Center for Molecular Magnetic Quantum Materials (M^2QM)
EFRC Director: Hai-Ping Cheng
Lead Institution: University of Florida
Class: 2018 – 2026

Mission Statement*: To provide the materials physics and chemistry understanding of molecular magnetic quantum materials essential for quantum and conventional computing beyond Moore's Law.*

Molecular magnetic materials (MMMs) are quantum materials, often with multiple exotic physical properties arising from their molecular spin states and their coupling to external fields and the environment. The objective of the Center for *Molecular Magnetic Quantum Materials* **(M^2QM)** is to discover, develop, and deliver the pivotal materials physics and chemistry knowledge of molecular magnetic quantum materials essential for quantum information technologies. M^2QM aims to transform molecular magnets (MMs) from promising building blocks into viable *quantum materials* that are useful both for coherent quantum information systems (QIS) and for quantum electron-spin devices.

M^2QM focuses on providing the crucial synthesis, characterization, aggregation and assembly, adaptation, and control needed for utilization of MMs as quantum materials. The central technological contexts are to develop technologies that enable quantum information processing for quantum computation, to impact problems critical to humanity, and to fulfil the potential for exquisite sensitivity and specificity of quantum sensing that utilizes quantum effects.

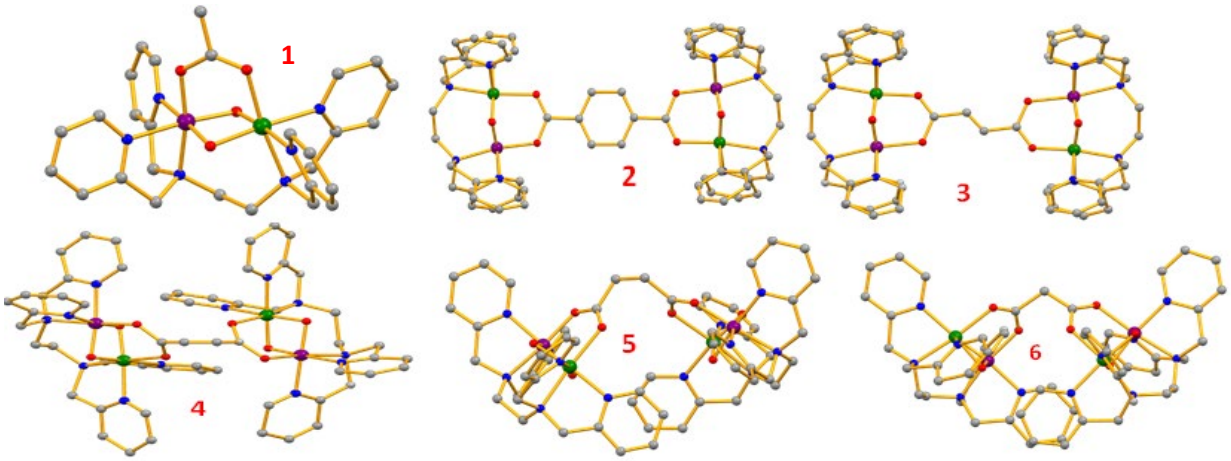

Fig.1 The [Mn_2] magnetic molecule with S=1/2 {1} and its conversion into dimers 2-6 by covalent linkage with a variety of dicarboxylates.

The Center provides a unique integration of advanced theory, innovative experiment, and expert chemical synthesis to design, probe, and control the quantum degrees of freedom of electron spins at the scale of molecules. Molecular spins offer the potential of almost limitless tunability via the techniques of coordination chemistry, with respect to coherence, energy gaps, and couplings. Furthermore, molecular qubits are completely identical and easy to create in large numbers. Figure 1 shows how a single spin center molecule can be linked chemically to create five different dimers. However, there remain many challenges for realizing quantum information (and other quantum) applications with molecules in practice. Those challenges primarily are related to control, addressing, and integration into technologies at larger scales while controlling decoherence.

M^{2}QM brings together experts in the synthesis of molecular magnets, characterization with unique spectroscopies, technological integration via surface and macromolecular chemistries, and computational and theoretical modeling of quantum properties, to carry out fundamental research to identify new and promising molecular platforms on which to make advances upon the specific challenges noted above.

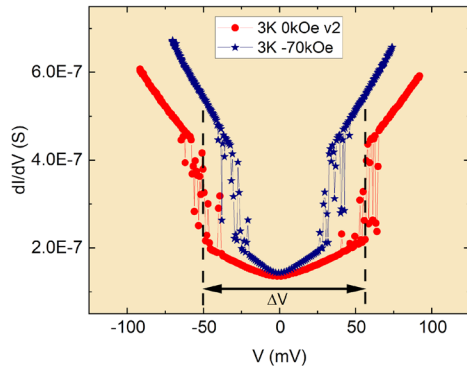

Fig. 2. Differential conductance plotted as a function of voltage bias shows field-dependent energy transitions between quantum states in an MnPc film.

We envisage three fundamental directions for the second M^{2}QM research term. First is to utilize the understanding of decoherence pathways gained in the first phase to design new MM systems with long coherence times. On those we will demonstrate two qubit gate operations at speeds that are fast compared to the coherence time. Second is to move from promising demonstrations of magnetoelectric couplings in bulk structures to a more focused design that exploits the relatively soft MM lattices and the tunability of individual MM spin configurations to achieve very strong magneto-electric coupling. Third is to demonstrate functional control of MM films and substrate interactions, for example, to achieve tunneling based control. All these directions will be supported by an intense theoretical and computational effort to simulate the quantum properties of individual molecules and aggregates, as well as machine-learning based discovery of new candidate molecules and aggregates. Figure 2 shows, for example, transport measurements of a MnPc thin film demonstrating transitions between quantum magnetic states are acquired using a 1 mV rms voltage modulation. A smaller voltage modulation should resolve additional energy levels in the transition regions.

M^{2}QM's quest to deepen and broaden the understanding of critical materials physics and chemistry of MMs for QIS is built upon accomplishments from the first funding period (EFRC class of 2018) and targeted at the fundamental science needed for eventual applications. That includes both quantum devices (qubits) and quantum-current (e.g., spin) systems. The strategy is pursued via three Thrusts, each an experimental-theoretical-computational team. Theory-computation efforts across the entire Center are enhanced via the Cross-cutting Theory-Computation team. M^{2}QM's bottom-up approach embodied in this organization is to synthesize MMs and linker molecules with high promise of properties useful for QIS, to achieve stable condensed assemblies of those molecules that preserve those desirable properties (chiefly spin-state control and coherence), and to demonstrate coupling, modulation, control, and coherence preservation required for QIS applications.

Center for Molecular Magnetic Quantum Materials (M^{2}QM)	
University of Florida	Hai-Ping Cheng (Director), George Christou, Arthur Hebard, Richard Hennig, John Stanton, Neil Sullivan, Samuel Trickey, Xiaoguang Zhang, Xiao-Xiao Zhang
Florida State University	Stephen Hill (associate director), Mike Shatruk
University of Central Florida	Talat Rahman
University of Texas at El Paso	Mark Pederson
Los Alamos National Laboratory	Vivien Zapf
California Institute of Technology	Garnet Chan

Contact: Hai-Ping Cheng, Director, m2qm.efrc@phys.ufl.edu, hping@ufl.edu
352-392-6256, www.efrc.ufl.edu