

# PhD Position in Theoretical Chemistry at Uni Vienna

The group of Leticia González at the Institute of Theoretical Chemistry, University of Vienna is offering a PhD position for a duration of 3 years (30 hours/week) starting as soon as possible. Information about the group can be found at <https://theochem.univie.ac.at/>.

You will work on light-induced reactions of transition-metal complexes in fields ranging from solar-energy harvesting to photocatalysis and photoemitters. To this aim, you will apply state-of-the-art theoretical methods and develop new computational strategies for their use in photodynamics simulations. Your work will establish a thorough understanding of the complex mechanisms of excited-state reactions of transition-metal complexes that combined with spectroscopic experiments from our collaborators will allow rational design of new and improved materials.

## Your Tasks

- Application of single and multi-reference quantum chemistry methods to study the electronic structure of transition-metal complexes
- Application of ab initio molecular dynamics methods to simulate the photodynamic processes
- Development of novel computational protocols for these simulations
- Preparation of scientific publications and dissemination of your results in international conferences
- Participation in teaching activities in theoretical chemistry at the undergraduate level

## Your Profile

- Master of science (chemistry, physics, computational science, or similar)
- Good knowledge in theoretical chemistry, especially on one or more of the following topics: excited-state quantum chemistry, ab initio molecular dynamics, quantum dynamics
- Hands-on experience with scientific computing and/or programming skills
- Strong communication, data presentation and data visualization skills
- Ability to work both independently and collaboratively.

**Interested?** Send a motivation letter, a CV and the names of two people who can tell about you, mentioning reference number 13069, either to the Job Center to the University of Vienna (<http://jobcenter.univie.ac.at>) or directly to me ([leticia.gonzalez@univie.ac.at](mailto:leticia.gonzalez@univie.ac.at)).

For more information on this position, please contact Prof. Leticia González:  
[leticia.gonzalez@univie.ac.at](mailto:leticia.gonzalez@univie.ac.at)