Physikalisches Kolloquium

Universität Augsburg
Mathematisch-Naturwissenschaftlich-Technische Fakultät

Prof. Marek Sierka

06.05.2024

Interplay of Digitization and Simulation in the Quest for New Functional Materials

In the first part of my talk I will give a general overview of our research activities in the area of computer-aided materials design. This includes the development of software infrastructure, material ontologies, digital workflows and semantic material data spaces for the systematic handling of hierarchical, process-dependent material data, as well as the development and application of machine learning tools for the design of materials with tailored properties.

In the second part I will focus on our developments in Density Functional Embedding Theory (DFET) for molecular and extended systems. DFET allows to reduce the computational cost for larger systems while achieving high accuracy by partitioning the systems into a larger part - "environment" - described by computationally efficient but less accurate methods, e.g. DFT, and a smaller, active part described by a computationally intensive and more accurate method, e.g. wave function theory (WFT) based methods. DFET provides an efficient way to study the ground and excited state properties of low-dimensional systems using high-level methods for the region of interest. In addition, our embedding scheme is coupled with a real-time time-dependent DFT (RT-TDDFT), which allows the study of the linear or nonlinear optical response of the embedded subsystem. The performance of our implementation is demonstrated by predicting excitation energies, absorption and high harmonic generation spectra in various test systems.