

MSE 2024

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Topic D: Digital Transformation

D03: Digital Materials: Experiments, simulation workflows, ontologies, and interoperability

Materials Science and Engineering is undergoing a major paradigm shift towards more efficient digitalization. Integration and reuse of data and knowledge from synthesis, production, characterization as well as of modelling activities open new perspectives for innovation. Emerging fields of Materials Informatics employing tools such as machine learning, big-data applications, statistical inference and Integrated Computational Materials Engineering (ICME) allow accelerating the discovery of new compositions and processes tailored to the production of materials with specific properties and microstructures. Efficient modeling and simulation of materials engineering processes is based on large amounts of heterogeneous experimental and simulation data. This data captures multiple scales, from atomistic to continuum, and a diversity of relevant physical, chemical and mechanical concepts such as thermodynamics, kinetics, functional and mechanical properties as well as metadata on materials history, data origin and provenance.

A key to enable the digitalization of materials and to leverage the advantages and opportunities of the digital age is an interoperable digital representation of materials and processes. An appropriate management of materials data requires the use of FAIR principles (findable, accessible, interoperable, and reusable). Digital workflows ensure the unity of materials data and used simulation protocols. They connect individual software tools, automatize the storage and curation of final simulation results as well as relevant intermediate steps and can, therewith, ensure the reproducibility of computational procedures. Ontologies are essential for formally representing universal materials science concepts, their interrelationships, and workflows. Application ontologies enhance identification, data integration and fully fledged complex simulation workflows. This will improve explainability and validation of real-life and simulated process designs. A unique identification and elucidation of entities and relations is required to meet the FAIR principles.

In this symposium, we call for an open discussion and exchange about the recent technical and scientific challenges involved in developing an interoperable representation of materials and processes. These include recent developments of ontologies, materials data schemas and software solutions that allow representation and integration of workflows, processes, and materials in a digitalized manner.

Symposium Organizer



Univ.-Prof. Dr.-Ing. Tilmann Beck
RPTU Kaiserslautern-Landau



Dr. Gerhard Goldbeck
Goldbeck Consulting Ltd



Dr. rer. nat. Tilmann Hickel
Max-Planck-Institut für Eisenforschung GmbH

