

ReferenceNr.: MCL_293

Materials Center Leoben Forschung GmbH (MCL) is a leading competence center in the field of materials research and technology. In this context, we support numerous companies in the production sector developing high-performance materials, manufacturing processes and products. By developing specific computer-aided technologies, we accelerate materials based innovation including the digitalization of the manufacturing chain as well as of products. Our portfolio includes cooperative research and development projects with international and national partners from the production and research sectors as well as several consulting, laboratory and simulation services in materials science.

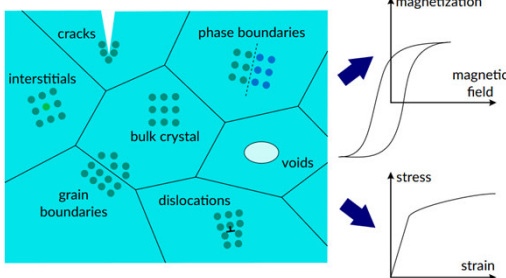
*Would you like to work in an innovative and international setting?
Then MCL is the perfect work place for you!*

Your Profile

You are a Master student in any of the computational sciences (computational materials science/physics/chemistry). The project requires knowledge in

- modeling techniques used in Machine-Learning (e.g., neural nets, Bayesian methods),
- programming (Python, C++),
- atomistic simulation,

and you are enthusiastic to develop and apply these methods to accelerate the design of innovative materials.



Tasks & Responsibilities

Machine-learning interatomic potentials (MLIPs) are a relatively new class of interatomic potentials aiming at atomistic simulations with quantum-mechanical accuracy—but a fraction of the cost. This now enables the calibration of models for macroscopic properties of alloys (for example, strength, fracture toughness, or magnetization) using material properties computed with MLIPs.

Such models depend on properties of material defects, such as stacking faults, grain boundaries, or dislocations. In this project, you will participate in the development of MLIPs to be used to simulate defects in alloys, and the development of automated protocols for constructing the MLIP training sets, as well as writing of a peer-reviewed journal article on the obtained results.

Our offer:



- flexible working hours
- further training/education
- employee events

A temporary employment contract for 6 months with immediate start and a gross salary of € 4,880.40 with normal working hours of 10.50 hours per week.

*Please send us your application and a detailed resume. We are looking forward to it!
We would like to especially encourage women to apply.*

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