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Research Data Infrastructures as Enablers for Materials Design

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Abstract

Suitable material solutions are of key importance in designing and producing components for engineering systems – either for functional or structural applications. Materials data are generated, transferred, and introduced at each step along the complete life cycle of a component. A reliable materials data space is therefore crucial in the digital transformation and an important prerequisite for machine learning in materials science.

Therefore, the consortium NFDI MatWerk aims to develop a sustainable infrastructure for the standardized digital representation of materials science and engineering (MatWerk). The goal is to seamlessly integrate decentralized data and metadata, experimental and computational workflows, and a materials ontology to maximize interoperability and reproducibility of materials data processing. To this end, data use profiles of participant projects from different sub-disciplines are analyzed to identify the most relevant scientific scenarios within MatWerk.

Similarly, the Plattform MaterialDigital (PMD) is committed to provide a prototypical infrastructure for the digitalization of materials in an industrial context implemented by decentralized data servers, semantic data schemas and digital workflows. The standards, methods, and tools developed within the PMD are deployed and consolidated within the context of currently more than 20 BMBF-funded academic and industrial research consortia. Scientific workflow environments represent a major focus area, including efforts to improve the definition and representation of digital workflows, as well as their distribution in form of a workflow store.

In this presentation we will describe the overarching visions behind these initiatives, their status, and progress of dissemination with a focus on the workflow activities and the connection between theoretical predictions and experimental solutions. Following the philosophy of both consortia, specific examples will be used to demonstrate innovative and pragmatic solutions.