NFDI for Catalysis-Related Sciences

B-1 Progress Report Part 1, <u>for Publication</u>

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General Information

Catalysis-related sciences are pivotal for efficient production across diverse industries. The NFDI4Cat consortium is dedicated to forging a robust research data infrastructure for catalysis-related sciences, spanning from molecular studies to large-scale production reactors. The consortium serves as a bridge between natural and engineering sciences, aligning with the DFG subject classification system, particularly review boards 321-324 and 403-406. Emphasis is placed on engineering sciences, especially Chemical and Thermal

Process Engineering (403-01) and Technical Chemistry (403-02), due to their critical role in catalytic processes.

NFDI4Cat's commitments encompass:

- Introducing standardised processes and support services.
- Developing specialised vocabulary.
- Fostering connections within the NFDI4Cat community and with international communities and other NFDIs.
- Enhancing digital and Research Data Management (RDM) skills.
- Establishing open, well-defined data structures and interdisciplinary metadata standards.
- Facilitating data collaboration among catalysis researchers.
- Providing software and tools for a distributed and hierarchical repository structure based on FAIR data principles.
- Connecting the repository network to national, European, and global research data services.

The NFDI4Cat team comprises 16 expert partners spanning catalysis and data science, high-performance computing, and machine learning. To enhance its structure, NFDI4Cat has introduced an Industry Advisory Board with a twofold mission: validating the relevance and impact of its deliverables for industrial members while strengthening ties with the industrial sector.

Important Links for NFDI4Cat's Outputs

Name	Description	Link
Website	Collection of news, events, and newsletters related to catalysis and its advancements	https://nfdi4cat.org/en/
Github	Public collection of tools and outputs	https://github.com/nfdi4cat
Zenodo	Collection of publications, presentations, posters, software, etc.	https://zenodo.org/communities/nfdi4cat/search?page=1&size=20
NFDI4Cat Meta Portal	Future access point to all digital resources	https://meta4cat.fokus.fraunhofer.de/
Ontology collection	Repository which lists several Ontologies relevant for Catalysis research.	https://github.com/nfdi4cat/Ontology-Overview-of-NFDI4Cat
Vocabulary guidelines for	A blueprint towards suggesting, adding, and editing content to the	https://zenodo.org/record/7669183

Name	Description	Link
NFDI4Cat	vocabularies developed throughout NFDI4Cat.	
Voc4Cat	A SKOS vocabulary for catalysis maintained by NFDI4Cat & friends	[nfdi4cat/voc4cat: A SKOS vocabulary for catalysis maintained by NFDI4Cat & friends (github.com)](#)
Data management plans & retention periods	The integration of open science into a digital economy, while considering legal European regulations, is a balancing act. Here research data management plans play a key role and have the potential to combine the interests of researchers as data producers and the public as data users in publicly funded projects.	https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/chem.202202720

Summary

Catalysis-related sciences, an intricate and interdisciplinary field, is pivotal for efficient production across various industries, addressing challenges like sustainable energy and climate change. However, data management in catalysis is fragmented, often localised to institutions or specific working groups. This fragmentation is exacerbated by the diversity within catalysis, encompassing heterogeneous, homogeneous, bio-, electro-, photocatalysis, reaction-, and process engineering. Recognizing the need for a unified approach, the NFDI4Cat consortium was established under the National Research Data Infrastructure (NFDI) initiative in October 2020. The consortium focuses on implementing FAIR principles—Findable, Accessible, Interoperable, and Reusable—in catalysis research data management. NFDI4Cat's mission is to lead the transition from the current state to **digital catalysis research** to generate the highest possible added value from catalysis research.

The consortium's vision is clear: **A connected community that leverages digital technologies and artificial intelligence for sustainable production of chemicals and energy carriers.** Over the past three years, NFDI4Cat has diligently worked on four foundational cornerstones, achieving notable successes that promise to have a transformative impact on the field of catalysis research:

Lifelong Availability of Catalysis Research Data
One of the foundational pillars of this vision is the creation of a shared and comprehensible knowledge base, guaranteeing enduring access to catalysis research data. The establishment

of the **NFDI4Cat Central Repository** is a significant step in this direction. At the same time, the **NFDI4Cat Meta Portal** is being developed as a beacon for metadata access. The introduction of **LARAsuite** and the establishment of **CarMeN** and **Adacta**, open source RDM systems under active development, aim to embody FAIR principles and streamline metadata collection.

Unified Data Exchange and Knowledge Structuring

In its pursuit of seamless communication and enhanced machine readability, NFDI4Cat has prioritised the development of common vocabularies, ontologies, and persistent identifiers. The introduction of the first version of the **Vocabulary Guidelines**, in tandem with a tool designed for crafting and managing SKOS-vocabularies using Excel and GitHub, sets a standard. **NFDI4Cat's ontology collection**, a repository highlighting key ontologies pertinent to Catalysis research, equips researchers with a unified linguistic platform and guidance in ontology selection. Additionally, the initiation of a prototype Persistent Identifier server, rooted in handle.net, has bolstered data findability and traceability capabilities.

Empowering the Catalysis Community

NFDI4Cat acknowledges the critical role of effective RDM for the catalysis community. To empower this community, the consortium initiated the development of the **RDM School of Catalysis**, specifically designed for emerging scientists. This ongoing initiative, enriched by forthcoming **educational videos** and **programming courses**, seeks to address the existing RDM knowledge void in the catalysis curriculum. To further inspire and motivate the community, the **Data Chemist Award** is being introduced in partnership with Chemistry Europe, aiming to recognize and celebrate exceptional work in the domain. Through these endeavours, NFDI4Cat aims to equip the community with the necessary training, tools, and awareness, ensuring that the consortium's work reaches its full potential impact.

Promoting Research Excellence and Collaboration

NFDI4Cat's commitment to research excellence was further exemplified by its focus on fostering industry collaboration while safeguarding intellectual property. The consortium developed a comprehensive **RDM plan** in line with the EU's guiding principle of '*as open as possible, as closed as necessary*.' To harmonise open science and digital economy, NFDI4Cat has implemented **retention periods** to fairly address the concerns of all parties involved.[1] In

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[1] Salazar, Abel, et al. "How Research Data Management Plans Can Help in Harmonizing Open Science and Approaches in the Digital Economy." Chemistry–A European Journal 29.9 (2023): e202202720.

the upcoming second half of the funding period, NFDI4Cat will focus on community accepted reward models.

NFDI4Cat is geared towards fostering research-oriented development, **ensuring that the research data management prerequisites of diverse specialist communities are met and made accessible to researchers on a national and international scale**. The mission, as delineated in the white paper [The Digitalization of Catalysis-related Sciences](#)[2], is to address the distinct needs of these catalysis communities. With permanent members actively engaged in the field, NFDI4Cat ensures that emerging community needs are continually integrated into its core activities. **NFDI4Cat has made significant strides in advancing digital research in catalysis related sciences branded as "digital catalysis" - from establishing robust data repositories to fostering educational initiatives**. While the consortium has achieved numerous milestones through collaborations, innovation, and a focus on community needs, challenges in interoperability, community acceptance, and technological adaptability remain. The multifaceted nature of catalysis demands ongoing refinement of data management tools. Moreover, ensuring tool functionality and user-friendliness is vital. As digital technologies evolve, NFDI4Cat must adapt to remain at the digital catalysis research vanguard. Collaborative integrations across projects and institutions, and outreach to the broader academic community, are areas requiring continued focus. NFDI4Cat is committed to addressing these challenges, aiming to benefit not just the catalysis community but the broader academic landscape.

Composition of the Consortium

Applicant institution

Applicant institution	Location	Duration
DECHEMA e.V.	Theodor-Heuss-Allee 25, 60486 Frankfurt	10/20 - 10/25

Co-applicant institutions

Co-applicant institutions	Location	Duration
Leibniz-Institut für Katalyse e.V. (LIKAT)	Albert-Einstein-Str. 29, 18059 Rostock	10/20 - 10/25

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[2] German Catalysis Society (GeCatS), March 2019

Co-applicant institutions	Location	Duration
Max-Planck-Institut für Dynamik komplexer technischer Systeme (MPI-DCTS)	Sandtorstraße 1, 39106 Magdeburg	10/20 - 10/25
Universität Greifswald (UHGW)	Institut für Biochemie, Felix-Hausdorff-Str. 4, 17487 Greifswald	10/20 - 10/25
Karlsruher Institut für Technologie (KIT)	Kaiserstraße 12, 76131 Karlsruhe	10/20 - 10/25
Universität Leipzig (UL)	Institut für Technische Chemie, Linnéstraße 3, 04103 Leipzig	10/20 - 10/25
Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)	Egerlandstr. 3, 91058 Erlangen	10/20 - 10/25
Technische Universität Dortmund (TUDO)	Fakultät für Bio - und Chemieingenieurwesen, Emil-Figge-Str. 68, 44227 Dortmund	10/20 - 10/25
Universität Rostock (UHRO)	Institut für Chemie, Albert-Einstein-Str. 3a, 18059 Rostock	10/20 - 10/25
Technische Universität Berlin (TUB)	Technische Universität Berlin, Insitut für Chemie, Sek. EW-K-01 (BasCat), Hardenbergstr. 36, 10623 Berlin	10/20 - 10/25
Technische Universität München (TUM)	Department Chemie, Lichtenbergstr. 4, 85748 Garching	10/20 - 10/25
Max-Planck-Institut für Chemische Energiekonversion (MPI-CEC)	Stiftstraße 34-36, 45470 Mülheim an der Ruhr	10/20 - 10/25
Technische Universität Braunschweig (TUBS)	Institut für Technische Chemie, Franz-Listz-Str. 35a, 38106 Braunschweig	10/20 - 10/25
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Co-applicant institutions	Location	Duration
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Applicant institution	Institution	Duration	ORCID
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Dr. Andreas Förster	DECHEMA e.V.	07/21 - 10/25	-

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