Vienna School of Mathematics

universität wien

Machine Learning Photochemistry with Low-Rank Tensor Approximation Techniques (University of Vienna, Supervisors: P. Marquetand, U. Stefanelli)

The PhD candidate will be concerned with the development and improvement of machine learning algorithms for the simulation of photo-chemical reactions. The candidate will be supervised by Philipp Marquetand (Theoretical Chemistry) and Ulisse Stefanelli (Mathematics), investigating the advantages of low-rank tensor approximation techniques, among others. The position is associated to the research platform "ViRAPID - Vienna Platform for Accelerating Photoreaction Discovery", where the candidate will work interdisciplinarily together with two other PhD students from chemistry and physics respectively.

The tasks comprise the development of new mathematical approaches and algorithms, quantum chemistry computations and excited-state molecular dynamics simulations. As the project is interdisciplinary, no applicant is expected to meet all requirements initially. Thus, the candidate will receive an in-depth training on the different techniques.

Applications have to be sent via the Job Center of the University of Vienna at the Reference number 10410. The deadline for application is **February 20, 2020**.