POTENTIALS

TECHNISCHE UNIVERSITÄT DARMSTADT

FACHGEBIET MATERIALMODELLIERUNG

PhD/Postdoc position immediately available for three years in the Materials Modelling Division at Technische Universität Darmstadt (Germany).

Topic: Interatomic potentials for amorphous solids from second principles.

Prerequisites:

- Master of Science in the field of Materials Science, Physics, Chemistry or comparable with good knowledge of Solid State Physics.
- Sound communication skills in English.
- Experience with molecular dynamics (MD) simulations, density functional theory (DFT) calculations and programming skills (preferably in python) are meriting.

Project description:

This project is part of a larger research initiative consisting of a total of six scientific projects that seek to generate, validate and quantify interatomic potentials in a systematic and thermodynamically consistent way.

At present, fitting schemes for interatomic potentials are starting from training data serving for the fitting process, that is related to energies and forces specific to a set of given atomic configurations (typically various crystalline bulk phases, including hypothetic and defective ones). The testing data set is similar to the training data set, but typically complemented by data describing more complex scenarios, like melting, diffusional transport, deformation behaviour or temperature-dependent free energies. Because of the vastness of the parameter space and the wide range of possible properties that might be of interest, it is, however, not clear when to conclude that the potential fitting is complete and that a suitable parameter set has been determined. At present no established universal validation scheme for potentials exists. Moreover, for most material classes, there is neither a parametrization that is covering both glassy and crystalline states in a fully realistic way.

In this project, the main objective is to devise robust strategies for the development of interatomic potentials, which are satisfyingly describing both, crystalline and amorphous states of matter, that can be extended to multi-component systems by using well defined training data set obtained from first-principles calculations. Specifically we will focus on Cu-Zr-(Al) and Si-O-(C) systems.

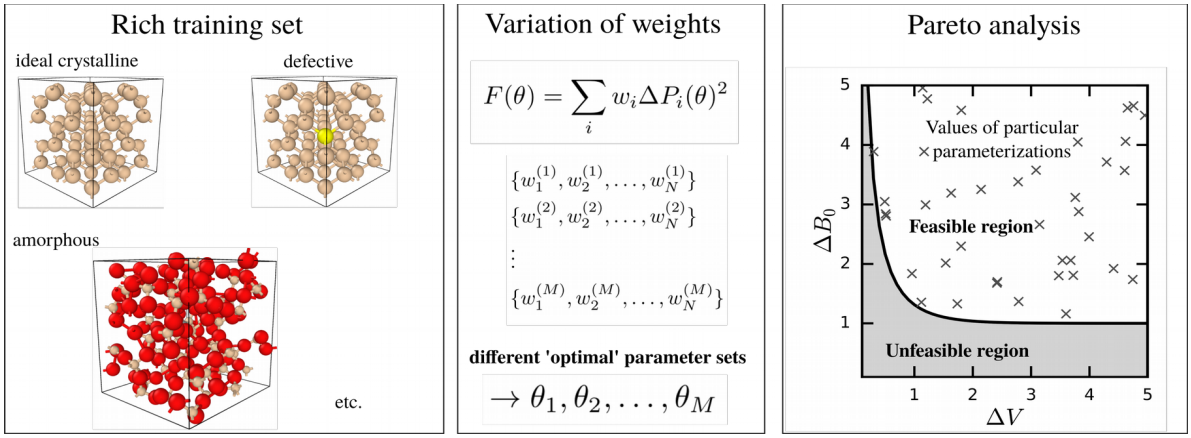

Figure 1. Strategy for deriving and quantifying the quality of various parameterizations of interatomic potentials describing both crystalline and amorphous states of matter. (i) A rich database containing in crystalline, defective and amorphous model geometries will be generated on the basis of DFT calculations. (ii) Interatomic potenitals will be fitted to reproduce these properties. Thereby, the weight for each property will be systematically varied, leading to a whole zoo of optimal parameter sets. (iii) These parameter sets will be categorized by means of Pareto analysis. Eventually various types of potentials (EAM, Tersoff, Neural-Network potentials, and second-principles potentials) will be explored.

Tasks: Figure 1 summarizes the strategy that will be pursued in this project. In detail, the successful candidate will

- refine and/or extend existing strategies for generating virtual amorphous structures from first-principles calculations in order to provide thermodynamically relevant and consistent training data sets for fitting of the potentials;
- use these data together with well-known training data sets for the crystalline phases in order to generate parameter families that can be classified in terms of their vicinity to the Pareto surface and thus allow for a validation and quantification of the quality of the potential;
- extend existing potentials for the binaries Cu-Zr and Si-O by adding a third component following the systematic approach described before;
- explore functional forms for second-principles and/or neuronal network potentials to obtain reliable and transferable interatomic potentials for amorphous/solid materials.

Duties: The successful candidate will

- perform all necessary scientific research;
- present results at regular group meetings and international conferences;
- participate in the teaching activities of the Materials Modelling Division.

Opportunities: The successful candidate will

- be part of a research initiative that aims at pioneering a systematic universal validation and quantification scheme for thermodynamically consistent interatomic potentials;
- work in an international research environment at TU Darmstadt;
- have the opportunity for a 2 month external visit abroad;
- get the possibility to obtain a doctoral degree in Materials Science.

Salary: According to the collective agreements on salary scales, which apply to the Technische Universität Darmstadt (TV-TU Darmstadt).

The Technische Universität Darmstadt intends to increase the number of female employees and encourages female candidates to apply. In case of equal qualifications applicants with a degree of disability of at least 50% will be given preference. The Technische Universität Darmstadt is certified as a family-friendly university and offers a dual career program.

Principle investigators of the Potentials initiative:
Prof. Dr. Karsten Albe, Technische Universität Darmstadt
Prof. Dr. Jörg Behler, Georg-August Universität Göttingen
Prof. Dr. Ralf Drautz, ICAMS Bochum (Speaker of the initiative)
Dr. Matous Mrovec, ICAMS Bochum
Prof. Dr. Jörg Neugebauer, Max-Planck Institut für Eisenforschung Düsseldorf
Dr. Alexander Stukowski, Technische Universität Darmstadt
Dr. Jochen Rohrer, Technische Universität Darmstadt

Contact, further information and application:
Dr. Jochen Rohrer, rohrer@mm.tu-darmstadt.de, +49 6151 16 21 893