



Contribution ID: 140

Type: **Talk**

NFDI-MatWerk: Use-case-driven development of research data infrastructure for materials science and engineering

Tuesday 25 March 2025 11:15 (10 minutes)

NFDI-MatWerk represents the communities of materials science and engineering, diverse in material scales, methodologies and technologies. A supporting infrastructure is built upon exemplary infrastructure use cases (IUCs), representing individual domain areas. Two such IUCs will be presented, also highlighting their use of ontologies in the materials science context:

IUC04 aims to ensure a model-driven (guided probing) collection of the relevant experimental and computational data to construct so-called defect-phase diagrams and their post-processing according to newly established simulation protocols. Another focal point is automatic semantic annotation of the computational data and its upload to an ELN system.

IUC17 has the aim of developing semantic representations describing crystalline structures and crystalline defects and their temporal evolution and to test if these descriptions are well designed and applicable for different types of simulations, experiments and microscopy. Another aspect covered is aiding domain scientists in implementing ontologies in their everyday research.

The built infrastructure services and solutions are currently in roll-out for the broader materials science and engineering community. To empower the community for FAIR research data management, NFDI-MatWerk is currently building several central services for learning, connecting and contributing to a FAIR data future.

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Session Classification: Talks - Collaboration with/in NFDI