Letter of intent

For the renewal application of NFDI4Cat

This document is a letter of intent, required as advance notification for renewal proposals in 2024, with which NFDI4Cat officials inform the DFG of our plan to submit a full renewal proposal.

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Formal details

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NFDI for Catalysis-Related Sciences

Acronym of the consortium

NFDI4Cat

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Objectives, work programme and research environment in the second funding period

Research area of the proposed consortium

Catalysis-related sciences are pivotal for the efficient production of a plethora of base and fine chemicals across diverse industries. NFDI4Cat is dedicated to forging a robust research data infrastructure for catalysis-related sciences through a comprehensive value chain from molecular studies to large-scale production reactors and entire plants. As catalysis-related research, the consortium aims to serve as a bridge between natural and engineering sciences, aligning with the DFG subject classification system, particularly review boards 321-324 (Natural Sciences) and 403-406 (Engineering Sciences). In this second phase of the NFDI4Cat project (NFDI4Cat 2.0), there will be a stronger emphasis on engineering sciences, particularly in areas that are critical to catalytic processes and their industrial applications.

While the primary focus of NFDI4Cat remains on catalysis and related engineering sciences, the consortium recognizes the importance of adapting to emerging research needs. Therefore, efforts will be made to:

- Incorporate New Disciplines: As catalysis research evolves, new scientific disciplines may become relevant. The consortium will remain flexible and inclusive, integrating new research areas as needed.
- Industry Collaboration: Strengthen partnerships with industry stakeholders to ensure the research data infrastructure meets practical needs and accelerates the translation of research into industrial applications.

Concise summary of the consortium's main objectives and task areas

NFDI4Cat 2.0 aims to shape the field of digital catalysis-related sciences by establishing a comprehensive and sustainable Research Data Infrastructure (RDI) covering the entire data value chain from molecular studies to large-scale production reactors. NFDI4Cat 2.0 will ensure that the RDI adheres to the FAIR principles (Findable, Accessible, Interoperable, Reusable). Additionally, NFDI4Cat 2.0 seeks to advance scientific discovery through a comprehensive Research Data Management (RDM). To achieve this, NFDI4Cat 2.0 will consolidate and enhance existing services and tools, providing stable and user-friendly digital tools, interfaces and services, that facilitate each step of the research data lifecycle. This initiative will ensure data integrity, security, and quality.

A crucial new aspect of NFDI4Cat 2.0 is the creation of data spaces[12] focused on highly relevant topics. These topics (use cases) will be identified through joint discussions with the community and the industry advisory board to ensure their relevance and impact. Through these efforts, NFDI4Cat 2.0 seeks to drive a transformative shift in how research data is managed in catalysis and related fields, promoting more efficient and innovative scientific discoveries and collaborations. Through focusing our efforts on use cases from highly relevant and actual areas, the second phase of NFDI4Cat aims to enhance the acceptance and adoption of standardized RDM processes among catalysis-related research and user communities.

NFDI4Cat 2.0 envisions a transformative advancement in research data management within catalysis and related fields, fostering more efficient and innovative scientific discoveries and collaborations on both national and international levels. The project will be underpinned by comprehensive educational initiatives and continuous training programs aimed at equipping both the next generation and current researchers with the skills needed to utilize the data infrastructure, tools, and services. The primary objectives of NFDI4Cat 2.0 include:

1. **Services and Tools:** NFDI4Cat 2.0 is committed to consolidate, expand, and refine its portfolio of user-friendly RDM tools and services. These enhancements aim to meet both general and specific needs within the catalysis research community and are strategically designed to support the entire lifecycle of research data, from data creation to preservation, improving both usability and integration across multiple platforms. NFDI4Cat 2.0 is committed to continuously broaden the range of available tools, also with respect to up-to-date developments in the field.
2. **Ontologies and Knowledge Graphs**: Developing robust ontologies and knowledge graphs, linking diverse data sets is crucial for the consortium. These efforts will enhance data interoperability and provide the foundation for a flexible, secure platform for data management. These developments will also help to find and close research gaps.
3. **Collaboration and Integration:** Promoting collaboration and integration within the research community and NFDI is a core focus of NFDI4Cat 2.0. Key tasks include collaboration with the different sections of NFDI, Base4NFDI and other consortia to enhance interoperability and resource sharing.
4. **Community Engagement and Involvement:** NFDI4Cat 2.0 will foster stronger partnerships with the community and industry stakeholders, to ensure that the RDI meets

[12] Otto, Boris; ten Hompel, Michael; Wrobel, Stefan (2022). "Designing Data Spaces - The Ecosystem Approach to Competitive Advantage" (PDF). Springer. ISBN 978-3-030-93974-8.

practical needs and accelerates the translation of research into industrial applications. Additionally, the project will remain flexible and inclusive by integrating new scientific disciplines, as the catalysis domain evolves, ensuring the infrastructure remains relevant and up-to-date with emerging research needs. NFDI4Cat 2.0 will also be in close contact with existing collaborative research centers, such as the Collaborative Research Center 1441 “TrackAct - Tracking the Active Site in Heterogeneous Catalysis for Emission Control” at KIT.

5. **Sustainable Organizational Model:** NFDI4Cat 2.0 will develop and implement a sustainable organizational model that supports long-term viability, participatory processes, and efficient use of human resources. This model will support ongoing developments and adoption of RDM practices within the consortium and beyond. Our model includes strategic plans for the operation of services, securing sustainable funding, and nurturing innovation. These strategies are crucial for providing a strong foundation for user-oriented development and advancing the field of catalysis.
6. **Access Rights, Confidentiality, and Integrity:** The creation of a unified framework for data protection will enhance the sovereignty, integrity, security, and quality of research data. This initiative will align with national and international data governance standards to maximize the reusability of research data.

The project structure of NFDI4Cat 2.0 encompasses seven Task Areas (TAs), each playing a crucial role in advancing our mission. Figure 1 illustrates this structure. Project Coordination (TA1) is depicted as an encompassing background layer, signifying its integral role in overseeing all project steps. The white rectangle in the centre represents TAs responsible for technical tasks (TA2-TA5), including the creation and development of data spaces, infrastructure, tools, and services. TA6 and TA7 focus on integrating new communities and enhancing user-oriented services, aiming for agile responses to community needs. Arrows between work packages indicate the flow of information, highlighting communication and interaction between TAs.

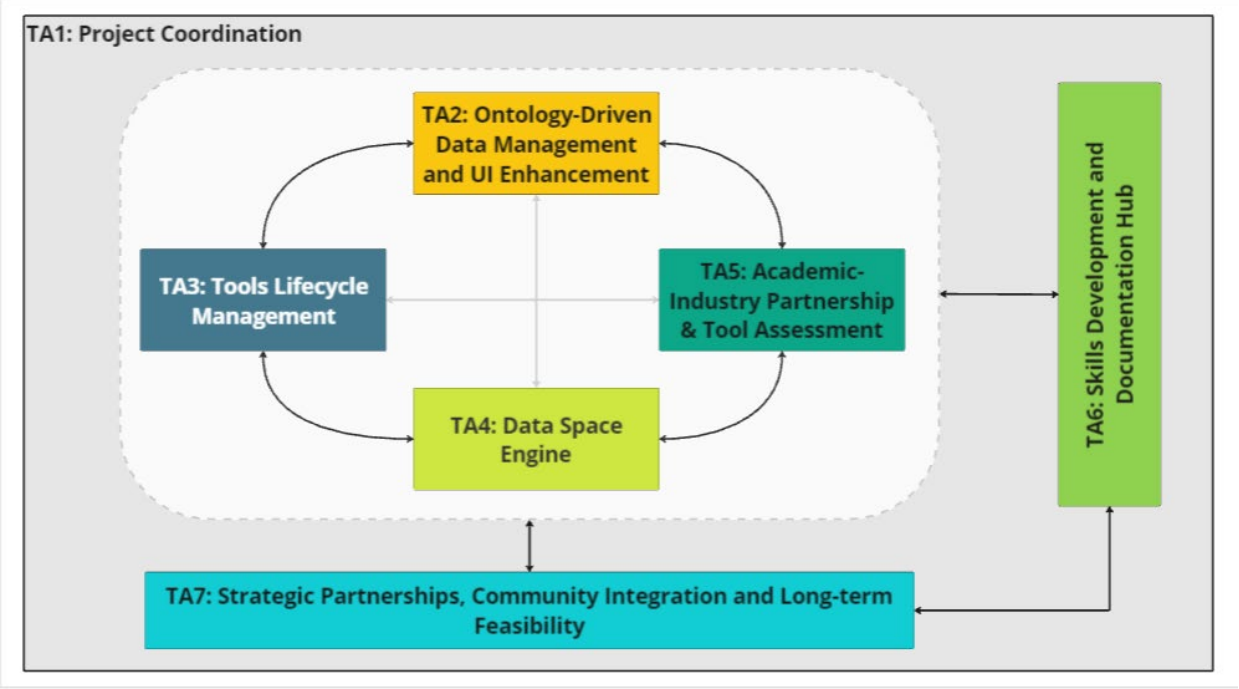

Figure 1: Schematic representation of NFDI4Cat 2.0 project structure, comprising seven Task Areas (TAs). The white elongated rectangle in the center represents the TA handling technical tasks. Arrows between work packages indicate the flow of information, emphasizing communication and interaction between TAs.

Brief description of the proposed use of existing infrastructures, tools and services that are essential to fulfil the objectives of the proposed consortium

One primary objective of NFDI4Cat 2.0 is to establish a comprehensive data space. This involves extending and better integrating all components developed in the first phase and creating data spaces within the community, guided by the selected use cases.

NFDI4Cat 2.0 builds on the idea of a research data commons, encompassing the federated infrastructure, tools and services developed and piloted in the first phase. This includes the 4Cat Meta Portal as a general access point for all digital resources including other repositories (e.g., Zenodo), the 4Cat Repository, and a Data Lake (currently under development) as common solutions for data storage, all operated on our 4Cat Cluster. This also spans all 4Cat Local Pilots, encompassing local Electronic Lab Notebooks (ELNs) and Laboratory Information Management Systems (LIMS), that have been put forward by different partner institutions in the first phase. The backbone of the overall infrastructure will be formed by a semantic layer. It builds on the vocabularies and ontologies developed in the first phase, providing a knowledge graph as a resource as well as tools and services for the community.

In the second phase, data spaces for catalysis-related sciences are envisioned, which will form the basis for collaboration between research institutions but also between research and industry.

It will build on existing standards to ensure interoperability, especially on national and European level. The 4Cat Data Spaces will provide the 4Cat Cockpit, a user-friendly digital tool designed to serve as a central access point. This cockpit will enable users to easily navigate and access all the data, infrastructures, tools, and services offered within the 4Cat Data Spaces. Different local and central components will be provided, considering the needs of the individual partners. Besides the components described in the last paragraphs, this will also include quality assessment services, which enable the evaluation of data and metadata, and AI methods and tools, which allow for the processing and analysis of data and metadata. Both were already piloted in the first phase and are planned to be more tailored to the domain-specific requirements of the community.

NFDI4Cat 2.0 will also ensure that the core services put forward within the Base4NFDI framework will be picked up and are being smoothly integrated in the 4Cat overall infrastructure. This especially holds for the IAM4NFDI service to ensure a fine-grained identity and access management, which is of ample importance for the community. This also includes the PID4NFDI service that enables a flexible persistent identifier management, also below the level of data sets. Further tools will also be integrated, where reasonable, also considering the infrastructures provided by other consortia, including NFDI4Chem, NFDI4Ing, FAIRmat and DAPHNE4NFDI.

Interfaces to other NFDI consortia: brief description of existing agreements for collaboration and/or plans for future collaboration

NFDI4Cat 2.0 is designed to integrate with and complement the efforts of other consortia within the NFDI framework and Base4NFDI. Our primary cooperation focus areas include tool and service development, community outreach, and the design of ontologies. NFDI4Cat 2.0 is committed to fostering collaboration across these domains and establishing structured interfaces with other consortia. NFDI4Cat have demonstrated successful collaboration and exchange with several consortia in the first phase, such as NFDI4Chem, NFDI4Ing, FAIRmat, NFDI-MatWerk, DAPHNE4NFDI, and NFDI4DataScience. These partnerships will be further developed and deepened in the next phase, ensuring robust and effective partnerships that drive innovation and progress.

To ensure a seamless integration and cooperation, NFDI4Cat 2.0 plans to involve key personnel from our partner projects as liaison officers. These individuals, including, for example, Annette Trunschke of FAIRmat will act as bridges, facilitating a continuous and efficient exchange of

information and resources. Their roles are crucial in maintaining clear communication channels and aligning project goals across consortia.

Additionally, NFDI4Cat will allocate personnel from co-applicant institutions to the NFDI Sections and to Base4NFDI. This strategy not only promotes information exchange but also enhances the interoperability of tools and services developed. This structured involvement ensures that all consortia benefit from shared knowledge and technological advancements, thus driving forward the collective mission of the NFDI network.

Through these concerted efforts, NFDI4Cat 2.0 aims to build robust, productive relationships with other consortia, leveraging collective strengths to advance the field of catalysis research within the NFDI framework.

International and national networking

Members of NFDI4Cat work closely with the German Catalysis Society (GeCats), Young GeCats, NachwuchsReaktionsTechnik (NaWuReT), and other catalysis-related organizations, fostering robust national cooperation. Moreover, the consortium was established with a clear vision to extend its reach beyond Germany, engaging in international collaborations to enhance the impact and effectiveness of its activity from the beginning. To achieve NFDI4Cat 2.0 goals, the consortium will enhance cooperative relationships with leading research institutions and initiatives worldwide. Notable international partners from the first phase include:

- IFPEN (France)
- NCCR Catalysis (Switzerland)
- Pacific Northwest National Laboratory (PNNL, USA)
- Allotrope Foundation, LLC (Washington, DC, USA)
- Hokkaido University (Japan)
- UK CatalysisHub (United Kingdom)
- Academy of Sciences of the Czech Republic (Czech Republic)
- Thematic Digital Competence Centre for Natural & Engineering Sciences (Netherlands)

One of the most successful examples of our international cooperation is the collaboration with the Thematic Digital Competence Centre for Natural & Engineering Sciences in the Netherlands. Together, we organized a workshop that brought together about 50 scientists from both countries. Over the course of two days, several new collaborations were initiated, particularly in the area of training and education. These efforts will pave the way for ongoing and future collaborative

workshops and exchanges aimed at concretizing and expanding our cooperative initiatives during NFDI4Cat 2.0.

Our commitment to aligning with international efforts is exemplified by our active engagement with the EOSC. NFDI4Cat's Mark Doerr is a member of the EOSC Technical and Semantic Interoperability Task Force, ensuring that our activities are in sync with broader European initiatives. This alignment allows us to contribute to and benefit from a unified European research data infrastructure, promoting interoperability and data sharing across borders.

Scientific exchange on RDM is a critical component of our strategy. We actively plan and finance various measures through the project, ensuring that our researchers can collaborate and learn from their international peers. These exchanges are crucial for fostering innovation and ensuring that our research remains relevant and impactful.