COMPUTATIONAL ANALYSIS
OF MAGNETIC MOLECULES

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Introduction to Research

- Two Molecules analyzed: $\text{Cr}_8\text{Gd}_8$ and $\text{Ni}_{21}\text{Gd}_{20}$ [1]

- Quantum Monte Carlo Method (QMC) used from the ALPS library [2][3].

- Motivation: Possible use in magnetic refrigeration
Magnetic Molecule
Cr$_8$Gd$_8$

- Ring like structure
- Alternating Cr-Gd atoms
- Two different bond lengths
- $[\text{Cr}_8\text{Gd}_8(\text{mda})_{16}(\text{CH}_3\text{COO})_8(\text{NO}_3)_8]\times\text{CH}_3\text{CN}$
Ni$_{21}$Gd$_{20}$

- Cage like structure
- Separate Ni lattice and Gd lattice connected at 6 points
- Results in 3 different bonds
  Ni-Ni  Gd-Gd Ni-Gd

\[
\text{[Ni}_{21}\text{Gd}_{20}(\text{OH})_{24}(\text{IDA})_{21}(\text{DPGA})_{6}(\text{C}_2\text{O}_4)_3(\text{NO}_3)_6(\text{CH}_3\text{COO})_3(\text{H}_2\text{O})_{12}]\cdot 5\text{Br}_5(\text{NO}_3)_4\cdot 20\text{CH}_3\text{OH}\cdot 30\text{H}_2\text{O}
\]
Ni$_{21}$Gd$_{20}$

- Cage like structure
- Separate Ni lattice and Gd lattice connected at 6 points
- Results in 3 different bonds Ni-Ni, Gd-Gd, Ni-Gd

$\text{[Ni}_{21}\text{Gd}_{20}(\text{OH})_{24}(\text{IDA})_{21}(\text{DPGA})_{6}(\text{C}_2\text{O}_4)_{3}(\text{NO}_3)_{6}(\text{CH}_3\text{COO})_{3}(\text{H}_2\text{O})_{12}]\text{Br}_5(\text{NO}_3)_{4}\cdot20\text{CH}_3\text{OH}\cdot30\text{H}_2\text{O}$

Energy levels $> 10^{18}$
The Quantum Monte Carlo Method

- **Heisenberg Model**

- **Computed using ALPS** [2][3]

- Has an uncertainty inversely proportional to the square of the number of Monte Carlo steps

- **Hamiltonian**

\[ \hat{H} = \sum_{i,j} J_{i,j} \hat{s}_i \cdot \hat{s}_j + \sum_i D_i \hat{s}_{iz}^2 - \sum_i g_i \mu_B H \hat{s}_{iz} \]

- Where \( J \) is the interaction strength
  - \( J > 0 \) Antiferromagnetism
  - \( J < 0 \) ferromagnetism

- \( D \) is the anisotropy

- \( g \) is the gyromagnetic ratio
Cr₈Gd₈ Analysis

T: Magnetic Susceptibility

Main data set to determine J parameters
Cr₈Gd₈ Analysis (cont)
**Cr\textsubscript{8}Gd\textsubscript{8} Analysis** (cont)

Magnetization vs. Field

Main data set to determine \( g \) and \( D \)
**Cr\textsubscript{8}Gd\textsubscript{8} Analysis (cont)**

Magnetization vs. Field

Main data set to determine g and D

Same parameters from Tχ
Ni$_{21}$Gd$_{20}$ Analysis
Ni$_{21}$Gd$_{20}$ Analysis (cont)

Clear minimum in the RMS Deviation

\[ J_2 = -0.03 \text{ Kelvin} \]
$\text{Ni}_{21}\text{Gd}_{20}$ Analysis (cont)
Ni$_{21}$Gd$_{20}$ Analysis (cont)
Ni$_{21}$Gd$_{20}$ Analysis (cont)
Ni$_{21}$Gd$_{20}$ Analysis (cont)

Same parameters from $T_X$
Ni$_{21}$Gd$_{20}$ Analysis (cont)
References


[2] B. Bauer et al. (ALPS collaboration)
- \textit{The ALPS project release 2.0: open source software for strongly correlated systems}

- \textit{The ALPS project release 1.3: open source software for strongly correlated systems}
- \textit{Journal of Magnetism and Magnetic Materials 310, 1187 (2007)}. 