

MSE 2024

24 - 26 Sep 2024 (Darmstadt)

dgm.de

Topic F: Functional Materials, Surfaces and Devices

F07: Data-driven and Machine Learning assisted materials research

Enabled by the exponential growth of data storage capacity and computational resources as well as the availability of open-source data analysis tools and Artificial Intelligence (AI), the fourth paradigm of science, namely data science, has taken off and impacts various disciplines including functional materials research. Large-scale combinational databases and impactful repositories are emerging, assisted by high-throughput synthesis/simulations and materials digitalization. Groundbreaking opportunities can be enabled by AI-assisted materials discovery, particularly promising for the highly disciplinary fields of functional materials research. It can guide the synthesis and discovery of new functional oxides and compounds with superior properties in fields of e.g. batteries, electrocatalysts, oxygen transport membrane and ferroic materials.

With the help of emergent data science and machine learning techniques, the composition -- processing -- microstructure -- property relationships of functional materials can be mapped out both forwardly and reversely, leading to forward inference and inverse design, respectively. For instance, the intrinsic physical properties can be statistically modelled using various types of descriptors derived from crystal structures, whereas the extrinsic properties can be statistically understood based on microstructure through Machine Learning surrogates. In particular, the inverse design of materials can be carried out based on high-throughput combinatorial screening, global optimization based on Bayesian optimization, and generative deep learning.

This symposium invites contributions from various domain expertise and on different length scales including synthesis, characterization, simulations and data analysis, who are in general data shareholders in the field functional materials research. It offers particularly a platform to exchange various application possibilities of data science tools and to showcase the best practice.

Symposium Organizer



Dr. Leopoldo Molina-Luna
Technische Universität Darmstadt



Prof. Dr. Bai-Xiang Xu
Technische Universität Darmstadt



Prof. Dr. Hongbin Zhang
Technische Universität Darmstadt

