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Molecular Qubit Frameworks: Spin Dynamics and Quantum Sensing Applications

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With atomic designability, fine tunability, and quantum coherence at room temperature, molecular electron spin qubits could enable unprecedented quantum information technologies. Molecular qubit frameworks (MQFs), i.e. crystalline and microporous materials comprising of molecular qubits, offer a versatile platform to engineer phononic, magnetic, and electronic environment surrounding electron spin defects, enabling precise control of spin relaxation time (T_1) and decoherence time (T_2). Their nanoscale pores further facilitate host-guest interactions, empowering quantum sensing of guest molecules.

In this talk, we will present our recent spin dynamics studies on MQFs. Through pulse electron paramagnetic resonance and vibrational spectroscopic characterization on a series of MQFs embedding semiquinone-like radicals (Figure 1), we show that hydrogen-bonded networks and their deuteration facilitate spin relaxation [1]. This finding motivated us to suppress spin relaxation by structural rigidification, synthesizing MQFs with T_1 and T_2 exceeding 300 μs and 1 μs at room temperature, respectively [2]. Analyzing anomalous and tunable spin relaxation in a chiral MQF, we discovered spin-phonon polarons, a new type of quasiparticles emerging from asymmetric spin-phonon coupling [3]. Finally, we will present quantum sensing of nuclear spins at room temperature in solution with MQFs via relaxometry and hyperfine spectroscopy [4].

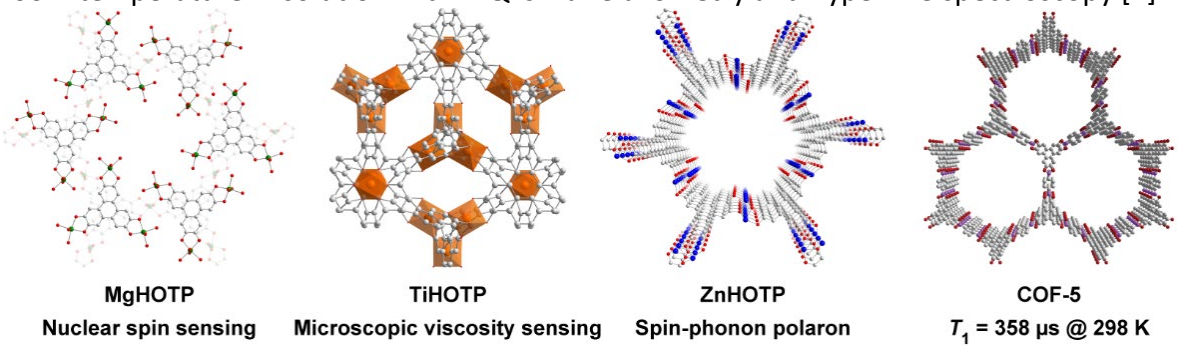


Figure 1. Molecular qubit frameworks.

References:

[1] A. Zhou et al., Nat. Commun. 15 10763 (2024).

[2] Z. Sun et al., J. Am. Chem. Soc. 147 31930 (2025).

[3] A. Zhou, R. Bi et al., arXiv:2506.04885 (2025).

[4] L. Sun, L. Yang et al., J. Am. Chem. Soc. 144 19008 (2022).