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<input type="checkbox"/>	Binding letter of intent (required as advance notification for proposals in 2019)
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<input type="checkbox"/>	Non-binding letter of intent (anticipated submission in 2021)

2 Formal details

Planned name of the consortium

- Consortium for Safety of Nanomaterials and Nanoproducts

Acronym of the planned consortium

- NFDI4NanoSafety

Applicant institution

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Spokesperson

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3 Objectives, work programme and research environment

Research area of the proposed consortium (according to the DFG classification system)

- 21 Biology, 22 Medicine, 31 Chemistry, 43 Material Science and Engineering

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

Nanomaterials are characterized by unique physical and chemical properties which make them desirable for several applications. Because of their nanoscale, the properties of nanomaterials are different from larger-scale particles. In some cases they could have a negative health impact. Focusing on safety aspects related to the application of nanomaterials and nanoproducts, the consortium works on a highly interdisciplinary basis and comprises institutes from the fields of materials science, medicine, toxicology and occupational safety. **Main objectives** of the NFDI4NanoSafety consortium are:

- Managing sustainably quality-assured data and provide it for re-use in a highly interdisciplinary research area
- Defining comprehensive metadata standards and quality criteria for research data
- Enabling a quick and unbiased overview of existing data sets, preferably error-corrected and quality-checked raw data
- Establishing standards for data preparation to support regulatory processes and meta-analyses (prediction)
- Increasing the quality and velocity of research by accessing existing data (and thus knowledge)
- Increasing the national and international cooperativeness by data sharing
- Increasing the efficiency in designing experiments by relying on existing research data and SOP
- Avoiding duplicate experiments (especially in case of animal testing) from the point of view of researchers, reviewers and research funding agencies

The consortium pursues these objectives in the following task areas:

1. Consortium management: managing and disbursing funds, serving as a contact for the DFG and the NFDI Directorate, and representing the consortium within the NFDI and externally.

2. Interoperable Metadata: Nanosafety research comprises several disciplines and stages in the life cycle of new materials. Inputs from chemistry, material science, biology and toxicology have to be considered. New materials are designed and characterized, their cell interaction and toxicology are investigated and data for regulatory processes are generated. Only with interoperable metadata, participating disciplines can understand and verify the data, transfer it into a different context, and assess their significance for their own work. Thus, the consortium will design and disseminate community-wide accepted metadata standards and organize their continuous review and further development in line with scientific requirements. Additionally, it will establish a nanosafety knowledge graph (as part of a larger NFDI-wide knowledge graph).

3. "Smart Lab" Environment: Research data play a crucial role in the analysis and assessment of the properties of nanomaterials as well as their safe production and application.

It is therefore crucial to document research data and the associated development process (provenance) comprehensively. In order to keep the effort for the researchers as low as possible and at the same time to improve the traceability and reproducibility of the results, the consortium aims at the provision of components for a largely automated data acquisition and processing in the laboratory from experimental design (SOP) to data evaluation. This includes implementing machine-interpretable standard operating procedures (SOP), interfaces to lab equipment, Electronic Laboratory Notebooks (ELN) and data repositories. Close cooperation with the corresponding working group of NFDI4Chem (and other consortia) is planned.

4. Data curation: Selection, normalization, annotation, metadata enrichment, publication, presentation and digital preservation of research data. The consortium plans to establish community-accepted curation criteria and provide several data curators to jointly operate a distributed data repository for published, quality-assured research data.

5. Community Involvement: organizing the committees of the consortium (User Forum, User Advisory Board, Scientific Advisory Board), liaising with working groups, learned societies and the community at large, and picking up requirements from the community (via user groups and feedback from training and education) and critically accompanying the implementation.

6. Education and Training: Comprehensive RDM requires cultural change. New job profiles such as data curators/stewards/scientists are needed in order to ensure the quality of research data and the adherence to the curation standards. The consortium will participate in the cross-cutting topic of curriculum development in the field of RDM. Further on, it will organize method- and tool-specific workshops and conferences, prepare tutorials and training materials and conducts surveys to identify relevant formats and topics for training and education. A cooperation with DaNa is envisioned, which provides information on applications, materials properties, toxicology, and environmental aspects of nanomaterials mainly to the public.

7. Outreach and Cross-cutting Topics: NFDI4NanoSafety is connected at a national level with MAK Commission, SKLM and relevant Leibniz Research Alliances. At an international level, the OECD, ECHA and EFSA are important partners in the field of standardization and regulation. A collaboration with the EU NanoSafety Cluster is foreseen as strategic partnership aiming to establish a general agreement on nanotoxicology in Europe as well as to provide a forum for discussion among industrial stakeholders and the general public. Cooperation with GoFAIR Implementation Networks related to the field of nanosafety research (e.g. Chemistry, GO NANO) will be established in order to support the FAIR principles also at an international level. Further on, the consortium will cooperate with other consortia and the NFDI in general regarding cross-cutting topics (see below).

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

For the recording of metadata along the life-cycle of research data, the Chemotion ELN will be adapted to the needs of the nanosafety community.

For data archival, identification and publication, established research data repositories like RADAR will be employed. RADAR currently is a generic data repository. It is envisioned to augment the RADAR metadata schema with Nanosafety-specific extensions to better support the needs of the research community.

For data storage and search, a range of specialized curated databases of interest to the community. The cross-disciplinary search will be based on the infrastructure provided by GeRDI. Relevant databases for NFDI4NanoSafety are:

- Crystallography Open Database (Open-access collection of crystal structures of organic, inorganic, metal-organic compounds and minerals, excluding biopolymers)
- RCSB PDB (Protein Data Bank archive-information about the 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease.)
- eNanoMapper proposes a computational infrastructure for toxicological data management of engineered nanomaterials (ENMs) based on open standards, ontologies and an interoperable design to enable a more effective, integrated approach to European research in nanotechnology.
- The European Union Observatory for Nanomaterials (<https://euon.echa.europa.eu>) provides information about existing nanomaterials on the EU market (safety, innovation, research, and uses)
- OpenRiscNet (data, analysis, modelling and simulation services for all areas of risk assessment)
- Open TG-GATEs (Omics & Protocols)
- Blast (biological sequences)

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

Nanosafety research is a cross-cutting topic by nature. Thus, we see strong links to at least four other consortia: NFDI4Chem (chemistry), NFDI4MSE (material science), NFDI4Health (medicine), and NFDI4AIRR (Immunology).

- **NFDI4Chem** focuses on the characterization of molecules and will provide infrastructure and services. Especially in the first step of designing and characterizing new nanomaterials, services of NFDI4Chem can be applied. This includes ELN, interfaces to

lab equipment and repositories standards. Metadata standards, which will be developed in NFDI4Chem, will be considered by NFDI4NanoSafety. Metadata standards developed by NFDI4Chem play an important role in the design of an interdisciplinary metadata format for nano-safety research. However, these need to be expanded to include aspects of materials science, biology, medicine, and toxicology.

- **NFDI4MSE** integrates physics, chemistry, mechanical and electrical engineering to develop novel materials, characterize and optimize them, develop processes to manufacture such materials, evaluate their lifetime and develop strategies to maximize the recyclability at end-of-life. The consortium aims at setting up a digital platform enabling access to raw and meta data and workflows as well as developing a materials ontology as well as further solutions for a digitized workflow. A strong collaboration between both consortia is envisaged and will help to synchronize and develop a common strategy for materials characterization and properties relevant for their applications in the biomedical field. This comprises aspects related to metadata standards and workflows as well as ontologies in order to enable interoperability.
- **NFDI4Health** focuses on the assembly and analysis of personal health data. The consortium aims at the standardization of metadata for clinical and epidemiological studies and datasets related to healthcare, the setup of data analysis services as well as archiving and improving the workflow for controlled access and sharing of such data. Regarding environmental data, NFDI4Nanosafety is looking forward to a close collaboration with NFDI4Health.
- **NFDI4AIRR** focuses on the adaptive immune system and the adaptive immune receptor repertoire (AIRR). It aims at building a network of repositories for data on the state of the adaptive immune system and services facilitating an integrated analysis of such data, including flow cytometry data, which is also relevant for nanosafety studies. A regular knowledge exchange between both consortia on technical aspects of management and storage of such data is envisaged that might lead to a shared storage infrastructure including specific metadata sets.

Cooperation talks were held with all four consortia mentioned. Each consortium covers important areas of nano-safety research, but can only partially do justice to the interdisciplinary approach of NFDI4NanoSafety. At the same time, the integration of nano-safety research into one of the four consortia would extend their focus far beyond their disciplinary and methodological limits and needs.

4 Cross-cutting topics

Please identify cross-cutting topics that are relevant for your consortium and that need to be designed and developed by several or all NFDI consortia.

Outreach and training across NFDI: see Task Area “Education and Training” above.

General principles of FAIR data management: The discovery and findability of datasets across disciplinary boundaries in a distributed infrastructure requires novel approaches such as semantic technologies. This requires an agreement on information models and vocabularies which have to be considered for the metadata standard. The resulting metadata schema will be transformed into an ontology which will form the core of a semantic knowledge graph. Knowledge graphs can be understood as large networks consisting of entities describing real or abstract objects based on their semantic structures (ontologies) and their relationships to each other. Knowledge graphs will be addressed in several other consortia as well. In order to design them in an interoperable way, close cooperation of many, if not all consortia within the NFDI is envisioned.

Software und Interfaces: The most obvious service provided by a research management infrastructure is the secure and reliable storage of research data. Aspects of scalability, efficiency, security and confidentiality require a highly distributed approach with a federation of interoperable repositories and databases. These systems need to fulfill a number of requirements:

- community-approved metadata standards
- standardized programming interfaces (API)
- immediate registration of research data, including persistent identifiers (EPIC, DOI)
- linked data representation for discovery
- unified authentication and authorization infrastructure
- long-term preservation measures according to community-defined selection criteria
- Simple local deployment, managed deployments or hosted solutions

The NFDI4NanoSafety consortium will define specifications for such repositories and databases to ensure the interoperability of the systems. Several of the aforementioned requirements will be addressed by many (if not all) other NFDI consortia, thus a collaborative approach will be taken to work out these definitions. At the same time, the NFDI4NanoSafety consortium will provide a reference implementation of a data repository both for local installation and as hosted service.

“Smart lab” concepts, which play a pivotal role for NFDI4NanoSafety, are also addressed by other consortia (e.g. NFDI4Chem).

Please indicate which of these cross-cutting topics your consortium could contribute to and how.

Additionally to the topics mentioned in the previous section, NFDI4NanoSafety can make a strong contribution towards interoperability. The consortium works on a highly interdisciplinary basis (materials science, medicine, toxicology and occupational safety). Therefore, the consortium can play an important hinge function between other consortia in these disciplines and contribute substantially to the creation of interoperable metadata standards that can be validated directly in nano-safety research use cases.