

NFDI for Catalysis-Related Sciences NFDI4Cat

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Catalysis is an interdisciplinary scientific technology field of strategic importance for the economy and the society as a whole. It is one of the most important core technologies for solving pressing challenges concerning climate change, supply of sustainable energy and supply of sustainable materials at the same time. Concrete examples of such pressing issues are the reduction or complete avoidance of CO₂ emissions, the valorization of plastic waste and CO₂ in chemical production, sustainable hydrogen generation, fuel cell technology, or feeding more than 7 billion people sustainably on this planet – they all require break-through advances in catalysis science and technology. To solve these pressing issues, a fundamental change is required in catalysis research, chemical engineering and process technology. A key challenge is to bring together the different disciplines in catalysis science and technology with the essential support of data scientists and mathematicians. The consortium aims to redefine catalysis research in the digital age and add new facets of digital empowerment. Core challenge is a fundamentally improved understanding in catalysis sciences, the creation of workflows in catalysis that build a bridge between theory/simulation and experimental studies in design, characterization and kinetics of catalysts and the related engineering aspects.

Key objectives that are considered essential for the success of the consortium have been identified:

Catalysis community-related

- a) Enable and support cross-disciplinary research in fundamental and applied catalysis to realise the vision from molecule to process
- b) Improve digital and RDM skills in community, consolidating and uniting existing efforts
- c) Establish, foster, and incentivise use of open well-defined data structures and metadata standards designed for interdisciplinary use
- d) Facilitate collaboration on data level (across institutional boundaries)
- e) Provide education and training in applied research data management and data science for catalysis in chemistry and chemical engineering

Technical

- a) Provide software to establish a distributed and hierarchical repository structure for experimental and theoretical data based on FAIR principles that balances privacy/confidentiality and open data sharing
- b) Connect this repository network to NFDI- as well as European- and world-wide services (e.g. ORCID, DOI, OpenAIRE)
- c) Provide a platform that allows seamless transition between private/local data, group/project/NFDI data and finally published data.
- d) Provide tools/software that help check the data quality (e.g. consistency and reproducibility)
- e) Objectives with respect to NFDI / special role of NFDI4Cat in NFDI
- f) Represent a stakeholder that can show case cross-NFDI consortia success due the strongly interdisciplinary and multi-scale nature of NFDI4Cat

As shown in figure 1, the continuous exchange of data and knowledge with other consortia is a major aim of NFDI4Cat. To enable this ambitious project NFDI4Cat signed the Berlin declaration in 2019 and the Berlin-Leipzig declaration in 2020. Furthermore, the future plan is to interact and connect the work and achievements with other initiatives to support also emerging consortia.

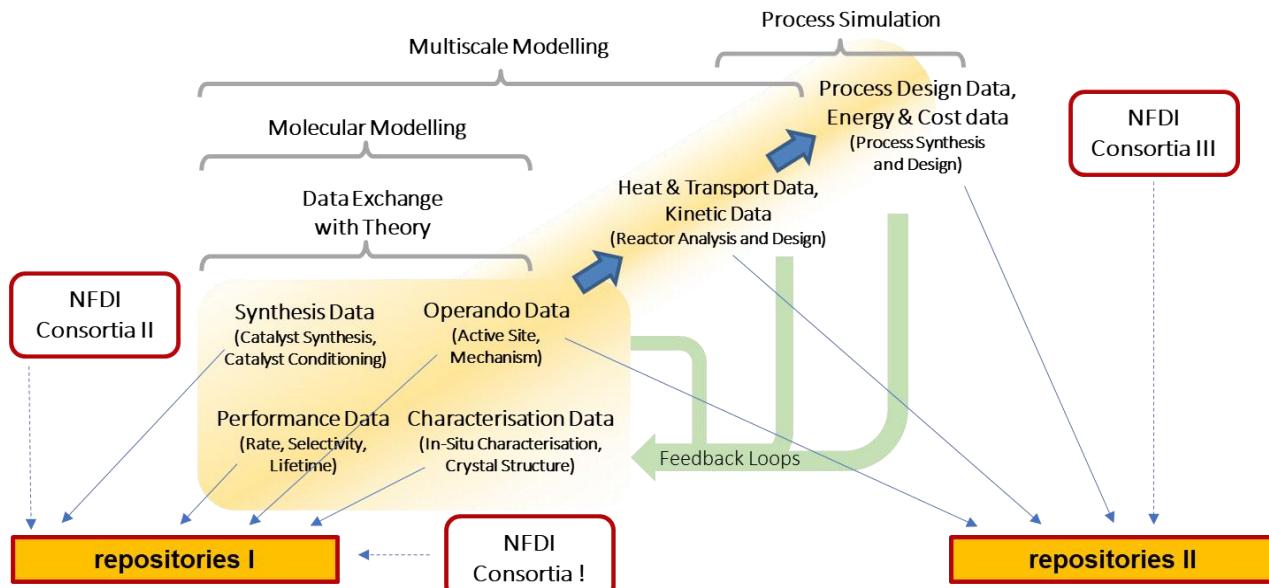


Figure 1. Digital Value Chain with Data from Catalysis Disciplines.

Current and planned collaborations include NFDI initiatives which focus on more general aspects of material science, chemistry and engineering. The chemical physics of surfaces of materials, chemical reactions at surfaces, and multi-scale modelling of heterogeneous catalysis will be explored in collaboration with FAIRmat. Together with NFDI4Chem, the digital approaches towards the digital representation of the chemistry of molecular compounds as well as standards, formats of analytical data and cross-cutting topics like ontologies, metadata formats will be discussed. Furthermore, the application of electronic laboratory notebooks (ELN) and the cross-linking of data repositories will be important intersections for NFDI4Chem and NFDI4Cat.

NFDI4Cat and NFDI4Chem share common interests in the following topics that will be addressed: in cooperation in the development of ontologies, meta-data formats and the cross-linking of data repositories. While NFDI4Chem focuses more on fundamental aspects in chemistry NFDI4Cat also covers the areas of technical chemistry and chemical engineering sciences.

Engineering aspects of catalysis, equipment characterisation and multiscale modelling will be approached within NFDI4Cat in close dialogue with NFDI4Ing. NFDI4Cat and NFDI4Ing will cooperate in the field of ontology development and metadata formats in order to harmonize the efforts in neighboring fields.

NFDI4Cat addresses all fundamental and applied aspects with its associated fields of technical chemistry and chemical engineering and enables and supports cross-disciplinary research to realise the vision from molecule to process. Special emphasis is placed on the cross-disciplinary nature of catalysis linking homogeneous, heterogeneous and bio-catalysis, building upon the chemical physics of surfaces of materials and chemical reactions at surfaces, a focus of FAIRmat.

NFDI4Cat and DAPHNE share common interests in characterization data on catalysts and therefore will develop joined schemes for connecting them to the functionality of materials.

DAPHNE focuses on data at large scale facilities which are of tremendous importance for operando and tomographic characterization of catalysts. IP-sensitive data are also relevant in DAPHNE and joint discussion will transfer experience from NFDI4Cat to DAPHNE. Joint workshops with the goal of establishing common examples, policies, best practice and guides for metadata catalogues, data repositories are planned.

Building strong connections with respect to the catalysis-related aspects of these consortia will further increase the success of NFDI4Cat. TIB as institutional library for science and technology can act as mediator for several planned initiatives in the area of chemistry related sciences. Together with other consortia like NFDI4Chem, a harmonization between the initiatives will be pursued; mutual learning through exchange will be fostered. In addition, the TIB within the consortia NFDI4Chem and FAIRmat is regarded as an important discussion partner for ontology engineering, vocabulary development and conceptual development for association of metadata in suitable formats.

By participating in the 2nd NFDI Conference, the consortium expects a higher visibility in the scientific community and, as a result, even closer thematic relationships with the consortia already recommended for funding, but also with those in the preparatory phase.

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