# NFDI-MatWerk

## Submission of Letter of Intent for Renewal Proposal in 2025

**Deutsche Forschungsgemeinschaft**
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## 1 Binding letter of intent as advance notification of a full renewal proposal

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|---|---|
| ☒ | Binding letter of intent (required as advance notification for renewal proposals in 2025) |

## 2 Formal details

- Name of the consortium

  **DE:** Nationale Forschungsdateninfrastruktur für Materialwissenschaft & Werkstofftechnik

  **EN:** National Research Data Infrastructure for Materials Science & Engineering

- Acronym of the consortium

  NFDI-MatWerk

- Applicant institution

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- Spokesperson

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*Highlighted in **bold** print: changes in the composition of the consortium compared to the progress report:*

- Co-applicant institutions (in alphabetical order)

  **Bundesanstalt für Materialforschung und -prüfung (new, formerly Participant)**
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- Participant institutions (in alphabetical order)

Deutsche Gesellschaft für Materialkunde e.V.

Deutscher Verband für Materialforschung und -prüfung e.V.

Gesellschaft für Angewandte Mathematik und Mechanik (GAMM)

Helmholtz-Zentrum hereon GmbH

**Hochschule Aalen (new)**

Leibniz-Institut für Neue Materialien gGmbH (INM) **(joined after progress report)**

Leibniz-Institut für Werkstofforientierte Technologien IWT

Max-Planck-Gesellschaft e.V., represented by the
Max Planck Computing and Data Facility

**Otto-von-Guericke-Universität Magdeburg (new)**

Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau

**Sächsische Landesbibliothek - Staats- und Universitätsbibliothek Dresden (new)**

**Technische Informationsbibliothek (new)**

**Technische Universität Berlin (new)**

Technische Universität Clausthal

Technische Universität Darmstadt

Universität Freiburg

Universität des Saarlandes **(formerly co-applicant)**

**Universität Kassel (new)**

Universität Paderborn

Universität Stuttgart

- Participant individuals (in alphabetical order of institution)

| Name | Institutional affiliation |
|---|---|
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| Dr. Stefan Klein | Deutsche Gesellschaft für Materialkunde e.V. |
| Prof. Dr.-Ing. Tilmann Beck | Deutscher Verband für Materialforschung und -prüfung e.V.<br>Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau |
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| Prof. Dr.-Ing. Florian Pyczak | Helmholtz-Zentrum hereon GmbH |
| **Prof. Dr. Tim Dahmen** | Hochschule Aalen |
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| Prof. Dr. Heike Leitte | Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau |
| Prof. Dr. Sandra Korte-Kerzel<br>**Prof. Dr. rer. nat. Ulrich Kerzel** | Rheinisch-Westfälische Technische Hochschule Aachen |
| PD Dr. Thomas Hammerschmidt<br>**Dr.-Ing. Sarath Menon**<br>**Prof. Dr.-Ing. Markus Stricker**<br>**Prof. Dr.-Ing. Alfred Ludwig**<br>**PD Dr. Rebecca Janisch** | Ruhr-Universität Bochum |
| **Katrin Stump** | Sächsische Landesbibliothek - Staats- und Universitätsbibliothek Dresden |
| **Prof. Dr.-Ing. Claudia Fleck** | Technische Universität Berlin |
| Prof. Dr. Nina Merkert | Technische Universität Clausthal |
| Prof. Dr.-Ing. Karsten Durst | Technische Universität Darmstadt |
| **Prof. Dr.-Ing. Markus Kästner** | Technische Universität Dresden |
| Prof. Dr. Hans-Georg Herrmann<br>**Prof. Dr. Christian Motz**<br>Prof. Dr. Frank Mücklich<br>**(formerly co-spokesperson)**<br>**Dr.-Ing. Flavio Soldera**<br>**Dr.-Ing. Florian Schäfer** | Universität des Saarlandes |
| Prof. Dr.-Ing. Felix Fritzen | Universität Stuttgart |
| Prof. Dr.-Ing. Gerson Meschut | Universität Paderborn |
| **Prof. Dr.-Ing. Wenwen Song**<br>**Prof. Dr. Benoit Merle** | Universität Kassel |
| **Dr. Irina Sens** | Technische Informationsbibliothek |

## 3 Objectives, work program and research environment in the second funding period

- **Research area of the proposed consortium** (according to the DFG classification system: http://www.dfg.de/subject-classification)

  4.31 – Materials Engineering

  4.32 – Materials Science

  4.12-02 – Mechanics

  4.12-03 – Lightweight Constructions

  4.51-03 – Construction Material Sciences, Chemistry, Building Physics

  4.51-05 – Applied Mechanics, Statics and Dynamics

  4.43 - Computer Science

  3.22 – Statistical Physics, Nonlinear Dynamics, Complex Systems, Soft and Fluid Matter, Biological Physics

  3.23 – Optics, Quantum Optics and Physics of Atoms, Molecules and Plasmas

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

The consortium NFDI-MatWerk supports the still young discipline of Materials Science and Engineering (MSE) in its effort to computationally and experimentally study, characterize, and control materials and their performance, as well as their processing and manufacturing. The ultimate goal of MSE research is to design and optimize materials with tailored properties and to maximize their usability along all steps of their life cycle. To this end, one major challenge particular to MSE data is their inherent interdisciplinary and multiscale character. To further support this mission, the Materials Science and Engineering community is closely collaborating with condensed matter physics (FAIRMat, Daphne), chemistry (NFDI4Chem, NFDI4Cat), mechanics/mathematics (MaRDI) as well as production technology (NFDI4Ing). This is caused by the strongly heterogeneous microstructures present in virtually all materials, ranging from chemical configurations and crystal defects at the atomistic level, through microscale deformations and secondary phases, up to macroscopic structures such as layers, pores and cracks. Furthermore, any process applied to a sample may change the material's microstructure and, thereby, its mechanical and functional performance.

Due to the vast number of different experimental, computational, and analytical methods to reveal these dependencies, essentially every lab developed its own data tools and services. This rapid but uncoordinated development has hampered the digital transformation in MSE as well as the implementation of FAIR principles. With the start of NFDI-MatWerk, we have steered the development of this infrastructure into a community-driven process. Based on the analysis of data usage profiles of many Participant Projects from different sub-disciplines, we have identified the most relevant scientific scenarios within MSE. The resulting Infrastructure Use Cases (IUC)

formed the backbone of NFDI-MatWerk, as they continuously guided and challenged the development of our infrastructure. By the inclusion of FlexFunds as a new organizational measure of NFDI-MatWerk we ensure that this community-driven strategy remains dynamic throughout the next funding period.

NFDI-MatWerk will continue with five Task Areas (TA) to bring the developments into a broader context and to advance the five most important objectives of NFDI-MatWerk: (i) to integrate and include all stakeholders with our Community Interaction (TA-CI); (ii) to provide solutions for a Materials Data Infrastructure (TA-MDI), able to host the representation of materials data and information according to FAIR principles; (iii) to easily develop, execute and share Workflows in Lab Environments (TA-WLE); (iv) to provide and integrate a unified Ontology in Materials Science (TA-OMS) with an increased coverage and interoperability, and (v) to allow for a community-driven Strategy Development (TA-SD) towards the digital transformation of MSE.

These objectives require a number of overarching activities in NFDI-MatWerk that will be central to the upcoming funding period. One of them is the development of an architecture aligning the MSE research data management ecosystem towards oneNFDI. Another one is the empowerment of the MSE community to leverage the advantages of artificial intelligence (AI) and machine learning (ML) tools, eliminating the need to develop proprietary workflows and data schemes for this purpose. NFDI-MatWerk also needs to support the MSE community in the development of semantics for materials and materials information architecture. In this way, the building, filling, and provision of a central MSE knowledge graph aligned to NFDIcore can become a community-driven effort and desire. Furthermore, NFDI-MatWerk will continue to collaboratively work on establishing quality criteria and processes for the curation of MSE data connected to the MSE knowledge graph.

For all these services and solutions, the acceptance and dissemination in the community will be decisive for the success of NFDI-MatWerk in the upcoming years. At the moment, the focus shifts from solution generation to implementation which requires more personnel devoted to this task in close collaboration with the participant projects. Therefore, the roll-out strategy of the first funding period will be substantially extended, ensuring scalability while taking into account the heterogeneity of MSE by implementing a federated FAIR research data infrastructure which works for the benefit of the full MSE community and beyond.

- **Brief description of the proposed use of existing infrastructures, tools and services that are essential in order to fulfil the planned consortium's objectives**

NFDI-MatWerk focusses not on creation but on integration of existing tools (e.g., ELNs, services, software, semantics…) into coherent and seamless solutions supporting the researchers' scientific workflows. In line with its federated design, data is primarily stored on local servers at the institutions where they are generated, reflecting current funding schemes. Where participating institutions are unable to provide specific services locally, central service instances are established by NFDI-MatWerk. For instance, we provide (1) a central registration of FAIR Digital Objects (FDOs) which requires generic infrastructure for minting persistent identifiers (PIDs) and a Data Type Registry (DTR), (2) storage and metadata management resources via Coscine (see here) and its backend DataStorage.nrw, funded by RWTH Aachen and North Rhine-Westphalia, (3) NFDI-MatWerk Data and Metadata repositories linked to KIT's Large Scale Data Facility (LSDF) [see here], supported through institutional and Baden-Württemberg funds and (4) collaborations with institutional and national computing centers via NHR and MPCDF and the JupyterHub Service, to fulfil the computational needs.

The NFDI-MatWerk semantic infrastructure consists of two parts: The MatWerk Ontology (MWO) and the MSE Knowledge Graph (MSE-KG). After supporting the proliferation of the NFDI4culture ontology to NFDI core ontology, MWO is now a modularized extension of NFDI-core and adopted by several other consortia to ensure top-level alignment and high-level data interoperability. MWO is the semantic backbone of the MSE-KG describing, e.g., resources and digital assets.

To allow the FAIR execution of complex protocols, integrated development environments (IDE) and workflow engines are employed, aiming at modularization to meet the needs of several communities. These protocols are restructured in workflow nodes to improve interoperability of workflows. A critical interface and tool for MSE users are Electronic Laboratory Notebooks (ELNs), where NFDI-MatWerk adopts a technology-neutral stance and rather pushes for interoperability and community standards within the ELN Consortium. Here we support the most widely used ELNs, e.g., OpenBIS, elabFTW and recently the ELN solution NOMAD platform.

Software development is hosted on public GitHub and GitLab repositories; data sharing facilitates using online repositories like Zenodo. To ensure data sovereignty, critical content is mirrored on Git servers maintained by RWTH Aachen and the git.nrw project, complementing public cloud usage. On the organizational level, NFDI-MatWerk leverages state-level initiatives such as bwFDM, HeFDI, and fdm.nrw to expand its network, and involve local RDM consultants, supporting rollout efforts at institutional levels. It also maintains close connection with the HMC platform, the AIMS project, and the MaterialDigital Network to advance semantic interoperability in materials science.

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

NFDI-MatWerk contributes in different ways to the overall NFDI development. This includes contributions to the governance of the NFDI association, as well as participation in NFDI sections and task forces, Base4NFDI and collaborations with other NFDI consortia. Here, NFDI-MatWerk serves as a bridge between consortia in natural and engineering sciences.

Many activities pushed forward by NFDI-MatWerk are shaping the vision of OneNFDI. Among them are the concepts for an NFDI architecture (work group “Architecture” in NFDI Section Common Infrastructure), for an overarching ontology (NFDIcore), or for interoperability between different ELN solutions (The ELN Consortium). There is an active cooperation for several Base4NFDI services, e.g., a strong personal involvement in the Identity and Access Management (IAM4NFDI) and a systematic exploitation of JupyterHub services (Jupyter4NFDI). Further, the FAIR-DO concept for a technical interconnection of discipline specific data spaces is a central activity in NFDI-MatWerk.

NFDI-MatWerk is part of the collaboration “Physical Sciences in NFDI” (FAIRmat, DAPHNE4NFDI, MaRDI, NFDI4Cat and PUNCH4NFDI) which organizes colloquia and workshops. Furthermore, NFDI-MatWerk is also participating in activities of the engineering consortia (NFDI4ING, DataScience, NFDIxCS, NFDI4Cat, NFDI4Chem, and others).

The link to FAIRmat is further established by a joint infrastructure use case (IUC), bringing the different perspectives of condensed matter physics and materials science on the same class of experiments into the same software environment. As a result, the FAIRmat database NOMAD is supported by the MatWerk-workflow manager pyiron and vice versa. Further interactions are on ELN solutions with NFDI4Chem and a regular exchange with NFDI4Cat and NFDI4BioImage (OMERO server). NFDI-MatWerk is in similar close collaboration with NFDI4Ing, with whom some of the data infrastructure solutions such as storage solutions, file transfer service, and metadata profile definitions as well as workflow standards are jointly developed and maintained. Several joint use cases have been identified and solutions have been implemented.

NFDI-MatWerk is highly active in the NFDI association. Christoph Eberl (IWM) is currently one of the elected spokespersons of the consortia assembly. Several members contribute to the different NFDI Sections, e.g., the Section Metadata, Terminology and Provenance to which NFDI-MatWerk prominently contributes. In the Section Industry Engagement Christoph Eberl (IWM) served as deputy speaker until May 2025 and continues to participate actively. Furthermore, members of NFDI-MatWerk are contributing to various Section Working Groups (e.g. Multi Cloud, Research Software, Ontology Harmonization) and NFDI Task Forces (e.g. Evaluation & Reporting, User Research, Governance & Sustainability, Metadata).

## 4 International and national networking

As described, NFDI-MatWerk is well integrated into the overall structure of NFDI. Beyond that we integrate BMBF-funded AI service centers as well as national innovation centers. Furthermore, we have a tight interaction with the MaterialDigital Initiative of the BMBF, which is strongly focussed on applied Materials Science and Engineering to support the digital transformation in industry. The German Materials Society is part of NFDI-MatWerk ensuring a close connection to the community.

On the European level and beyond, there are numerous connections: NFDI-MatWerk works with common architecture concepts such as the FDO. This allows interconnection with national (like NFDI) and international (like EOSC and Gaia-X) infrastructures while preventing the creation of data silos. Cooperation with EOSC has been established via KIT: Members of NFDI-MatWerk actively participate in the newly launched Nanoscience Foundries and Fine Analysis Europe (NFFA) PILOT project—an extension of the NFFA-Europe project. The Service Coscine is part of the EOSC FIDELIS Network for trustworthy Repositories. Fraunhofer IWM and BAM were instrumental in founding the European Materials Modelling Council (EMMC) and support the ontologies developed therein. Founding members Gerhard Goldbeck and Emanuele Ghedini are part of the Advisory Board of NFDI-MatWerk (see website). Fraunhofer IWM is also involved in the European Advanced Materials Initiative 2030. NFDI-MatWerk is well embedded in the international MSE community (e.g., U.S. National Institute of Standards and Technology or Japanese National Institute for Materials Science; Swiss EMPA platform for Materials Science and Technology) as well as in international research data initiatives. To ensure harmonization, NFDI-MatWerk appointed an International Scientific Advisory Board that meets bi-annually and participates in NFDI-MatWerk conferences as well as project meetings where it stays continuously informed about progress within the consortium. Scientists from NFDI-MatWerk are strongly involved in the Research Data Alliance (RDA). Furthermore, members actively participate in the Materials Research Data Alliance (MaRDA). MaRDA council member Catherine Brinson serves on the Advisory Board of NFDI-MatWerk. The International Data Space Association network has defined a reference architecture for creating and operating virtual data spaces, where collaborations have been initiated through Fraunhofer Society. In addition, members of NFDI-MatWerk actively engage with international materials science communities by organizing international conferences, workshops, and symposia at topic-related events such as annual Material Science and Engineering conferences or bi-annual Federation of European Materials Societies (FEMS EuroMat) conference series.