

**Type of Position:** PhD (praedoc 75%, University of Vienna, Austria)

**Research Area:** Theoretical Chemistry

**Principle Investigator (PI):** Prof. Dr. Leticia González

**Name of Institute:** Institute of Theoretical Chemistry  
University of Vienna, Austria

**TRR234-C3: Integration of photocatalytic components in complex environments** (González)

This subproject aims at modelling photocatalytic components in explicit solution and block-copolymers matrices in order to quantifying the impact that the environment has on the different molecular components. We are interested in looking at photophysical properties of the photosensitizers, such as absorption and emission properties, or their time-dependent response to excitation, finding how embedding modifies reactivity, redox potentials, catalytic cycles, regeneration and degradation pathways, and in general at the catalytic mechanisms. In particular, we will look into water oxidation polyoxometallates as well as single-metal coordination complexes as catalysts.

**Short description of the Job:** In close collaboration with synthetic inorganic chemists and physical chemists, the candidate will use molecular dynamics, non-adiabatic dynamics and advance quantum chemistry, to characterize catalysts and photosensitizers, understand the activation, oxidation, regeneration and possible degradation pathways of the chosen catalysts and discover relaxation pathways of photosensitizers.

The successful applicant will have strong interest in theoretical and computational chemistry, catalysis and inorganic chemistry. Ideally, she/he has some previous knowledge in quantum chemistry, multiscale techniques, or molecular dynamics. She/he should be highly motivated to work in an interdisciplinary and international team and should have excellent written and oral communications skills in English.