

Press Release

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Materials Science and Engineering institutions collaborate on implementing a distributed research data infrastructure

Five years of funding for the consortium NFDI-MatWerk

In a collaborative effort to tackle the enormous challenge of building a common National Research Data Infrastructure NFDI, entire research areas across Germany are working together in subject-specific consortia. As one of ten consortia in the second round, NFDI-MatWerk is now receiving five years of funding for Materials Science and Engineering. The Fraunhofer Institute for Mechanics of Materials is the spokesperson for this consortium, in which the Max-Planck-Institut für Eisenforschung (MPIE) is also involved. Together with 10 other applicants and 15 associated institutions, the researchers are driving forward the digitalisation of materials research.

The Gemeinsame Wissenschaftskonferenz GWK, a decision-making body with representatives of the German Federal Government and the States, decided on July 2, 2021 to fund the NFDI-MatWerk consortia. It followed the recommendation of the expert panel and the German Research Foundation DFG. The first funding phase for NFDI-MatWerk is planned to go from October 2021 to September 2026. A total of 18 consortia applied for funding in various scientific areas in this second round for the National Research Data Infrastructure NFDI in a competitive process, 10 of which were recommended for funding.

"To develop customised materials for complex technologies and to fully consider the heterogeneous internal structure of materials, it is necessary to closely integrate different disciplines within and beyond materials science and engineering. To enable researchers in these disciplines to work together, a common national research data infrastructure is essential. Only in this way can research results and the tools used to generate them be exchanged, merged and published without much effort.", explains Dr. Tilmann Hickel, research group leader in the department "Computational Materials Design" at the MPIE and co-spokesperson in the NFDI-MatWerk consortium.

Materials are the basis for our modern technology

The aim of materials science and materials engineering is to characterize the physical mechanisms in materials and to develop resource-saving high-performance materials with the most ideal properties possible for the respective application. Manufacturing processes are investigated accordingly and designed so that materials and component systems have the necessary service life and can be used in a circular economy and consuming as little resources as possible. Materials' experts optimize from the atomistic scale to the macro or component level. Processing steps influence the internal material structure on the various scales and thus determine the mechanical and functional properties. Today, research groups still use their own tools and standards for data processing and storage for the data they generate through experiments and simulations. Therefore, sharing data and software tools is unfortunately a tedious task.



The Materials Science and Engineering community is developing a common research data infrastructure

"Many excellent scientists have already developed tools and standards that they use in their respective research groups. Instead of now working on similar challenges in parallel as before, we want to develop an infrastructure in NFDI-MatWerk that is so easily accessible and networked that in future the first step before investigating a new material property will be to run tools in programme libraries. Through NFDI-MatWerk, research in the field of materials science can be considerably more efficient in the future.", says Prof. Jörg Neugebauer, director of the MPIE department "Computational Materials Design".

The consortium covers more than 80 percent of the Materials Science and Engineering community

The NFDI-MatWerk consortium, coordinated by the Fraunhofer Institute for Mechanics of Materials IWM, consists of experts from the fields of materials science and materials engineering as well as mechanics. The applicant institutions are:

- Deutsches Forschungszentrum für Künstliche Intelligenz GmbH DFKI
- FIZ Karlsruhe Leibniz-Institut für Informationsinfrastruktur GmbH
- Forschungszentrum Jülich GmbH
- Fraunhofer-Gesellschaft für angewandte Forschung e.V.
 - Fraunhofer-Institut für Werkstoffmechanik IWM
 - Fraunhofer-Institut für Werkstoff- und Strahltechnik IWS
- Friedrich-Alexander-Universität Erlangen-Nürnberg
- Karlsruher Institut für Technologie KIT
- Max-Planck-Institut für Eisenforschung GmbH, MPIE
- RWTH Aachen University
- Technische Universität Bergakademie Freiberg
- Universität des Saarlandes

The associated institutions are:

- Albert-Ludwigs-Universität Freiburg
- Bundesanstalt für Materialforschung und -prüfung
- Christian-Albrechts-Universität zu Kiel
- Deutsche Gesellschaft für Materialkunde e.V. (DGM)
- Deutscher Verband für Materialforschung und -prüfung e.V. (DVM)
- Gesellschaft für Angewandte Mathematik und Mechanik e. V. (GAMM)
- Helmholtz-Zentrum Geesthacht
- Leibniz-Institut für Werkstofforientierte Technologien IWT
- Physikalisch-Technische Bundesanstalt Braunschweig und Berlin (PTB)
- Ruhr-Universität Bochum
- Technische Universität Clausthal-Zellerfeld
- Technische Universität Darmstadt
- Technische Universität Kaiserslautern
- Universität Paderborn
- Universität Stuttgart



The Max-Planck-Institut für Eisenforschung is contributing in particular with its expertise in the digital representation of workflows, in the simulation of materials and in software development. In a TaskArea on this topic, the exchange and semantic description of data together with the associated metadata and workflows in a digital environment for materials is being advanced. This should ensure the usefulness of research results long after a research project has ended. In order to achieve this goal, the Integrated Development Environment for Simulation Workflows pyiron [pyiron.org] was created at the MPIE and is being continuously developed to meet the requirements of the NFDI.

About the National Research Data Infrastructure

The National Research Data Infrastructure (NFDI) has the objective to systematically index, edit, interconnect and make available the valuable stock of data from science and research. So far, these data have mostly been available in a decentralized, projectrelated, or temporary form. The Federal Government and the States fund the NFDI jointly. Digital data storage is an indispensable prerequisite for treating new research generating findinas. and making innovations (Nationale issues. Forschungsdateninfrastruktur NFDI). In November 2018, the Federal and State governments decided to establish a National Research Data Infrastructure NFDI and intend to fund up to 30 consortia in total. In the final stage, up to 85 million euros per year are to be made available for this purpose.



NFDI-MatWerk aims to integrate decentralised expertise through a uniform data language and standardised interfaces. In this way, scientists will be able to work together in the future, independent of time and place, and generate new kinds of knowledge. Copyright: Fraunhofer-Institut für Werkstoffmechanik IWM



The international team of the Max-Planck-Institut für Eisenforschung conducts advanced basic materials research for the fields of mobility, energy, infrastructure, medicine and digitalisation. The focus lies on nanostructured metallic materials as well as semiconductors, which are analysed down to their atomic and electronic scales. This enables the MPIE team to develop new, tailor-made structural and functional materials embracing their synthesis and processing, characterization and properties, as well as their response in engineering components exposed to real operating environments.

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