TUD Dresden University of Technology, as a University of Excellence, is one of the leading and most dynamic research institutions in the country. 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 Mechanical Science and Engineering, Institute of Materials Science**, the **Chair of Materials Science and Nanotechnology** (Prof. Cuniberti) offers a position as

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

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

starting at the **earliest possible date**. The position is limited to 36 months with the option of extension. The period of employment is governed by the Fixed Term Research Contracts Act (Wissenschaftszeitvertragsgesetz – WissZeitVG). The position aims at obtaining further academic qualification (usually PhD). Balancing family and career is an important issue. The position is generally suitable for candidates seeking part-time employment. Please indicate your request in your application.

**Tasks:** The aim of the research work within the **Collaborative Research Center CRC1415 “Chemistry of synthetic 2D materials”** is to combine quantum mechanical (QM) methods with state-of-the-art machine learning (ML) techniques to investigate and predict the electronic and magnetic properties of the building blocks in two-dimensional (2D) polymers (e.g., (a)chiral covalent organic frameworks). This will enable us to define data-driven design rules that will be integrated into generative AI frameworks for the design of novel 2D polymers with desired QM properties for catalysis and energy storage. The computational work will be performed in close collaboration with synthetic chemists at TU Dresden to validate the synthesis of the novel materials, ensuring an interdisciplinary working environment. The project would require the candidate to perform extensive QM calculations using density functional theory and to develop python-based tools for data analysis. Additionally, further development of ML-based computational workflows to explore structure-property and property-property relationships will be a key task. To this end, the successful applicant will be integrated into the research activities of CRC1415 and at the Chair of Prof. Cuniberti.

**Requirements:** university degree (Master/Diploma) in physics, chemistry, materials science, engineering or similar. Knowledge and practical experience in quantum mechanical methods as well as in machine learning approaches (force field development, generative models) are required. A high degree of commitment, interdisciplinary thinking, the ability to work in a team and independently, as well as excellent communication and writing skills in English are required. Previous hands-on experience with Fortran, Python, and PyTorch is highly desirable. Previous computational experience in research projects concerning organic molecules and materials is desirable, but not a prerequisite. 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 your Curriculum Vitae (max. 4 pages), motivation letter (max. 1 page), transcripts of bachelor or master degree (in English or German), and a recommendation letter from a senior/junior research scientists by **September 16, 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](https://securemail.tu-dresden.de) by sending it as a single pdf file to [jobs.nano@tu-dresden.de](mailto:jobs.nano@tu-dresden.de) or to: **TU Dresden, Fakultät Maschinenwesen, Institut für Werkstoffwissenschaft, Professur für Materialwissenschaft und Nanotechnik, Herrn Prof. Gianaurelio Cuniberti, 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](https://tu-dresden.de/karriere/datenschutzhinweis).