Exploring molecular quantum bits

University of Stuttgart
Institute for Theoretical Chemistry

Project type
B.Sc. / M.Sc.

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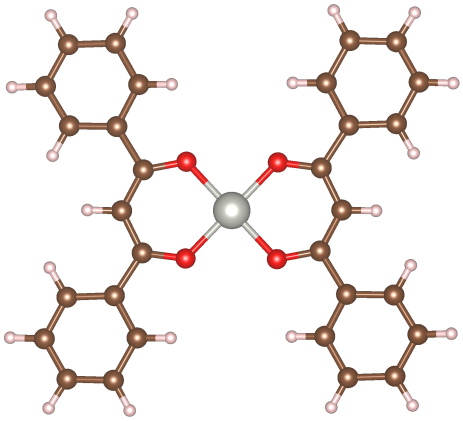
Motivation

Quantum science is one of the emerging key technologies of the coming decade. The aim is to exploit quantum effects for applications like sensing, simulation, communication, and computing. The central object in this technology are quantum bits, which unlike classical bits can assume a superposition of 0 and 1, thus opening new perspectives for the solution of certain 'hard' problems.

Spins in open-shell molecules provide a rather natural way to implement quantum bits. The main challenge consists in understanding and controlling the mechanisms that limit the lifetime of the quantum state, the memory time T_m. This is the time during which the spin can remain in a defined superposition state.



Topic

In this project, we will investigate a prototypical molecular quantum bit. You will learn how to apply various quantum chemical methods to compute the molecular structure and the properties of the molecule and how more advanced properties like hyperfine couplings and their modifications by vibrations are computed. You will also be introduced into the techniques to further analyze these properties and to obtain estimates for the lifetimes of the spin states of these molecules.