

PhD position (f/m/d): AI-supported accelerated design of sustainable catalysis materials



ReferenceNo.: MCL_280

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.

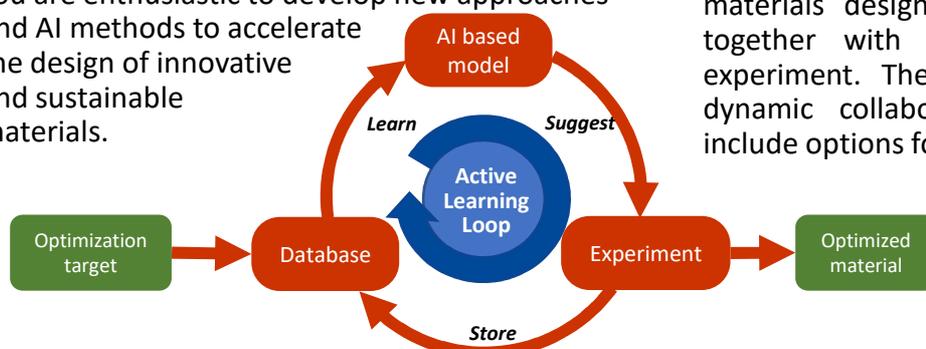
*Would you like to work in an innovative and international setting?
Then MCL is the perfect work place for you!*

Your Profile

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

- programming (e.g., python),
- atomistic simulation (e.g., DFT, LAMMPS).

You are enthusiastic to develop new approaches and AI methods to accelerate the design of innovative and sustainable materials.



Tasks & Responsibilities

The aim of the project is to develop combined computational/experimental workflows for an **AI-supported design of sustainable catalysis materials** free of rare earth elements.

You will apply **active learning design loops for materials design** informed by ab initio modeling and machine-learned interatomic potentials to find promising new materials. The multi-scale materials design workflows will be developed together with experts from simulation and experiment. The research will take part in a dynamic collaborative scientific network and include options 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 € 52,862.74 (40h/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.*

bewerbung@mcl.at