CSC-RUB PhD Project Proposal

Title: Atomic cluster expansion for water at surfaces

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: Ralf Drautz, Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-University Bochum

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 the computation of complex chemical rearrangements.
The simulation of electrocatalytic reactions for hydrogen formation at surfaces is challenging. Many machine learning potentials have great difficulties to describe the transition metal catalyst surface in contact with water and the reactants in a uniform manner.

Study objective:
We will work towards simulating hydrogen formation in electrocatalytic reactions. To this end an atomic cluster expansion machine learning potential will be parameterized for water in contact with a transition metal surface. Then the water – metal interface will be studied with molecular dynamics simulations. Time permitting ions will be parameterized and embedded in water.

Expected Results:
The key result will be an efficient machine learning interatomic potential for water in contact with a transition metal surface. Transferable knowledge and computer code will be generated that will enable the fast, largely automated parameterization of related materials systems.

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.