1 Binding letter of intent as advance notification of a full proposal

☑	Binding letter of intent (required as advance notification for proposals in 2021)

2 Formal details

- **Planned name of the consortium**

  InnoMatSafety - Consortium for the safety of innovative materials

- **Acronym of the planned consortium**

  InnoMatSafety

- **Applicant institution**

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- **Participants**

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3 Objectives, work programme and research environment

Research area of the proposed consortium

205 Medicine, 322 Chemical Solid State and Surface Research, 323 Physical Chemistry, 325 Biological Chemistry and Food Chemistry, 406 Materials Science

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

The consortium addresses the research area of innovative materials and their impact on human health and the environment. Innovative materials include nanomaterials as well as other materials that exhibit novel properties independent of a defined size-range. They might possess deviating toxicological profiles compared to those of conventional materials. This requires strategies to assess and predict potential hazard and risk along their life-cycle as only safe materials applications can support sustainable innovations. The topic demands contributions from various disciplines. Correspondingly, the consortium works on an interdisciplinary basis and comprises members from the fields of chemistry, physics, materials science, toxicology, medicine, biology, and information sciences. The research field of materials safety is hallmarked by a vast variety of material types and approaches to characterise their intrinsic and toxicological properties. There is an urgent need to develop appropriate test systems and testing schemes supporting scientific understanding, appropriate materials design as well as regulatory needs. Consolidation of research data and their efficient use/re-use are mandatory for the further advancement of the field. A major challenge in this interdisciplinary and heterogeneous field is the establishment of community-wide accepted standards for acquisition, description, curation, and storage of research data. Our vision is to support the design and advanced risk assessment of innovative materials through data-rich concepts like safe-by-design, adverse outcome

pathways, computational modelling, and meta-analyses. To this end, we will establish a reliable and sustainable research data infrastructure which interlinks datasets along the data flow in the field of innovative materials safety. To realise this vision, we have set ourselves these objectives:

- Establishing community-approved metadata standards, vocabularies and ontologies as well as quality criteria for research data in the field of innovative material safety.
- Enabling seamless access to both high quality data and machine-readable operating procedures, furthering data reuse and efficient experimental design.
- Supporting the digital transformation of all processes in the research workflow from material design up to toxicological assessment.
- Promoting RDM and FAIR data as relevant competencies within the community and as an integral part of professional curricula.
- Creating an ethical and legal framework with a focus on community-specific aspects of intellectual property rights, animal studies, and genetic engineering.

We strive to provide reliable data for evaluation, decision-making and regulation throughout the data lifecycle according to the FAIR principles.

TA #	TA Name	TA core responsibility
1	Governance/Management	Providing guidance to the consortium and supporting the task area leaders in fulfilling their objectives; promoting cross-cutting development and providing legal support within the consortium
2	Description standards and quality criteria	Providing modular-based and interoperable description standards and a comprehensive concept for research data quality assurance and guidance on minimal data requirements and completeness
3	Digitized (meta-)data acquisition, documentation and transfer	Providing machine-readable (S)OPs, APIs for seamless lab-device to ELN data transfer and machine-readable (S)OP and lab-devices integration
4	Networked repositories and databases	Developing a federated network of repositories/databases within the framework of the NFDI
5	Training and Dissemination, Community involvement	Enabling the cultural change in collecting and re-using data by communicating the goals, services, and results of the initiative, by adapting to the community needs, educating next and current generation researchers, and facilitating cross-disciplinary networking across the community

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

InnoMatSafety will take advantage of its strong national and international networking and cooperate closely with established European infrastructures such as eNanoMapper. In addition, the consortium partners included EUON/DaNa, the AdvancedNano GOFAIR Implementation Network (EU), as well as ICSD, and CSD for the analysis of crystallographic data.

The InnoMatSafety consortium aims to create a distributed infrastructure of existing, networked repositories/databases for data archival, publication and retrieval, including:

- data.eNanoMapper (Chemistry/Health Science):
- Open TG-GATEs (Toxicogenomics)
- NanoCommons Knowledge Base (Nanomaterials Safety)
- ToxCast (Toxicology)

Due to its central role for organisations that manage scientific data on chemicals in a regulatory context, the consortium plans to integrate IUCLID (International Uniform Chemical Information Database) as a key software to record, store, maintain and exchange data on intrinsic and hazard properties of chemical substances.

In order to define requirements for toxicological datasets and data quality, the consortium will closely interact with the DFG Permanent Senate Commission for the Investigation of Health Hazards of Chemical Compounds in the Work Area (MAK Commission) and the DFG Permanent Senate Commission on Food Safety (SKLM). The consortium plans to describe the data by a modular metadata scheme (a blueprint for such a scheme has been developed by some of the partners in the NanoS-QM project (https://nanosqm.leibniz-nanosicherheit.de/), based on existing scientific and regulatory relevant standards. Furthermore, the development of an overarching ontology is planned, adapted to the requirements of the community and integrated in ELNs that are already used by some partners such as eLabFTW, openBIS or Chemotion.

Wherever possible and appropriate, we will reuse infrastructure components from other, already established consortia - as stated in the Leipzig-Berlin declaration - as well as results from the NFDI sections (see "4 Cross-cutting topics")).

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

With **NFDI4Chem**, we plan to cooperate closely in the adaptation and further development of electronic laboratory notebooks (ELN) and the connection of laboratory equipment to ELN via corresponding interfaces.

We intend to work together with **NFDI4Ing** in the development of metadata schema and operating procedures concerning materials characterisation and materials safety data, in the description of workflows and the development of ontologies.

With **NFDI4Cat**, we have a joint interest in innovative and safe catalytic materials. The implementation of Safe-by-Design approaches in the field of catalysis by use of data on materials properties and safety and concepts for standardisation of such data will be discussed.

InnoMatSafety can benefit from the work of **NFDI4Matwerk** in the area of material characterisation. At the same time, InnoMatSafety's "safe-by-design" approach in particular complements parts of the NFDI4Matwerk work programme. An exchange regarding the documentation of data (e.g. by use of ELN), the development of metadata standards, as well as data requirements for predictive modelling (Safe by Design) is envisaged.

With **4Immuno**, we share a common interest in interoperable and modular metadata standards and quality criteria for measurements, e.g. for methods like cytometry.

We will develop joint use-cases with **DeBioData** on the efficacy and toxicity of innovative materials used in the field of drug delivery and thereby evaluate interoperability of our data description standards.

4BIOIMAGE addresses important methods relevant to several consortia, including InnoMatSafety. We will cooperate in developing metadata standards and ontologies for relevant microscopy techniques (e.g., confocal laser scanning microscopy) as well as in knowhow transfer and training in the field of microscopy, especially image analysis, and in defining joint interfaces to ELN.

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.

InnoMatSafety sees several topics that can be better addressed across consortia. For this reason, the consortium supports cross-cutting activities as described in the Leipzig-Berlin declaration. In addition, we see active participation in the establishing sections of the NFDI as being central to the success of our initiative as well as of the NFDI as a whole. More specifically, we see overlapping interests in the fields of interoperable metadata, knowledge graph and vocabularies, legal and ethical issues, authentication and authorisation infrastructure, and services for long-term preservation of research data. In addition, we see synergies with other consortia in the areas of electronic laboratory notebooks (ELN) and the connection of laboratory equipment with ELN.

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

The interdisciplinary approach of InnoMatSafety already ensures that metadata standards and technical interfaces are interoperable across the boundaries of individual sub-disciplines. Through the diverse connections to other consortia, InnoMatSafety takes this connecting approach even further and thus contributes to the realisation of a single NFDI with cross-disciplinary discovery and re-use of research data. Furthermore, InnoMatSafety contributes to the simplification of the documentation of experimental procedures with the concept of machine-readable, modular standard operating procedures, which can be reused in other disciplines.