Consortium for the Safety of Innovative Materials (InnoMatSafety)

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The consortium *InnoMatSafety* 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 from a defined size-range. Accordingly, innovative materials might possess toxicological profiles deviating from the ones of conventional materials. This requires strategies to assess and predict potential hazard and risk along their life-cycle as only safe materials applications can be exploited to 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, materials science, biology, medicine, toxicology, and occupational safety. 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 the 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 field are the establishment of standards for acquisition, curation, and storage of heterogeneous research data. This can only be enabled by a smart research data management infrastructure.

Due to its interdisciplinary nature and the variety of analytical methods employed in the research area, **data types** are very heterogeneous and comprise the following datasets:

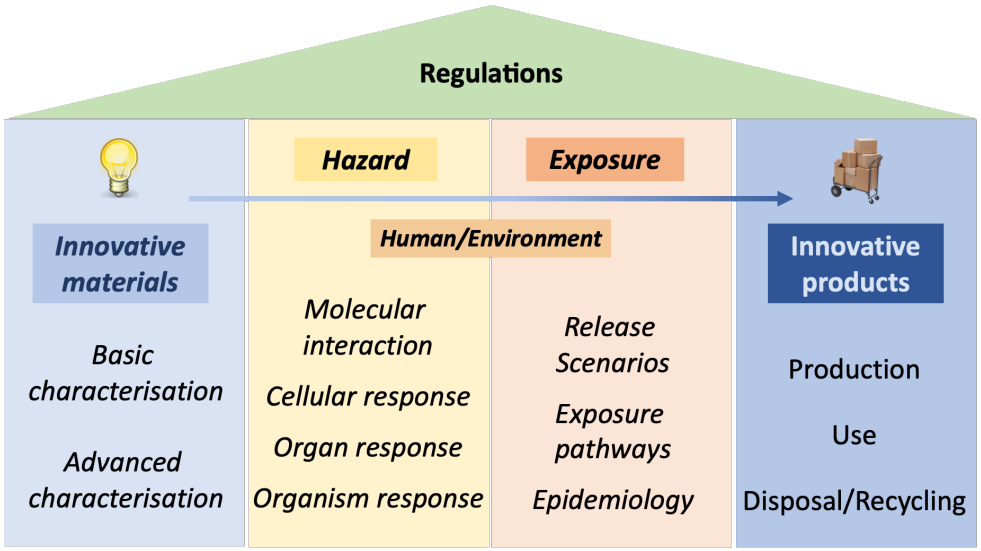

Figure: Data sets (*in italics*) used in the field of Innovative Materials Safety.

Our vision is to develop and establish a stable, secure, reliable and sustainable research data management infrastructure in the field of innovative materials safety. This will allow users across disciplines to access, store and re-use quality-assured data and information anytime and anywhere. The initiative will contribute to standardisation and digitisation of processes

starting from the planning of research projects, acquisition of data, up to their publication, collection, curation, and dissemination. The consortium focuses on the following **measures and services**:

- Developing (meta-)data standards that work across the involved disciplines and support regulatory needs
- Developing and publishing machine-readable and fine-granular (standard) operating procedures for research, materials development and regulation
- Creating a federation of interoperable domain-specific repositories/databases for storing, sharing, finding and re-using research data, including (meta)data from ELN
- Engaging with the community in order to increase data literacy, foster the FAIR data principles, integrate RDM and data science into curricula, and disseminate the services provided by the consortium
- Creating an ethical and legal framework that provides guidelines and policies regarding the use of personal data, animal testing, terms of use and intellectual property

InnoMatSafety faces **specific challenges in data management**. First of all, 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. Thus, the safety assessment of innovative materials requires more comprehensive, contextual and fine-granular information in comparison to conventional chemical substances. This information also comprises extensive metadata related to the materials characterisation, properties of biological models, as well as hazard and exposure assessment. Further re-use of data, e.g. for risk assessment, is limited as the description of data is currently often incomplete or the data are inaccessible. In 2014, forty databases on innovative materials-related information were in operation. In 2019, most of those databases were either discontinued or contained little data[1]. Most databases are 'data silos' lacking interoperability.

The consortium brings together experts in the safety of innovative materials active at the various levels from materials research to regulatory aspects and extensive **expertise in research data management**, represented by FIZ Karlsruhe - Leibniz-Institute for Information Infrastructure, which has extensive expertise in building and operating research data management systems. Several partners of InnoMatSafety are part of the Leibniz-Research Alliance Nanosafety,[2] in which a research data infrastructure for nanosafety research has been conceptualised. 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).

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 public, which is complemented on a national level by the DaNa project.[3] Learned societies and professional

[1] https://www.nanosafetycluster.eu/
[2] https://www.leibniz-nanosicherheit.de/en/
[3] https://www.nanopartikel.info/

organisations such as DECHEMA and the German Society of Toxicology[4] 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] Open TG-GATEs, Blast,[6] OpenRiscNet and NanoObservatory[7] and integrate these databases into the envisioned data federation. Researchers from InnoMatSafety partner institutions are appointed members of the MAK[8] as well as the SKLM Commission[9] and will ensure close cooperation with these bodies. The consortium has close links with relevant Leibniz Research Alliances, such as the "NanoSafety Research Alliance", "Health Technologies" and "Bioactive Compounds and Biotechnology". InnoMatSafety aligns to and complements other NFDI consortia, in particular 4Chem, 4Health, 4MSE, FairMat, 4Cat, BioDiversity, 4AIRR and MaRDI. 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, 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 of the other consortia so far.

InnoMatSafety addresses various **cross-cutting topics**. The end-to-end digitalisation of data collections from material characterisation to regulatory activities requires interoperable data and processes along the innovation cycle, including tools that minimise the necessary documentation effort for researchers. These challenges 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 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, identifying mutual interests and potential fields of collaboration, and information on (technical and legal) cross-cutting topics (e.g. which consortia will address which topics[10]). How will the NFDI cover transdisciplinary research areas?

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[4] https://www.toxikologie.de/
[5] http://www.enanomapper.net/
[6] https://blast.ncbi.nlm.nih.gov/Blast.cgi
[7] https://euon.echa.europa.eu/
[8] Permanent Senate Commission for the Investigation of Health Hazards of Chemical Compounds in the Work Area
[9] DFG Senate Commission on Food Safety
[10] see also DOI 10.5281/zenodo.3457212

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