

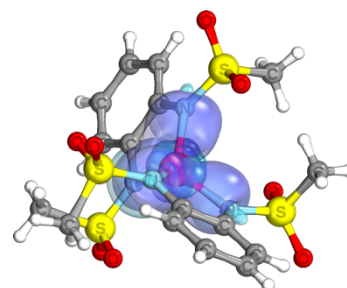
**PHD-POSITION FOR MODELLING OF MOLECULAR QUANTUM BITS
(m/f/d, E13 TV-L, temporary for the duration of 3 years)**

The University of Stuttgart represents outstanding, world-renowned research and first-class teaching in one of Europe's most dynamic industrial regions. As a reliable employer, the university supports and promotes the academic careers of its researchers. It is proud of its employees, who currently come from over 100 different countries. The university is a partner for knowledge and technology transfer and focuses on multidisciplinary.

The Institute for Theoretical Chemistry was founded more than 50 years ago as the first research institution in Germany with this dedicated focus. Today three independent research groups cover a number of topical themes in theoretical chemistry ranging from high-accuracy methods for electronic and vibrational structure to machine-learning models to treat condensed phase problems. The institute also contributes to the SimTech cluster of excellence at the University of Stuttgart.

The project:

Applications for this project are invited by the research group of Professor Köhn. The task is to further develop theoretical models to understand the properties of molecular quantum bits. These are molecular systems with unpaired spins, like (poly)radicals or transition metal complexes, which are of interest as building blocks for molecule-based quantum technologies like quantum sensing or quantum information processing. Particular interest lies on the understanding of the lifetimes of quantum states, which is determined by interactions with vibrational degrees of freedom. The project will include close collaboration with experimental groups from, e.g., physical or inorganic chemistry, as well as with groups from physics.

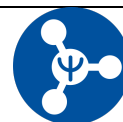


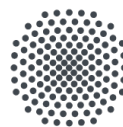
Your tasks:

- You will study the properties of the molecular quantum bits by a range of quantum-chemical methods (from DFT to multireference correlation methods).
- You implement new concepts to understand the complex interactions in these systems, e.g by developing spin Hamiltonian models or using concepts from machine learning.
- You support the research of our experimental partners by tailored model simulations and communicate the results to them.
- In addition, you will participate in the teaching activities at the institute at the undergraduate level.

Your qualifications:

- Very good Master of Science degree (or equivalent) in Chemistry or Physics or closely related fields.
- A strong background in quantum mechanics and electronic structure theory.
- Hands-on experience with scientific computing and basic programming knowledge, e.g. using Python.
- Excellent English skills (spoken and written).
- Ability to work independently and self-responsibly both on your own and in a team. In this respect, strong skills in communication, and data presentation and visualization are essential.





We offer:

- An inspirational and supportive research environment at our institute and the University of Stuttgart with ample networking opportunities and much room for your own research ideas.
- An interdisciplinary nationally and internationally well-connected research team.
- Fully funded conference and work-shop visits.

Please submit your complete application, including one-page motivation letter, academic CV, one letter of reference, as well as academic certificates and transcript of records to

apply@theochem.uni-stuttgart.de

until December, 15, 2023. If you have any questions regarding this application, please contact us via the same email address.

At the University of Stuttgart, we actively promote diversity among our employees. We have set ourselves the goal of recruiting more women scientists and employing more people with an international background, as well as people with disabilities. We are therefore particularly pleased to receive applications from such people. Regardless, we welcome any good application.

Women who apply will be given preferential consideration in areas in which they are underrepresented, provided they have the same aptitude, qualifications and professional performance. Severely disabled applicants with equal qualifications will be given priority.

As a certified family-friendly university, we support the compatibility of work and family, and of professional and private life in general, through various flexible modules. We have an employee health management system that has won several awards and offers our employees a wide range of continuing education programs. We are consistently improving our accessibility. Our Welcome Center helps international scientists get started in Stuttgart.

