NFDI MatWerk

National Research Data Infrastructure for Materials Science and Engineering
NFDI-MatWerk

The challenge in Materials Science and Engineering (MSE)

The multiscale and multidisciplinary nature of materials leads to complex scientific workflows and highly dimensional data. The scientific findings resulting from these workflows are communicated primarily as documents, where the content is semantically unaligned, unstructured and neither machine readable nor machine understandable.

NFDI-MatWerk's approach

NFDI-MatWerk develops a FAIR research data infrastructure for the MSE community in Germany. To meet the FAIR principles, the consortium aims to integrate i) workflows and ii) semantic descriptions, and to develop the necessary iii) software and iv) infrastructure solutions for decentralized research data processing.

Task Area
Materials Data Infrastructure

The Task Area Materials Data Infrastructure develops and maintains the infrastructure for the management of materials data and metadata by using the FAIR Digital Object concept.
The service architecture developed within NFDI-MatWerk can be easily adopted by other NFDI communities.
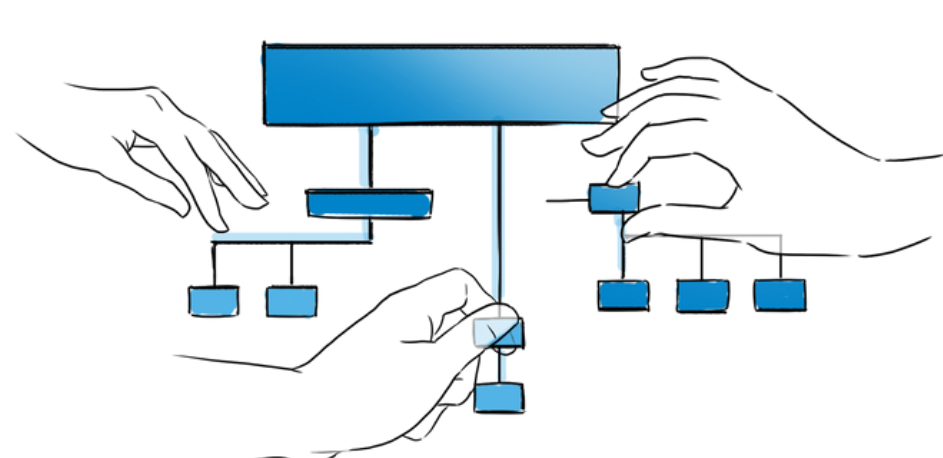
IUC 02 — **Focus Infrastructure Use Case**
Framework for the curation and distribution of reference data sets

Latest developments
- Shared Service Architecture
- FAIR Digital Object Technical Process Workflow - demonstrator for IUC 02
- Metadata Extraction and Mapping Service
- Vocabulary Service EVOKS

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5 Task Areas
> 20 Participant Projects
17 Infrastructure Use Cases (IUCs)

One vision:
Amplifying materials knowledge by FAIR research data management

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Task Area
Workflows and Software Development
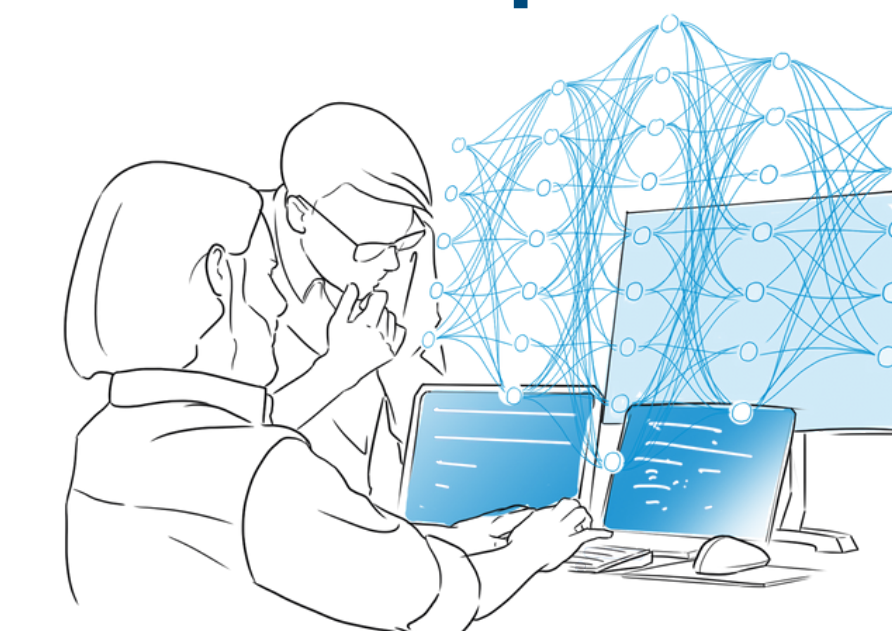
The Task Area Workflows and Software Development provides software solutions, in which FAIR data, corresponding metadata and FAIR workflows in MSE are
- shared between institutions,
- made long-term available, and
- semantically and quantitatively described in a reliable, reproducible and machine usable form.

IUC 04 — **Focus Infrastructure Use Cases**
Model-driven data space exploration

IUC 09 — Infrastructure interfaces with condensed-matter physics (collaboration with FAIRmat)

Latest developments
- Integrated Development Environment PyIron
- PASTA Electronic Lab Notebook (ELN)
- Chaldene - Jupyter Notebooks
- Demonstrators for IUC 04 and IUC 09
- User Journey Indentation - demonstrator

Task Area
Ontologies for Materials Sciences

A lack of structured (meta)data hinders a researchers ability to find, access, interoperate, and reuse data - all of which are significant drawbacks for data-driven approaches and increased research sustainability.
The aim of the Task Area Ontologies for Materials Science is
- to aid the development of semantic descriptions in the materials science domain (e.g., for certain experiments or processes), as well as
- the design and implementation of a MSE Knowledge Graph (MSE KG).

IUC 17 — **Focus Infrastructure Use Case**
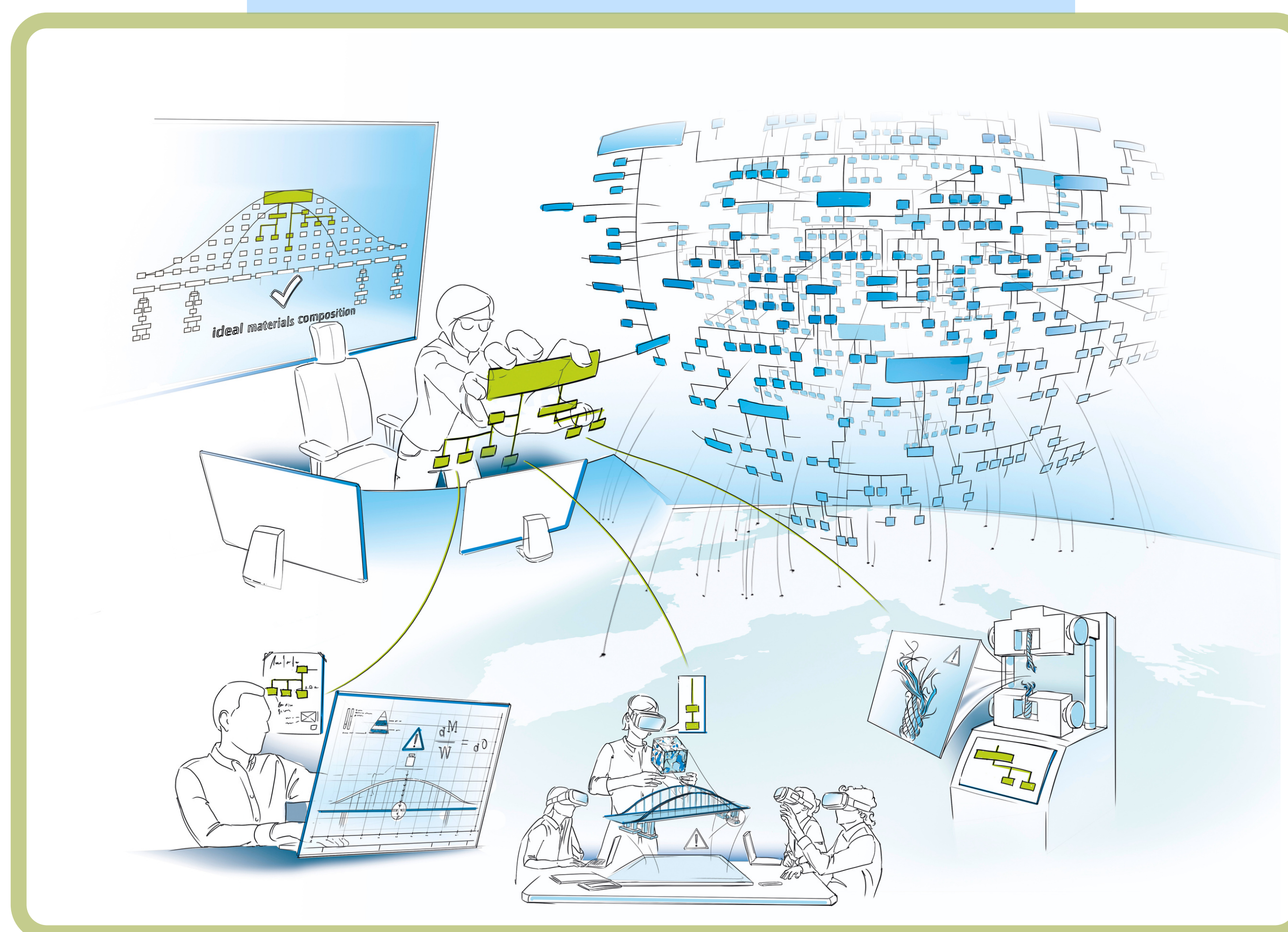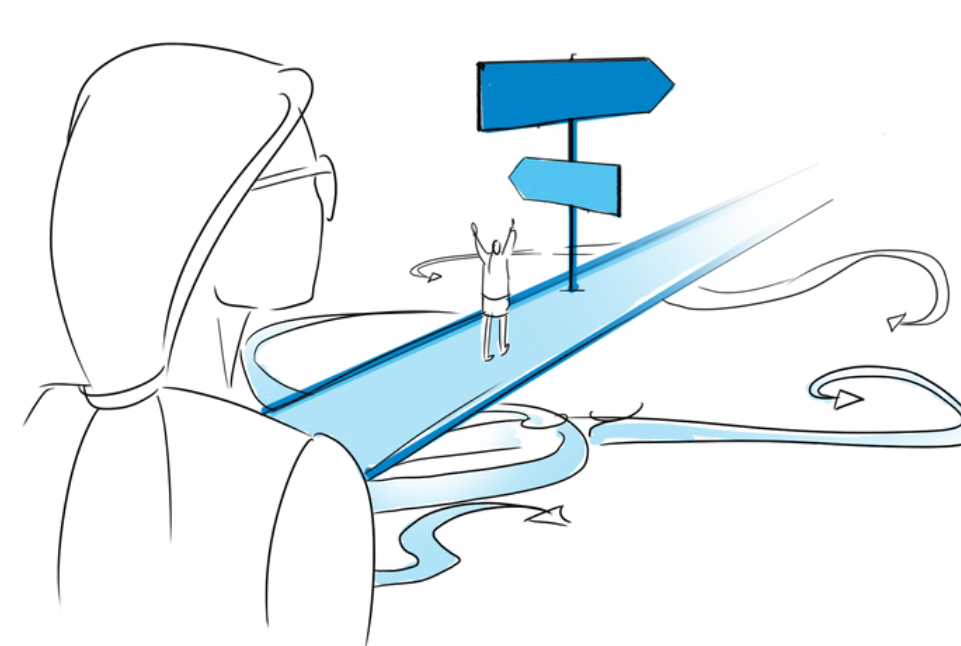Ontologies for defects in crystals

Latest developments
- MSE KG - Demonstrator
- Ontologies for Defects - IUC17 online demonstrator
- Linked Open Data - Working Group
- Harmonized semantics in Electron Microscopy - Repository

Task Area
Strategy Development

The Task Area Strategy Development aims to
- establish transparent and community-driven decision-making processes,
- involve the scientific community in the infrastructure development process,
- develop incentives and good scientific practices for a successful (cultural) change process, and
- ensure the legal and financial framework.

What are IUCs?
Infrastructure requirements resulting from various research scenarios (e.g., Participant Projects) are collected and specified in the form of Infrastructure Use Cases (IUCs). IUCs provide research-relevant usage profiles („queries") with real data and workflows that allow realistic testing during and at the end of development periods.

Task Area
Community Interaction

The Task Area Community Interaction aims to foster dynamic information exchange and collaboration from NFDI-MatWerk to the MSE community. The objectives are
- to ensure active involvement and a dynamic interchange of ideas among the MSE community members, and
- to facilitate learning and skill enhancement including training sessions, interactive webinars, and educational content about research data management (RDM), Electronic Lab Notebooks and further.

The offer is aimed at a variety of levels, from students and technical professionals to seasoned researchers.

Latest developments
EUSMAT Summer School (09/2023)
Winter School with TU Dresden & Fraunhofer IWS (12/2023)

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CoRDI
Conference on Research Data Infrastructure