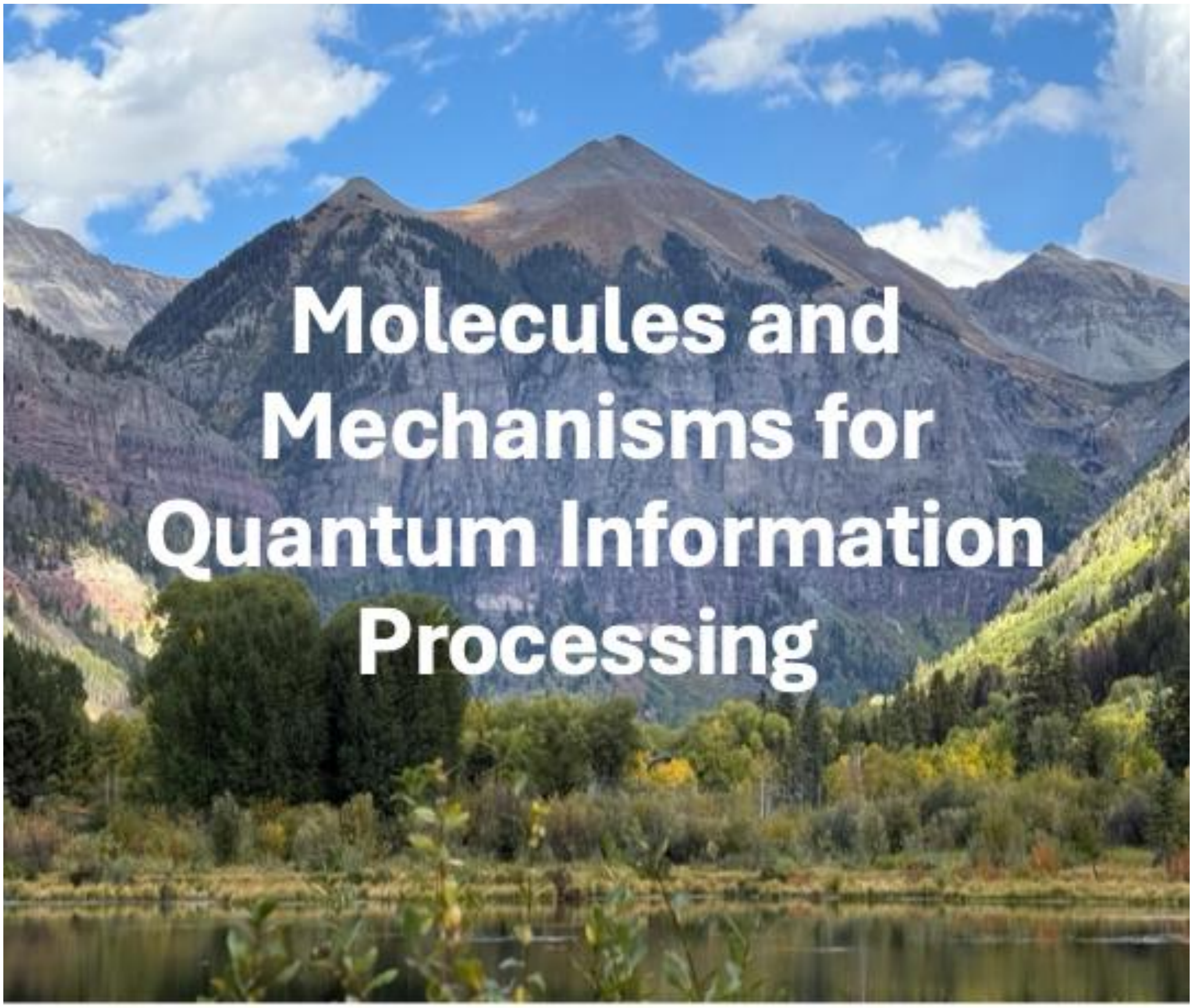

Molecules and Mechanisms for Quantum Information Processing

Co-Chairs: Michael R. Wasielewski
and Natia Frank

October 06-10, 2025

Telluride Science & Innovation Center
300 S Townsend St. Telluride, CO 81435

Workshop Details

Molecules and Mechanisms for Quantum Information Processing
10/06/2025 - 10/10/2025
Michael R. Wasielewski
Natia Frank

Meeting Description:
Controllable quantum systems are under active investigation for quantum computing, secure information processing, non-volatile memory, and quantum sensing. Within the context of quantum information science, quantum computing, communications and sensors all rely on the fundamental unit of a qubit which possesses at least two well-defined quantum states that can be prepared and addressed independently. Superposition and entanglement of qubit states can lead to complex gates for quantum operations, making the control of entanglement particularly interesting. Solid state qubit platforms with long decoherence times have been integrated into quantum computing technologies and current quantum sensors,. The challenges however of precise control over position and entanglement in these systems suggest that chemical approaches to qubit design may have distinct advantages. The ability to address, interrogate, and read out the properties of an individual molecular qubit in isolation and subsequently within an array through spectroscopy and molecular design allows for fundamental insight into the quantum properties necessary for the implementation of molecular-based qubits in quantum information applications.

Notes:
We wish to ensure an intimate workshop setting, with no more than 20 to 25 participants. If you are interested in attending, but have not received an invitation, please contact the workshop organizer before registering.

Telluride Science is about expanding the frontiers of science, exploring new ideas, and building collaborations. The workshop schedule will allow for substantial unstructured time for participants to talk and think. All participants are expected to stay for the entire duration of the workshop. Scientists are encouraged to consider bringing family or friends. Telluride offers a number of options for children's camps (including Telluride Academy, Aha School for the Arts, and Pinhead Institute). There is more information on childcare, camps, and family activities on Telluride Science's website. Feel free to contact Telluride Science's staff to help with any planning and/or coordinating care.

Meeting Venue:
Telluride Science & Innovation Center
300 S Townsend St. Telluride, CO 81435

Acknowledgements:
We thank the Telluride Science Research Center for their tireless support of education and research in science. We also thank the Royal Society Philosophical Transactions for generous funding.

Molecules and Mechanisms for Quantum Information Processing
Registered Meeting Participants

Bittner, Eric	University of Houston
Earley, Justin	Arizona State University
Flatté, Michael	University of Iowa
Frank, Natia L.	University of Nevada-Reno
Fuchs, Gregory	Cornell University
Hadt, Ryan G.	Caltech
Herrera, Felipe	Universidad de Santiago de Chile
Johnston-Halperin, Ezekiel	The Ohio State University
Kopp, Sebastian M	Northwestern University
Maurer, Peter	University of Chicago
Poh, Yong Rui	University of California San Diego
Schatz, George	Northwestern University
Shushkov, Philip	Indiana University
Slageren, Joris van	University of Stuttgart
Weiss, Leah	University of Chicago
Zadrozny, Joseph	The Ohio State University

Molecules and Mechanisms for Quantum Information Processing

SCHEDULE

Monday Oct 06		
7:30-9:00	Badge Pickup & Breakfast available at site	
9:00-9:10	Opening Remarks	
Session 1		
9:10-9:40	Sebastian Kopp, Northwestern University	Rational Design and Optically Detected Coherent Spin Control of Organic Molecular Color Center Qubits
9:40-10:20	Natia L. Frank, University of Nevada Reno	Optical Gating of Spin Dynamics in Isotropic Spin qubits
10:20-10:40	Coffee Break	
10:40 -11:20	Ryan Hadt, Caltech	Coupling Light to Molecular Electron Spins for Quantum Sensing
11:20-12:00	Eric R. Bittner, University of Houston	Synchronization of Quantum States: Exploring how noise, topology, and dimensionality affect quantum phase coherence
12:00 – 14:00	Lunch	
Session 2		
14:00-14:40	Justin Early, Arizona State University	Copper Nanoclusters as Systematically Tunable Platforms for Molecular Qubit Physics
14:40-15:00	Philip Shushkov, Indiana University	Spin relaxation in molecular qubits
15:00-15:20	Coffee Break	
15:20-16:30	Discussion	

Tuesday Oct 07		
7:30-9:00	Breakfast available at site	
Session 3		
9:00-9:40	Felipe Herrera, Universidad de Santiago de Chile	Atomistic Decoherence of Molecular Spin Qubits
9:40-10:20	Joseph Zadrozny, The Ohio State University	Molecular Tailoring of Spin-To-Environment Interactions
10:20-10:40	Coffee Break	
10:40 -11:20	George Schatz, Northwestern University	Understanding Single Photon Emission In Transition Metal Dichalcogenides; Transfer Of Entanglement From Photons To Electrons During Two-Photon Absorption
11:20 -14:00	Break and Lunch	
Session 4		
14:00-14:40	Yong Rui Poh, University of California San Diego	Organic Diradicals as Resources for Quantum Information Science

14:40-15:20	Ezekiel Johnston-Halperin, The Ohio State University	Understanding the materials basis for ultra-low loss quantum magnonics in the coordination compound vanadium tetracyanoethylene
15:20 -15:40	Coffee Break	
15:40 -16:30	Discussion	
18:00	Group Dinner at "Rustica"	*Please sign up at TSRC office before Tuesday morning.*

Wednesday Oct 08		
7:30-9:00	Breakfast available at site	
Session 5: Hybrid Systems and Assemblies		
9:00-9:40	Peter Maurer, University of Chicago	From diamond defects to protein-based qubit sensors
9:40-10:20	Joris Van Slageren, University of Stuttgart	Molecular Qubit Assemblies
10:20-10:40	Coffee Break	
10:40 -11:20	Leah Weiss, University of Chicago	A synthetic spin-photon interface with rare-earth molecules at telecommunications wavelengths
11:30 -13:30	Lunch	
Afternoon:		
13:30-16:00	*Group Hike (meet at TSRC center at 1:30 pm)*	

Thursday Oct 09		
7:30-9:00	Breakfast available at site	
Session 6:		
9:00-9:40	Michael Flatté, University of Iowa	Enhancement of Microwave to Optical Quantum Transduction in Molecular Materials via a Magnon Mode
9:40-10:20	Gregory Fuchs, Cornell University	Quantum and nonlinear magnonics based on the molecule-based ferrimagnet vanadium tetracyanoethylene
10:20-10:40	Coffee Break	
10:40 -12:00	Group Discussion	Grand challenges in the field (Where we have come and where we need to go)
12:00 -14:00	Lunch	
Session 7:		
14:00-15:00	Working and Collaboration sessions	

Synchronization of Quantum States: Exploring how noise, topology, and dimensionality affect quantum phase coherence

Eric R. Bittner*

Department of Physics, University of Houston

ABSTRACT: When we think of noise in quantum systems, we usually picture it as the great spoiler—washing out delicate superpositions and destroying entanglement. But the story is more interesting. Just as pendulum clocks on the same wall can spontaneously tick in unison, quantum systems can also synchronize, sometimes because of the noise in their environment rather than in spite of it. In this talk, I will explore how the structure of noise, the connectivity of a system, and even its dimensionality and topology, shape the way quantum states maintain—or lose—phase coherence. Drawing on examples that range from pairs of coupled spins to extended lattices and topological chains, I will show how correlations in the environment can protect certain collective modes, leading to unexpected resilience against decoherence. Along the way, we will see how ideas from classical synchronization, network theory, and topological physics converge in the quantum realm. The broader message is that noise and dissipation, usually treated as adversaries, can sometimes be harnessed as resources—pointing toward new strategies for stabilizing coherence in quantum devices and materials.

Copper Nanoclusters as Systematically Tunable Platforms for Molecular Qubit Physics

Asish Kumar Dehury, Venkatesan Kathiresan, Justin D. Earley

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ABSTRACT: Superatomic metal clusters provide unique opportunities to combine atomic-like electronic properties with scalable synthetic approaches for quantum information applications. While gold nanoclusters have demonstrated diverse magneto-optical behaviors spanning molecular to metallic regimes[1,2], the systematic exploration of copper nanoclusters as quantum coherent systems remains largely unexplored. We present copper nanoclusters as a novel class of tunable qubit systems that enable controlled perturbation of superatomic electronic structure while maintaining the framework necessary for systematic molecular physics investigations.

Following established synthetic protocols[3], we produce atomically precise copper nanoclusters including a 5-atom copper core passivated with ascorbic acid ligands ($Cu_5[AA]_4$) and a 25-atom copper core passivated with glutathione ligands ($Cu_{25}[GSH]_{20}$), providing systematic access to the transition from molecular orbital to band structure regimes through controlled variation of cluster nuclearity and ligand environment. Continuous-wave EPR reveals strong Cu^{2+}-like signals with distinct g-value anisotropy and hyperfine coupling patterns indicating evidence of supermolecular d-orbital character and a doublet ($S = ½$) ground state that persists across the two cluster compositions. These observations indicate that $Cu_5[AA]_4$ and $Cu_{25}[GSH]_{20}$ nanoclusters possess the requisite electronic and spin structure characteristics for coherent magnetic sublevels.

Copper nanoclusters provide systematic access to electronic structure modifications while maintaining structural integrity, directly addressing a central challenge in molecular qubit research where property changes often introduce uncontrolled variables. This platform extends beyond current size and ligand variations to encompass nanocluster chain assemblies for extended quantum networks, mixed metallic core compositions for tailored electronic properties, and controlled access to plasmon behavior in larger clusters. Building on established relationships between cluster architecture and magnetic behavior, these capabilities position copper nanoclusters as a versatile foundation for systematic molecular qubit design, enabling precise investigations of quantum coherence across multiple length scales and electronic regimes.

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Enhancement of Microwave to Optical Quantum Transduction in Molecular Materials via a Magnon Mode

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Department of Applied Physics and Science Education, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

ABSTRACT: Recently a method of enhancing microwave to optical quantum transduction via a magnon mode was proposed based on erbium dopants in a wide band gap solid state insulator[1]. However, low-loss magnetic materials based on organic constituents (i.e. V[TCNE]$_2$) offer potential advantages over the initial proposal based on inorganic materials. The ability to hybridize the microwave excitation with the uniform mode of the magnetic material allows much higher transduction rates (i.e. 1000 x faster at the same optical pump Rabi frequency) than devices without magnetic components. In addition the range of device parameters (i.e. microwave detuning) is greatly expanded over the range allowable for entirely paramagnetic spin centers. Finally, and perhaps most importantly, the use of magnetic material changes the conditions for the microwave and the optical resonators; specifically mode volume matching is no longer required. Here the type of desirable magnetic interactions in materials systems will be identified and a presentation of potential directions, using erbium optical transitions to match telecom wavelengths, will be described. This is an important step towards realizing high-fidelity entangling operations between remote qubits and will provide additional control of the transduction through perturbation of the magnet.

Work done in collaboration with T. O. Puel and was supported as part of the Center for Molecular Quantum Transduction (CMQT), an Energy Frontier Research Center funded by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award No. DE-SC0021314.

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Optical Gating of Spin Dynamics in Isotropic Spin qubits

Subrata Ghosh, Khetpakorn Chakarawet, Harini Wimalasekera, Devon Adecer, , R. David Britt, Steve Hill, Natia L. Frank*

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The optical manipulation of spin quantum states provides an important strategy for quantum control with both temporal and spatial resolution for quantum computing, sensing and communications. While significant progress has been made in the discovery of molecular spin-based qubits with long decoherence times, current challenges are focused on molecular quantum sensors that have long decoherence times, (achieved by isolation from the bath) and strong coupling to the environment (achieved by strong coupling to the bath) required for sensing of external field or analytes. We report here a strategy for coupling molecular spin-based qubits to the bath without sacrifice of decoherence times. Photochromic ligands that undergo isomerization in response to changes in solvation, electric field, temperature, or light can be used to modulate electron transfer-coupled spin transition processes, spin-orbit coupling, and metal-ligand covalency in bound transition and lanthanide metal ions. Visible light irradiation (λ_{exc} = 550-600 nm) of a spirooxazine cobalt−dioxolene complex induces photoisomerization of the ligand that in turn triggers a reversible intramolecular charge-transfer coupled spin- transition process at the cobalt center between a low-spin Co(III)−semiquinone doublet and a high-spin Co(II)−bis-semiquinone sextet state. Determination of the spin relaxation and decoherence times of the low-spin Co(III)−semiquinone doublet state reveal slow spin dynamics and decoherence, and a change in the population of the SQ state ($m_s \pm 1/2$) qubit state with light modulation.[1] Extension of this strategy to low-spin transition metal ($S = 1/2$) leads to reversible changes in spin relaxation rate, decoherence time, and g-value with changes in photochromic ligand state, providing a robust strategy for quantum sensing in molecular spin-based qubits.

Quantum and nonlinear magnonics based on the molecule-based ferrimagnet vanadium tetracyanoethylene

Gregory D. Fuchs

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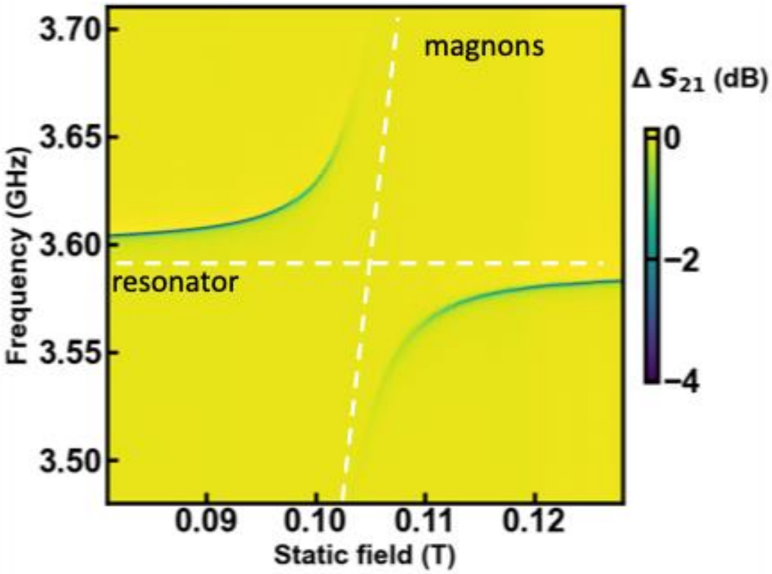
ABSTRACT: As we progress in the second quantum revolution, a natural question we ask is – is there a role for magnonics in quantum information platforms? Building on a decade of foundational work in this areas from many groups worldwide, I will discuss our efforts to develop new the roles for magnonics in quantum technologies. A major challenge is mitigating loss, since loss is the enemy of quantum coherence. First I'll discuss our experimental efforts to establish a scalable cavity magnonics platform based on the ultra-low loss molecule-based ferrimagnet vanadium tetracyanoethylene V[TCNE]x [1]. Then, I'll describe our approach to a cavity-magnonics implementation of the optomechanical-type nonlinear Hamiltonian [2]. Using this nonlinear interaction, we theoretically show how driving magnons that are coupled to a microwave electromagnetic resonator can enable resonator cooling and quantum squeezing. This approach can work with any low-loss magnetic material, here we describe it implementation with yttrium iron garnet (YIG) and V[TCNE]x. Finally, I'll describe our experiment working using NV centers to quantitatively measure the precession angle of V[TCNE]x microstructures [3].



The spectrum of a V[TCNE]$_x$ microstructure coupled to a lumped-element superconducting resonator with cooperativity exceeding 1000.

References

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Coupling Light to Molecular Electron Spins for Quantum Sensing

Ryan G. Hadt

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ABSTRACT: Spin-photon interfaces enable powerful strategies for quantum state initialization, manipulation, and readout, key functionalities for emerging quantum technologies. While these capabilities have been demonstrated in solid-state systems such as color centers and rare-earth dopants, molecular platforms remain largely untapped, despite advantages deriving from their synthetic tunability and environmental versatility. Moreover, the control of quantum states in solid-state materials typically relies on pulsed microwaves, which can limit spatial and temporal resolution compared to fully optical approaches. This talk will describe our recent demonstration of all-optical, picosecond-resolved measurements of molecular electron spin decoherence in Ir(IV) complexes under ambient, biologically relevant conditions.[1] These capabilities enable unique mechanistic interrogation of spin decoherence processes, informing chemical design strategies to prolong molecular decoherence times by more than an order of magnitude. Additionally, this talk will discuss our ability to expand optical addressability into the tissue transparency window and probe complex chemical dynamics in solution, broadening the potential for *in vivo* quantum sensing. Together, these advances position molecular spin-photon interfaces as a promising frontier in quantum information science.

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Atomistic Decoherence of Molecular Spin Qubits

Felipe Herrera

Department of Physics, Universidad de Santiago de Chile, Santiago, Chile.

ABSTRACT: Low-spin open-shell molecules are promising qubit platforms for quantum processing [1] given their long spin coherence timescales, comparable with diamond color centers, and the possibility of integrating qubit arrays into crystalline structures using established chemistry. To fully untap the potential of molecular qubits, a microscopic quantum mechanical understanding of the decoherence and relaxation processes that limit spin coherence is essential. Current approaches to this problem based on electronic structure methods are fundamentally limited in their ability to model multiple sources of quantum noise [2]. To address this issue, we developed a dynamical stochastic approach to construct the Redfield tensors that determines the open system dynamics of molecular spin qubits based on Haken-Strobl theory [3], to predict qubit relaxation (T_1) and decoherence (T_2) timescales over a broad range of temperatures and magnetic fields.

The proposed model involves a fluctuating molecular gyromagnetic tensor due to spin-lattice interaction and local magnetic fields due to hyperfine interactions with a spin reservoir. The bath spectral densities are parametrized using a small number of measurements of T_1 times. Using a vanadium-based spin qubit as a case study, the model predictions are shown to agree quantitatively with experiments [4]. To reduce the number of free parameters in the theory, we built ab-initio spin-lattice spectral density based on trajectories of phonon-induced fluctuations of the gyromagnetic tensor, obtained from atomistic modeling of a recently developed copper porphyrin qubit [5]. Complementing the model with a phenomenological spin-bath spectral density, we reproduced the measured magnetic field and temperature dependence of the T_1 and T_2 times of a copper porphyrin lattice for the first time. Our methodology is universally applicable to other molecular spin qubits and can assist in the microscopic characterization of quantum magnetometers and two-qubit gates based on open-shell molecules.

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Understanding the materials basis for ultra-low loss quantum magnonics in the coordination compound vanadium tetracyanoethylene

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The study of quantum magnonic interactions relies implicitly on the ability to excite and exploit long lived spin wave excitations in a magnetic material. That requirement has led to the nearly universal reliance on yittrium iron garnet (YIG), which for half a century has reigned as the unchallenged leader in high quality-factor (high-*Q*), low loss magnetic resonance, and more recently in the exploration of coupling between magnonic and spin or superconducting degrees of freedom in prototype quantum devices. This pride of place is not due to a lack of interest in other high-*Q* magnetic materials, but rather the systematic failure to identify another material system exhibiting low-loss magnetic excitations. In recent years, we have demonstrated that the ultra-low loss molecular ferrimagnet vanadium tetracyanoethylene ($V(TCNE)_2$) is poised to unseat YIG as the material of choice for quantum applications. For example, recent results have demonstrated the integration of patterned magnetic structures into superconducting resonators, yielding strong photon-magnon coupling in the microwave regime in an integrated circuit architecture [1], and the creation of a double disk structure that can be quantitatively read out using nitrogen vacancy (NV) centers in diamond [2].

Fully realizing the potential of these proof-of-principle measurements, however, will require advances in our understanding of the origin of the magnetism and ultra-low damping in $V(TCNE)_2$ and related materials. Here I will discuss results demonstrating fully spin polarized band structure [3] and a high level of porosity [4]. These observations begin to paint a picture of the surprising combination of strong local exchange, and consequent strong magnetic ordering, alongside an exceptionally low saturation magnetization that suppresses dipole coupling. Further, the demonstration of encapsulation of $V(TCNE)_2$ thin films using atomic layer deposition (ALD) of Al_2O_3 [5] allows for close approach with, e.g., magnetic force microscopy (MFM), facile characterization via optical spectroscopy, and more flexible integration into solid-state device fabrication protocols. Taken together, these advances represent a new era of magnetic characterization and materials development that promises the investigation of a new class of high T_C, low M_s, highly porous, and ultra-low loss magnetic materials that are particularly well suited for applications in quantum information and related fields.

[1] Q. Xu *et al.*, Advanced Science **11**, 2310032 (2024).
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Rational Design and Optically Detected Coherent Spin Control of Organic Molecular Color Center Qubits

Sebastian M. Kopp[1], Shunta Nakamura[1], Yong Rui Poh[2], Jonathan R. Palmer[1], Kathryn R. Peinkofer[1], Brian T. Phelan[1], Joel Yuen-Zhou[2], Matthew D. Krzyaniak[1], and Michael R. Wasielewski[1]

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ABSTRACT: Molecular optical-spin interfaces are emerging as promising alternatives to solid state defects such as diamond nitrogen vacancy centers for quantum information science applications.[1,2] In this work, we report an optical-spin interface in organic molecular qubits consisting of two luminescent tris(2,4,6-trichlorophenyl)methyl (TTM) radicals connected via the *meta*-positions of a phenyl linker.[3,4] Optical polarization of the $|T_0\rangle$ sublevel of the triplet ground state is achieved by spin-selective excited-state intersystem crossing from the $|T_+\rangle$ and $|T_-\rangle$ sublevels of the triplet excited state. Addition of a methyl substituent to the phenyl linker increases the predicted excited-state intersystem crossing spin selectivity from 80% to 97% while reducing the electronic coupling between the TTM subunits. This is supported experimentally by an order of magnitude increase in the optically detected magnetic resonance contrast and longer excited-state lifetimes. We demonstrate coherent microwave manipulation of the spin polarized ground state populations and coherences using optically detected Rabi nutations, Hahn echo formation, and echo decay measurements at 85 K in a nuclear-spin rich solvent matrix. This marks a crucial step towards leveraging the favorable spin relaxation times of organic molecules for applications as quantum sensors at temperatures that heretofore have been difficult to achieve by molecular color centers. In addition, we demonstrate that the optical-spin interface of organic diradicals is preserved in doped crystals with favorable spin relaxation times up to room temperature. We combine pulse light ODMR schemes with coherent microwave manipulations of the doped crystals to improve the ODMR contrast and present an in-depth understanding of the spin polarization and relaxation processes present in the molecular color centers.

References

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4. S. M. Kopp et al., *J. Am. Chem. Soc.* **2025**, *147*, 22951–22960.

From diamond defects to protein-based qubit sensors

Peter Maurer

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Abstract: Spin qubits provide unmatched sensitivity for quantum sensing, but most solid-state platforms remain difficult to integrate with biology. Recent advances point to a new frontier: molecular and protein qubits that combine nanoscale size, optical addressability, and biocompatibility. I will present two emerging approaches. First, pentacene molecules scaffolded on hexagonal boron nitride create surface molecular qubits with coherence times up to 188 μs, enabling deterministic placement into van der Waals heterostructures and coupling to nearby spins. Second, genetically encodable fluorescent-protein qubits, only ~3 nm in size, exhibit coherence and optical readout comparable to defect spins in diamond while being seamlessly deployable inside living cells. Together, these platforms establish a new class of molecular quantum sensors that unify quantum engineering and biology, opening pathways toward probing biochemical dynamics and developing next-generation diagnostics.

Organic Diradicals as Resources for Quantum Information Science

Yong Rui Poh, Joel Yuen-Zhou

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ABSTRACT: Electron spins are promising resources for quantum information science, and molecules offer additional advantages of high tunability and scalability. In particular, organic molecules host electron spins that are relatively long-lived, offering more avenues for engineered interactions with its environment. In the first half of my talk, I will discuss our recent works on designer organic diradicals that can function as optically addressable molecular spin qubits [1-3]. These light-initiated platforms have traditionally been hosted in metallic complexes and our design principles for an organic analogue have been supported by ab initio calculations and experimental implementations [4-5]. In the second half of my talk, I will discuss how diradicals in the excited state, also known as radical pairs or electron donor-acceptor complexes, can be harnessed for chiral resolution under an applied magnetic field [6]. The principles are analogous to the chirality-induced spin selectivity (CISS) effect, whereby a broken time-reversal symmetry is intricately linked to a broken mirror symmetry via the electron spin. Through these theoretical endeavours, we hope to motivate further explorations of spin dynamics to achieve unprecedented quantum information goals, such as quantum sensing and quantum control.

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Understanding Single Photon Emission in Transition Metal Dichalcogenides; Transfer of Entanglement from Photons to Electrons During Two-Photon Absorption

George C. Schatz

Northwestern University, Evanston IL 60201 USA

The first part of this talk concerns the development of single or multiple layers of transition metal dichalcogenides (TMDs) for applications as single photon emission (SPE), with emphasis on the use of theory and computations to provide a basis for designing and interpreting experiments. We begin by talking about the emission properties of TMD's, mostly focusing on WSe_2, and the use of chemical functionalization and strain to activate strong single photon emission. Here we find using density functional theory that diazonium functionalization quenches most of the emission through energy transfer processes, leaving behind the longest wavelength emission which shows excellent SPE properties. We also identify specific defects in WSe_2 that are responsible for the emission, and we show why this doesn't happen for WS_2. Theory has also proven useful in explaining the temperature dependence of SPE, and nitrogen plasma effects.

The second part of this talk is concerned with the transfer of entanglement from entangled photons to entangled electronic states in two-photon absorption, here described with a Lindblad master equation approach with simple models of the photons and electrons. This work uses entanglement entropy results to show that for realistic dephasing rates, there can be a positive correlation between photon and electron entanglement.

Spin relaxation in molecular qubits

Philip Shushkov

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The interaction of the electronic spin and molecular vibrations mediated by spin-orbit coupling governs spin relaxation in molecular qubits. We derive a dynamic molecular spin Hamiltonian that includes both adiabatic and non-adiabatic spin-dependent interactions, and we implement the direct computation of its matrix elements using density functional theory and analytical derivative theory. The dynamic molecular spin Hamiltonian contains a novel spin-vibrational orbit interaction with non-adiabatic origin together with the conventional molecular Zeeman and dipolar spin interactions with adiabatic origin. The new spin-vibrational orbit interaction represents a non-Abelian Berry curvature on the ground-state electronic manifold and generates an effective magnetic field in the ground-state electronic spin dynamics. Furthermore, we develop a spin relaxation rate theory that estimates the spin relaxation time via the two-phonon Raman process and the molecular crystal vibrational dynamics. The application of the dynamic molecular spin Hamiltonian together with the spin relaxation rate theory to S=1/2 molecular qubits demonstrates that the spin relaxation time at elevated temperatures is dominated by the non-adiabatic spin-vibrational orbit interaction. The computed spin relaxation rate and its magnetic field orientation dependence are in agreement with experimental measurements. Analysis of the influence of the molecular electronic structure on the strength of the spin-vibrational orbit interaction charts new avenues for the improvement of the spin-coherent properties of molecular systems.

Molecular Qubit Assemblies

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ABSTRACT: Paramagnetic molecules that may be employed as molecular qubits have been shown to possess long coherence times in the three digit microsecond regime, in nuclear-spin-poor and dilute matrices, such as doped solids and frozen solutions.[1] To make progress toward implementing quantum technologies with such molecules, a long road lies ahead.

A first step is the preparation of two- and other few-qubit assemblies.[2] This is essential for the implementation of two-qubit gate operations. Ideally, the interaction between the two qubits should be switchable, e.g., by light excitation. To this end, we have prepared dimers of the TEMPO radical which are bridged by anthracene moieties, using different coupling strategies.[3] Time-resolved absorption measurements reveal different intersystem crossing efficiencies. The coupled nature of the photoexcited three-spin system was unambiguously demonstrated by time-resolved EPR measurements.

For quantum computing and quantum simulation, extended two-dimensional arrays of qubits are required. As a first step in this direction, we have prepared self-assembled monolayers (SAMs) of TEMPO-molecules using a modular approach.[4] Careful analysis demonstrated clean SAM formation. EPR measurements on intact SAMs revealed sizable coherence times. Recent investigations with other radicals substantiated and enhanced on these findings.[5]

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A synthetic spin-photon interface with rare-earth molecules at telecommunications wavelengths

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Quantum control and readout of polyatomic molecules is a frontier for quantum information science. The tunability, nanometer size, and portability of chemically synthesized molecules presents an opportunity for bottom-up design of quantum materials with possible applications from quantum sensing in non-standard environments to synthetic quantum interconnects. With this motivation, we have developed a proof-of-principal molecular spin qubit using a central rare-earth ion (erbium) coordinated by organic ligands. We have shown that this molecular architecture combines a coherent ground-state spin and a high-resolution spin-photon interface at telecommunications frequencies [1]. We have further demonstrated optical control of spin polarization and readout that is both spin- and site-selective, distinguishing between electronic spin states and occupation of distinct physical sites within a solid-state molecular crystal. Compatibility with state-of-the-art photonic and microwave devices provides an opportunity for development of hybrid molecular quantum technologies and optimization by chemical design.

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Molecular Tailoring of Spin-To-Environment Interactions

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Abstract: Understanding how spins interact with their local environment is an important fundamental step toward novel quantum sensing platforms that exploit spins. In this presentation, I will focus on electronic spins on molecules and understanding how they interact with the environment, both from a chemical standpoint (e.g. interactions with local solvents or other molecules) and from a spectroscopic standpoint (e.g. frequency/field dependence of applied microwaves). I will explicitly focus on metal ions for the talk, like V(IV) and Ni(II). Metal-ion spins have magnetic resonance characteristics that are entwined with electronic structure, and hence relatively tiny changes to physical structure can produce large changes in magnetic characteristics. Recent work in our lab exploiting these changes to study magnetic noise and low-frequency sensitivity will be discussed.