

Symposium AI-driven Materials Design: Recent Developments, Challenges and Perspectives (SYMD)

jointly organised by
the Metal and Material Physics Division (MM),
the Magnetism Division (MA),
the Surface Science Division (O),
the Crystalline Solids and their Microstructure Division (KFM), and
the Semiconductor Division (HL)

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In a surprisingly short time, AI (artificial intelligence) has demonstrated its transformative potential in materials science by integrating machine learning algorithms and generative models to predict and optimize material properties. High-throughput computational frameworks powered by AI enable rapid screening of vast chemical spaces, significantly reducing the time and cost associated with traditional experimental approaches and providing new physical insights. By leveraging large data sets and sophisticated algorithms, researchers have successfully uncovered hidden patterns and relationships in material behavior, leading to the discovery of novel materials with superior mechanical, electrical, magnetic, or catalytic properties.

The interdivisional symposium highlights the latest advances and success stories in AI and data-driven materials design, focusing on both machine learning and generative approaches. Leading experts in the field present the latest methods in AI used to predict material properties, optimize manufacturing processes, and accelerate the discovery of new materials. Key topics include the development and application of machine learning models, highthroughput computational techniques, and the integration of AI with experimental and theoretical methods, as well as current challenges and future perspectives.

Overview of Invited Talks and Sessions

(Lecture hall H1)

Invited Talks

SYMD 1.1	Mon	15:00–15:30	H1	Learning physically constrained microscopic interaction models of functional materials — ●BORIS KOZINSKY
SYMD 1.2	Mon	15:30–16:00	H1	GRACE universal interatomic potential for materials discovery and design — ●RALF DRAUTZ
SYMD 1.3	Mon	16:00–16:30	H1	Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction — ●NONG ARTRITH
SYMD 1.4	Mon	16:45–17:15	H1	Inverse Design of Materials — ●HONGBIN ZHANG
SYMD 1.5	Mon	17:15–17:45	H1	Data-Driven Materials Science — ●MIGUEL MARQUES

Sessions

SYMD 1.1–1.5	Mon	15:00–17:45	H1	AI-driven Materials Design: Recent Developments, Challenges and Perspectives
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