

Two fully funded 3-year PhD positions in coupled-cluster theory development

Interested in thinking deeply about electronic structure? One of the most interesting problems in electronic structure is strong electron correlation. It appears in bond breaking, transition-metal chemistry, and catalysis. We are looking for two motivated PhD students to join the FWF ASTRA Merit project “Coupled-Cluster Methods for Strongly Correlated Materials”. You will be supervised by Dr. Pavel Pokhilko, the Principal Investigator (PI) of the project. With his guidance and support, each student will work on an individual project focused on the development of new coupled-cluster methods for strongly correlated systems. Subsequently, you will apply these methods to magnetic materials and catalysts.

You will experience the full cycle of electronic-structure method development:

- Development of coupled-cluster and many-body methods.
- Strong electron correlation and magnetism.
- Applications to realistic systems.
- Industry-level C++ programming.

Desired qualifications:

- An MSc degree (or equivalent) in chemistry, physics, or a related field. The degree must be obtained before the start of the employment.
- Good written and spoken English. German skills are not required.
- Knowledge of quantum mechanics and quantum chemistry.
- Experience in programming.

We especially welcome applicants from all over the world who enjoy mathematical reasoning and difficult conceptual problems.

What we offer:

The anticipated start is **January 1, 2027**. In exceptional circumstances, some flexibility regarding the starting date may be possible.

Dr. Pokhilko’s team will be embedded in Prof. Leticia González’s group at the University of Vienna. You will have a unique opportunity to interact with group members working on a broad range of scientific problems, such as semiclassical nonadiabatic dynamics, quantum dynamics, photocatalysis, solvation, and other actively investigated areas. The group offers a friendly and welcoming international working environment with multiple opportunities for cooperation. The University of Vienna is the largest university in Austria. Located in the heart of Vienna, you’ll find something for every taste—from a vibrant cultural scene and diverse cuisine to easy access to nature, all within a walkable city.

You will have opportunities to attend conferences and present your research.

The position is fully funded (30h per week—maximum for PhD candidates in Austria) with an employee's gross annual salary of € 39649 per year (before taxes), in accordance with the FWF guidelines. In Austria, salaries are paid in 14 installments per year. The contract is for 1 year, renewable up to 3 years in total upon mutual agreement. The contract has full social benefits including health insurance.

Application:

To apply, please contact Dr. Pavel Pokhilko directly at **pavel.pokhilko@univie.ac.at** and attach a cover (motivation) letter, CV, and academic transcript. In the cover letter, describe your motivation to join the project, specify your previous experience, and provide contact details for two references. Early applications are encouraged and will be reviewed immediately.