Chair of Materials Engineering of Additive Manufacturing
TUM School of Engineering and Design
Technical University of Munich

HiWi Position

Computational Materials Design with Focus on Programming, Simulation, and High-Throughput Methods

Motivation

Modern materials research is increasingly driven by computational methods, automation, and data-intensive workflows. This project applies programming and high-throughput simulation techniques to computational materials science using Ni-based alloys as a representative system. These alloys are widely used in demanding applications, where improving mechanical performance remains a key challenge.
The CALculation of PHAse Diagrams (CalPhaD) methodology provides a robust framework for modeling thermodynamic and kinetic processes. By combining CalPhaD with automated, high-throughput workflows, this project aims to efficiently explore large compositional spaces and extract insights from simulation data.

Objective

The goal is to develop and apply computational and data-driven methods for materials design, with a strong emphasis on programming, automation, and high-throughput simulations. The project will focus on building scalable workflows to predict phase stability, microstructure evolution, and their impact on mechanical performance.

A central aspect is the development of reproducible pipelines for large-scale simulations and data analysis, enabling efficient exploration of composition–property relationships.

Tasks

- Development of scripts and automated workflows for high-throughput simulations
- Implementation and execution of computational models (e.g., CalPhaD-based tools)
- Handling and analysis of large simulation datasets
- Data visualization
- Documentation

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Your profile

- Strong interest in programming; experience with Python or similar languages is highly desirable
- Interest in data-driven methods and high-throughput approaches
- Familiarity with computational materials science is a plus
- Experience with CalPhaD-based software (e.g., Thermo-Calc, MatCalc) is an advantage but not required
- Ability to work independently and in a structured manner
- Good proficiency in English (written and spoken)

Contact

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