Seminar Title: Isolation of Zr^{III} Aryloxides: A New Class of Molecular Qu*d*its
Speaker: Maggie Mahaney, Department of Chemistry, University of Rhode Island
Date: November 21, 2025 (2:00–3:00 PM, Beaupre 105)

The second quantum revolution has been marked by the development of computing technologies capable of coherently controlling quantum states—at the heart of which lies qubits, the basic informational unit in quantum information science (QIS). Like classical bits, qubits assume the $|0\rangle$ and $|1\rangle$ states but can also assume superpositions of these states. Quantum computers therefore have the potential to perform certain tasks (quantum chemistry calculations, measurement, secure communications, etc.) much more efficiently than classical computers. Current state-of-the-art qubits are largely fabricated with solid-state approaches, which suffer from fast decoherence times due to environmental sensitivity and difficulty in addressing single qubits within a bulk array. Molecular qubits, on the other hand, can overcome these challenges because of the “bottom-up” nature of chemical synthesis: With targeted ligand design, molecular qubits can be uniquely tailored to each QIS application.

This seminar will present our development of rare Zr^{III} aryloxide complexes as a new class of molecular qubits. The unpaired electron spin on the Zr^{III} center can be coherently controlled as a qubit; however, hyperfine coupling to the nuclear spin of the ^{91}Zr isotope (I = 5/2, 11.2%) expands the accessible state space in these multi-level molecular qu*d*its. Encoding information in the additional electronuclear states should improve computational error rates and latency when using a single qu*d*it compared to a multi-qubit array. Pulsed EPR experiments confirmed our Zr^{III} aryloxide complexes do, indeed, act as qu*d*its. Spin-lattice relaxation times up to 87 ms and spin coherence times up to 123 μs were also observed, marking these complexes as some of the best molecular qubits observed to date and highlights the promise of Zr^{III} ions for future molecular qubit development.