Chemistry for Quantum Information Science

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The unique combination of atomic-scale tunability, reproducibility, and chemical specificity make paramagnetic molecules a paradigm-shifting category of materials. This capability has the potential to be transformative for developing a bespoke quantum ecosystem, as, for example, the requirements for a node within a quantum communications network are distinct and potentially orthogonal to those for a quantum sensor. Our team imbued molecular qubits with the same read-out approach as defect-based systems. To achieve this, we envisioned an inverse design problem whereby we mimicked the electronic structure with an orthogonal physical structure. Using transition metal chemistry, we designed the ground state, excited states and dynamics based on straightforward ligand field analysis. By coupling optical read-out with spatial precision, we seamlessly integrated a new class of materials with existing read-out technology. Translating this discovery towards application requires a second set of proof-of-concept demonstrations. Critical amongst them are increasing coherence time across a wide temperature range. One component of achieving that is gaining more insight into phonon modes and their contributions to coherence properties.