Magnetic Coordination Complexes for Quantum Information Processing

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Molecular qubits have emerged as a promising platform for quantum information processing, combining spin physics with the synthetic versatility of coordination chemistry. Molecular architectures allow deterministic control over spin placement, symmetry, and exchange interactions, enabling the rational design of tailored quantum properties. However, decoherence driven by spin–phonon interactions and environmental couplings remains a major challenge. This work pursues three main objectives:

1. Enhancing spin coherence: Strategies to increase coherence times in paramagnetic metal complexes rely on rational tuning of the coordination sphere. By adjusting local symmetry and ligand-field strength, the degeneracy of electronic states can be lifted and magnetic anisotropy finely tuned. This enables the emergence of clock transitions that cancel some decoherence pathways. These effects are probed using a combination of Electron Paramagnetic Resonance (EPR) technique and SQUID magnetometry measurement. [1]

2. Spin control via electric fields: Spin–electric coupling is investigated in low-symmetry frustrated triangles using a home-built electric-field-modulated EPR setup. [2], [3] This approach aims to understand and optimize spin–electric coupling in those systems. This provides insight into the mechanisms that enhance electric-field control of spin states, complementary to conventional magnetic-field manipulation.

3. Optical spin initialisation and readout: Light-induced processes are explored to enable optical addressing and coherent control of spins. [4] Fluorescence and Raman spectroscopy provide detailed insight into how molecular structure and local environment affect spin dynamics.

This work contributes to developing a toolkit to identify and control the key molecular ingredients for realizing effective molecular qubits.

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