Contribution ID: **91**   Type: **TALK**

Towards Standardizing Catalysis and Beamline experiments at HZB

Monday 4 November 2024 10:30 (20 minutes)

Advanced catalysts are key to sustainable energy, reducing emissions, and improving resource efficiency. However, the synthesis of novel catalysts usually involves a unique blend of scientific methods, precise catalyst formulations, and the empirical knowledge of scientists. Additionally, the wide variety of techniques performed at different beamlines in synchrotron radiation facilities, along with continuously changing sample environments, produces highly heterogeneous data.

In this work we present the efforts to develop a common (meta)data schema that combines existing international community-driven standards in order to integrate and make such heterogeneous data FAIR (Findable, Accessible, Interoperable, and Reusable) at HZB catalysis labs and BESSY II.

This common schema for managing catalysis and beamline (meta)data is built with LinkML, an internationally adopted framework for building data models that are both human-readable and machine-actionable, particularly useful in linked data and semantic web technologies. We use voc4cat –a SKOS vocabulary for catalysis emerged from NFDI4Cat –and NeXus –a common data exchange format for X-ray, neutron, and muon experiment, being developed as an international standard –to enhance and standardize data related to catalysis experiments and beamline operations. Our ultimate goal is aiming for data that is consistently formatted and integrated across different sources and systems. To ensure consistency and interoperability, we test the schema by integrating it with electronic laboratory notebook (ELN) workflows using NOMAD, an open-source data management platform developed by FAIRmat.

This effort intrinsically supports the data management milestones of the ROCK-IT (Remote, Operando Controlled, Knowledge-driven, and IT-based) project, funded by the Helmholtz Association, which exemplifies the practical application of FAIR principles at BESSY II and demonstrates how state-of-the-art IT can significantly enhance control and insights with a focus on catalysis experiments.

Please specify "other"

In addition, please add 3 to 5 keywords.

Catalysis, NeXus, LinkML

Please specify "other"

For whom will your contribution be of most interest?

Scientists and technicians who maintain and operate research infrastructure for data generation

Please assign yourself (presenting author) to one of the following groups.

Primary author: VELAZQUEZ SANCHEZ, Ana (HZB)

Co-author: PATEL, Sonal Ramesh (HZB)

Presenters: VELAZQUEZ SANCHEZ, Ana (HZB); PATEL, Sonal Ramesh (HZB)

Session Classification: Session A1

Track Classification: Connecting research data: 4. Metadata annotation and management