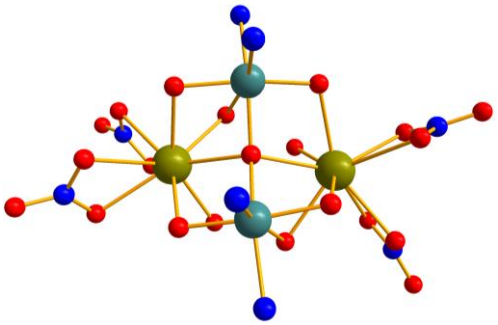
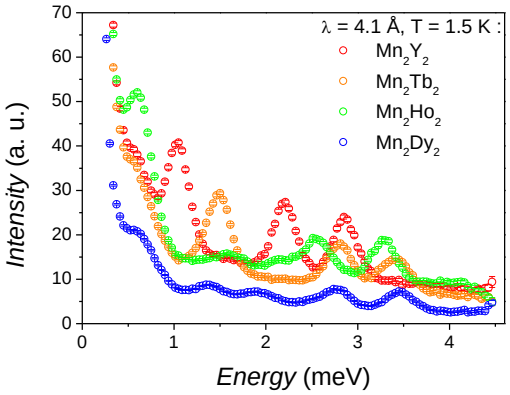
Bachelor/Master Thesis Project

Efficient Large Scale Simulation of Magnetism in Single Molecule Magnets



Molecular nanomagnets are an ideal opportunity to study quantum mechanics in small, finite systems, and a large variety of non-trivial quantum effects can be observed. Excellent inelastic neutron scattering data can be recorded experimentally, which helps us to identify which quantum effect is dominating in a particular molecular nanomagnet. Examples are the quantum harmonic oscillation of magnons, quantum tunneling, and spin frustration. Although the Hamiltonian of molecular nanomagnets is in principle known, the variety of non-trivial quantum effects leads to a number of open fundamental questions.



In our group we study the subgroup of the molecular nanomagnets called Single Molecule Magnets (SMMs). They allow us to realize data storage and quantum bits near the nanoscale, which is highly attractive for applications and is a main motivation for studying them. The best SMMs incorporate Lanthanide metal ions with partially filled 4f atomic shells. However, Lanthanide ions unfortunately require a large number of parameters for describing their magnetism, which results in a dramatic increase in the computational time for simulating them.

The aim of this thesis is to improve our existing simulation code such as to massively reduce the computational cost in what we call "linked fits". We expect performance improvements by several orders of magnitude by using sparse matrix techniques, iterative numerical methods, and possible GPU based computing. This will enable the study of the magnetism of families of Lanthanide-based SMMs.

Interested?

Then don't hesitate to come for a coffee on the second floor of the Physik Hochhaus!

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