

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



ReferenceNr.: MCL_283

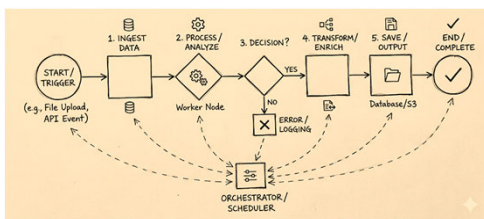
Materials Center Leoben Forschung GmbH (MCL) is a leading competence center in the field of materials research and technology. In this context, we support numerous companies in the production sector developing high-performance materials, manufacturing processes and products. By developing specific computer-aided 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 informatics or any of the computational sciences (e.g., computational materials science/physics/chemistry, applied mathematics). The project requires knowledge in programming (e.g., python) and APIs.

Knowledge about workflow orchestration systems (argo workflows, pyiron, AiiDA) is appreciated. You are enthusiastic to develop new approaches and computational tools to accelerate the design of innovative and sustainable materials using state-of-the-art approaches from AI, IT and data science.



Tasks & Responsibilities

The aim of the project is to develop and implement a computational framework to run a **“workflow of workflows”** for complex, automated, digital materials design tasks. The tasks include identification of relevant workflows, APIs, and events and their integration into an event-driven meta-orchestration layer that links multiple workflows together. These “workflow of workflows” will be tested for use cases from materials development, **involving AI-based approaches** combined with physics-based simulations.

The work will be done in close collaboration with MCL’s software development team and experts in materials simulation and experiment. The research will take part in a collaborative scientific network and include **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 € 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.*

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