



PhD Position

Atomistic modelling and simulation of high entropy alloys

Description

A new class of metallic alloys, the so-called high entropy alloys (HEAs), has promising and previously unprecedented structural, mechanical and thermal properties, which will be part of a national research network. The aim of the PhD project is to enable materials design of novel refractory high entropy alloys for high-temperature applications by predictive multiscale models.

Computer simulations (**density functional theory**) are used to study atomic-scale fluctuations, which influence the mechanical properties and thermal stability of high entropy alloys. The simulations are done in strong collaboration with an experimental work at the same institute for the validation of the simulation approach.

Tasks

You will:

- Perform ab-initio simulations on high-performance computing facilities.
- Develop new simulations methods.
- Compare simulation, theory and experiments.
- Present results at international conferences.
- Collaborate with academic project partners.

Requirements / Selection criteria

- Excellent university degree in science or engineering (materials science, physics, engineering mechanics or a related subject).
- Proactive and enthusiastic young scientist with excellent communication skills in English.
- Basic programming skills (C++, Fortran or Python)

Institute

Institute for Applied Materials IAM-WBM
Group: Computational Nanomechanics of Materials

Starting date

As soon as possible

Contact/ Information

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How to apply

E-mail (with CV, References, Transcript of Records)