

PhD Project: Microscopic Simulation of Solvation

To develop an accurate method for the atomistic simulation of complexes in solution we are looking for a physicist or chemist with a solid background in theory as well as programming experience. The project relies on a statistical approach to the distribution of solvent molecules around the solute. This classical approach to the structure of a molecular solvent will be coupled with a quantum mechanical method for an accurate description of the solute. Parallel algorithms for an efficient implementation of the method will be developed together with the Department of Informatics (Scientific Computing) and a theory group at a leading university in the USA. Applications aim at case studies in catalysis and environmental chemistry. The International Graduate School of Science and Engineering at TUM supports this international cooperative project by means of a generous scholarship.

For further information or submission of your detailed application please contact Prof. N. Rösch, Theoretical Chemistry and Catalysis Research Center, TU München, Garching, Germany, Email roesch@mytum.de, Tel. +49.89.289.13619