sample names**

International XAFS DB Portal

Material name containing: 銅

[Q1426 : Copper](#)
[Q1412 : Copper acetate](#)
[Q2319 : Copper bis\(2,2,6,6-tetramethyl-3,5-heptanedionate\)](#)
[Q1393 : Copper chromite](#)
[Q1409 : Copper fluoride](#)
[Q1428 : Copper molybdate](#)
[Q889 : Copper nickel](#)
[Q1413 : Copper nitrate, hydrous](#)
[Q1417 : Copper nitride](#)
[Q1410 : Copper phthalocyanine](#)
[Q1433 : Copper tungstate](#)
[Q1851 : Copper\(I\) chloride, anhydrous](#)
[Q3840 : Copper\(I\) electrolyte solution](#)
[Q1427 : Copper\(I\) iodide, anhydrous](#)
[Q1415 : Copper\(I\) oxide](#)
[Q3679 : Copper\(I\) selenide](#)
[Q1416 : Copper\(I\) sulfide](#)
[Q3668 : Copper\(II\) Sulfide](#)
[Q1411 : Copper\(II\) acetylacetonate](#)
[Q1418 : Copper\(II\) bromide, anhydrous](#)
[Q1422 : Copper\(II\) carbonate](#)
[Q1421 : Copper\(II\) chloride, anhydrous](#)
[Q1420 : Copper\(II\) chloride, hydrous](#)

MatVoc Explorer
Materials Vocabulary

Select Dictionaries Loose Search

Showing 1 result:

NIMS XAFS DB Project Materials Dictionary > Chemicals > Inorganic materials > Pure metal > Copper

Q1426: Copper

Vocabulary ID <http://matvoc.nims.go.jp/entity/Q1426>

Language	Label	Description	Alias
English	Copper	BENTEN-registered chemicals, Cu-foil	Cu-foil, Copper, 7440-50-8
Japanese	銅	BENTEN登録済み化学物質、Cu箔	Cu箔

Semantic Relatives

International XAFS DB Portal, IXDB



③ Select

“Q1426 : Copper”

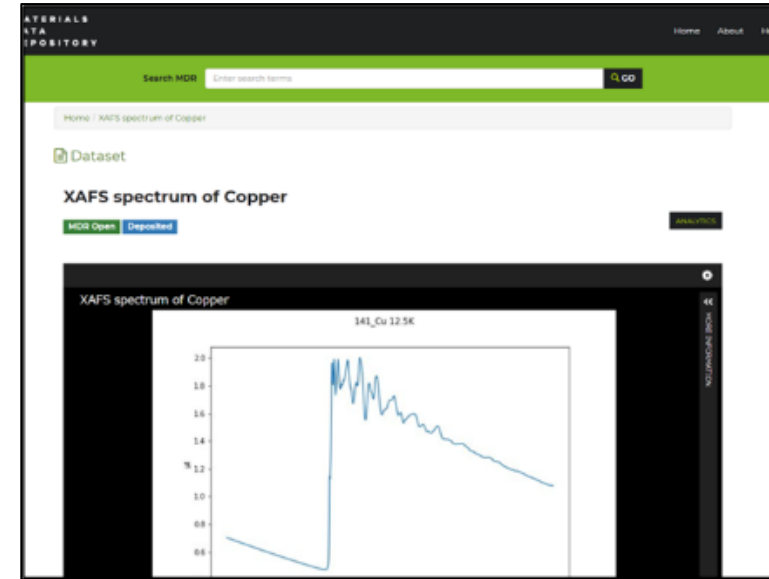
Display a list of links to spectra

International XAFS DB portal

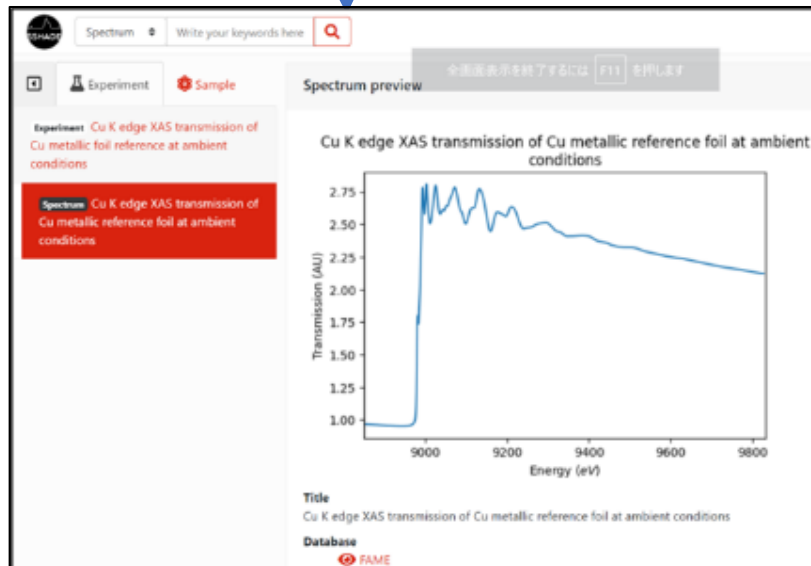
Links for Copper

- <https://mdr.nims.go.jp/concern/datasets/w3763b36m> (Aichi Synchrotron Radiation)
- <https://mdr.nims.go.jp/concern/datasets/hm50tv733> (Hokkaido University)
- <https://xaslib.xrayabsorption.org/spectrum/275/> (IXAS)
- <https://xaslib.xrayabsorption.org/spectrum/89/> (IXAS)
- <https://xaslib.xrayabsorption.org/spectrum/91/> (IXAS)
- <https://xaslib.xrayabsorption.org/spectrum/92/> (IXAS)
- <https://mdr.nims.go.jp/concern/datasets/4f053k50s> (KEK)
- <https://mdr.nims.go.jp/concern/datasets/6t02m512> (KEK)
- <https://mdr.nims.go.jp/concern/datasets/70795b6j> (KEK)
- <https://mdr.nims.go.jp/concern/datasets/8f06g579t> (KEK)
- <https://mdr.nims.go.jp/concern/datasets/gm80hz547> (KEK)
- <https://mdr.nims.go.jp/concern/datasets/kk91fp694> (KEK)
- <https://mdr.nims.go.jp/concern/datasets/th83m2688> (KEK)
- <https://mdr.nims.go.jp/concern/datasets/vh53x0039> (KEK)
- <https://mdr.nims.go.jp/concern/datasets/zk51vm676> (KEK)
- <https://mdr.nims.go.jp/concern/datasets/2227ms449> (Spring-8)
- <https://mdr.nims.go.jp/concern/datasets/2z10ws744> (Spring-8)
- https://www.sshade.eu/data/spectrum/SPECTRUM_OP_20180117_002 (SSHADE/FAME)
- https://www.sshade.eu/data/spectrum/SPECTRUM_OP_20230216_001 (SSHADE/FAME)
- https://www.sshade.eu/data/spectrum/SPECTRUM_OP_20230216_001C (SSHADE/FAME)

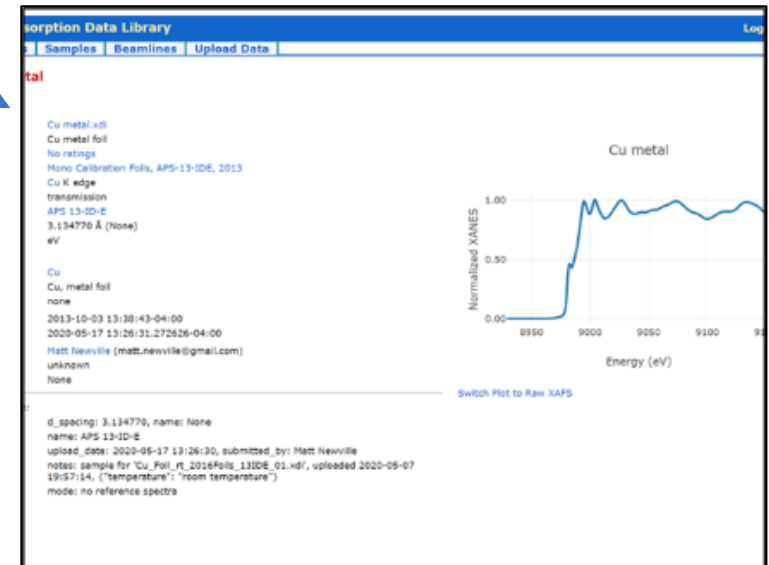
Related HAXPES



Japan:
MDR
XAFS DB



France:
SSHADE/
FAME



US:
XASLIB

Principle of IXDB

<https://ixdb.jxafs.org/>



Fluctuations in search terms (Material names),
such as chemical formulas,
Japanese/English names and aliases

→ ① Convert to QID (Material ID)



NIMS Material Vocabulary
Management Infrastructure

“銅”、“Cu”...

Q1426

③ To each DB

IXDB portal



Q1426

URL
Facility



XASLIB (277spectra)

<https://xaslib.xrayabsorption.org/elem/>



SSHADE/FAME (516spectra)

<https://www.sshade.eu/db/fame>



MDR XAFS DB
(2,263 spectra)

<https://doi.org/10.48505/nims.1447>

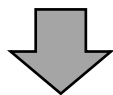


Metadata converted into knowledge
in graph database (RDF)

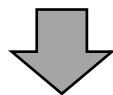
→ ② Integrated search using QID

From Vocabulary Unification to Knowledge Unification

Various repository data,
international databases



Unified representation of knowledge

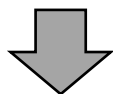


Even if the data sources are different, if it's XAFS,
they can be placed under the same framework

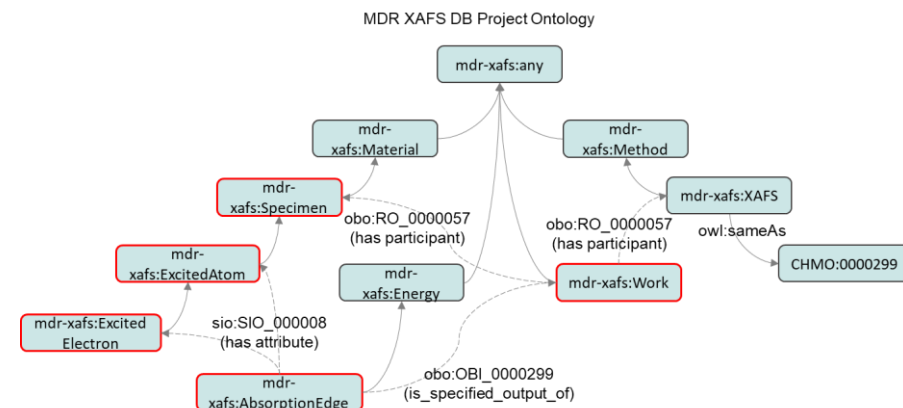
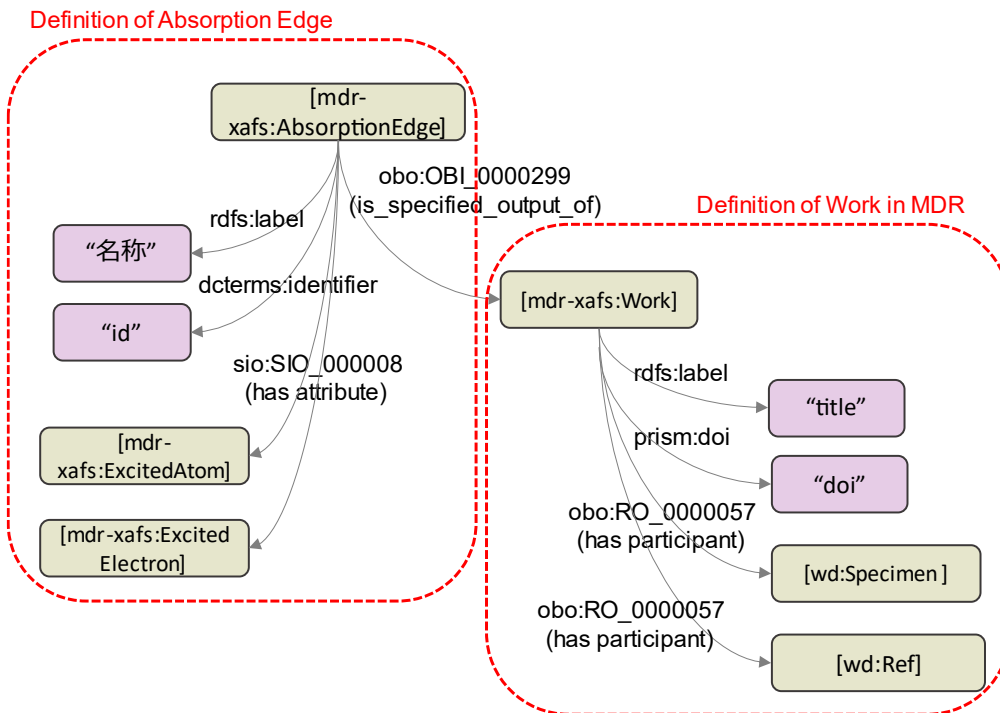
Ontology concept

Application:

Cross-search for synchrotron radiation data
(inner-shell knowledge integration)



Cross-search for XAFS + HAXPES (implemented)



Summary



- **Achieved Integrated XAFS databases of Japan**
 - SPring-8, KEK PF, Hokkaido Univ., Ritsumeikan SR, Aichi-SR, SAGA-LS
 - NIMS MDR for FAIR-based & Data-driven utilization
- **Metadata initiatives**
 - Common metadata format, proposed by Japanese XAFS Society*
 - * Need to collaborate with XDI, NXxas (NeXus) for future standardization
 - Value management in MatVoc → flexible cross-search
- **International XAFS DB portal** <https://ixdb.jxafs.org/>
 - Achieved cross-searching of Japan, US, Europe XAFS databases
 - #Spectra = 3,104, #Element = 62 (Li-U), #Absorption edge = 116
 - Expansion of MatVoc + Ontology for Knowledge unification
 - Cross-search of XAFS-HAXPES was also implemented

**Welcome
Everyone's
Participations!**