Theoretical study of GdW_{10} and GdW_{30} molecules energy transitions and experimental fitting.

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Single Ion Magnets (SIM) are appealing for theoretical research given their simple Hamiltonian. A very promising family of SIM involves lanthanide atoms encapsulated by polyoxometalates (POMs), which represent a class of mononuclear lanthanoid complexes known for their intriguing single-molecule magnetic properties[1]. In this study, we investigated the Hamiltonian characteristics of two specific POMs, GdW_{10} and GdW_{30} [2], and examined the underlying physical phenomena governing their energy transitions. Our analysis aimed to provide accurate predictions and enhance the theoretical-experimental consistency in the understanding of these systems. Our final goal is to combine lanthanide SIM with superconducting and magnonic circuits for quantum computing and sensing applications.

References

[1] Cardona-Serra S, Clemente-Juan JM, Coronado E, Gaita-Ariño A, Camón A, Evangelisti M, Luis F, Martínez-Pérez MJ, Sesé J. Lanthanoid single-ion magnets based on polyoxometalates with a 5-fold symmetry: the series [LnP5W30O110]12- (Ln3+ = Tb, Dy, Ho, Er, Tm, and Yb). J Am Chem Soc. 2012 Sep 12;134(36):14982-90. doi: 10.1021/ja305163t. Epub 2012 Aug 30. PMID: 22894703.

[2] Jenkins, Duan, Diosdado, García-Ripoll, Gaita-Ariño, Giménez-Saiz, Alonso, Coronado, & Luis. (2017). Coherent manipulation of three-qubit states in a molecular single-ion magnet. Physical Review B, 95(6). https://doi.org/10.1103/PHYSREVB.95.064423

Figures

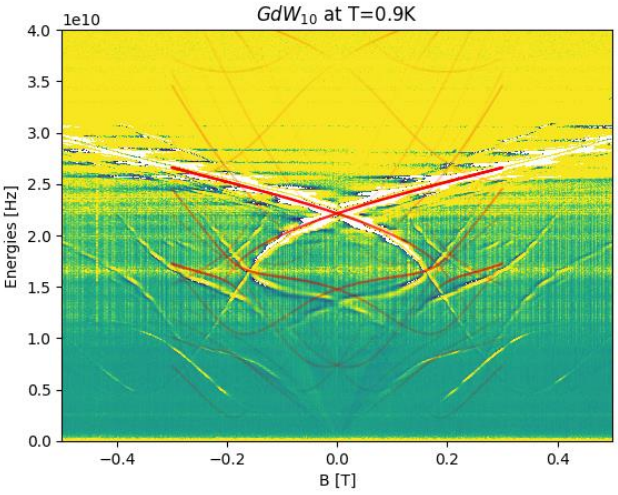

Figure 1: Plot of the theoretical energy levels transition on the experimental measure.