PhD/Postdoc position available in the Materials Modelling Division at Technische Universität Darmstadt, Germany

**Topic:** Automated calculation of phase diagrams from interatomic potentials used in materials science

**Duration:** Up to 3 years, full-time position

**Requirements:**
- Master of Science in the field of Materials Science, Physics, Chemistry or similar, with good knowledge of statistical physics and thermodynamics of materials
- Sound communication skills in English
- Prior experience with atomistic modelling techniques (e.g. classical molecular dynamics (MD), density functional theory (DFT), Monte-Carlo methods) and software engineering projects (Python language)

**Project description:**

The predictive power of materials simulations based on classical interatomic potentials (e.g. molecular dynamics) depends on the transferability and quality of the underlying interaction models, which typically represent an approximation of the true (i.e. ab initio) atomic interactions. This project seeks to develop novel validation methods and tools for assessing the performance of such empirical interatomic potentials. A stringent validation test would be to calculate the predicted phase diagrams for the solid and liquid phases of single- and multi-component systems. Such a test would immediately reveal whether a given potential shows artifacts such as the absence of thermodynamically stable phases, the occurrence of unphysical "ghost" states, or inaccurate transition temperatures. However, presently available approaches to compute phase diagrams are numerically too expensive to be applied routinely, particularly when targeting an accuracy of a few K, comparable to experimentally derived phase diagrams. We plan to develop innovative approaches and software tools that allow to compute accurate phase diagrams at a fraction of the presently necessary computational effort.

The project is part of a German research initiative with six scientific projects that all seek to generate, validate and quantify interatomic potentials in a systematic and thermodynamically consistent way. More specifically, the advertised position is part of a joint project of the Materials Modelling Division at TU Darmstadt and the Max Planck Institute for Iron Research in Düsseldorf (with Professor J. Neugebauer as Co-PI). Furthermore, Professor Paul Erhart at Chalmers University in Gothenburg, Sweden, is going to serve as an external collaborator.

**Tasks:** The successful candidate will have to
- benchmark existing computational sampling schemes for calculating phase transitions and other thermodynamic properties from interatomic potential models;
- develop adaptive protocols and computational tools for high-throughput, automated phase diagram calculations with built-in convergence checking;
- implement these protocols in the pyiron (pyiron.github.io) simulation platform for use by the other projects of the initiative and eventual dissemination among the scientific community;
- publish the developed methodologies in scientific journals;
- collaborate with and coordinate the work with the partner research group at the Max Planck Institute;
- present results at regular group meetings and international research conferences;
- actively participate in the teaching activities of the Materials Modelling Division.
Opportunities: The successful candidate will
- be part of a new 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 research stay (e.g. in Gothenburg);
- get the chance to obtain a doctoral degree in Materials Science.

Salary: According to the collective agreements on salary scales that 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

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