physikalisches Kolloquium

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AI-guided materials optimization and development

Mo. 16.6.25
16:00 Uhr
Ort: H34

Materials are the foundation of technological advancements that shape our modern society. Their continuous development enables new applications and products, while the discovery of novel materials addresses key societal challenges like clean energy production, sustainability, global prosperity, health, and wellbeing.

I will present artificial intelligence (AI) solutions for two extreme data regimes. For CO_2 to methanol conversion in the context of carbon capture and recovery, experimental data is scarce, but computational data plentiful. I will illustrate how we utilized machine-learning solutions from the Open Catalyst Project (OCP) to compute nearly a million adsorption energies of catalytically relevant molecules on different metals surfaces. We used the corresponding adsorption energy distributions as descriptors for catalytically interesting systems and propose new catalysts.

In biomaterials science, data is also scarce. I will introduce AI-guided workflows based on Bayesian optimization and the Aalto Materials Digitalization (AMAD) platform to facilitate efficient data collection. We used these workflows to optimize the hydrothermal extraction of lignin and lignin-carbohydrate complexes from birch wood. Each lignin sample is characterized with 2D nuclear magnetic resonance (NMR) spectroscopy and property measurements such as antioxidant activity or glass transition temperature. From the resulting holistic dataset, we extracted structure-property-process relationships with machine-learning that offer insight into how lignin can be further modified for value-added applications.

AI-guided workflow for adaptive materials optimization and characterization illustrated for biopolymers extracted from wood