

Consortium for the Safety of Innovative Materials (InnoMatSafety)

Spokesperson: Dr. Annette Kraegeloh, INM – Leibniz Institute for New Materials, Campus D2 2, 66123 Saarbrücken,
annette.kraegeloh@leibniz-inm.de

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. Major challenges in this interdisciplinary and heterogeneous field are the establishment of community-wide accepted standards for acquisition, description, curation, and storage of research data.

Due to its interdisciplinary nature and the variety of analytical methods employed in the research area, **data types** are very heterogeneous and comprise datasets collected in various sub-disciplines (Figure 1):

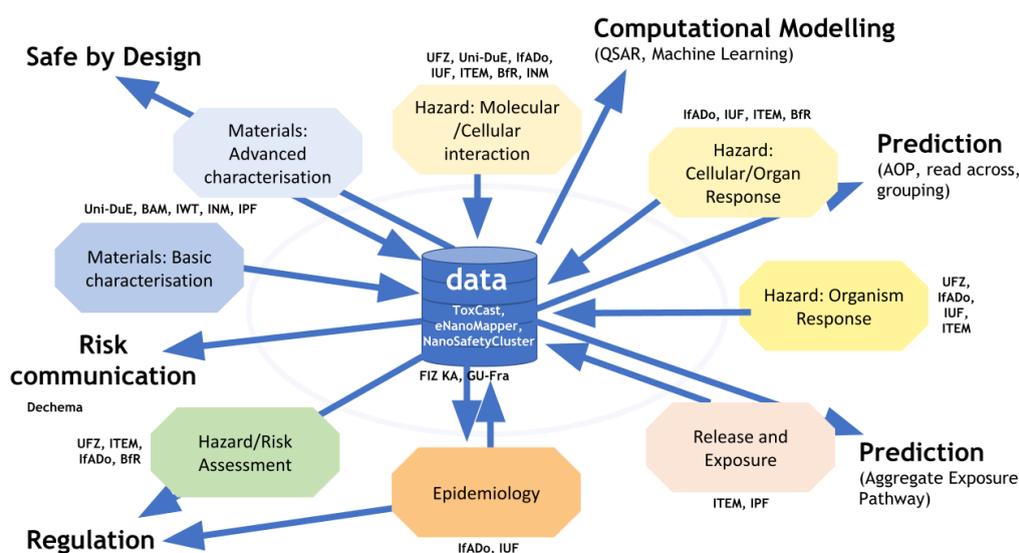


Figure 1: Envisioned InnoMatSafety data flow, indicating main tasks of the engaged sub-disciplines.

Our vision is to implement a reliable and sustainable research data infrastructure which interlinks datasets along the data flow. This will 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. Central **measures and services** include:

- 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.
- Promote 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.

InnoMatSafety faces **specific challenges in data management**. Innovative materials are described by complex datasets representing their chemical, physical, and toxicological properties. These properties might change along the materials life cycle and in dependence on the environmental conditions. The transformation towards advanced toxicity testing approaches demands the identification of mechanistic information in conjunction with the development of relevant and predictive models and test systems¹. The safety assessment of innovative materials, including hazard and exposure assessment, requires more contextual, comprehensive and fine-granular information compared to conventional chemical substances and traditional testing approaches. Necessary information is related to the materials of interest, biological models, endpoint readout and data analysis as well as hazard and exposure assessment. Currently, re-use of such data, e.g. for prediction, modelling or risk assessment, is limited as the description of data is currently often incomplete or data are inaccessible. In 2014, forty databases on innovative materials-related information were in operation. In 2019, however, most of those databases were either discontinued or contained little data². Most databases are 'data silos' lacking interoperability.

The consortium brings together experts in the safety of innovative materials, working at the different phases from materials research to regulatory aspects. **Expertise in research data management** is provided by FIZ Karlsruhe, Goethe University Frankfurt, and fdm.nrw. Several InnoMatSafety members cooperate in the BMBF-funded project NanoS-QM, developing and evaluating quality criteria and description standards for research data in the field of nanosafety research. The description standards will be translated into metadata formats and integrated into Electronic Lab Notebooks (ELN). Additionally, InnoMatSafety partners are co-applicants in the NFDI consortia 4Chem, 4MatWerk, and 4Ing.

InnoMatSafety will cooperate with **relevant (international) partners and existing infrastructures**. The Organization for Economic Co-operation and Development (OECD), the European Chemical Agency (ECHA) and the European Food Safety Authority (EFSA) are important partners in the field of standardisation and regulation. The EU NanoSafety Cluster provides a forum for discussion among industrial stakeholders and the general

¹ doi: 10.14573/altex.1803011

² <https://www.nanosafetycluster.eu/>

public, which is complemented on a national level by the DaNa project.³ Learned societies and professional organisations such as DECHEMA and the German Society of Toxicology⁴ provide links to the various scientific communities represented in the consortium. BfR and BAM will ensure the link to regulation and availability of materials. InnoMatSafety will harmonise interfaces and description standards with the providers of eNanoMapper,⁵ ToxCast, Open TG-GATEs, OpenRiskNet and NanoObservatory⁶ and link these databases both into the envisioned data federation and EOSC. Researchers from InnoMatSafety partner institutions are appointed members of the MAK⁷ as well as the SKLM Commission⁸ and will ensure close cooperation with these bodies. The consortium has close links with relevant Leibniz Research Alliances, such as the “Leibniz Research Alliance NanoSafety”⁹, currently preparing a reorganisation as Leibniz-Research Alliance Advanced Materials Safety and “Health Technologies”. InnoMatSafety aligns to and complements other NFDI consortia, in particular 4Chem, 4Health, 4MatWerk, 4Cat, 4Immuno, Neuroscience, 4BIOIMAGE and DeBioData. A close exchange with these consortia is foreseen with regard to data formats, metadata standards, data structures, programming interfaces and tooling/services (e.g. ELNs, interfacing with laboratory equipment).

InnoMatSafety has several **interfaces to the NFDI at large**. Due to its interdisciplinary nature, the consortium can act as a hinge to other consortia and validate the interoperability of metadata schemas across several subjects (chemistry, materials science, physics, toxicology) by means of concrete use cases. InnoMatSafety, thus supports a major goal of the NFDI, namely the re-use of data across disciplinary boundaries. Additionally, InnoMatSafety covers toxicology and regulatory issues which are not addressed in any other consortium so far.

The digital transformation of the innovation cycle from material characterisation to regulatory activities requires interoperable data and processes as well as tools that minimise the necessary documentation effort for researchers. These **cross-cutting topics** have to be met by other consortia. Of particular interest to InnoMatSafety are:

- Smart Labs, Electronic Lab Notebooks, Lab automation
- Interoperable metadata, knowledge graph and vocabularies
- Legal and ethical issues
- Authentication and Authorisation Infrastructure
- Services for long-term preservation of research data

With its interdisciplinary approach, InnoMatSafety can **contribute to cross-cutting topics** such as interoperable metadata schemata as well as modular and machine-readable Standard Operating Procedures (SOP) and their integration into ELN.

Expectations for the NFDI conference include networking with other consortia, revealing mutual interests and potential fields of collaboration, and identifying cross-cutting topics¹⁰.

³ <https://www.nanopartikel.info/>

⁴ <https://www.toxikologie.de/>

⁵ <http://www.enanomapper.net/>

⁶ <https://euon.echa.europa.eu/>

⁷ Senate Commission for the Investigation of Health Hazards of Chemical Compounds in the Work Area, see http://www.dfg.de/en/dfg_profile/statutory_bodies/senate/health_hazards/

⁸ DFG Senate Commission on Food Safety, see

http://www.dfg.de/en/dfg_profile/statutory_bodies/senate/food_safety/index.html

⁹ <https://www.leibniz-nanosicherheit.de/en/>

¹⁰ see also DOI [10.5281/zenodo.3457212](https://doi.org/10.5281/zenodo.3457212)

Members of the planned consortium:

Spokesperson	Institutional affiliation
PD Dr. Annette Kraegeloh Head Nano Cell Interactions group annette.kraegeloh@leibniz-inm.de	INM – Leibniz Institute for New Materials, Campus D2 2 66123 Saarbrücken
Co-Spokesperson	Institutional affiliation
Matthias Razum Head e-Research Matthias.Razum@fiz-karlsruhe.de	FIZ Karlsruhe - Leibniz-Institute for Information Infrastructure Hermann-von-Helmholtz-Platz 1 76344 Eggenstein-Leopoldshafen
Members of the planned consortium	Institutional affiliation
PD Dr. Andrea Haase Dr. Blair Johnston Fibre and Nanotoxicology	Bundesinstitut für Risikobewertung (BfR) Max-Dohrn-Straße 8-10 10589 Berlin
PD Dr. Christoph van Thriel Neurotoxicology and Chemosensation Department of Toxicology	IfADo – Leibniz Research Centre for Working Environment and Human Factors Ardeystraße 67 44139 Dortmund
PD Dr. Klaus Unfried Environmentally-induced Skin and Lung Aging Dr. Roel Schins Particles, Inflammation and Genome Integrity	IUF – Leibniz Research Institute for Environmental Medicine Auf'm Hennekamp 50 40225 Düsseldorf
Prof. Dr. Lutz Mädler Dr. Norbert Riefler Particles and Process Engineering	IWT – Leibniz Institute for Materials Engineering Badgasteiner Str. 3 28359 Bremen
Dr. Harald Bresch Department: Materials and the Environment Competence Center nano@BAM Dr. Thilo Muth eScience	Bundesanstalt für Materialforschung und -prüfung (BAM) Richard-Willstätter-Straße 11 12489 Berlin
Dr. Sylvia Escher In Silico Toxicology	ITEM – Fraunhofer Institute for Toxicology and Experimental Medicine Nikolai-Fuchs-Straße 1 30625 Hannover
Prof. Dr. Matthias Epple Inorganic Chemistry	University of Duisburg-Essen Universitätsstraße 7 45141 Essen
Dr. Magdalene Cyra Dr. Matthias Fingerhuth Landesinitiative für Forschungsdatenmanagement-fdm.nrw	University of Duisburg-Essen fdm.nrw c/o Universitätsbibliothek Universitätsstraße 9 45141 Essen
Dr. Dana Kühnel Bioanalytical Ecotoxicology	Helmholtz-Zentrum für Umweltforschung GmbH - UFZ Permoserstraße 15

	04318 Leipzig
Dr. Christoph Steinbach Dr. Nils Bohmer Dr. Nadja Möller	Dechema e.V. Theodor-Heuss-Allee 25 60486 Frankfurt am Main
Prof. Dr. Lena Wiese Database Technologies and Data Analytics Institute for Computer Science	Goethe Universität Frankfurt Robert-Mayer-Straße 10 60629 Frankfurt am Main
Dr. Katja Nau Process Optimization, Information Management, Applications (PIA) Institute for Automation and Applied Informatics (IAI)	Karlsruhe Institute of Technology (KIT) Hermann-von-Helmholtz-Platz 1 76344 Eggenstein-Leopoldshafen
Prof. Dr. Brigitte Voit Scientific Director IPF and Head Institute Macromolecular Chemistry Dr. Ron Dockhorn Theory of Polymers	IPF – Leibniz Institute of Polymer Research Dresden Hohe Straße 6 01069 Dresden
Prof. Dr. Franziska Boehm Intellectual Property Rights in Distributed Information Infrastructures	FIZ Karlsruhe - Leibniz-Institute for Information Infrastructure Hermann-von-Helmholtz-Platz 1 76344 Eggenstein-Leopoldshafen