

# PhD position in atomistic simulation of H in Ni-base superalloys with machine-learning interatomic potentials

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## Stellenbeschreibung

The Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) is looking for a **research associate (m,f,x) in atomistic simulation of H in Ni-base superalloys with machine-learning interatomic potentials, for 3 years, 29,8725 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.

The urgent need to decarbonise our society leads to core challenges in the transition from fossil to H-based fuels that affect also gas turbines for power generation. It is becoming increasingly critical that hydrogen (H) is integrated into materials design principles and in lifetime predictions of engineering parts. The goal of this project on Ni-based superalloy is to reveal the influence of H on the microstructure, the interaction of H with different alloying elements and the influence of H on creep. The PhD student will perform large-scale atomistic simulations with accurate accounting for H-metal interactions. This includes density-functional theory calculations and the development of machine-learning interatomic potentials based on the atomic-cluster expansions. The PhD project is embedded in a collaboration with experimental partners at the Ruhr-University Bochum (creep experiments of H-charged samples) and the Max-Planck-Institute for Sustainable Materials, Dusseldorf (H-sensitive scale-bridging characterization) and the industry partner ThermoCalc, Sweden (thermodynamic modelling).

### Your tasks:

- High-throughput density-functional theory calculations for H in Ni-base superalloys
- Development of machine-learning interatomic potentials for H in Ni-base superalloys on the basis of the atomic cluster expansion
- Large-scale atomistic simulations of the influence of H on phase stability and mechanical properties

- Close collaboration with experimental partners (Ruhr-University Bochum and Max-Planck-Institute for Sustainable Materials, Dusseldorf) and with industrial partner (ThermoCalc, Sweden)

## Anforderungsprofil & Qualifikationen

### Your profile:

- We expect a very good MSc degree in physics, chemistry, materials science or related disciplines with strong background or interest in software development, atomistic simulation and machine learning

### Our offerings:

- Challenging and varied tasks with a high level of personal responsibility
- Team-oriented cooperation in a committed, international and appreciative team
- a dynamic environment
- an open working atmosphere
- a job in the heart of the lively Ruhr metropolitan region with its diverse cultural offerings

### 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:

Thomas Hammerschmidt, Phone: +49234 32 29375

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: 3755 until 28.10.2024, send by e-mail to the following address: [thomas.hammerschmidt@rub.de](mailto:thomas.hammerschmidt@rub.de)**

## Vorteile für Mitarbeitende

- Sport- und Freizeitangebote
- Weiterbildungsmöglichkeiten
- Vergünstigtes Jobticket
- Arbeitsplatz in lebendiger Metropolregion

## Stellenmerkmale

Beschäftigungsart	<b>Wissenschaftliche:r Mitarbeiter:in</b>
Beschäftigungsumfang	<b>Teilzeit (befristet)</b>
Home Office	<b>Nein</b>
Bewerbungslink	<a href="https://jobs.ruhr-uni-bochum.de/jobposting/bd9f134568acc42aec651f5317abf1a4f5d5d285?ref=stellenwerk">https://jobs.ruhr-uni-bochum.de/jobposting/bd9f134568acc42aec651f5317abf1a4f5d5d285?ref=stellenwerk</a>

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## Kontaktdaten


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Kontakt

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Webseite

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