FY 2020 Energy Frontier Research Centers

Quantum Information Science Awards

Center for Molecular Quantum Transduction (CMQT)
Director: Michael R. Wasielewski, Northwestern University
Co-PIs: Danna Freedman (Northwestern; Deputy Director), Mark Hersam (Northwestern), Matthew Krzyaniak (Northwestern), Xuedan Ma (Northwestern), George Schatz (Northwestern), Nathaniel Stern (Northwestern), Roel Tempelaar (Northwestern), Emily Weiss (Northwestern), Nathalie de Leon (Princeton), Gregory Fuchs (Cornell), Michael Flatté (University of Iowa), Randall Goldsmith (University of Wisconsin, Madison), Ezekiel Johnston-Halperin (Ohio State University), Jeffrey Long (University of California, Berkeley), Joel Yuen-Zhou (University of California, San Diego)

Quantum Sensing and Quantum Materials (QSQM)
Director: Peter Abbamonte, University of Illinois, Urbana-Champaign
Co-PIs: Barry Bradlyn (UIUC), Tai C. Chiang (UIUC), Taylor Hughes (UIUC), Angela Kou (UIUC), Vidya Madhavan (UIUC), Fahad Mahmood (UIUC), Nadya Mason (UIUC), Philip Phillips (UIUC), Daniel Shoemaker (UIUC), Dale Van Harlingen (UIUC), Tom Devereaux (SLAC), Benjamin Feldman (SLAC), Kathryn Moler (SLAC), David Reis (SLAC), Zhi-Xun Shen (SLAC), Mariano Trigo (SLAC), Dirk Morr (University of Illinois, Chicago)

Center for Molecular Quantum Transduction (CMQT)
EFRC Director: Michael R. Wasielewski
Lead Institution: Northwestern University
Class: 2020 – 2024

Mission Statement*: To develop the fundamental scientific understanding needed to carry out quantum-to-quantum transduction through a bottom-up synthetic approach, which imparts atomistic precision to quantum systems.*

Quantum-to-quantum transduction is the coherent exchange of information between quantum systems, which is an essential element of quantum information science. To achieve this goal, **CMQT** explores the underlying interactions among quantum spins, excitons, and vibrational excitations of molecules and molecular materials that are relevant to molecular quantum-to-quantum transduction. **CMQT** comprises an interdisciplinary team of chemists, physicists, and materials scientists with the individual expertise and collective breadth to create knowledge in this emerging area.

Why use molecules and why now? To date, research in spin-based QIS has demonstrated success by harnessing and exploiting defects in solids. Using molecule-based systems offers the advantages of structural reproducibility, atomic scale spatial control, structural modularity, and access to uniquely molecular degrees of freedom (DOFs), i.e. the various pairwise interactions between photons, excitons, magnons, phonons, spins, and charges (**Fig. 1**). The number of quantum DOFs available in molecular systems make them attractive targets for quantum transduction, as quantum information can be transferred coherently between DOFs.

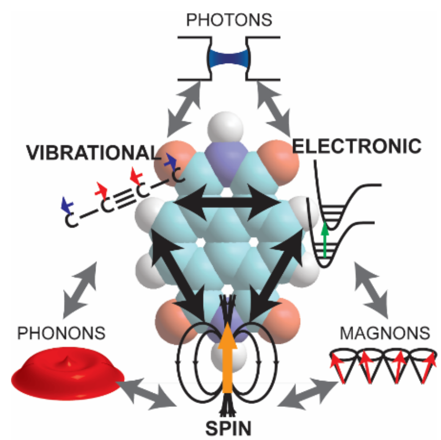

Fig. 1. Synergistic **CMQT** research directions. Thrust 1 focuses mainly on spin and electronic DOFs. Thrust 2 adds phononic and magnonic DOFs. Thrust 3 adds photonic and vibrational DOFs.

Molecular architectures provide unmatched flexibility for tailoring the properties that are critical to quantum transduction, and molecular synthesis affords the opportunity to build novel molecular materials from the bottom-up, both of which are at the heart of our proposed research. Thus, molecular systems offer an exceptional opportunity to explore the interface between quantum systems essential for sensing, communication, and computation.

CMQT exploits recent breakthroughs from our team including landmark coherence times and stabilities of molecular qubits and quantum materials, the ability to create hybrid qubits, and resonant photonic architectures. As we move forward, our approach includes both ensemble-level studies to rapidly understand interactions, and development of *single-molecule* methods to interface molecular QIS with other QIS platforms. We are also leveraging cutting-edge physical measurement techniques with high spatial, temporal, and spectral resolution to understand how to transition quantum-to-quantum transduction from the ensemble to the single molecule level.

Our goals are embodied by three cross-cutting Thrusts with closely integrated approaches and team synergies that progressively exploit the flexibility and tunability of molecular architectures to address quantum-to-quantum transduction at increasing length scales. Individually, the Thrusts each pose and answer fundamental questions relevant to quantum transduction in different regimes, ranging from local to long-distance. Taken together, the Thrusts develop a transformative integrated framework for how molecules can facilitate quantum transduction at all the scales relevant for quantum information science.

Thrust 1. Localized Molecular Quantum-to-Quantum Transduction (co-Leaders: Fuchs and Freedman). *The goal of this Thrust is to develop new mechanisms and strategies to coherently couple localized molecular DOFs and thus lay the foundation for molecular quantum-to-quantum transduction.* Designer molecular qubits with long coherence times and tunable interactions enable quantum state transduction between molecular quantum states demonstrated at the ensemble level to be transitioned rapidly to quantum measurement at the single molecule level. We are exploring synthesis and measurements that leverage atomic precision to enable quantum transduction through local interactions.

Thrust 2. Distributed Molecular Quantum-to-Quantum Transduction (co-Leaders: Johnston-Halperin and Long). *The goal of this Thrust is to demonstrate quantum transduction within distributed molecular quantum systems.* Thrust 2 explores quantum transduction in ensembles of tailored molecular qubits including those developed in Thrust 1 that interact *via* spin-magnon coupling to delocalized, highly coherent, magnon modes in molecule-based magnetic thin films. This approach bridges the length scales of single molecules with those of state-of-the-art solid-state quantum systems.

Thrust 3. Multiscale Molecular Quantum-to-Quantum Transduction (co-Leaders: Goldsmith and Weiss). *The goal of this Thrust is to use the combination of flying qubits (photons) and molecular DOFs to achieve quantum transduction over multiple length scales within hierarchical quantum systems.* Thrust 3 incorporates the molecular systems established in Thrusts 1 and 2 into photonic structures to demonstrate coherence transfer between multiple molecular DOFs and between these DOFs and photons, including producing heralded photons necessary to probe quantum aspects of energy-important light-harvesting processes, such as natural and artificial photosynthesis.

Achieving molecular quantum-to-quantum transduction is necessarily an interdisciplinary effort, requiring the scope of an EFRC to assemble the necessary expertise in the design and synthesis of molecular and solid-state materials, the capacity to measure coherent quantum states at the single quantum level, and the ability to seamlessly incorporate theory and modeling of materials and measurement schemes with the experimental constraints of real systems. **CMQT** is working toward meeting this challenge.

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Cornell University	Gregory Fuchs
University of Iowa	Michael Flatté
University of Wisconsin, Madison	Randall Goldsmith
Ohio State University	Ezekiel Johnston-Halperin
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Quantum Sensing and Quantum Materials (QSQM)
EFRC Director: Peter Abbamonte
Lead Institution: University of Illinois, Urbana-Champaign
Class: 2020 – 2024

Mission Statement*: To develop three new quantum sensing techniques—scanning qubit microscopy, two-electron Einstein-Podolsky-Rosen (EPR) spectroscopy, and nonlinear x-ray optics—and use them to study local and nonlocal quantum observables in quantum materials.*

The EFRC on Quantum Sensing and Quantum Materials (QSQM) will apply new types of quantum sensing technique to measure and correlate local and nonlocal quantum observables in three families of quantum materials central to DOE's energy mission: exotic superconductors, topological crystalline insulators, and strange metals.

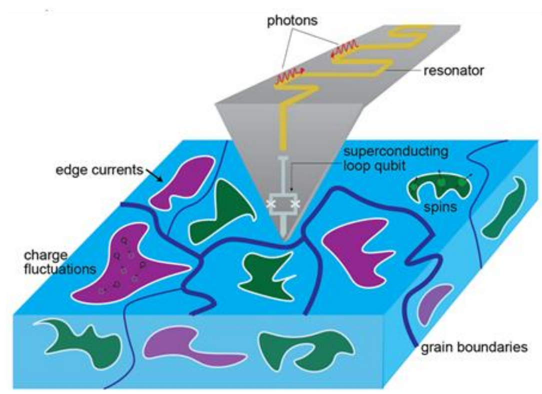

Figure 1 Conceptual illustration of a scanning qubit microscope, which consists of a tip-mounted flux qubit that may be scanned in close proximity to a heterogeneous quantum material.

To carry out this mission, we plan to develop three new, cutting-edge quantum sensing instruments. The first is a **scanning qubit microscope (SQM)**, which consists of a single flux qubit integrated into a tip that may be scanned over the surface of a material, as illustrated in Fig. 1. The state of a qubit is exceedingly sensitive to charge and flux noise, making an SQM a highly sensitive probe of local charge and spin fluctuations near surfaces or interfaces.

The second instrument is a **two-electron EPR spectrometer**, which uses correlated Einstein-Podolsky-Rosen (EPR) pairs of electrons to reveal hidden global interactions in materials. This instrument, illustrated in Fig. 2, can be operated in two different modes. In the first, double photoemission, the sample is illuminated with ultrafast XUV photon pulses that eject correlated electron pairs from the surface. The angle-and energy-distribution of these pairs can be used to reconstruct the anomalous Green's function of the material. In the second, two-electron Rutherford scattering, time coincident ultrafast electron bunches are scattered off one another near a material surface, revealing the renormalized interaction between quasiparticles.

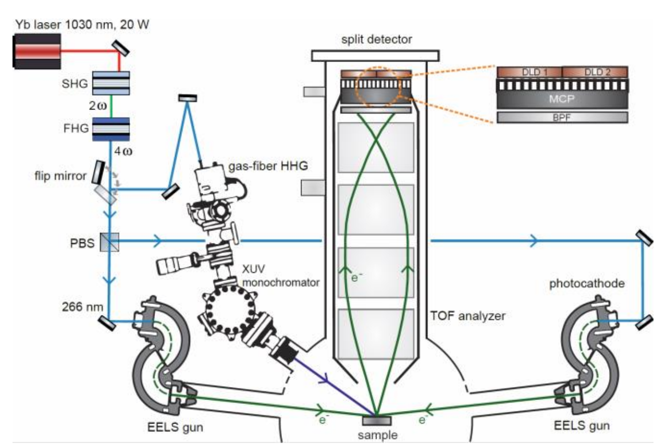

Figure 2 Conceptual illustration of a two-electron, time-of-flight, Einstein-Podolsky-Rosen spectrometer, which uses coherent pairs of electrons to detect valence band phenomena in quantum materials.

The third, **x-ray four-wave mixing** instrument uses correlated pairs of photons to measure the nonlinear optical response of materials at nonzero momentum. Illustrated in Fig. 3, this experiment is carried out at a free-electron laser facility, such as the LCLS facility at SLAC National Accelerator Laboratory. This instrument will directly measure the global geometry of Hilbert space of a material, revealing previously undetected topological phenomena, and will also identify new broken symmetries in materials that reveal exotic and previously unobserved phases of matter.

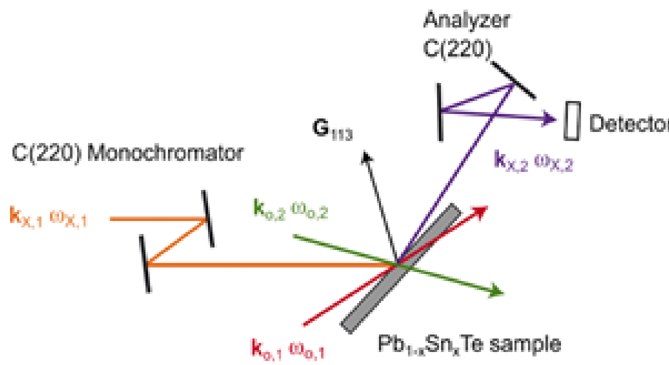

Figure 3 Conceptual illustration of an x-ray four-wave mixing experiment, which uses coherent pairs of photons to measure the nonlinear optical properties of quantum materials at nonzero momentum.

The new quantum sensing techniques we develop will enable us to unravel the most compelling mysteries of quantum materials. Scanning qubit microscopy will allow us to detect not only localized electronic states but also sources of dissipation and dephasing in materials over a wide frequency range. It will measure the frequencies of excitations and fluctuations in materials with unprecedented sensitivity. It will enable us to determine whether corner states and hinge states exist in higher-order topological insulators, whether new types of zero-energy states emerge at domain walls in unconventional superconductors, and reveal how strange metals screen charge.

Two-electron EPR spectroscopy will improve our scientific understanding of all materials in which interactions play a nontrivial role, including magnetic materials, strange metals, doped Mott insulators, interacting topological phases, and charge and spin density wave materials. It can directly reveal the pairing boson in most unconventional superconductors, as well as the mechanism behind other types of Fermi surface instabilities in quantum materials.

Nonlinear optics is widely known to be a highly sensitive probe of broken symmetries in materials. However, such measurements have always been restricted to small momenta. Our momentum-resolved x-ray nonlinear optics instrument will allow us to detect new categories of phenomena including the predicted nonlinear axion optical response in topological crystalline insulators, and whether charge carriers in strange metals flow independently or via collective hydrodynamic transport.

Together, these schemes will provide new knowledge about interacting and topological materials, facilitate the discovery of new materials, and define new directions for future spectroscopic probes.

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