Accurate and efficient density matrix renormalization group-based methods for extended molecules

Quantum chemical computations nowadays play a fully-fledged role in chemical research. Computational chemistry helps to analyze and explain experimental observations, supports design of novel materials, and allows for predicting properties of new molecules. Despite the huge progress in development of novel computational methods, there are, however, several classes of chemical problems which are still awaiting a more reliable theoretical description. A long-standing problem and a challenge for existing methods are chemical systems suffering from *quasidegeneracy*, also known as systems with strongly correlated electrons.

Many important chemical problems fall into the category of *quasidegeneracy* e.g. homolytic bond breaking/formation, open-shell and excited electronic states, transition-metal complexes, and transition states of chemical reactions. Impressive progress in development of density functional theory (DFT) methods notwithstanding, they are not reliable if applied to chemical problems with *quasidegeneracy*. The density matrix renormalization group (DMRG) method, on the other hand, is dedicated to accounting for *quasidegeneracy* in efficient manner. It misses, however, an important chunk of electron correlation, the so called dynamic correlation. Consequently, applicability of DMRG to chemical systems is still limited.

The aim of the proposed project is development and implementation of new computational tools based on DMRG, which are suitable for extended strongly correlated molecules and their application to challenging problems such as the electronic structure of biologically relevant transition metal complexes. In order to achieve this aim, we plan to develop dynamic correlation correction tailored to DMRG and quantum embedding methods which will significantly extend applicability of DMRG to large systems. Another critical goal of the project are fast computational algorithms for the new methods and their efficient parallel implementation in quantum chemistry software.

New computational tools will break the accuracy- and system size-limits of the currently available DMRG-based approaches. They will be applied in the course of the project to investigate challenging real-world chemical problems.