

Type of Position: Postdoctoral researcher 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

Duration: 12 months

TRR234-C3: Development of multiscale fragment-based excitonic models (González)

This subproject aims at further developing our home developed surface hopping code so that dynamics of multi-component systems can be modelled in the presence of complex environments. We aim at developing and implementing a multi-scale fragment-based excitonic model able to describe potential energy surfaces within our SHARC (surface hopping including arbitrary couplings) code that include energy and charge transfer processes between individual components.

Short description of the Job: The candidate should be experienced with software development and nonadiabatic molecular dynamics in order to develop an excitonic model and charge transfer model that exploits vibronic coupling models. Such novel method will be applied to photosensitizers and catalysts in complex environments.

The successful applicant will have strong interest in theoretical and computational chemistry, experience in programming and method development, as well as background on excited states, multiscale approaches and possibly energy and charge transfer processes. 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.