

Technische Universität Dresden (TUD), as a University of Excellence, is one of the leading and most dynamic research institutions in Germany. Founded in 1828, today it is a globally oriented, regionally anchored top university as it focuses on the grand challenges of the 21st century. It develops innovative solutions for the world's most pressing issues. In research and academic programs, the university unites the natural and engineering sciences with the humanities, social sciences and medicine. This wide range of disciplines is a special feature, facilitating interdisciplinarity and transfer of science to society. As a modern employer, it offers attractive working conditions to all employees in teaching, research, technology and administration. The goal is to promote and develop their individual abilities while empowering everyone to reach their full potential. TUD embodies a university culture that is characterized by cosmopolitanism, mutual appreciation, thriving innovation and active participation. For TUD, diversity is an essential feature and a quality criterion of an excellent university. Accordingly, we welcome all applicants who would like to commit themselves, their achievements and productivity to the success of the whole institution.

At the **Faculty of Chemistry and Food Chemistry**, the **Chair of Theoretical Chemistry** offers a position as

Research Associate / PhD Student / Postdoc (m/f/x)

(subject to personal qualification employees are remunerated according to salary group E 13 TV-L)

starting **as soon as possible**. The PhD Student position entails 65% of the fulltime weekly hours and is, subject to the availability of resources, limited to 3 years. The Postdoc position entails 100 % of the fulltime weekly hours and is limited to 2 years. The period of employment is governed by the Fixed Term Research Contracts Act (Wissenschaftszeitvertragsgesetz - WissZeitVG). The position offers the chance to obtain further academic qualification (usually PhD).

Tasks: The project aims at developing and employing density-functional based and data-driven methods for designing (i) novel ionic high-entropy and (ii) two-dimensional compounds. The successful candidates will leverage dedicated machine learning techniques for thermodynamic and electronic analysis. An accurate description of thermodynamic stability is crucial for materials design especially for ionic systems such as oxides. While currently used density-functional approaches have limited predictive power, the candidate will develop a novel universal data-driven method combining the merits of previous correction schemes and machine learning to design ionic high-entropy and novel two-dimensional materials and their electronic and magnetic properties. The work will be carried out in close collaboration with various local and international collaborators necessitating a strong commitment to scientific communication and networking.

Requirements: a university degree (M. Sc. or equivalent) and if applicable a PhD degree in chemistry, physics or theoretical/computational materials science and profound knowledge in computational and theoretical physics/chemistry. Capability of excellent communication, team work – also with experimental partners – is essential. Good scripting and programming skills (C++, Python). Skills in machine learning, high-performance computing, solid-state physics/chemistry, materials thermodynamics, 2D compounds, and density-functional theory (VASP, Quantum Espresso) are welcome.

What we offer: We offer a position with a competitive salary in one of Germany's most attractive research environments. TU Dresden provides outstanding working, research, and networking possibilities. The positions will be in the established Dresden-concept Research Group "Autonomous Materials Thermodynamics" of Dr. Rico Friedrich at the Chair of Theoretical Chemistry (Prof. Thomas Heine) and Helmholtz-Zentrum Dresden-Rossendorf. An overview of the research of the group can be

found at <https://hzdr.de/automatlab>. It maintains strong ties with the local experimental groups of TU Dresden and the institutes of the DRESDEN-concept network. The chair hosts its own computer cluster and has full access to the high-performance computing (HPC) infrastructure at ZIH Dresden, one of Germany's leading HPC centres. Dresden, the capital of the State of Saxony, is a city with a beautiful historical centre and offers a high standard of living with high ratings in housing, safety, and healthcare.

TUD strives to employ more women in academia and research. We therefore expressly encourage women to apply. The University is a certified family-friendly university and offers a Dual Career Service. We welcome applications from candidates with disabilities. If multiple candidates prove to be equally qualified, those with disabilities or with equivalent status pursuant to the German Social Code IX (SGB IX) will receive priority for employment.

Please submit your detailed application including a motivation letter, curriculum vitae with publications (if any), copies of academic certificates, and contact details (including email addresses and phone numbers) of two references by **April 19, 2024** (stamped arrival date of the university central mail service or the time stamp on the email server of TUD applies), preferably via the TUD SecureMail Portal <https://securemail.tu-dresden.de> by sending it as a single pdf file **named "Application_PhD_Automat_your_Last_and_First_name.pdf"** and the **subject line "Application PhD Automat Lastname Firstname"** to rico.friedrich@tu-dresden.de or to: **TU Dresden, Fakultät Chemie und Lebensmittelchemie, Professur für Theoretische Chemie, z. Hd. Dr. Rico Friedrich, Helmholtzstr. 10, 01069 Dresden, Germany**. Please submit copies only, as your application will not be returned to you. Expenses incurred in attending interviews cannot be reimbursed.

Reference to data protection: Your data protection rights, the purpose for which your data will be processed, as well as further information about data protection is available to you on the website: <https://tu-dresden.de/karriere/datenschutzhinweis>.