TECHNISCHE UNIVERSITÄT WIEN

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EINLADUNG zum IFP-SEMINAR

Software tool for comprehensive transport data analysis: Introduction and practical use cases

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Host: Ernst Bauer

Termin: Mittwoch, 28. Februar 2024, 16:00 Uhr

Ort: TU Wien, Freihausgebäude
Wiedner Hauptstraße 8-10, 1040 Wien
Seminarraum DC rot 07 (roter Bereich, 7. OG)

Vor dem Vortrag gibt es ab 15:30 Kaffee und Kekse

Abstract:

Linking the fundamental physics of band structure and scattering theory with macroscopic features, such as measured temperature dependencies of thermoelectric transport, is essential for a fundamental understanding of thermoelectric phenomena and ensures more targeted and efficient experimental research. Nonetheless, many experimental results in the field of thermoelectricity are only interpreted qualitatively, yielding only superficial understanding of the collected data.
In this talk, a comprehensive fitting tool to analyse temperature-dependent thermoelectric properties, particularly the Seebeck coefficient, resistivity, and Hall coefficient within the parabolic-band model, is presented. To ensure a broad and convenient applicability of the tool, an easy-to-use, open-source software is introduced and briefly explained. The interactive user interface, presenting the active fit as well as the effective band structure in real time, allows for the user to predict doping-related changes by modifying the respective parameters, which returns the predicted transport properties and related quantities like the temperature-dependent chemical potential or carrier concentration. This will help to reach a better understanding of the interplay of band theory with the transport properties and has the potential to accelerate thermoelectric research. In addition, a neural network assists the user by predicting initial parameters sufficiently accurate to execute the fit.
To demonstrate the potency of the fitting tool, various Fe_2VAl-based materials are analysed with respect to their band-structure and scattering parameters and compared with predictions from DFT calculations.