CSC-RUB PhD Project Proposal

Title: Atomic cluster expansion for the prediction of multi-component phase diagrams

Sector of research: Dr. rer. nat. or Dr. Ing.

Degree awarded: Physics or Mechanical Engineering

Keywords: Atomistic Modelling and Simulation, machine learning potentials, high-throughput calculations, density functional theory, free energy computation, phase stability, high-entropy alloys, active learning, materials design

Supervisor of PhD project: Prof. Dr. Ralf Drautz, Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-University Bochum, e-mail: ralf.drautz@rub.de

Research focus of supervisor:

Our research has three main objectives:

1. to obtain effective interatomic interactions from fundamental theories of the electronic structure;

2. to employ effective interatomic interactions in large scale and long-time atomistic simulations for obtaining effective models and parameters;

3. to develop data-driven and high-throughput atomistic simulation methods for model validation and the discovery of novel materials.

Interatomic potentials are obtained by systematically coarse graining density functional theory to effective models of the interatomic interaction. Potentials are employed in atomistic simulations for predicting structural stability and mechanical, kinetic and thermodynamic properties of materials.

Automated workflows together with high-throughput calculations are used to explore chemical phase space, to validate trends in structural stability predicted by simplified models and for a systematic analysis of interatomic potentials. Density functional theory calculations and statistical machine learning are employed for computational materials design and to assist and guide experimental research.

Publications:

Automated free energy calculation from atomistic simulations, S. Menon, Y. Lysogorskiy, J. Rogal, R. Drautz, arXiv preprint arXiv:2107.0898

Design of refractory compositionally complex alloys with optimal mechanical properties, A. Ferrari, Y. Lysogorskiy, R. Drautz, Physical Review Materials 5 (6), 063606 (2021)

Performant implementation of the atomic cluster expansion (PACE) and application to copper and silicon, Y. Lysogorskiy, C. van der Oord, A. Bochkarev, S. Menon, M. Rinaldi, et al., npj Computational Materials 7 (1), 1-12 (2021)

Atomic cluster expansion of scalar, vectorial, and tensorial properties including magnetism and charge transfer, R. Drautz, Physical Review B 102 (2), 024104 (2020)

Atomic cluster expansion for accurate and transferable interatomic potentials, R. Drautz, Physical Review B 99 (1), 014104 (2019)

Summary of research plan:

Background: Numerous contributions to the design and development of novel materials have been made with atomistic simulations based on density functional theory. To date most of the density functional theory screenings are limited to materials at zero temperature and with few chemical species only. In particular it is difficult to explore basic quantities of interest in materials science, such as phase diagrams.
Recent progress in machine learning potentials means that accurate surrogate models may be derived from density functional theory. The machine learning potentials, here the atomic cluster expansion (ACE), was shown to be accurate and computationally efficient, which enables sampling for free energy calculations, phase equilibria and phase diagrams. However, the parameterization of machine learning potentials for multi-component materials remains a tremendous challenge. While today hundreds of thousands of density functional calculations can be carried out automatically, the chemical complexity of multi-component alloys as described by machine learning potentials means that a direct parameterization is not possible.

Study objective:
We will focus on the parameterization of a multi-component metallic alloy that stretches across the hcp – bcc stability boundary, such as the refractory bcc metals Mo, Nb and V together with hcp elements Ti and Zr. To this end high throughput DFT calculations will be carried out to sample the composition space as exhaustively as possible. In parallel the atomic cluster expansion basis functions will be sparsified iteratively. In this way a machine learning potential that covers the complete alloy phase space will be developed. Then, the phase diagram of the alloy will be predicted based on atomistic simulations alone.

Expected Results:
The key result will be an efficient machine learning interatomic potential for a multi-component alloy together with its predicted phase diagram. This has not been achieved to date and will form the basis for the publication of several papers. Furthermore, transferable knowledge and computer code will be generated that will enable the fast, largely automated parameterization of other multi-component alloys and the computation of their phase diagrams.

Methods:
machine learning potential, atomic cluster expansion, density functional theory, sampling and screening, high-throughput computation, materials data science, free energy computation/reversible scaling

Candidate Requirements: MSc in Physics, Materials Science, Chemistry, or a related discipline. Strong mathematical and programming skills. Keen interest to conduct research in a team and on your own. Willingness to learn. Motivation to push boundaries. Good frustration tolerance. Good English language skills.

Motivation for CSC application (max 250 words): The PhD candidate will be embedded in a thriving and enthusiastic team that develops machine learning interatomic potentials in collaboration with leading research groups from around the world. The PhD candidate will be integrated into the ICAMS graduate school. Methodological training will be available as required.