

# Master Thesis: Active Learning Algorithms for Simulating Dislocations in Metals

Reference No.: MCL\_234

Materials Center Leoben (MCL) supports numerous companies in the production sector developing high-performance materials, manufacturing processes and products. MCL designs specific computer-aided technologies in order to accelerate innovation processes in manufacturing companies as well as to support the digitalization of the value chain and 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.

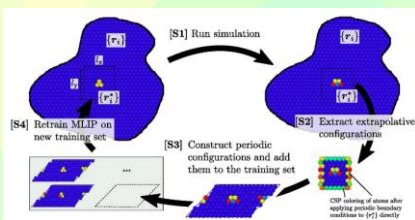
## Machine-Learning potentials for Dislocations

*These topics inspire you or you are already familiar with them?  
Then you are the right person for this position!*

### What are we looking for....

A motivated master student from materials science, physics, or computational sciences (e.g., computational mechanics, applied mathematics) with one (or more 😊) of the following skills

- crystallography/atomic-scale mechanics,
- atomistic simulation,
- linear algebra/machine-Learning methods,
- programming (Python, C++).



### Your challenge...

Machine-learning potentials are a relatively new class of interatomic potentials aiming at atomistic simulations with quantum-mechanical accuracy—but a fraction of the cost. In this work, you will extend an active learning algorithm for training such potentials to dislocations in metals. More precisely, your challenge is to

- develop algorithms for constructing training sets for the machine-learning potential to be used in simulations of fcc dislocations,
- testing and validation of the developed algorithms.

The precise tasks may depend on your background and personal preferences.

### Our offer

An employment with immediate start and a gross salary of € 3.000,- for six months.

*Please send your complete application documents by email.  
We are looking forward to knowing you!*

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