

Institute of Thermomechanics, Czech Academy of Sciences

invites you to a lecture within the lecture series **Institute of Thermomechanics Seminar**

Theory-guided defect engineering based on quantum-mechanical calculations

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Defects are omnipresent, and defect-free states exist only as approximative idealizations of the complex reality around us. Specifically in materials science, defects can be not only tolerated (as nearly unavoidable) but also exploited within various defect-engineering approaches. Indeed, defects offer a potentially unlimited playground for fine-tuning materials properties in contrast to the defect-free state, which is only one. Quantum-mechanical calculations have proved to be an excellent guide in this uncharted territory. Focusing specifically on the magnetic materials, both point defects and extended defects may have a profound impact on a variety of properties, including structural, elastic, or thermodynamic ones. Importantly, the impact can be, in fact, positive when defective systems outperform their perfect counterparts.

The talk will exemplify these facts in the case of our recent projects, which were focused on defects in magnetic intermetallic compounds as well as disordered alloys. The former will be represented by Fe₃Al-based intermetallics, the latter by Fe-based superalloys. Special attention will be paid to mutual interactions of defects with different spatial dimensions, such as point-defect impurities interacting with planar grain (antiphase) boundaries, or extended defects existing in materials exhibiting different levels of chemical disorder.

**The lecture will be held on Wednesday, May 20th, 2026 at 11:00 a.m.
in the building of the Institute of Thermomechanics (Lecture Hall),
Dolejškova 5, 182 00 Prague 8**

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