

The Faculty of Chemistry at the Georg-August-Universität Göttingen welcomes applications for two

### Ph.D. positions (f/m/d)

at the Theoretical Chemistry group (Group of Prof. Reinhard Maurer). The positions are remunerated with 65% E 13 TV-L (corresponding to 25.87 hours per week) with a limited contract of 4 years. The positions should be filled by 01.09.2026 at the latest. Salary: Pay grade 13 TV-L (65%).

#### Your duties

- You will conduct individual and collaborative research projects in theoretical chemistry and computational simulation,
- continually update your own knowledge and understanding in the field and translate knowledge of advances in the subject area into research activity,
- write up research work for publication,
- present information on research progress and outcomes to team members and collaboration partners,
- contribute positively to a collegiate research environment by supporting students and engaging in group activities such as meetings and seminars,
- contribute to teaching of courses as defined in Section 31 of the Higher Education Act of Lower Saxony (NHG) and administering of examinations.

#### Your profile

- You hold (or are in the process of concluding) a Master's degree in Chemistry, Physics or a related discipline,
- ability to work collaboratively and effectively within an interdisciplinary and diverse team,
- You have experience in academic writing.
- You have an interest and background in surface chemistry, quantum chemistry, or computational simulation.
- You have an excellent command of written and spoken English.
- experience with programming (e.g. Python, Julia) and simulation methods (e.g. molecular or quantum dynamics) is advantageous.

This post is designed to serve in fostering young researchers and scientists and give the successful applicant the opportunity to pursue a doctoral degree.

Another requirement for employment is a commitment from the doctoral supervisors to supervise the successful applicant in the doctoral program within the framework of the GAUSS doctoral program.

We are looking for Ph.D. students working in the following areas:

**Project 1:** Simulation of catalytic nanoparticles and their interaction with adsorbed molecules for light-induced chemical reactions. This project will involve state-of-the-art electronic structure calculations and mixed quantum-classical dynamics simulation tools to study industry-relevant reactions such as CO hydrogenation or ammonia decomposition. A key outcome of this project will be the design, through doping, of nanostructured catalytic materials with high reaction selectivity and efficiency, along with a deep understanding of the underlying correlation between material structure and electronic properties. You will contribute to the development of new dynamic software and machine learning methods for the computational design of novel catalytic materials.

**Project 2:** Development of novel quantum mechanical (QM) and quantum embedding based methods to simulate excited states at metal-organic interfaces. In this role, you will carry out first-principles calculations, design and implement advanced embedding techniques, and integrate these into spectroscopic prediction workflows and machine-learning surrogate models to enable accurate simulations of excited-state dynamics for small molecules interacting with complex surfaces.

**Who we are:** In the Maurer group, we aim to develop computational simulation methodology to study quantum phenomena at surfaces with applications ranging from photocatalysis, to nanotechnology and electrochemistry. Our goal is to combine electronic structure theory, molecular and quantum dynamics methodology, and machine learning methods to achieve an accurate yet computationally feasible description of complex phenomena in materials and at solid/gas and solid/liquid interfaces. You will join a large, international and interdisciplinary research group that provides a collaborative and supportive environment.

The University of Göttingen is an equal opportunities employer and places particular emphasis on fostering career opportunities for women. Qualified women are therefore strongly encouraged to apply in fields in which they are underrepresented. The university has committed itself to being a family-friendly institution and supports their employees in balancing work and family life. The mission of the University is to employ a greater number of severely disabled persons. Applications from severely disabled persons with equivalent qualifications will be given preference.

The documents are to be submitted by electronic form (single PDF file) to the e-mail [rmaurer@chemie.uni-goettingen.de](mailto:rmaurer@chemie.uni-goettingen.de) . The deadline for submission is 20:00 (CET) on Thursday May 14, 2026.

If you have any questions, please contact us via e-mail [rmaurer@chemie.uni-goettingen.de](mailto:rmaurer@chemie.uni-goettingen.de) .



**Please note:**

With submission of your application, you accept the processing of your applicant data in terms of data-protection law. Further information on the legal basis and data usage is provided in the Hinweisblatt zur Datenschutzgrundverordnung (DSGVO) <https://www.uni-goettingen.de/hinweisdsgvo>

Link to Georg-August-Uni website with the official job posting:

<https://www.uni-goettingen.de/de/644546.html?details=3296>