WWU MÜNSTER

FACHBEREICH PHYSIK

Graduiertenkolleg 2149
Research Training Group

Allgemeines Physikalisches Kolloquium

Donnerstag, 28.04.2022 um 16 Uhr c.t.

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Design of finite temperature materials properties enabled by innovative digital concepts

Since the function of materials is controlled by properties and processes on the atomic scale, ab initio based high-throughput methods are valuable strategies in materials design. For computational efficiency, they are however often restriction to T=0K calculations, while many technologically relevant materials properties and thermodynamic stabilities change when going from low to high temperatures. On the other hand, the constantly increasing performance of digital tools for simulation and data-driven science enables more targeted material development including these kinds of finite-temperature effects. A flexible infrastructure, including data management and workflow solutions is required to make this symbiosis user-friendly efficient. Within this presentation, examples from ab initio thermodynamics for the design of phase stabilities in hard-magnetic alloys and defect-phases in advanced high-strength steels will be demonstrated. We will discuss physical concepts with a focus at the impact of magnetic excitations. At the same time, the examples will be used to derive requirements and present solutions for a digital infrastructure. An outlook will be given to current strategies with the NDFI initiative NFDI-MatWerk.