CATALYSIS RDM – FROM ONTOLOGIES TO ELECTRONIC LAB NOTEBOOKS

Prepared For:
ACM/IEEE JOINT CONFERENCE ON DIGITAL LIBRARIES
Catalysis research is interdisciplinary, data are generated in several sub-steps and, thanks to new tools, in large quantities. Considering the wide variety of potential data types in catalysis, research data management is an important part of moving catalysis research into a digital future.

Currently, data management in catalysis is mostly organized at the working group level or, at most, at the institute level and is based on local conventions. As a result, much of the data remains unused.

NFDI4Cat has created this 90-minute workshop to help you understand the importance of Research Data Management (RDM), present some key tech skills in catalysis research, and and show you ways to start shaping the future of RDM.
PROGRAMME

RDM in Catalysis Research (20 min)
Given the wide variety of potential data types in catalysis, research data management is an important component of moving catalysis research into a digital future. This session will provide an overview of the current state of the art in catalysis and conclude with some recent developments and best practices from NFDI4Cat.

Discussion (10 min)

Catalysis & Ontologies (15 min)
Why are ontologies so important? This session provides an introduction to ontologies and introduces the workflow and tools developed by NFDI4Cat to achieve the best results.

Discussion (5 min)

Hands-On Ontologies (15 min)
In this practice-oriented module, we will present a real-world example from the field of catalysis illustrating the application or development of ontologies.

How do I choose the right ELN? (20 min)
There is no one-size-fits-all solution when it comes to electronic lab notebooks (ELN). Nevertheless, we would like to take this opportunity to give you some tips on key parameters and determining factors that you should consider when selecting an ELN.

Discussion (5 min)
OUR SPEAKERS

M. Sc. Michael Liebau
Leipzig University
PhD student for "Research Data Management"

Prof. Norbert Kockmann
TU Dortmund University
Leader of the Task area "Ontology Development and Metadata Standards"

M. Sc. Alexander Behr
TU Dortmund University
PhD student for "Ontology Development and Metadata Standards"

Dr. Mark Greiner
Max Planck Institute for Chemical Energy Conversion
Leader of the Task area "Data Analysis, Quality Management and Re-Use"
We are a community-driven and user-centred initiative working to secure the digital future of catalysis and catalysis-related sciences.

NFDI4Cat consists of 16 experienced project partners from all areas of catalysis and the disciplines of reaction and process engineering. The catalysis and engineering competences are complemented by expertise in the fields of data science, high-performance computing and machine learning.

NFDI4Cat is here to help you improve your research through:
» Findable, Accessible, Interoperable and Reusable (FAIR) data,
» better data quality, and
» improved data management supporting Open Science.

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