PhD position in theoretical chemistry at Uni Vienna

In the group of Philipp Marquetand at the Institute of Theoretical Chemistry, University of Vienna, a PhD position is available with a duration of 3 years (30 hours/week) starting August 2022 or later. Information about the group can be found at [http://marquetand.net/](http://marquetand.net/) and [https://theochem.univie.ac.at/](https://theochem.univie.ac.at/).

You will work on photochemistry simulations of processes on time scales of picoseconds and beyond. To this aim, you will develop and implement path-integral approaches and related methods for nonadiabatic dynamics, which you will interface with parameterized potentials / machine learning potentials. Possible applications include but are not limited to simulations of photochemical processes taking place in proteins, DNA or dye-sensitized solar cells.

**Your tasks:**

- Development of excited-state dynamics approaches for long-time-scale simulations in the gas phase and the condensed phase
- Application of the newly developed methods to molecular systems of photochemical interest.
- Preparation of scientific publications
- Participation in teaching as defined by the collective agreement, student services, and administration.

**Your profile:**

- Master of science (chemistry, physics, computational science or similar), ideally with a publication record.
- Good knowledge in theoretical chemistry, especially on one or more of the following topics: excited-state quantum chemistry, machine learning, molecular dynamics, thermostats, path-integral methods.
- Programming skills, preferably Python, Julia, Fortran.
- Hands-on experience with scientific computing, working on the Linux command line
- Strong communication, data presentation and visualization skills. Therefore, English is required, German is an advantage.
- Ability to work both independently and collaboratively.

For more information on this position, please contact Dr. Philipp Marquetand: philipp.marquetand@univie.ac.at