Researcher (f/m/d): Development & application of machine-learning potentials for materials design

ReferenceNo.: MCL_278

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.

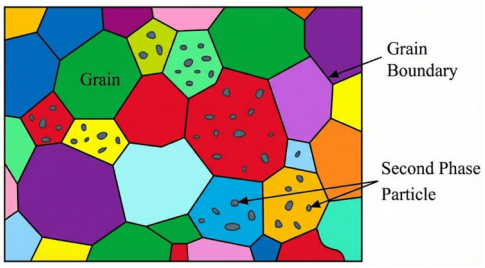
Would you like to work in an innovative and international setting?
Then MCL is the perfect work place for you!

Your Profile

You have or will shortly receive a PhD degree in any of the computational sciences (e.g., computational materials science/physics/ chemistry, applied mathematics). The project requires knowledge in

- programming (e.g., C/C++, Python),
- atomistic simulation,

and you are enthusiastic to develop and apply new AI methods to model material microstructures and by that accelerate the design of innovative materials.



Tasks & Responsibilities

Machine-learning interatomic potentials (MLIPs) have been a breakthrough for providing the quantitative accuracy of quantum mechanics to large-scale atomistic simulations. However, they suffer from a very high complexity (e.g., millions of parameters) when applied to systems with a large chemical space, also involving other quantum-mechanical phenomena like magnetism.

You will explore with MLIPs atomistic systems of microstructural features up to date infeasible with first principles methods, adapt and apply new approaches for MLIPs, and develop microstructure models e.g., for grain boundaries. This is key to design novel advanced materials. The research takes place in a collaborative and international scientific network and allows for research stays abroad.

Our offer:

- flexible working hours
- further training/education
- home office
- employee events
- cooperation with Firmenradl

A permanent employment contract with immediate start and a gross salary per year of at least € 65,684.64 (40h/week). The project is planned for a duration of at least 3 years.

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

bewerbung@mcl.at