

Atomistic computation of phase diagrams

Online seit 30.01.2025 | 2025-01-30-923368 | Wissenschaftliche:r Mitarbeiter:in

Stellenbeschreibung

The Chair of Atomistic Modelling and Simulation at ICAMS is looking for a **research associate (m,f,x), for 4 years, 39.83 hours per week, TVL E13**

The Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) focuses on the development and application of a new generation of simulation tools for multi-scale materials modelling with the aim of reducing development cost and time for new materials. The different length scales from the atomic structure to macroscopic properties of materials are bridged by an interdisciplinary team of scientists from engineering, materials science, chemistry, physics and mathematics.

Machine learning interatomic potentials enable the representation of atomic interactions with quantum mechanical accuracy. The efficiency of machine learning interatomic potentials allows for simulations with thousands of atoms and millions of time steps, which can be exploited for the computation of free energies. With the advertised position we are targeting the computation of complete multicomponent phase diagrams from machine learning interatomic potentials, including all relevant contributions to the free energy of the competing phases.

Your tasks:

- Theory of phase transformation and phase diagram calculation from atomic interactions
- Development of efficient strategies and algorithms for the computation of phase diagrams
- Implementation and application of software for semi-automated computation of phase diagrams from interatomic potentials

Anforderungsprofil & Qualifikationen

We expect an excellent or very good doctoral degree (PhD) in physics, chemistry, materials science or related disciplines and a strong expertise in code development, atomistic simulation, machine learning and statistical mechanics, in particular:

- Background in atomistic theory
- Proven track record in thermodynamic simulation of materials
- Strong expertise in code development
- Experience with machine learning

Our offerings:

- Challenging and varied tasks with a high degree of personal responsibility
- Support from and collaboration with competent colleagues
- team-oriented collaboration in a committed, international and appreciative team
- a friendly and cooperative environment
- Options for location-flexible work

Additional information:

At the request of the applicant (m,f,x), the staff council may be involved in selection interviews. <https://www.wpr.ruhr-uni-bochum.de/>

If the position is funded by third-party funds the employee has no teaching obligation.

German language courses are offered by the University Language Center (ZFA) in the field of German as a Foreign Language (DaF).

<https://www.daf.ruhr-uni-bochum.de/sbgk/index.html.en>

You can find information about TVL at: <https://oeffentlicher-dienst.info/>

The Ruhr-Universität Bochum is one of Germany's leading research universities, addressing the whole range of academic disciplines. A highly dynamic setting enables researchers and students to work across the traditional boundaries of academic subjects and faculties. To create knowledge networks within and beyond the university is RUB's declared aim.

The Ruhr-Universität Bochum stands for diversity and equal opportunities. For this reason, we favour a working environment composed of heterogeneous teams, and seek to promote the careers of individuals who are underrepresented in our respective professional areas. The Ruhr-Universität Bochum expressly requests job applications from women. In areas in which they are underrepresented they will be given preference in the case of equivalent qualifications with male candidates. Applications from individuals with disabilities are most welcome.

Contact details for your application:

Prof. Dr. Ralf Drautz, Phone: +49234 32 29310

Travel expenses for interviews cannot be refunded.

For information on the collection of personal data in the application process see:
<https://www.ruhr-uni-bochum.de/en/information-collection-personal-data-application-process>.

We are looking forward to receiving your application with the specification ANR: 4225 until 10.02.2025, send by e-mail to the following address: atom-office@icams.rub.de

Please get in touch with the contact person named above if you would like to use an alternative application channel.

Vorteile für Mitarbeitende

- Vergünstigtes Jobticket
- Arbeitsplatz in lebendiger Metropolregion

Stellenmerkmale

Beschäftigungsart	Wissenschaftliche:r Mitarbeiter:in
Beschäftigungsumfang	Vollzeit (befristet)
Home Office	Nein
Bewerbungslink	https://jobs.ruhr-uni-bochum.de/jobposting/ae628a168cded2bd42ce715aae4806a467de8294?ref=stellenwerk

Kontaktdaten

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<https://uni.ruhr-uni-bochum.de/de/stellenangebote>