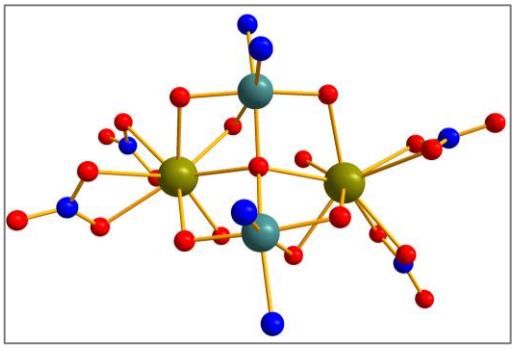
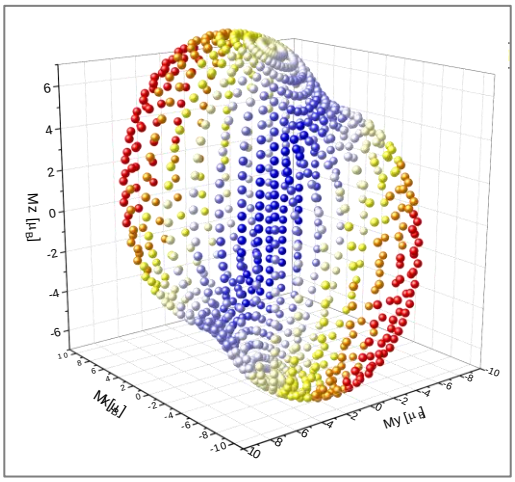
Bachelor/Master Thesis Project

Efficient Large Scale Simulation of the Powder Magnetisation in Single Molecule Magnets



Molecular nanomagnets provide us with a fantastic playground for experimentally testing the quantum mechanics and quantum statistics of well-defined collections of interacting quantum objects. Despite their small number of spins, and their in principle known Hamiltonian, molecular nanomagnets display a great variety of non-trivial collective quantum behavior.

A particular sub class of molecular nanomagnets is that of the Single Molecule Magnets (SMMs), which provide us with the opportunity to realize data storage and quantum bits at the molecular scale, and which are thus of interest from a fundamental scientific point of view as well as for applications in quantum information technologies. The most promising SMMs contain Lanthanide metal ions, but using Lanthanide ions presents us with a fundamental challenge: Numerical simulation and fitting of available experimental data can quickly become prohibitive, in terms of computational time. Most experimental data are recorded on powdered samples, which requires a numerical integration over the sphere in order to obtain the "powder average". This is the most time consuming part in the numerical simulation, and any improvement will result in dramatically enhanced abilities to analyze the experimental data and unravel underlying physics.



The aim of this thesis is to explore and develop advanced numerical integration methods to improve our existing simulation code, and to then apply it to the investigation of a SMM.

What do you learn?

- Quantum Magnetism
- C - based Coding
- Numerical Simulation

Interested?

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