Helmholtz-Zentrum Dresden-Rossendorf e.V.

With cutting-edge research in the fields of ENERGY, HEALTH and MATTER, around 1,500 employees from more than 70 nations at Helmholtz-Zentrum Dresden-Rossendorf (HZDR) are committed to mastering the great challenges facing society today. The Center for Advanced Systems Understanding (CASUS) is a German-Polish research center for data-intensive digital systems research. We invite you to be part of our diverse and international team at CASUS in Görlitz. The Department of Machine Learning for Materials Design is looking for a

Postdoc (f/m/d): Machine Learning for Materials Modeling.

Scope of Your Job In this role, you will contribute to ongoing research efforts in developing scalable machine learning models for applications in materials science. Your tasks include contributing to the development of the Materials Learning Algorithms software package and applying machine learning models beyond the scope of machine learning interatomic potentials. Target applications include heterogeneous materials and nanoscale electronics.

City: Görlitz; Starting date (earliest): 01/07/25; Duration: two years; Remuneration: TVöD Bund; Reference number: 2025/69; Closing date: 31/05/25

Working field

- Data Generation: Generate datasets using first-principles simulations software (density functional theory and related codes)
- Automated Workflows: Utilize automated workflows on high-performance computing systems for efficient data generation
- Model Development: Develop transferable machine learning models and apply them to answer questions in materials science
- Collaboration: Collaborate with peers, both within and beyond the research group, on related research topics
- Mentoring: Supervise and mentor junior group members
- International Engagement: Collaborate with our international partners
- Dissemination: Present your scientific findings at academic venues and publish research in peer-reviewed journals

Requirements

- Completed university studies (PhD) in the field of Physics, Computer science, Materials science, Chemistry, or a related field
- Proficiency in programming languages (Python, C/C++, Julia)
- Background in machine learning methods
- Experience in developing, training, and tuning machine learning models
- Prior exposure to collaborative software development and version control systems (Git)
- Experience with electronic structure and molecular dynamics simulation codes

(VASP, QuantumEspresso, CP2K, LAMMPS)
- Motivation to work collaboratively in a team-oriented environment
- Excellent communication skills

What we offer

- A vibrant research community in an open, diverse and international work environment
- Scientific excellence and extensive professional networking opportunities
- Salary and social benefits in accordance with the collective agreement for the public sector (TVöD-Bund) including 30 days of paid holiday leave, company pension scheme (VBL)
- We support a good work-life balance with the possibility of part-time employment, mobile working and flexible working hours
- Numerous company health management offerings
- Employee discounts with well-known providers via the platform Corporate Benefits
- An employer subsidy for the "Deutschland-Ticket Jobticket"

Application

We look forward to receiving your application documents (including cover letter, CV, diplomas/transcripts, etc.), which you can submit via our online-application-system: https://www.hzdr.de/db/Cms?pNid=490&pLang=en&pOid=74651

More information at https://stellenticket.de/193751/TUBS/
Offer visible until 15/05/25