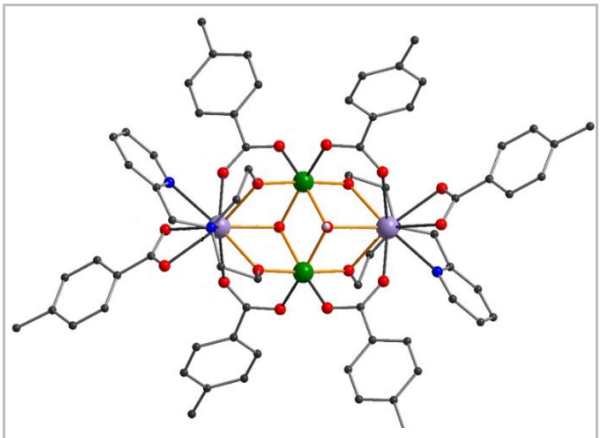
Master Project

Ligand Field Parameterization in Single Molecule Magnets using Machine Learning Methods

Single-Molecule Magnets (SMMs) allow us to realize data storage and quantum bits at the nanoscale, which is highly attractive for applications and is a main motivation for studying them. They belong to the class of Molecular Nano Magnets, which give us a unique possibility to experimentally study a large variety of non-trivial quantum effects in small, finite systems, and to address a number of open fundamental questions. Examples of such effects are quantum tunneling and toroidal moments.



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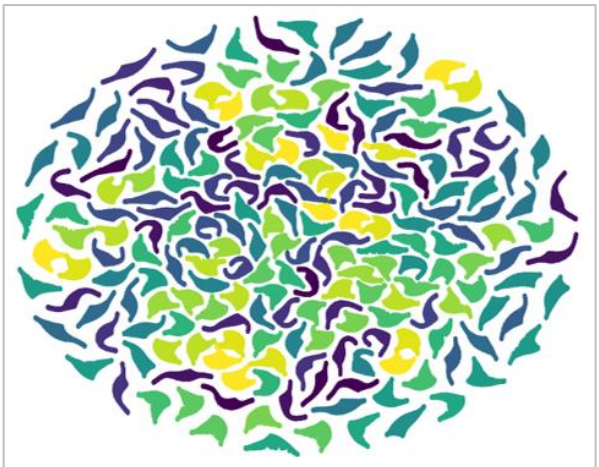
Lanthanide-based SMMs in particular demonstrate promising magnetic retention due to large inherent anisotropies. The effect on their magnetic properties due to the surrounding ligand structure can be parameterized by a set of 27 parameters arising from ligand field theory. Experimental data such as magnetization and susceptibility curves, however, are typically featureless for these materials. Multiple distinct parameter sets can describe the data to equal accuracy, making the inverse problem of determining model parameters a formidable challenge.



t-SNE plot of magnetic data

In this thesis, the over-parameterized inverse problem is tackled using various Machine Learning methods such as Autoencoders and Invertible Neural Networks. Physics-informed regularizers as well as numerical techniques relevant to inversion like Markov Chain Monte Carlo can be investigated.

What do you learn?

- Quantum Magnetism
- Numerics and Deep Learning
- Inverse Problems

Interested?

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