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Funded Project

CDIF-4-XAS: Describing X-Ray Spectroscopy Data for Cross-Domain Use

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Implemented by

Science and Technology Facilities Council
PSDI PHYSICAL SCIENCES DATA INFRASTRUCTURE
CARDIFF UNIVERSITY
PRIFYSGOL CAERDYDD
CatalysisHub
COMMITTEE ON DATA CODATA INTERNATIONAL SCIENCE COUNCIL
DAPHNE 4NFDI
HZB Helmholtz Zentrum Berlin
HMC

Funded by the European Union

CHALLENGE ADDRESSED

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Large Scale Facilities

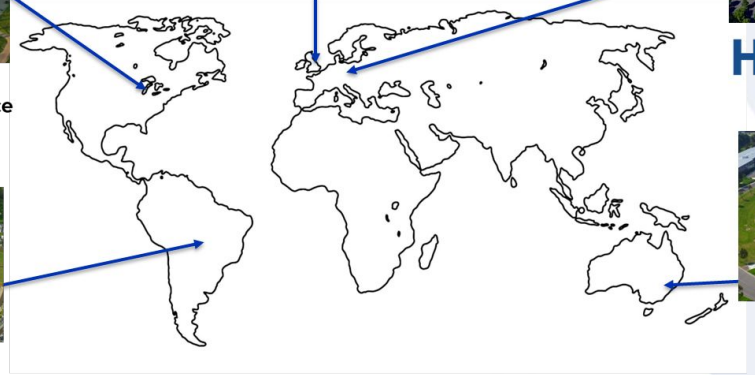
Argonne NATIONAL LABORATORY | Advanced Photon Source
Chicago, U.S.A

diamond
Harwell, UK

HZB BESSY II Light Source
Berlin, Germany

LNLS
Campinas, Brazil.

ANSTO
Clayton, Australia.



Large quantities of XAS data
Custom data collection software

XAS Laboratory Equipment

Commercial

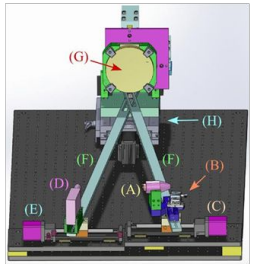
easyXAFS

hpspectroscopy

SIGRAY

Custom made

University of Sheffield
STX - Scanning Transmission XAS user facility

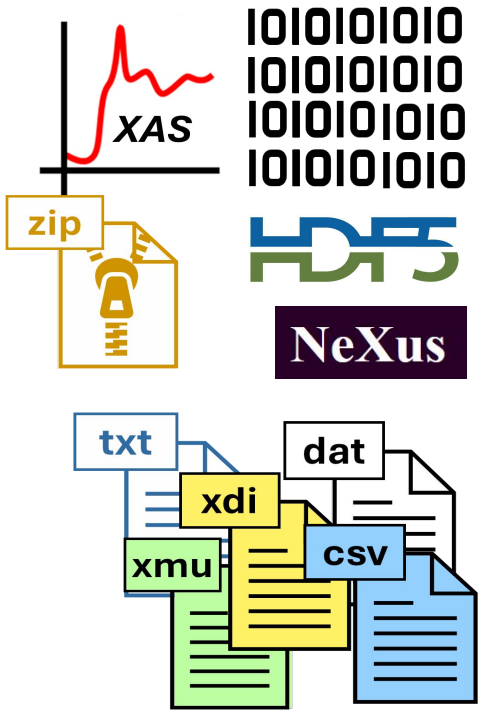


Munich Institute of Biomedical Engineering
Munich Compact Light Source (MuCLS)

XAS data in custom formats

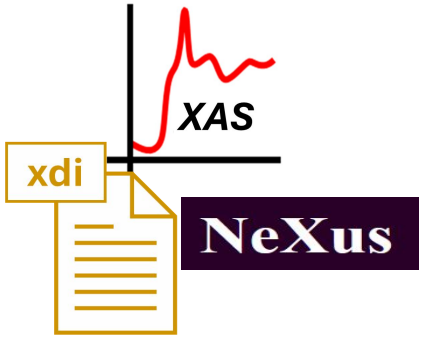
- Improving the transfer, interoperability and reusability of X-ray spectroscopy data and metadata.
- Enabling new science through combining X-ray spectroscopy data at scale across infrastructures.

CHALLENGE ADDRESSED



- Goal: Support cross-domain interoperability of X-ray Absorption Spectroscopy (XAS) data.
- Problem: Diverse formats and tools for storing XAS data and metadata, making the data difficult to integrate or interoperate.
- Solution: CDIF-4-XAS profile to enable consuming and producing standardized XAS data.
- Demonstration: Implementation in Galaxy.

SOLUTION



- XAS domain survey: identify XAS Community standards.
- Mapping: create a common mapping framework to integrate data using different standards
- Innovation: mapping of binary (non-text) data (CDIF mostly used on text data formats).
- Implementation Plan: create Galaxy tools

- We have published two deliverables for phases one and two in Zenodo: https://zenodo.org/communities/cdif-4-xas/records
- Overview of X-Ray Absorption Spectroscopy standards, vocabularies (and ontologies), data formats and practices (DOI: 10.5281/zenodo.14920226)
- CDIF-4-XAS: Mappings from Community Standards to CDIF (DOI: 10.5281/zenodo.17421917)

RESULTS

Publish CDIF-4-XAS tools in Galaxy instances:

- https://materialsgalaxy.stfc.ac.uk/
- https://usegalaxy.eu/

Support adoption:

- Create tutorials and training materials.
- Examples with data, and packaged research objects.

Promotion:

- Shared with the research community trough publications and demonstrations at workshops and conferences.

TEAM

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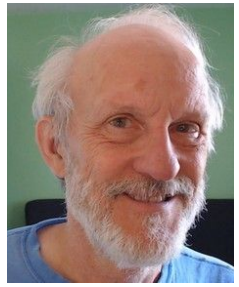
Slava Tykhonov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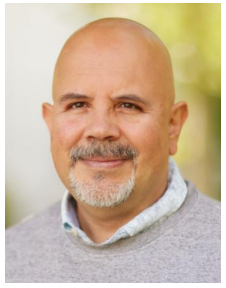
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