

PhD position for three years in the field of electronic structure theory and materials modeling:

Molecular quantum materials offer a unique platform to study fundamental physical effects caused by strong electron correlation, while also having the potential for large-scale applications due to their simple chemical modification, potentially low production cost, and versatile mechanical properties.

Due to the complex interactions in these materials, understanding how the charge and spin degrees of freedom of electrons interact at the microscopic level is difficult. However, this understanding is essential for identifying the descriptors that allow for the systematic modification of existing and the design of new materials with enhanced properties or even properties on demand. The goal of this project is to develop a theoretical framework that allows for systematically improvable ab initio simulations of these materials.

Your role:

- Develop and apply state-of-the-art electronic structure methods to simulate organic quantum materials.
- Method development, i.e., quantum embedding techniques and diagrammatic electronic structure approaches
- Software development and high-performance computing applications.

Your background:

- Master's degree in chemistry, physics, materials science, or a related field.
- Strong background in theoretical chemistry, quantum chemistry, and/or electronic structure theory.
- Programming experience (preferably Python); familiarity with Linux and high-performance computing.
- Excellent problem-solving skills and the ability to work both independently and in a team.
- Strong written and spoken English skills.

What to expect:

- A dynamic, highly motivated young research group with close scientific mentoring.
- Access to international collaborations and an interdisciplinary research environment at the DESY campus.
- Training opportunities, including participation in summer/winter schools and conferences.
- Access to state-of-the-art computing facilities.
- Living in the vibrant city of Hamburg with a rich cultural

scene and an international atmosphere.

Website:

<https://www.chemie.uni-hamburg.de/institute/ac/arbeitsgruppen/toelle.html>