Basic Energy Sciences

Quantum Information Science Awards Abstracts

Creating and Probing Large Gap 2D Topological Insulators for Quantum Computing|
Ray Ashoori, Joe Checkelsky, Liang Fu, Nuh Gedik, and Pablo Jarillo-Herrero1

Generation and Remote Distribution of Quantum Entanglement in Solids
David Awschalom, Andrew Cleland, Aashish Clerk, Giulia Galli, Alan Dibos, Joseph Heremans, Alex High, Xuedan Ma, Gary Wolfowicz, Xufeng Zhang, and Tian Zhong

Design, Control and Application of Next Generation Qubits
Arun Bansil, Claudio Chamon, Adrian Feiguin, Liang Fu, Eduardo Mucciolo, and Qimin Yan

Programmable Quantum Materials (Pro-QM) Energy Research Frontiers Center (EFRC)
D.N. Basov, Ana Asenjo Garcia, Cory Dean, James Hone, Michal Lipson, James Shuck, Andrew Millis, Abhay Pasupathy, Xavier Roy, Xiaodong Xu, David Cobden, Daniel Gamelin, Jiun-haw Chu, Matthew Yankowitz, and Di Xiao

Building the Quantum Material Press: An Enabling Nanoscience Facility for Quantum Information Science
Charles T. Black, Greg Doerk, Suji Park, Jerzy T. Sadowski, Young Jae Shin, Aaron Stein, and Kevin G. Yager

The Institute for Quantum Matter Energy Research Frontiers Center
Collin Broholm, N. Peter Armitage, Robert Cava, Natalia Drichko, Seyed Koohpayeh, Yi Li, Tyrel M. McQueen, Satoru Nakatsuji, Predrag Nikolic, Brad Ramshaw, Nitin Samarth, Oleg Tchernyshyov, and David Vanderbilt

Nanofabrication Toolset for Correlating Coherence to Structure in Quantum Information Systems
Stefano Cabrini, D. Frank Ogletree, Adam Schwartzberg, Shaul Aloni, Alexander Weber-Bargioni, David Prendergast, and Andrew Minor

Molecules Functionalized with Cycling Centers for Quantum Information Science
Wesley C. Campbell, Anastassia N. Alexandrova, Justin Caram, John M. Doyle, Eric R. Hudson, Nick Hutzler, and Anna Krylov

Molecular Magnetic Quantum Materials Energy Frontier Research Center
Hai-Ping Cheng, Garnet Chan, George Christou, Arthur Hebard, Richard Hennig, Stephen Hill, Talat Rahman, Neil Sullivan, John Stanton, Samuel Trickey, Vivien Zapf, and Xiaoguang Zhang

Two-Dimensional Quantum Gas with Real Time Control of Complete Hamiltonian
Cheng Chin (PI), Kathryn Levin (Co-PI), Jonathan Trisnadi, Mickey McDonald, Mingjiamei Zhang, and Han Fu

Porting Classical Approaches for Quantum Simulations to Quantum Computers
Bryan K. Clark

Control of Energy Transport and Transduction in Photosynthetic Down-Conversion
David F. Coker, Gregory D. Scholes, Ksenia Bravaya, and Sahar Sharifzadeh, Francesco Segatta, Justin Provazza, Catrina Oberg, James Gayvert, and Ariel Cohen

Creating and Interfacing Designer Chemical Qubits
Danna E. Freedman, William Dichtel, Jeffrey Long, Mark Hersam, James Rondinelli, and Michael Wasielewski

Simulating Long-Time Evolution of Driven Many-Body Systems with Next Generation Quantum Computers
James Freericks, and Alexander Kemper

Quantum Entanglement Between a Solid-State Spin and Trapped Ion via a Photonic Link
Kai-Mei Fu, and Boris Blinov

Coherent Spin-Magnon Coupling for Quantum-to-Quantum Transduction
Gregory D. Fuchs, Daniel C. Ralph, Michael E. Flatté, and Ezekiel Johnston-Halperin

Studying light-matter interactions and energy transfer at the nanoscale with a trapped-ion quantum computer
Hartmut Haeffner, Mohan Sarovar, and Birigitta Whaley

Resource-Efficient Quantum Simulations on NISQ Devices: Advancing the State-of-the-Art
Itay Hen and Amir Kalev

A Route to Molecular Quantum Technologies Using Endohedral Metallofullerenes
Stephen Hill and Jianyuan Zhang

Space-Time Quantum Information from the Entangled States of Magnetic Molecules
Wilson Ho, William J. Evans, Ruqian Wu3

Design & Assembly of Atomically-Precise Quantum Materials & Devices
Jennifer Hoffman, Julia Mundy, Boris Kozinsky, and Taylor Hughes

Deterministic Placement and Integration of Quantum Defects
Han Htoon, Edward Bilejec, Yongqiang Wang, Jennifer A. Hollingsworth, Sergei Tretiak, Igal Brener, David Bruce Burckel, and Andrew C. Jones

Atom-defect Hybrid Quantum Systems
Ania Bleszynski Jayich, Kunal Mukherjee, David Weld, and Norman Yao

Understanding and Controlling Entangled and Correlated Quantum States in Confined Solid-state Systems Created via Atomic Scale Manipulation
Stephen Jesse, Ondrej Dyck, Andy Lupini, Mina Yoon, Prineha Narang, and Dirk Englund

Molecular Control of Spin-Entangled Triplet Excitons from Singlet Fission
Justin Johnson, Obadiah Reid, Brandon Rugg, Chris Chang, Brian Fluegel, Natalie Pace, Niels Damrauer, Kori Smyser, Joel Eaves, and John Anthony

ECRP: Emergent properties of magnons coupled to microwave photons
M. Benjamin and Jungfleisch

Quantum Computing Algorithms and Applications for Coherent and Strongly Correlated Chemical Systems
Sabre Kais, Yong P. Chen, Libai Huang, David Mazziotti, and John Anderson2

Parametrically Induced Quantum Engineering (PIQUE)
Archana Kamal, Leonardo Ranzani, Diego Ristè, José Aumentado, and Raymond W. Simmonds

Frontiers in Quantum Metrology and Transduction
Mark Kasevich, Jason Hogan, Benjamin Lev, Amir Safavi-Naeini, Monika Schleier-Smith, and Jelena Vuckovic

Designing Quantum Algorithms and Hardware for Chemistry and Materials
Christopher Monroe, Jungsang Kim, Kenneth Brown, Jianfeng Lu, Thomas Barthel, Vladimir Manucharyan, Alexey Gorshkov, Maxim Vavilov, and Ivar Martin

Quantum Probes of the Materials Origins of Decoherence
S. Kolkowitz, V. Brar, J. Choy, J. DuBois, M. Eriksson, L. Faoro, M. Friesen, A. Levchenko, V. Lordi, R. McDermott, K. Ray, and Y. Rosen

Embedding Quantum Computing into Many-Body Frameworks for Strongly Correlated Molecular and Materials Systems
Karol Kowalski, Wibe A. de Jong, Travis Humble, Nathan Wiebe, and Dominika Zgid

Nanoscale Quantum and Classical Sensing for Superconducting and Topological Quantum Information
Ben Lawrie, Eugene Dumitrescu, Gabor Halasz, Matt Brahlek, Peter Maksymovych, and Chengyun Hua

Quantum Sensed Nuclear Magnetic Resonance Discovery Platform
Michael Lilly, Edward Bielejec, and Andrew Mounce

Materials for Ultra-Coherent, Mobile, Electron-Spin Qubits
Stephen Lyon, Mark Dykman, M. David Henry, and Eric Shaner

Photon Qubit Entanglement and Transduction
Xuedan Ma, Xufeng Zhang, Stephen Gray, David Czaplewski, Axel Hoffman, and Daniel Rosenmann

Direct Observation of Fractional Quantum Hall Quasiparticle Braiding Statistics via Interferometry
Michael Manfra

Hybrid Quantum/Classical Algorithms for Photochemistry and Nonadiabatic Dynamics
Todd J. Martinez, Edward Hohenstein, Dmitry Liakh, Alexander McCaskey, Abraham Nitzan, Robert Parrish, David Reichman, and Joseph Subotnik

Simulating Strongly Correlated Molecules with a Superconducting Quantum Processor
Nicholas J. Mayhall, Edwin Barnes, Sophia E. Economou, David Pappas

Center for Novel Pathways to Quantum Coherence in Materials
Energy Research Frontiers Center (EFRC)
Joel E. Moore (Director), James Analytis, Stefano Cabrini, Michael Crommie, Peter Ercius, Naomi Ginsberg, Alessandra Lanzara, Jeffrey Neaton, Joseph Orenstein, Ramamoorthy Ramesh, Eli Rotenberg, Feng Wang, Chao Yang, Norman Yao, David Awschalom, Aashish Clerk, Giulia Galli, Supratik Guha, F. Joseph Heremans, Martin Holt, Jiwoong Park, Xufeng Zhang, Dmitri Basov and Ania Bleszynski Jayich

Quantum States in Layered Heterostructures Controlled by Electrostatic Fields and Strain
Stevan Nadj-Perge, Andrei Faraon, Marco Bernardi,
Julia Greer, Gil Refael

Enhancing Entanglement: Non-Markovian and Floquet Reservoir Engineering in Many-Qubit Superconducting Quantum Circuits
Oskar Painter and Aash Clerk

Integrated Development of Scalable Materials Platforms for
Topological Quantum Information Devices
Vlad Pribiag, Paul Crowell, Sergey Frolov, Noa Marom, and Chris Palmstrøm

An Ion-Trap Quantum Simulator for Exotic 2D Materials
Philip Richerme, Gerardo Ortiz, and Babak Seradjeh

Thin Film Platform for Rapid Prototyping of Novel Materials with Entangled States for Quantum Information Science
Christopher Rouleau, Gyula Eres, Rama Vasudevan, David Geohegan, Alexander Puratzky, Kai Xiao, and An-Ping Li

Developing Molecular f-Element Quantum Materials with Strong Electron Correlations
Eric J. Schelter, Corwin Booth, and Jochen Autschbach

QUINTESSENCE: Quantum Instrumentation for Novel Techniques Applying Entanglement and Spinpolarization for Studies with Low Energy Coherent Electrons
Andreas Schmid, Alexander Stibor, D. Frank Ogletree, Alex Weber-Bargioni, Andy Minor, Colin Ophus, and Jim Ciston

Planar Systems for Quantum Information
Jie Shan, James Hone, Allan H. MacDonald, Kin Fai Mak, and Tony F. Heinz

Optical Generation and Manipulation of Spin Qubits
David A. Shultz and Martin L. Kirk

High-Coherence Multilayer Superconducting Structures for Large Scale Qubit Integration and Photonic Transduction
Irfan Siddiqi, Stefano Cabrini, D. Frank Ogletree, Alex Weber-Bargioni, Andrew Minor, Norman Yao, and
William Oliver

Topological Phases of Quantum Matter and Decoherence
Nikolai Sinitsyn, W. Zurek, S. Lin, V. Zapf, D. Yarotksi, L. Cincio, P. Coles, V. Chernyak, and A. Bleszynski Jayich

Intrinsic Topological Superconductors for Next-Generation Quantum Systems
Susanne Stemmer, Leon Balents, Stephen Wilson, and Andrea Young

Hybrid Quantum Systems: Spins, Photons and Superconducting Qubits
Hong Tang, Steve Girvin, Peter Rakich, Robert Shoelkopf, Liang Jiang, Rufus Cone, and Charles Thiel

ECRP: Coherent Control of Strongly Interacting Spins in the Solid-State
Jeff Thompson

Controlled Synthesis of Solid-State Quantum Emitter Arrays for Quantum Computing and Simulation
Jelena Vuckovic, Dirk Englund, Tony Heinz, Mikhail Lukin, Nicholas Melosh, Hongkun Park, and Susanne Yelin

Systems for Transducing Entanglement between Photons and Electron Spins
Michael R. Wasielewski, Emily A. Weiss, Theodore Goodson III, and Shaul Mukamel

QPress: Quantum Press for Next-Generation Quantum Information Platforms
Amir Yacoby, Philip Kim, Pablo Jarillo-Herrero, Joe Checkelsky, Efthimios Kaxiras, Alan Aspuru-Guzik, and Willian Wilson

Quantum Computing Enhanced Gutzwiller Variational Embedding Approach for Correlated Multi-Orbital Materials
Yongxin Yao, Feng Zhang, Noah Berthusen, Niladri Gomes, Cai-Zhuang Wang, Kai-Ming Ho, and Peter P. Orth

ECRP: The Emergent Photophysics and Photochemistry of Molecular Polaritons: a Theoretical and Computational Investigation
Joel Yuen-Zhou

Creating and Probing Large Gap 2D Topological Insulators for Quantum Computing

Ray Ashoori (PI),[1] Joe Checkelsky,[1] Liang Fu,[1] Nuh Gedik,[1] and Pablo Jarillo-Herrero[1]

Topological insulators have unusual electronic properties. The interior of a piece of topological insulator material behaves as an electrical insulator while the edges conduct electricity. New techniques make it possible to create atomically thin flakes of topological insulator materials and to place and stack them with other materials to create larger electronic structures. Theorists have proposed using such structures to produce qubits with topological protection against decoherence. The information processing elements would exist at the conducting edges of the flakes. Now, there is a hunt for materials with properties for making robust topological qubits. In this quest, it is imperative to develop theories for materials and then to screen materials for the features needed for effective creation of topological qubits: (1) low disorder to preserve the integrity of topological edge states; (2) a large topological energy scale ("band gap") to allow for high temperature operation; and (3) either intrinsic superconductivity or the capacity to develop it via proximity from an adjacent layer.

Development and screening of candidate topological insulator materials for use in qubits requires a detailed understanding of their electronic properties. Unfortunately, in many candidate topological insulator materials it has proven difficult to make good (ohmic) electrical contacts for characterization by transport measurements. Even in cases where ohmic contacts exist, ordinary measurements of electrical transport do not probe the bulk in these systems when they are electrically tuned into a topologically insulating state. Further limiting the understanding of these systems, direct probes of the electronic bands in these 2D topological systems are lacking, due to either the small size of flakes of these materials or due to their destruction in exposure to air in transporting these materials to characterization facilities.

Work in this award will involve synthesis of candidate topological insulators and probing them with a combination of methods that can yield a detailed determination of their electrical properties without the need for direct electrical contact. The measurements include (1) a novel pulsed quantum tunneling method that permits very high resolution electronic structure determination; (2) a capacitance method that can make precision measurements of the thermodynamic properties of the electronic system; 3) methods for laser-based angle resolved photoemission spectroscopy for determination of the electronic bands in the material; and (4) a THz technique that can determine the topological properties of the material.

This work brings together theoretical prediction, synthesis, and measurement of samples of different 2D topological insulator materials that potentially contain the key features for higher temperature topological quantum computation. Theoretical efforts will be aimed not only at predicting materials and related device architectures but also to provide feedback to the above studies for improved synthesis and fabrication schemes to improve quantum system properties. The team assembled here offers complimentary expertise in synthesis of bulk, thin film, and atomically thin exfoliated materials with applicability to a wide variety of candidate systems for the next generation of robust quantum information systems.

[1] Massachusetts Institute of Technology

Generation and Remote Distribution of Quantum Entanglement in Solids

David Awschalom,[1] Andrew Cleland, [1] Aashish Clerk[1], Giulia Galli,[1] Alan Dibos, [2] Joseph Heremans,[1] Alex High,[1] Xuedan Ma, [2] Gary Wolfowicz,[1] ,Xufeng Zhang,[2] Tian Zhong[3]

The 'Generation and Remote Distribution of Quantum Entanglement in Solids' effort at Argonne National Lab and Fermi National Accelerator Laboratory continues to realize large-scale entanglement networks based on solid-state quantum systems. This requires development of novel experimental and theoretical strategies for the establishment of a real-world quantum network from the ground up. We will present our efforts characterizing a 30-mile-long, fiber-optic link in the Chicago metro area to investigate new methods for generating and controlling quantum entanglement using solid-state quantum systems. In particular, we will discuss the first steps toward characterizing the optical fiber losses for each quantum channel and the necessary timing synchronization protocols needed to stabilize the fiber channel at each end. We will also update details of the fiber-compatible cryogenic optical experiments installed at the Argonne node, and other technical elements including frequency down conversion and photonic device fabrication for improved photon collection and detection efficiency. These are necessary components to improve the entanglement rate along with long-lived solid-state nuclear spin memories to protect the quantum information while the entanglement swap is performed remotely. The current efforts will not only provide a real-world testbed for quantum science, but also open new technological possibilities for long-distance entanglement networks.

[1] Center for Molecular Engineering and Materials Science and Engineering, Argonne National Laboratory; Pritzker School of Molecular Engineering, University of Chicago

[2] Center for Molecular Engineering and Center for Nanoscale Materials, Argonne National Laboratory

[3] Center for Nanoscale Materials, Argonne National Laboratory; Pritzker School of Molecular Engineering, University of Chicago

Design, Control and Application of Next Generation Qubits

Arun Bansil,[1] Claudio Chamon,[2] Adrian Feiguin,[1] Liang Fu,[3] Eduardo Mucciolo,[4] and Qimin Yan[5]

The technologies for manipulating and storing information quantum mechanically, which are currently based on Josephson-junctions, ion-traps, and qubits generated by defect spins in solids are often hindered by the decoherence processes arising from inevitable couplings to the environmental degrees of freedom. Topological qubits, however, are inherently more robust to decoherence effects, and should be able to sprint ahead once various practical barriers have been overcome. At the present early stage of the development of the field, it is important to continue to explore a variety of architectures and materials beyond the conventional paradigms in order to seed breakthroughs toward building a scalable quantum computer. With this motivation, we are pursuing a comprehensive theoretical research program with four interconnected thrusts as follows.

- A materials discovery effort in two-dimensional compounds in search of materials that could support Majorana zero modes as well as materials that could support defect structures suitable as qubits.
- Exploration of architectures for topological quantum computation by investigating both superconducting Majorana qubits and robust platforms for braiding, consisting of new "meta-materials" built of arrays of Majorana qubits.
- Investigation of properties of hybrid metal-organic qubits based on transition-metal centers in graphene, and molecular crystals of polyaromatic complexes with various atoms embedded at their centers.
- Study of decoherence effects in the presence of dispersive spin baths.

We are using a full spectrum of theoretical and numerical approaches to address various key issues, which range from first-principles computations to the exact treatment of many-body systems using density-matrix-renormalization group, and data-driven high-throughput approaches using a materials database and machine-learning.

[1] Majorana superconducting qubit: C. Schrade and L. Fu, Physical Review Letters 121, 267002 (2018).

[2] Obstacles to quantum annealing in a planar embedding of XORSAT: P. Patil, S. Kourtis, C. Chamon, I. E. R. Mucciolo, and A. E. Ruckenstein, Physical Review B 100, 054435 (2019).

[3] Scalable fermionic error correction in Majorana surface codes: O. Viyuela, S. Vijay, and L. Fu, Physical Review B99, 205114 (2019).

[1] Department of Physics, Northeastern University, Boston MA 02115
[2] Department of Physics, Boston University, Boston MA 02215
[3] Department of Physics, Massachusetts Institute of Technology, Cambridge MA 02139
[4] Department of Physics, University of Central Florida, Orlando FL 32816
[5] Department of Physics, Temple University, Philadelphia, PA 19122

Programmable Quantum Materials (Pro-QM)
Energy Research Frontiers Center (EFRC)

D.N. Basov (Director),[1] Ana Asenjo Garcia,[1]
Cory Dean,[1] James Hone,[1] Michal Lipson,[1]
James Shuck,[1] Andrew Millis,[1]
Abhay Pasupathy,[1] Xavier Roy,[1]
Xiaodong Xu,[2] David Cobden,[2]
Daniel Gamelin,[2] Jiun-haw Chu,[2]
Matthew Yankowitz,[2] Di Xiao[3]

Quantum materials (QMs) manifest the many roles of topology, dimensionality and strong correlations in defining macroscopic observables. The vision for this Energy Research and Frontier Center on Programmable Quantum Materials is to discover and deploy new forms of quantum matter controllable by external stimuli, atomic-layer assembly, magnetic proximity, and nanomechanical manipulation, with the goal of effectively programming their quantum properties.

The particular materials systems we will focus on are the transition metal dichalcogenides (TMDCs) and 2D-halides, two large classes of layered van der Waals (vdW) solids combining a vast range of properties with an unprecedented degree of controllability. The key novelty of the Pro-QM approach is developing strategies for transforming QMs into desired states with tailored quantum properties not attainable in common metals or semiconductors. In parallel, we will investigate the formation of on-demand macroscopic coherent states. Pro-QM will engineer coherent phenomena and robust quantum fluids formed by excitons and exciton-polaritons in vdW heterostructures. The research objectives rely on two cross-cutting themes: i) creation of new tailored materials and architectures hinging on combinations of vdW atomic layers assembled in complex heterostructures; and ii) transformative advances in experimental imaging tools for probing optoelectronic and magnetic properties at native length- and time-scales.

This ambitious program calls for an outstanding team with diverse and complementary expertise. Our team combines emerging (untenured) leaders together with senior researchers with extensive track records of collaborative and impactful research underpinning the field. Guided by concrete and compelling scientific goals and technical approaches, this team will act as cohesive squad in which all members have well defined roles.

The impact. The goals of Pro-QM EFRC are daring in their experimental and intellectual reach, and promise disruptive impact on a range of Grand Challenges for fundamental energy research. A concerted EFRC effort is imperative for making the desired leaps documented through numerous collaborative publications and patent disclosures.

[1] Columbia University
[2] University of Washington
[3] Carnegie Mellon University

Building the Quantum Material Press:
An Enabling Nanoscience Facility for Quantum Information Science

Charles T. Black,[1] Greg Doerk,[1] Suji Park,[1] Jerzy T. Sadowski,[1] Young Jae Shin,[1]
Aaron Stein,[1] and Kevin G. Yager[1]

The Quantum Material Press (QPress) is an ongoing project to develop a first-of-its-kind facility for automated synthesis of layered heterostructure materials by assembly of atomically thin, two-dimensional (2D) components. With integrated and AI-enabled capabilities for *in-situ* characterization and fabrication, the QPress will accelerate discovery of next-generation materials for quantum information science (QIS). This research will yield enhanced understanding of layered materials and the exfoliation process and will ultimately deliver a revolutionary science tool for fabricating and studying quantum heterostructures.

The QPress will be operated at the Center for Functional Nanomaterials at Brookhaven National Laboratory as a valuable resource for the QIS research community. We are strongly collaborating with colleagues at Harvard and MIT, who in parallel are investigating the underlying QPress basic science, including: synthesis of new van der Waals materials, analytics for heterostructure discovery, *in-situ* characterization methods, and applying the QPress to topological superconductivity and quantum simulation.

In recent progress on the project, we have shown the ability of simple robotic motion systems to replace human action in exfoliating van der Waals crystals into distributions of 2D flakes. We have investigated the role of stamp properties, motion profiles, and application of thermal fields. We have also developed an automated cataloger based on software control of an optical microscope, coupled to machine-vision software for identification and classification of exfoliated 2D material flakes. We will next integrate these modules into the QPress cluster tool and deploy data analytics to enable highly automated workflows for 2D materials stacking.

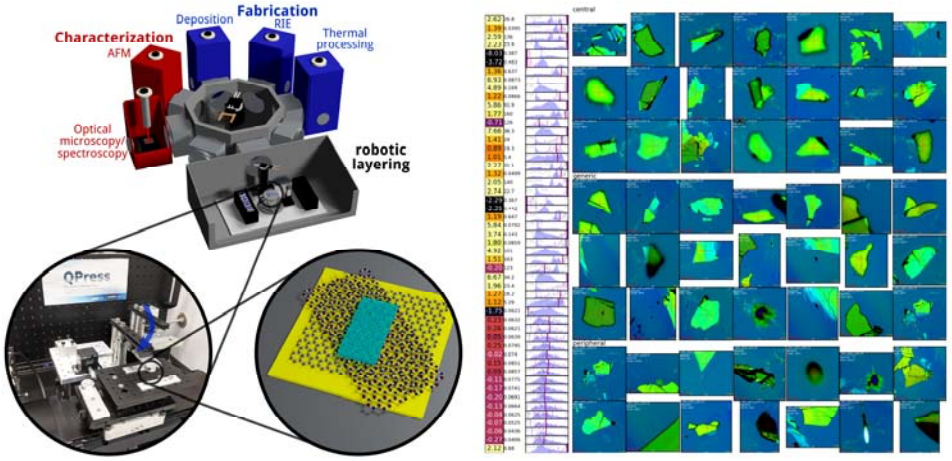


Figure. (Left) The QPress will be a cluster tool, connecting modules for characterization (red) and fabrication (blue), and robotic exfoliation/stacking, thereby enabling the creation of QIS heterostructure materials. (Right) Example image resulting from automated identification, clustering, and classification of 2D material flakes from optical microscopy images. Results of this kind will be aggregated into a searchable materials library.

[1] Center for Functional Nanomaterials, Brookhaven National Laboratory (BNL)

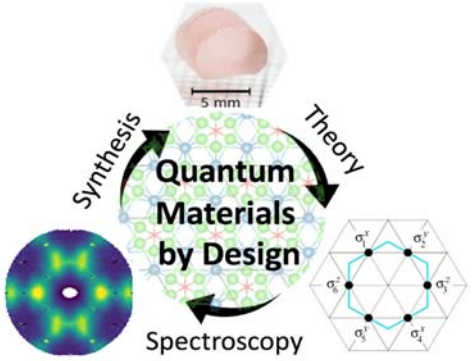
The Institute for Quantum Matter Energy Research Frontiers Center

Collin Broholm (Director),[1] N. Peter Armitage,[1] Robert Cava,[2] Natalia Drichko,[1] Seyed Koohpayeh,[1] Yi Li,[1] Tyrel M. McQueen,[1] Satoru Nakatsuji,[3,1] Predrag Nikolic,[4,1] Brad Ramshaw,[5] Nitin Samarth,[6] Oleg Tchernyshyov,[1] David Vanderbilt[7]

The discovery and characterization of quantum materials is one of the grand challenges of 21st century physical science. New materials, developed though a deep understanding of their underlying physics, will play an essential role in extending the information technology revolution and confronting the unprecedented growth in global energy needs. Despite many important advances, quantum materials continue to present deep fundamental challenges. How can we predict and control the collective properties of 10^{23} electrons in a solid? What novel quantum dominated states of matter, and electronic and magnetic properties may ensue? The opportunities for fundamental discoveries that could transform technologies are bountiful as we extend our ability to understand and control collective quantum phenomena in materials.

The Institute for Quantum Matter Energy Frontier Research Center consists of a collaborative team of scientists that spans the materials-by-design triad of materials discovery and synthesis (single crystals and thin films), advanced experimentation (neutron scattering, optical spectroscopies, transport, ultrasound, and high magnetic field techniques) and theory (analytical and numerical). The Institute is pursuing four types of quantum matter that have not previously been realized: **Topological magnetic semimetals, quantum spin liquids, monopole superconductors, and axion insulators.** Each target presents distinct challenges with deep intellectual connections. There are also crosscuts between areas in terms of the techniques and methods used so that successes in one area advance others.

As we make progress in the realization and characterization of quantum materials, their unique physical properties present opportunities for breakthrough applications in energy and information. These include practical superconductivity for energy storage and distribution, materials with emergent quantum coherent particles for quantum information processing, systems that afford the possibility to control magnetic degrees of freedom with electrical drive, and new platforms for energy efficient electronics. IQM is motivated by the fundamental challenges that correlations and topology present but as our understanding of interacting electrons progresses, we shall also bring the application potential of quantum materials into focus.



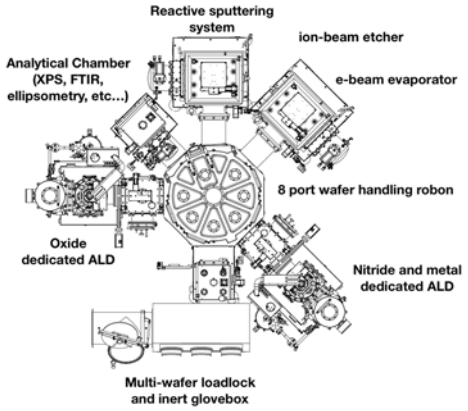
The IQM mission: To realize, understand, and control revolutionary quantum materials and structures where quantum effects such as entanglement and coherence find collective macroscopic manifestations.

[1] Johns Hopkins University
[2] Princeton University
[3] University of Tokyo
[4] George Mason University
[5] Cornell University
[6] Pennsylvania State University
[7] Rutgers University

Nanofabrication Toolset for Correlating Coherence to Structure in Quantum Information Systems

Stefano Cabrini,[1] D. Frank Ogletree,[1] Adam Schwartzberg,[1] Shaul Aloni,[1] Alexander Weber-Bargioni,[1] David Prendergast,[1] Andrew Minor[1]

The fundamental unit of quantum computation and sensing is the qubit, and many physical systems have been investigated for practical realization. These include superconducting Josephson junction circuits, color centers, and isolated cold atoms or ions. Superconducting qubit circuits (SCQBs) being one of the most promising avenues to quantum computation. However, there are limitations to their practical application due to noise sources which shorten their functional "qubit lifetime" (described by two parameters: the energy relaxation time (T1) and the dephasing time (T2)). In this project we are building a suite of integrated, high-fidelity fabrication instrumentation that will allow new communities of users to investigate the fundamental limits of state-of-the-art quantum systems at the Molecular Foundry. We will enable users to understand existing systems and design new ones by creating a quantum fabrication toolset for directed growth of conventional and novel materials, advanced lithography and pattern transfer paired with in- and ex-situ surface characterization. We are developing three new key capabilities at the Molecular Foundry:



Schematic of proposed cluster system containing multiple material growth/deposition systems with advanced in-situ characterization and inert sample loading and manipulation.

1. A robotic fabrication cluster system with materials deposition, including atomic layer and physical vapor depositions, ion etching, and analytical characterization instrumentation, all automated by and contained within a vacuum sample handling robot (see figure).
2. A high-resolution electron beam writing system will allow quantum device patterning with complete flexibility in feature shape, density and size, enabling nanoscale feature control.
3. A low temperature transport measurement system will allow for the investigation of novel materials for superconductors and dielectrics and "close the loop" between design and fabrication.

The new electron beam writing system has been delivered and installation is currently underway. The robotic cluster system is in the midst of procurement and a request for proposals will be published shortly with an expected order date of early 2020 and delivery date of mid-2021. To develop insight into SCQB materials and fabrication we have begun a new research thrust using existing fabrication and characterization capabilities at the Molecular Foundry. Using atomic layer deposition, cross-sectional TEM, x-ray photoelectron spectroscopy and careful control of device processing we have found significant impurities at the superconductor interface which strongly impact resonator performance. As the proposed capabilities come online, we will be able to gain further insight into materials challenges such as these, as well as develop new fabrication processes and materials to significantly improve on existing SCQBs. This knowledgebase and new instrumentation will be an invaluable resource for the Molecular Foundry user community.

[1] Molecular Foundry, Lawrence Berkeley National Laboratory

Molecular Magnetic Quantum Materials
Energy Frontier Research Center

PI: Hai-Ping Cheng,[1] Co-PIs: Garnet Chan,[2] George Christou,[1] Arthur Hebard,[1] Richard Hennig,[1] Stephen Hill,[3] Talat Rahman,[4] Neil Sullivan,[1] John Stanton,[1] Samuel Trickey,[1] Vivien Zapf,[5] Xiaoguang Zhang[1]

The Center for Molecular Magnetic Quantum Materials (M^2QM) aims to provide the pivotal materials physics and chemistry understanding of molecular magnetic quantum materials essential for quantum and conventional computing beyond Moore's Law. The *overarching goal* is to turn molecular magnets into quantum materials useful for both quantum information devices and for quantum-current-based digital devices. Stated in a longer-term perspective, the vision of M^2QM is to understand and exploit the rich complexities of molecular magnetic systems as foundational ingredients for quantum information technologies. Organized into three thrust areas, we focus on magneto-electric couplings[1,2], quantum superposition and entanglement of molecular spin states[3,4], and spin-charge coupling on surfaces and interfaces[5]. Our fundamental theory crosscutting research takes on tasks essential to the general interests of all thrusts and beyond[6]. In this presentation, I highlight recent progress on several specific projects in the M^2QM Center, including the phase diagram of the Mn-taa system and its physical origins, magnetic coupling and control in two-center magnets, transport characteristics of Mn_{12} supported on graphene, and decoherence behavior in finite size molecules.

References

1. *Magnetoelectric behavior via a spin state transition,* Shalinee Chikara, Jie Gu, X.-G. Zhang, Hai-Ping Cheng, Nathan Smythe, John Singleton, Brian Scott, Elizabeth Krenkel, Jim Eckert, and Vivien S. Zapf, *Nature Comm*. 10, 4043 (2019).
2. *Three Jahn-Teller states of matter in spin-crossover system Mn(taa),* Jie-Xiang Yu, Dian-Teng Chen, Jie Gu, Jun Jiang, Long Zhang, Yue Yu, Xiao-Guang Zhang, Vivien Zapf, and Hai-Ping Cheng (submitted).
3. *Molecular spins for quantum computation*, A. Gaita-Ariño1, F. Luis, S. Hill and E. Coronado, Nature Chem. https://doi.org/10.1038/s41557-019-0232-y.
4. *Magnetic coupling pathway and pressure dependence of Mn_3-dimers*, Jie-Xiang Yu, George Christou, and Hai-Ping Cheng (submitted).
5. *Electronegative ligands enhance charge transfer to Mn12 single-molecule magnets deposited on graphene*, Xiaochen Zhu, Ashlyn Hale, George Christou and Arthur F. Hebard (under review).
6. *Spin Decoherence in Molecular Qubits: Insights from Quantum Many-Body Simulations,* Jia Chen, Cong Hu, John F. Stanton, Stephen Hill, Hai-Ping Cheng, and Xiao-Guang Zhang (submitted).

[1] University of Florida
[2] California Institute of Technology
[3] Florida State University
[4] University of Central Florida
[5] Los Alamos National Laboratory

Two-dimensional quantum gas with real time control of complete Hamiltonian

Cheng Chin (PI),[1] Kathryn Levin (Co-PI),[1]
Jonathan Trisnadi,[1] Mickey McDonald,[1] Mingjiamei Zhang,[1] Han Fu[1]

We report our progress toward the realization of a new experimental platform, called "Quantum Matter Synthesizer" (QMS) based on ultracold atoms in a two-dimensional lattices. This platform will allow for a dynamic control of the many-body systems at single atom level, and will be realized by integrating several new technologies to control and manipulate atoms:

1. In situ imaging of individual atoms in a 2D quantum gas

The QMS equips with two microscopes with high numerical aperture, which allow us to distinguish individual atoms in the lattice. In addition, a powerful laser cooling scheme will be employed to keep atoms in the ground state during the imaging. We expect that the sample will remain in the quantum degenerate regime after imaging.

2. Control of individual atoms based on an array of optical tweezer

We will employ a digital micromirror device to generate as many as 1,000 independent optical tweezers. Each one of the tweezers will move one atom to a new location, and a collection of the tweezers can generate arbitrary patterns of atoms in the optical lattice.

3. Control of pair-wise interactions between two atoms

A new technique, called optical Feshbach resonance, will be employed to modify the interactions between two atoms by focusing far-detuned laser light on them. We have shown that optical Feshbach resonance can locally address few atoms and operate at the time scale of 10 nano-seconds. Full spatio-temporal control of atomic interactions will be implemented in the QMS.

Our first goal in the coming year is to arrange 225 atoms in an array of 15x15 lattice sites. Vacancies or double occupancies will be removed by optical tweezers; the pattern of the atoms will be confirmed based on in situ imaging. Our next step will be to integrate optical Feshbach resonance to locally modify interatomic interactions in the sample.

[1] University of Chicago

Porting classical approaches for quantum simulations to quantum computers

Bryan K. Clark[1]

One of the most promising applications for quantum computers is the simulation of quantum systems ranging from molecules to materials. Such simulations are difficult to run on classical computers because of their exponential cost in processing time, which currently restricts the size of exact simulations to systems of approximately 50 electrons. Classically, this exponential difficulty is dealt with by developing alternative approximation techniques, such as fixed-node quantum Monte Carlo and the density matrix renormalization group [1]. Unfortunately, these approximations are often not accurate enough. While in principle, quantum computers overcome this problem, the standard exact quantum computing techniques are unusable for today's era of noisy quantum computers [2]; new quantum algorithms are needed.

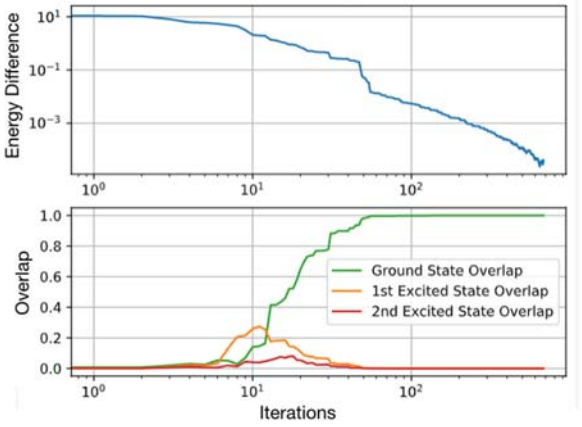


Figure 1: Improved variational quantum eigensolver optimization showing the energy difference (top) and fidelity (bottom) from the ground state of the XXZ Hamiltonian as a function of iterations for a 3-layer circuit.

The objectives of this research are to develop quantum computing algorithms for simulating molecules and materials by porting the classical approximation techniques used on classical computers to quantum computers. In addition, this research will establish how to make these algorithms simultaneously leverage existing large classical parallel computing resources in concert with small quantum machines. Some recent progress toward this goal includes improving the optimization methodology for variational quantum eigensolvers [3] on variational quantum circuit ansatz (see preliminary results in Figure 1). In addition, we have begun to construct new algorithms to leverage classical machines to determine how to set up promising initial quantum states on a quantum computer.

[1] DM Ceperley and BJ Alder. Quantum monte carlo for molecules: Greens function and nodal release. The Journal of chemical physics, 81(12):5833–5844, 1984; Steven R. White. Density matrix formulation for quantum renormalization groups. Phys. Rev. Lett., 69:2863–2866, Nov 1992.

[2] Dave Wecker, Bela Bauer, Bryan K Clark, Matthew B Hastings, and Matthias Troyer. Gate-count estimates for performing quantum chemistry on small quantum computers. Physical Review A, 90(2):022305, 2014; John Preskill. Quantum computing in the nisq era and beyond. Quantum, 2:79, 2018

[3] Jarrod R McClean, Jonathan Romero, Ryan Babbush, and Al´an Aspuru-Guzik. The theory of variational hybrid quantum-classical algorithms. New Journal of Physics, 18(2):023023, 2016.

[1] University of Illinois at Urbana Champaign

Control of Energy Transport and Transduction in Photosynthetic Down-Conversion

PI & Co-PIs: David F. Coker,[1] Gregory D. Scholes,[2] Ksenia Bravaya,[1] and Sahar Sharifzadeh[3]
Key Personnel: Francesco Segatta,[1] Justin Provazza,[1] Catrina Oberg,[2] James Gayvert,[1] and Ariel Cohen[3]

The project will develop experimental and theoretical capability that aims to control energy transport and transduction at the molecular level, focusing on multi-chromophore photosynthetic light harvesting pigment-protein complexes that down-convert initial electronic excitation by manipulating local environmental coupling and dissipation. Two different control mechanisms will be explored: (1) manipulating the nature of the chromophores, their excited state couplings, and interactions with local environment, and (2) we will study how initial state preparation and non-equilibrium driving of these complex, noisy systems might be enabled using ultrafast nonlinear spectroscopy with shaped laser pulses to monitor mechanism and potentially control function.

To accomplish these goals the team will first develop computational protocols that combine statistical mechanical simulations with first principles quantum calculation of coarse-grained model Hamiltonian ensemble parameters, together with dissipative quantum dynamical techniques to enable prediction of non-linear spectroscopic responses of multi-chromophore light harvesting systems, focusing on modeling the effects of pulse shaping and initial state preparation on signals.

The theoretical team includes the **quantum dynamics and non-linear spectroscopy modeling group** (Coker, Segatta, Provazza) who are developing simulation tools for combining first principles model Hamiltonian ensemble data with non-perturbative dissipative quantum dynamical simulation methods to compute 2D electronic spectroscopy, and transient absorption signals, enabling exploration of the influence of pulse shaping on initial state preparation and the subsequent dynamics probed in these signals. The **first principles quantum model Hamiltonian group** (Bravaya, Gayvert, Sharifzadeh, Cohen) are developing and extending multi-reference configuration interaction excited state quantum chemistry methods that can treat multi-electron excitations, and the influence of inhomogeneous solvation in complex protein environments as well as many-body perturbation theory approaches that can treat these phenomena and provide benchmark studies. Our theory groups are working in close collaboration with the **shaped pulse nonlinear spectroscopy experimental group** (Scholes, Oberg) who are implementing shaped pulses to control preparation of initial vibronic excited states and probe subsequent dynamics. The use of our first principles non-equilibrium driven open quantum system dynamics approach will enable open loop quantum control for predicting initial state preparation. Direct comparison with experimental signals will provide detailed mechanistic interpretation of state preparation capability.

The Scholes group has access to various structurally characterized mutants and chimeras. These will be characterized spectroscopically, modelled theoretically, and provide the basis for detailed studies of the influence of local structural modification on couplings and environmental interactions that influence control mechanisms.

[1] Department of Chemistry, Boston University
[2] Department of Chemistry, Princeton University
[3] Department of Electrical and Computer Engineering, Boston University

ECRP: Using Ultrafast Entangled Photon Correlations to Measure the Temporal Evolution of Optically Excited Molecular Entanglement

Scott Cushing[1]

Entangled photons can be created by splitting one photon into two lower energy photons via the process of spontaneous parametric down-conversion. The resultant pair of photons, however, can still act as one photon in subsequent light-matter interactions. For example, an entangled photon pair has a molecular absorption cross section close to that of a single photon, will only leave the same side of a 50:50 beamsplitter, and diffract at half their wavelength. The goal of this project is to measure how the entangled photons' properties are temporally transferred to a molecular spin state. This includes measuring how quantum and classical decoherence routes control entanglement, the timescale of these processes, and whether or not these quantum states can be transferred to a secondary, electronically coupled system. To probe these questions, a few-femtosecond, few-photon entangled spectrometer will be constructed. The proposal will answer fundamental questions about entangled light-matter interactions as well as create new avenues in ultrafast spectroscopy through the application of entanglement.

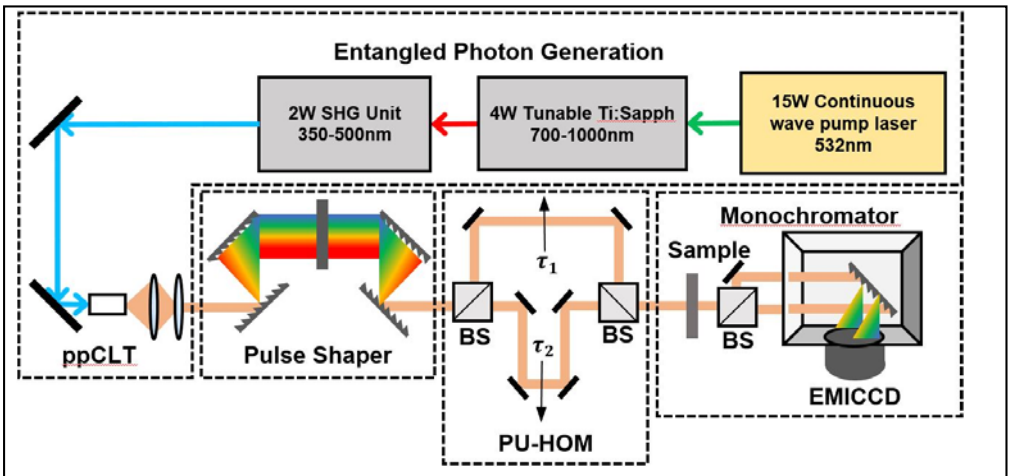


Figure 1. Schematic of the entangled photon spectrometer. The ppCLT is a periodically poled congruent lithium tantalate waveguide; BS is a beam splitter; EMICCD is an intensified electron multiplying camera, PU-HOM is a simplified schematic of a phase-unlocked Hong-Ou-Mandel interferometer.

[1] Division of Chemistry and Chemical Engineering, California Institute of Technology

Q4Q: Quantum Computation for Quantum Prediction of Materials and Molecular Properties

Rosa Di Felice (PI),[1] Anna I. Krylov,[1] Marco Buongiorno Nardelli,[2] Marco Fornari[3]

Computational studies have boosted knowledge and progress in chemistry and materials science, by enabling prediction of novel phenomena in molecules and materials, which is at the core of DOE's mission. While computers have undergone enormous progress in the last 3 decades, the underlying silicon technology is coming to a critical stage and the scientific community is looking for alternatives. Quantum computation (QC) is a potential option. Quantum information theory has made great progress in producing a mature formulation of concepts, theorems and algorithms. Yet, the field of quantum computation has been frustrated by the difficulty of fabricating useful hardware. Two other significant issues for the development of quantum computing have been: the hindrance to identify breakthrough applications and the difficulty of mastering both quantum computer science and chemistry/materials science. However, these hurdles are beginning to be overcome. The two research areas identified for their potential synergy with quantum hardware and software targeted in this project are "controlling the quantum dynamics of nonequilibrium chemical and materials systems" and "unraveling the physics and chemistry of strongly correlated systems". The quantum devices that are currently accessible to users implement two different schemes for quantum computation: (a) gate-model quantum computation (GMQC) in IBM and Rigetti cloud hardware and (b) adiabatic quantum optimization (AQO) in D-Wave commercial hardware. We are using all these platforms to solve simple problems in chemistry and materials science.

AQO: we estimate the formation energies of small molecules (such as H_2, LiH, HeH^+) on D-Wave quantum annealers, using both the D-Wave 2X installed at USC and D-Wave 2000. We provide comparisons of the effectiveness of the quantum annealers with respect to classical computers and QMQC. We also apply the quantum annealers to learn binding affinities for transcription factors to DNA. Furthermore, we use various kinds of graphs to build materials models and solve the graphs by finding the ground state of an Ising Hamiltonian on D-Wave. In all these cases, we explore different embedding parameters to find the optimal performance.

GMQC: we compare the efficiency and stability of IBM and Rigetti quantum devices and simulators to compute the ground state of simple di-atomic molecules, using the variational quantum eigensolver. The performance is also assessed against AQO. We practice with available quantum software pyQuil, QISKIT and OpenFermion for electronic structure calculations. We aim at building the interface of these software packages with Q-CHEM for hybrid computation. We plan to explore novel algorithms beyond the molecular ground state.

[1] University of Southern California
[2] University of North Texas, Denton
[3] Central Michigan University

Quantum Chemistry for Quantum Computers

Francesco A. Evangelista,[1] Alán Aspuru-Guzik,[2] Garnet K.-L. Chan,[3] Gustavo E. Scuseria,[4]
James D. Whitfield,[5] Dominika Zgid [6]

Over the past fifty years, quantum chemistry has had a transformative impact on chemistry and materials science by enabling the computational prediction of properties and reactivity of molecules and materials. Two factors have made this success possible: i) the development of efficient theories of electronic structure and ii) the steady growth of computing power. Nevertheless, quantum chemistry methods are currently unable to tackle strongly correlated molecules and materials, owing to the exponential complexity of the fundamental physics of these systems. Quantum computers, which manipulate information using quantum mechanical principles, offer a solution to this problem. With the rapid development of quantum computing hardware and a recent preliminary demonstration of quantum advantage (computing power superior to that of classic hardware), there is a realistic expectation that quantum computing will have a transformative effect on chemistry simulations in the near future. A crucial step to translate these early successes into advances in the chemical sciences is the development of new quantum computing algorithms for chemistry.

The objective of this research is to create quantum chemistry methods for strongly correlated molecules and solids that will run on quantum computers with a modest number (50–100) of quantum bits (see Figure 1 for a summary of the four project thrusts). We are developing new quantum algorithms for many-electron simulations based on quantum imaginary- time evolution (Motta et al., Nat. Phys. 2019) and its real-time variant, and developing efficient fermionic mappings for quantum chemistry computations. To leverage the power of small quantum devices, we are developing downfolding approaches for applications to large-scale systems and embedding methods for solids. These new algorithms ad methods are being implemented in open-source software. We are also developing standard benchmarks for testing the accuracy and computing power of new quantum hardware. And in collaborations with industry partners, we are validating prototypes of quantum computers using these new methods. More generally, this project paves the way to applications of quantum computers to study strongly correlated systems critical to the mission of the DOE, such as transition metal catalysts, high-temperature superconductors, and novel materials that are beyond the realm of classical simulation.

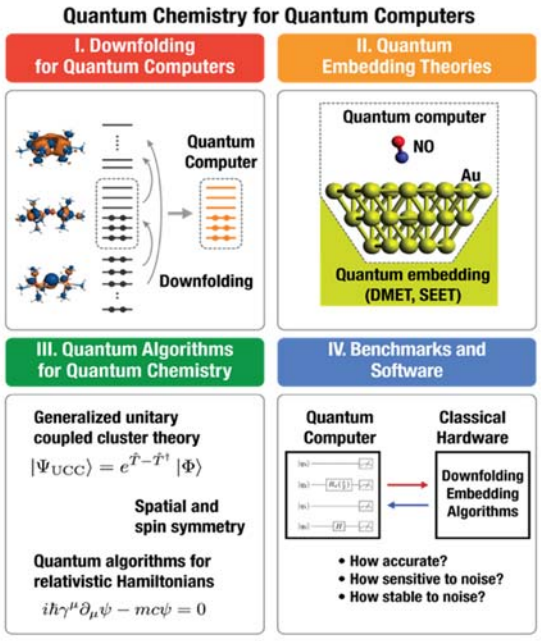


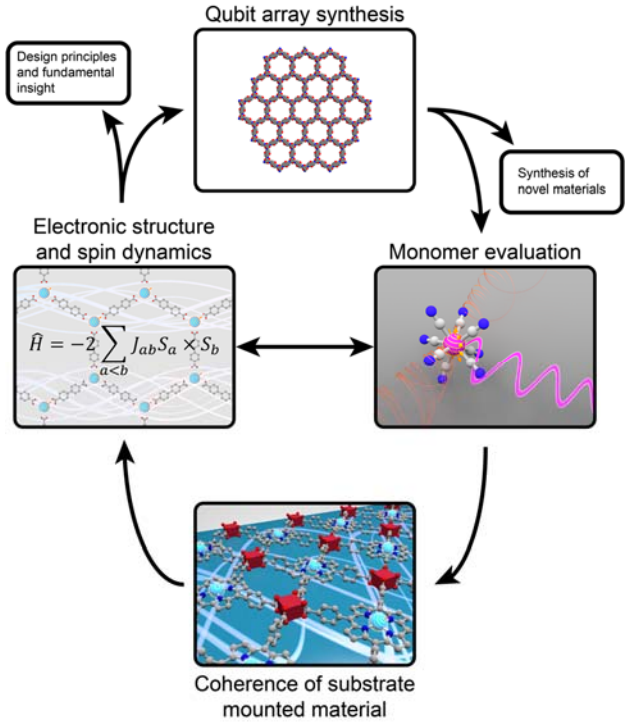
Figure 1. The four project thrusts.

[1] Emory University
[2] University of Toronto
[3] California Institute of Technology
[4] Rice University
[5] Dartmouth College
[6] University of Michigan

Creating and Interfacing Designer Chemical Qubits

PI: Danna E. Freedman,[1] **Co-PI**: **William Dichtel**,[1] **Jeffrey Long**[2] **Mark Hersam**, [1] **James Rondinelli**,[1] **Michael Wasielewski**[1]

The transformative ability of chemistry to impact quantum information science lies within the intertwined combination of atomic-scale control and the ability to produce arrays of qubits from a single synthetic process. Advances in synthetic chemistry and control over molecular-based materials will be harnessed to establish new framework-based qubit platforms. The goal of this project is the chemical synthesis of an atomically-precise array of qubits integrated with a 2D substrate primed for system integration. The team will seek to imbue qubits with spatial precision by designing bottom-up arrays of qubits using an interdisciplinary materials theory and synthetic chemistry approach within an iterative paradigm based on active exchange of data and materials among team members with synthesis, computation, and qubit characterization. Specifically, chemical synthesis will be used to create metal-organic and organic radical-based arrays of qubits that are interfaced with surfaces of functional 2D materials with compositions, geometries, dimensionalities guided by electronic-structure theory. The outcome will be a platform of highly tunable molecular qubits and qubit arrays. The main objectives are to: (a) Create a defect-free network of qubits; (b) Interface qubits with surfaces; and (c) Generate fundamental insight into quantum properties of the qubit networks. Success in the objectives will be assessed by determining the synthetic control over the qubit-qubit interactions and the viability of the qubit arrays for quantum information science.



[1] Northwestern University
[2] University of California, Berkeley

Simulating long-time evolution of driven many-body systems with next generation quantum computers

James Freericks (PI),[1] Alexander Kemper (co-PI)[2]

We are on the cusp of entering the world of quantum computing for applications to science. While quantum computers have already existed for a few years, the current hardware is far from ideal–they do not have many qubits, the results are prone to errors, and they cannot run computer codes with large gate counts. The objective of our work is to find the best applications for cutting-edge science that can be studied on current and near-term quantum computers, and then design and run these algorithms in the most robust fashion with respect to potential errors. Key to our current work is simulating dynamics exactly, which is possible for small systems.

We present results in two directions: (i) describing the behavior of driven-dissipative quantum systems; and (ii) measuring low-energy states of quantum magnets. In (i), we benchmark dissipative dynamics for a noninteracting system via a master equation approach implemented with high fidelity using quantum hardware. Specifically, we modeled an infinite noninteracting system coupled to an infinite fermionic bath. Based on the solution of the problem using the Lindblad formalism, we were able to obtain the correct steady state on IBM hardware by constructing the Kraus maps directly. For this small system, a (still difficult) qubit reset is not required.

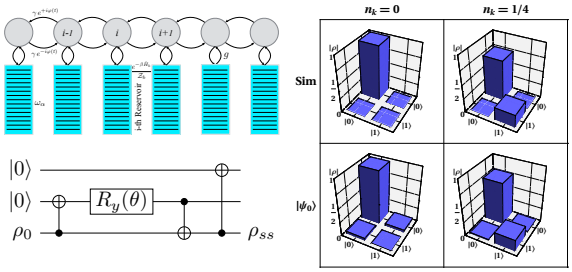


Fig. 1: Simulating an infinite (noninteracting) driven-dissipative system by coupling to an infinite reservoir. Left: schematic of sites coupled to infinite fermionic baths and circuit for proof of principle. Right: Density-matrix results from IBM hardware for one k-point, showing >99% fidelity.

In (ii) we have demonstrated the possibility of evaluating low-energy excited state spectra on quantum hardware. We have mapped out the magnon spectra using a Lehmann representation of the correlation function for a 4-site Heisenberg model entirely using quantum computers. Although the direct results are quite noisy, by utilizing simple error corrections and leveraging the power of Fourier transforms, reasonable results may be obtained. Tantalizingly, the time evolution in this approach was possible without the use of Trotterization, suggesting that more general improvements to time evolution may be possible for larger systems.

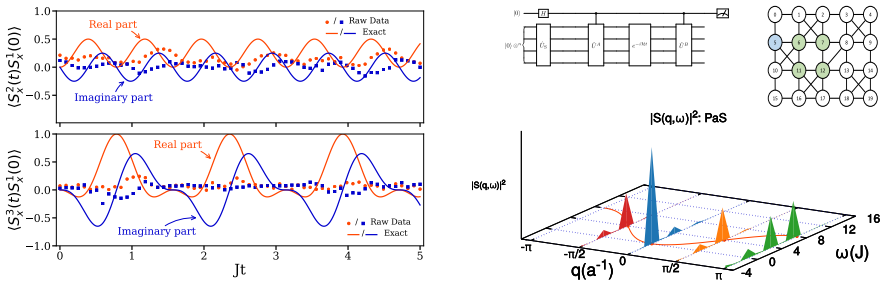


Fig. 2: Calculating spin-spin correlation functions on IBM quantum hardware. Left: raw data. Right: circuit, layout, and obtained magnon spectra. arXiv: 1909.05701.

[1] Georgetown University
[2] North Carolina State University

Quantum entanglement between a solid-state spin and trapped ion via a photonic link

Kai-Mei Fu,[1] Boris Blinov[1]

One of the main limiting factors in the development of quantum computers is engineering a single qubit system which excels at all the requirements for quantum computing. In contrast, efficient transduction between qubit systems may lead to hybrid-qubit quantum computers in which different qubits may specialize in memory, operations, and interconnects, eliminating the need for a single qubit to excel on all fronts. In our work we plan to create, for the first time, entanglement between a single isolated Yb+ atom suspended in space by an electric field, the ideal qubit for quantum memory, and a single electron spin in the semiconductor ZnO, a candidate for fast qubit operations. The scheme is enabled by the nearly-identical optical transition frequencies in these disparate quantum systems. Future applications of this hybrid system that utilizes three types of qubits, single semiconductor spins, single atoms and single photons, may include quantum repeaters and quantum networks, and new types of quantum computing platforms.

[1] University of Washington

Molecules Functionalized with Cycling Centers for Quantum Information Science

Wesley C. Campbell,[1] Anastassia N. Alexandrova,[2] Justin Caram,[2] John M. Doyle,[3] Eric R. Hudson,[1] Nick Hutzler,[4] Anna Krylov[5]

The emerging quantum technology stems from two simple observations: that information is physical (Shannon), and that therefore information is also quantum (Feynman). Many of the pioneering steps in the field of quantum information processing and quantum sensing have been taken by ultracold, gas-phase atoms that can be controlled at the quantum level because they contain narrow-band optical cycling transitions -- subsets of states that are fully connected despite the presence of spontaneous emission.

We are designing and developing the tools to add this quantum information functionality to a diverse set of systems ranging from gas-phase molecules to surfaces. With very few exceptions, molecules that are known to optically cycle conform to the template of an alkaline earth atom bound to a halide (or halide-like group). How these features change when the molecule is ionized, when there are multiple optical cycling centers on a single molecule, or when one end of the molecule is bound to a surface have implications for the applicability of this scheme in a wide array of environments. We will discuss extensions of this theme as well as some variants that do not fit this mold. Some of the lessons these species provide have led to new directions for this work and concepts for molecular quantum information processors.

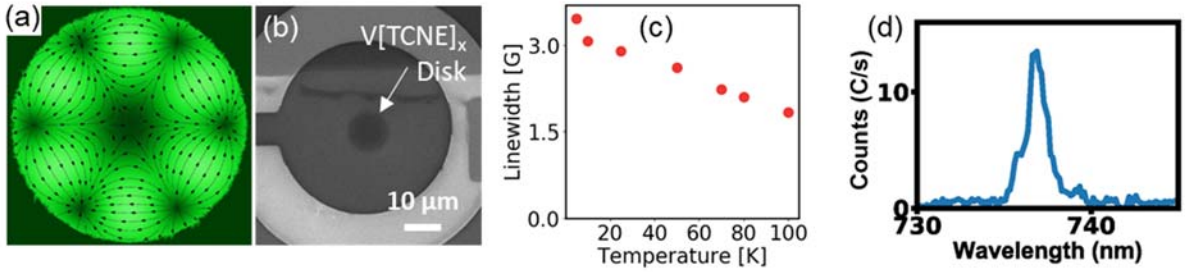
[1] UCLA Physics & Astronomy
[2] UCLA Chemistry & Biochemistry
[3] Harvard Physics
[4] Caltech Physics
[5] USC Chemistry

Coherent spin-magnon coupling for quantum-to-quantum transduction

Gregory D. Fuchs,[1] Daniel C. Ralph[1], Michael E. Flatté[2], Ezekiel Johnston-Halperin[3]

Our project seeks to create and study coherent coupling between qubits based on isolated defect spins in diamond and the magnons of patterned vanadium tetracyanoethylene ($V[TCNE]_x$) – an ultra-low damping organic-based magnet. The resulting hybrid quantum system will be used to create entanglement between spins that are mutually coupled to a magnon mode or it to form a bus between isolated diamond spins and a superconducting circuit via strong resonator-magnon coupling. Additionally, diamond defect spins such as nitrogen-vacancy (NV) centers can be entangled with photons via their coherent optical transition, enabling quantum-to-quantum from the microwave to the optical regime. Key scientific and technical challenges include (i) understanding the best geometries for coupling, (ii) developing the growth and patterning of an ultra-low damping magnon modes at low temperature, (iii) the fabrication of highly-coherent, shallow defect spins with narrow optical transitions and (iv) the integration, characterization and optimization of spin-magnon coupling. Furthermore, this hybrid quantum system must be able to operate at temperatures below 100 mK.

During this period our team has made progress on all of these challenges, taking an integrated approach. To address (i) Flatté has led a theoretical effort to calculate magnon modes of a normally magnetized $V[TCNE]_x$ disk from Maxwell's equations and the Landau-Lifshitz equation. The results showing the resulting microwave fringe field of a whispering gallery like mode is shown in Fig. 1a, which serves to increase the coupling rate by reducing the modal volume. Experimentally, we have developed an integrated process to grow, pattern, encapsulate and characterize $V[TCNE]_x$ integrated with diamond membranes containing shallow NV centers and microwave antennas (Fig. 1b). A key aspect of $V[TCNE]_x$ is its low damping, which equal to or below that of the best ferromagnetic insulating materials at room temperature. We have recently shown that this result persists to low temperature (Fig. 1c) in $V[TCNE]_x$ thin films. We attribute the modest linewidth increase to inhomogeneous anisotropy introduced by mismatched of thermal expansion between $V[TCNE]_x$ and the substrate. Measurements of patterned structures, that should not show this effect, are underway. In addition to implantation and characterization of shallow NV centers, we are also examining the performance of SiV centers with shallow implantation depths (Fig. 1d). Although NV centers have superior spin coherence at room temperature, silicon-vacancy (SiV) centers in diamond have superior optical performance and are less sensitive to electric field noise. At the T < 100 mK, the SiV center spin coherence should recover to a value comparable with NV centers, enabling both superior optical properties and excellent spin coherence. An examination of the low temperature spin coherence of shallow SiV centers is in progress.



[1] Cornell University
[2] University of Iowa
[3] The Ohio State University

Studying light-matter interactions and energy transfer at the nanoscale with a trapped-ion quantum computer

Hartmut Haeffner[1], Mohan Sarovar[2], Birigitta Whaley[1]

A grand challenge in materials sciences is to control energy transfer and dissipation at the nanoscale. Meeting this challenge requires progress in understanding of how nanoscale structure influences these phenomena. Although detailed quantum mechanical models exist that capture the structure and physics of materials and molecular species, solving these models to calculate the relevant emergent phenomena has so far proven difficult.

A quantum simulator, capable of implementing a realistic model of the system of interest, could provide insights into these processes in regimes where numerical treatments fail. We model such transfer processes using an ion-trap quantum simulator. Sites within molecular complexes are encoded in the electronic states of the ions while the molecular vibrational degrees-of-freedom are represented by the thermal vibrational motion of the ion crystal. In addition, the state of electromagnetic fields is encoded in the vibrations of the ions. Thus, the full process of light absorption and transport to a specific site can be studied.

Theory activities are designed to both complement and inform the experiments such that the project will bring new understanding to energy transduction and transport in materials. Possible applications of this understanding are improvements to the design of new photodetectors and photovoltaic systems.

[1] University of California, Berkeley
[2] Sandia National Laboratories, Livermore

Resource-Efficient Quantum Simulations on NISQ Devices: Advancing the State-of-the-Art

Itay Hen[1], Amir Kalev[2]

The simulation of quantum many-body systems is a central challenge in Physics, Chemistry and Material Sciences as well as in other areas of science and technology. Devising efficient simulation algorithms is a task that is as important as it is demanding. It will serve to advance our understanding of phenomena associated with the dynamics of non-equilibrium chemical and materials systems, unravel the physics and chemistry of strongly correlated electron systems and so much more. To date however, no classical algorithms are known to efficiently simulate quantum many-body systems. Quantum algorithms offer a way around the classical bottlenecks by way of `digitizing' the time evolution of the system in question on a circuit. However, present-day quantum computing devices only allow for the programming of small and noisy quantum circuits, which places severe constraints on the types of applications these devices may be used for in practice. To take full advantage of the computing power of present, and near-future, quantum information processors as quantum simulators, it is paramount to devise quantum algorithms whose resource efficiency is tightly optimized to run on small noisy circuits. Here, we propose to theoretically develop and experimentally benchmark a novel algorithmic approach for resource-efficient Hamiltonian simulations that, we argue, will supersede the current state-of-the-art. The proposed technique utilizes aspects of quantum Hamiltonian simulation that to date have not been taken into account in existing Hamiltonian simulation algorithms, specifically, prior knowledge of the structure of the Hamiltonian and, perhaps more importantly, its relation to the initial state of the system, to further reduce the resource cost of the simulation. We will show that this additional information allows for a series expansion of the quantum time-evolution operator that takes advantage of this information, which has so far been disregarded. The advantages of this new approach translate, in turn, to a more efficient, or resource-lean, Hamiltonian simulation technique as compared to the existing state-of-the-art. This effort will have in addition an equally important experimental component within which the proposed technique will be benchmarked on currently available quantum devices and where the capabilities as well as limitations of noisy intermediate-scale quantum (NISQ) hardware will be determined.

[1] University of Southern California
[2] University of Maryland

A Route to Molecular Quantum Technologies Using Endohedral Metallofullerenes

Stephen Hill[1] and Jianyuan Zhang[2]

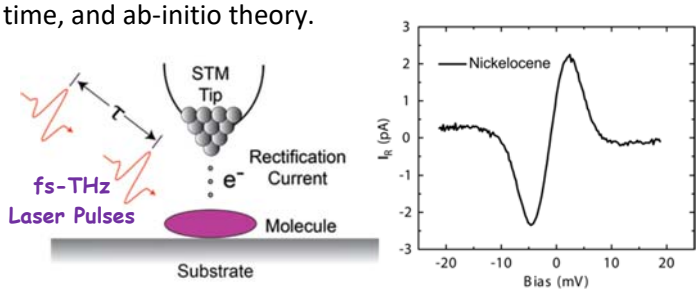
In the search for physical realizations of the basic units for practical quantum computing (quantum bits or qubits), the bottom-up molecular approach is highly promising. This project focuses on fundamental studies of a unique class of metal-organic hybrid molecules, so-called endohedral metallofullerenes (EMFs), in which quantum information can be encoded into the magnetic (spin) states associated with lanthanide (Ln) atoms that are encapsulated within robust carbon cages (fullerenes). This approach promises significant advantages over other current magnetic qubit targets based on inorganic molecules and solids. First and foremost, the fullerene cage provides a rigid environment devoid of elements that possess magnetic nuclei (the ^{12}C nucleus is non-magnetic), thereby protecting the encapsulated atoms from well-known and stubborn noise sources – random vibrations and fluctuating magnetic fields due to nearby nuclei – that can easily erase fragile quantum information states. Equally important is the focus on carbon-based molecules, which opens up the vast toolbox of organic molecular chemistry. This will allow for large-scale synthesis of chemically identical species, with exquisite control over the quantum information states of the associated endohedral Ln atoms. Meanwhile, chemical functionalization of the periphery of the EMF cage will provide potential routes to scaling-up into more complex quantum circuits via molecular self-assembly, and possibilities for rapid optical encoding and read-out of quantum information via attachment of optically active organic groups. Finally, the quantum computational resources that are attainable within a single EMF molecule containing multiple Ln atoms (up to three) with large magnetic moments (e.g. Gd^{3+}) are expected to be considerable in comparison to inorganic transition metal counterparts. Therefore, the project aims to demonstrate the implementation of simple quantum algorithms on individual Ln EMF qudits (the generalization to base d of a qubit), something that is not possible on a single molecular qubit. Synthetic efforts aim to: (1) realize accurate and targeted tuning of the magnetic quantum states of encapsulated Ln ions, thus enabling precise, high-fidelity qubit manipulation using advanced microwave magnetic resonance techniques; and (2) enable responsiveness to other external stimuli (light, current, etc.) for localized/selective qubit readout and control. The project will leverage unique electron spin resonance (ESR) instrumentation available at the US National High Magnetic Field Laboratory (NHMFL), both for precisely characterizing the magnetic states of candidate Ln-EMF molecules, and for demonstrating practical quantum logic operations. Collectively, these efforts will lead to a seamless feedback loop encompassing structural design, chemical synthesis, spectroscopic characterization, and quantum operation, to establish fundamental understanding of the design rules for EMF-based molecular qubits/qudits with desired properties, paving the way towards next-generation quantum technologies.

[1] Department of Physics and National High Magnetic Field Laboratory, Florida State University
[2] Department of Chemistry and Chemical Biology, Rutgers University

Space-Time Quantum Information from the Entangled States of Magnetic Molecules

Wilson Ho,[1] William J. Evans,[2] Ruqian Wu[3]

The ability to vary and control the quantum properties of single magnetic molecules arises from the large variations that are possible in the elemental composition and structure of organometallic molecules. These variations include choices in the transition and rare earth metal atoms and the attached organic framework that isolate the magnetic centers from the environment but also couple to them. Because the electron spins can form two-level systems and have long coherence times, they are potential candidates for quantum information processing as qubits. Furthermore, the sensitivity of the electron spin to the magnetic field and other nearby spins enables it to be configured for sensing and imaging. This collaborative project combines synthesis, measurement, and theory of magnetic molecules as qubits, sensors, and imaging agents by studying the energies and spatial distributions of quantized excitations, the length of time the quantum states remain superposed and entangled, and the different factors that cause dephasing and degradation of coherence. The magnetic excitations in molecular systems, from a single molecule to molecular lattices, are measured by inelastic electron tunneling and terahertz laser induced rectification current spectroscopies with the laser scanning tunneling microscope (laser-STM). The coherent superposition and entanglement of the magnetic states are created and tracked in time by terahertz (THz) and near-IR femtosecond laser pulses coupled with the STM. Measurement with simultaneous spatial and temporal resolution enables a basic understanding and system control at the atomic scale. A variety of molecular complexes that have a magnetic atom sandwiched between two rings of carbon atoms will be synthesized, measured, and calculated. The two rings isolate the central magnetic atom from its environment, which would increase the length of time the spin quantum states remain superposed and entangled. An important goal of the planned research is to maximize this time for information processing based on the quantum states by optimizing the composition and structure of molecules. The sandwiched metal atom in these molecules can be a transition metal, a rare earth metal, or uranium to provide rich spin correlation effects. The possibility of ligand substitution allows alterations of the molecular motions that affect the strength of the spin-vibrational coupling and the time duration of the spin coherence in molecular qubit states. Reversible electron transfer from the STM tip to the bridging molecule in bimetallic rare earth magnetic molecules allows electrical control of the spin correlation between the two magnetic atoms within the complex. This research lays the foundation for optimizing the composition, structure, and interaction of magnetic molecules as carriers of quantum information by combining chemical synthesis, measurement in space-time, and ab-initio theory.



Schematic diagram of a femtosecond THz laser combined with a low temperature scanning tunneling microscope, and a rectification spectrum induced by the THz laser of a single magnetic nickelocene molecule adsorbed on Cu(001) surface.

[1] University of California, Irvine
[2] University of California, Irvine
[3] University of California, Irvine

Design & Assembly of Atomically-Precise Quantum Materials & Devices

Jennifer Hoffman,[1,2] Julia Mundy,[1] Boris Kozinsky,[2] Taylor Hughes[3]

The PIs are developing a platform of new materials to be used in quantum information devices. The efforts integrate theoretical and experimental approaches within a tight feedback loop to predict, design, realize, and characterize new materials platforms and device architectures based on "Xenes" – single layers of atoms arranged in a honeycomb lattice, analogous to carbon-based graphene, but with heavier elements such as stanene, bismuthene, and plumbene. To functionalize these Xenes into devices, the investigators will decorate the Xenes with "adatoms" such as halogens or magnetic atoms. They will employ high-throughput computational materials screening to identify promising adatoms or molecular groups that possess the desired functionality. Scanning probe lithography – the technique of dragging sharp tip across a surface with picometer precision – will be used to pattern the Xene layers with arrays of specific adatoms or molecules. The different adatoms can locally stabilize distinct quantum states of matter, whose boundaries can be used to transport spin or charge. Scanning tunneling microscopy, which uses an atomically sharp tip to measure tiny currents of a few thousands of electrons, will be used to immediately detect the effect of individual atomic placement on the emergent quantum states. The investigators envision qubit systems that are reconfigurable in situ by dragging single atoms. The proposed research could result in novel quantum device capabilities currently envisioned including increased resolution in imaging and detecting; advanced cryptography for secure communication; and unprecedented computational capabilities that far exceed today's classical computing limits to handle "big data."

[1] Department of Physics, Harvard University
[2] School of Engineering & Applied Sciences, Harvard University
[3] University of Illinois at Urbana Champaign

Deterministic Placement and Integration of Quantum Defects

Han Htoon,[1] Edward Bilejec,[2] Yongqiang Wang,[1] Jennifer A. Hollingsworth,[1] Sergei Tretiak,[1] Igal Brener,[2] David Bruce Burckel,[2] Andrew C. Jones[1]

Solitary defects with quantum mechanical states mimicking those of trapped ions have been delivering many breakthroughs in quantum information science (QIS). However, to date, research on defect-derived quantum functionality has primarily relied on serendipitously discovered, naturally formed defects, which not only distribute randomly in host materials but also exhibit diverse optical and quantum coherence properties. As a result, integration of defects into electronic/photonic nanodevices – an essential step for realizing most QIS technologies – can only be achieved by very complex, costly, and time-consuming approaches that place a bottleneck on the progress of QIS research. This project aims to establish new quantum science infrastructure based in the Center for Integrated Nanotechnologies (CINT) that will address the need for: (1) Deterministic creation of atomic defects capable of mimicking trapped ions in a wide variety of host materials; (2) Understanding correlations between the atomic structure of defects and their quantum functionalities; and (3) Integration of these defects into photonic/electronic devices. We propose to achieve (1) via two complementary strategies based on top-down, ion implantation technologies and bottom-up, scanning probe-enabled chemical quantum defect creation.

Toward establishing ion beam based top-down defect implantation, we have acquired two new ion beam systems: (1) Raith Velion focused ion beam (FIB) system capable of implanting quantum defects with 20-30 nm precision at 10 kV accelerating voltage or above, and (2) Colutron Ion Source and Beamline, which is designed to provide ultra-low energy implantation (<500 eV) that will enable impurity doping in 2D materials, as well as a low energy nitrogen source for defect center production. Both systems are expected to be operational in early 2020. An *in situ* single-defect optical characterization system is also being constructed inside the FIB system to deliver an unprecedented 100% deterministic defect creation capability ("one functional defect per one site").

The bottom-up chemical defect creation strategy is based upon recent discoveries that quantum defects can be introduced in single wall carbon nanotubes and 2D layered semiconductors through covalent chemical functionalization. A new CINT staff scientist, Andrew Jones, is currently constructing a novel dual scanning probe microscopy system capable of delivering the chemical reactants required for the functionalization with a target precision of <50 nm. The system will also allow *operando* optical monitoring to ensure creation of single quantum defects deterministically. We have also developed new photo-reactive covalent chemical functionalization chemistry and demonstrated its utility via photo-lithography based deterministic defect placement.

While these novel QIS infrastructures are still under development, we are serving CINT users in deterministic creation of defects using the existing focused ion beam system (nanoImplanter) and in placement of quantum emitters using a commercial dip-pen lithography system. Theoretical analyses have also been performed toward understanding chemical quantum defect implantation/creation. These works together have led to more than 10 peer reviewed publications in various stages of submission. This project has enabled ~20 new CINT user projects from world-leading QIS research groups in 2018 and 2019.

[1] Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos NM 87545
[2] Center for Integrated Nanotechnologies, Sandia National Laboratories, Albuquerque, NM 87185

Atom-defect Hybrid Quantum Systems

Ania Bleszynski Jayich,[1] Kunal Mukherjee,[2] David Weld,[1] Norman Yao[3]

We are developing a hybrid quantum system combining the benefits of atoms and defects, realizing a composite quantum technology platform with capabilities well beyond those of its constituent parts. Individual adatoms deposited onto a diamond surface in a highly controlled, cryogenic, and ultra-high vacuum environment are coherently coupled to subsurface NV centers, enabling creation and manipulation of quantum states in strongly interacting hybrid atom-defect clusters. By leveraging the strengths of its constituent parts, NV centers and individual atoms, this hybrid architecture presents several important advantages that directly address the two primary challenges facing any quantum technology: 1) engineering of robust and scalable interactions and 2) decoherence. Crucially, the proposed quantum system features extreme materials control over both the constituents and the quantum interface between them. Non-invasive probing of adatoms in a metal-free environment should enable the realization of unprecedentedly long coherence times for adatom spins. This will enable quantitative probing and control of surface-mediated decoherence processes which represent a nearly universal challenge to all quantum computing architectures. With its localization at the surface, the NV-adatom system forms an ideal nanoscale quantum sensor. Leveraging our ability to assemble and address adatoms on a clean 2D surface, a specific metrological application we will pursue is probing novel states of matter in 2D interacting spin systems. The convergent expertise of our team (experimental and theoretical aspects of quantum control of atoms and defect centers, and atom-by-atom materials synthesis) is vital to the success of this ambitious proposal.

[1] Physics Department, UC Santa Barbara
[2] Materials Science Department, UC Santa Barbara
[3] Physics Department, UC Berkeley

Understanding and Controlling Entangled and Correlated Quantum States in Confined Solid-state Systems Created via Atomic Scale Manipulation

Stephen Jesse,[1] Ondrej Dyck,[1] Andy Lupini,[1] Mina Yoon,[1] Prineha Narang,[2] Dirk Englund[3]

Success of quantum information science requires the capability to tailor and control minute interactions in coupled quantum states of a system, protect them from perturbations, establish connections to the macroscopic world, and understand their behavior at a fundamental level. Here we will address these challenges by utilizing the sub-atomically focused electron beam of a scanning transmission electron microscope (STEM) to manipulate the local atomic structure and chemistry in low-dimensional materials. The experimental efforts are integrated with multifaceted predictive theory to help interpret measurements and guide materials choices and atomic scale design. We aim to create, enhance, and stabilize entangled and correlated states through direct control over dopant and vacancy position and material geometry to locally tune bandgaps, electronic wavefunctions, and phonon modes, and to provide conditions under which topological effects emerge to form protected quantum states.

A key enabling component of this work centers on enhancing scanning transmission electron microscopy (STEM) as a platform for atomic scale manipulation to allow directed fabrication of specific defects and arrays of defects in designed patterns. To this end, we have developed a new electronics platform that allows for high-speed acquisition, control, and in-line analysis and decision making for STEM. We have demonstrated arbitrary scanning to focus energy where needed to either induce transformations or do fast, sparse, low-dose imaging with real-time compressive sensing and neural net-based feature finding. We have also developed a rapid beam energy changing protocol that has decreased by 20-fold the time needed to change between regimes above and below sample damage thresholds. In previous work, we have shown the ability to directly dope graphene with silicon atoms at precise locations, move specific dopants within a suspended single layer of graphene, and combine multiple dopants together. We have recently extended aspects of this control to several other atomic species including Ti, Fe, Ag, Co, Ni, Pt, and Cr. Of particularly note are results with Cr-doped graphene that suggest strain and slight variations in atomic arrangements of alter local magnetic and electronic properties opening exciting opportunities creating graphene-based quantum systems. The fact that we experiment and model at the same spatial scales allows for a tight coupling between the two. We have used this to seek out several material systems that are likely to exhibit single-photon emission or topological properties and to predict properties of fabricated defect structures. We have recently made advances in modelling capabilities including development of novel first-principles calculations of defect-phonon coupling, GPU-accelerated method to predict correlated light-matter interactions, and a new scheme for correcting electronic potentials in DFT calculations to minimize periodic interactions.

We are working to directly address open questions in the materials physics of atomic scale solid-state quantum systems through direct control of matter at the atomic scale. We manipulate, modify, and model atomic structures to gain a deeper understanding of the physics governing their behavior.

[1] Oak Ridge National Laboratory, Oak Ridge, TN 37831
[2] Harvard University, Cambridge, MA 02138
[3] Massachusetts Institute of Technology, Cambridge, MA 02139

Molecular Control of Spin-Entangled Triplet Excitons from Singlet Fission

Justin Johnson,[1] Obadiah Reid,[1,2] Brandon Rugg,[1] Chris Chang,[1] Brian Fluegel,[1] Natalie Pace,[1] Niels Damrauer,[2] Kori Smyser,[2] Joel Eaves,[2] John Anthony[3]

Understanding the entanglement that results from the production of two electron-hole pairs, or excitons, via singlet fission (SF) has relevance for quantum information science (QIS). The unique nature of the spin coherence that couples the two spin-triplet excitons born from SF could lead to its persistence for microseconds and beyond at room temperature. A deeper understanding of the nature of the entangled triplet pair state may lead to the opportunity to leverage its unique properties in QIS schemes for which significant challenges currently exist.

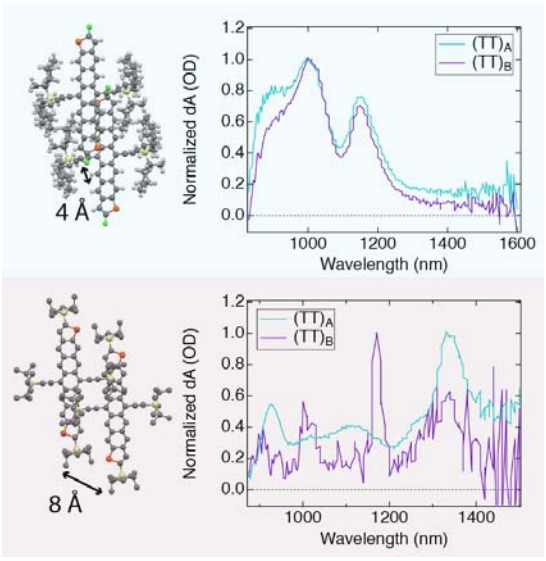


Figure 1. TSBS (upper) and TIPS (lower) substituted pentadithiophenes. Left, closest intermolecular interactions in the crystal and right, transient spectra associated with intermediate and final triplet pair species.

Our recent activities have included developing time-resolved electron paramagnetic resonance (TrEPR) spectroscopy for the detection and evaluation of triplet pair states. These data have been correlated with transient absorption data that possess unique spectral features that can be assigned as arising from these spin states. In particular, we have focused on a series of pentadithiophenes (Figure 1) that show a range of intermolecular couplings and also transient behaviors. Our understanding of the energetics of the triplet pair manifold and the kinetics of population flow within it is being enhanced with electronic structure and dynamics calculations that illustrate the influence of molecular orientation and coupling. We have expanded from the model system of pentadithiophene toward various other acene derivatives that exhibit "dimer-like" behavior in the solid-state. Comparison with isolated covalently bound dimers is also being made as we build a library of pentacene dimer structures with varying bridge length and identity.

We are supporting these core activities with other experimental technique development, including low temperature magnetic field dependent fluorescence for determination of triplet pair exchange splitting. Additionally, we have developed an optically detected magnetic resonance experiment in which detection can be not only fluorescence but also photoinduced absorption, which will allow us to specifically track triplet pair state population under the influence of resonant excitation to produce spin sublevel transitions.

[1] National Renewable Energy Laboratory (NREL)
[2] Department of Chemistry, University of Colorado Boulder
[3] Department of Chemistry, University of Kentucky

ECRP: Emergent properties of magnons coupled to microwave photons

M. Benjamin Jungfleisch[1]

Studying the emergent properties of hybrid quantum material platforms holds the promise to advance quantum technologies, and to revolutionize our understanding of controlling quantum mechanical interactions. A new direction emerged in recent years when it was realized that magnons, the elementary quanta of spin waves, could be used as one building block in the quantum toolbox. Determining the specific mechanisms for the generation and control of hybrid quasiparticles based on magnons could potentially lead to the ability to engineer new materials for quantum coherent processing and quantum computers. The goal of this project is to achieve precise control of light-matter interaction in magnetic hybrid systems and nanostructures, where the light part is carried by microwave photons, and the matter component is carried by magnons in engineered magnetic metamaterials. This research will implement new measurement techniques and undertake systematic studies of new material systems for efficient control of magnon-photon coupling. The underlying mechanisms of the interaction of magnons with photons will be determined, as these interactions are essential for utilizing magnons as coherent information transduction platform between carriers. This project explores the mechanism by which nonuniform magnons interact with photons in the strong coupling regime, determines the spatial distribution of the hybrid excitations, and identifies how to dynamically and spatially control the interaction. It is therefore essential to broaden the range of material platforms, as well as the measurement techniques that can be applied to understand the mechanisms of magnon-photon coupling. Specific goals include: (1) Exploring the dispersion and collective properties of the magnon-polaritons in new materials; (2) Realization of magnonic hybrids with non-zero wavevector and the effective control of the magnon-polariton properties through an engineered magnonic band structure; (3) Determining the mechanisms by which spin-transport phenomena interact with electromagnetic fields in the strong coupling regime. Overall, this research will result in a wealth of new knowledge about the physics of magnonic hybrid systems and the control of their emergent properties. The activities of this project are expected to impact the fundamental understanding of magnon-polaritons, and lay the foundation to create novel spintronic devices, which could be used in quantum information science.

[1] Department of Physics and Astronomy, University of Delaware

Quantum Computing Algorithms and Applications for Coherent and Strongly Correlated Chemical Systems

Sabre Kais (PI),[1] Yong P. Chen,[1] Libai Huang,[1] David Mazziotti,[2] John Anderson[2]

A central challenge of science is the design and synthesis of "efficient" molecules and materials, that is molecules and materials that can efficiently transfer and store energy and/or information or generate new molecules through chemical reactions. The appearance of these desirable properties in molecules and materials, however, frequently coincides with the emergence of exponential complexity in their many-electron wave functions, known as strong electron correlation. The advent of publicly available quantum computing hardware with programmable interfaces has led to an explosion of interest in developing and applying quantum algorithms to chemistry problems. We aim specifically to develop and apply quantum computing algorithms to (a) describe strongly correlated "efficient" molecules and materials at a computational cost that scales non-exponentially with the number of atoms and electrons and (b) elucidate reaction mechanisms in complex chemical systems through Markovian and non-Markovian open quantum systems techniques. For transition-metal coordination polymers we will use quantum-computing algorithms, synthesis, and experimental measurements to develop modular materials with novel catalytic, magnetic, and spin-related properties. For molecular aggregates we will through a combination of quantum computing algorithms and experiment exploit the analogy between the Holstein polaron in superconducting circuits and vibronic coupling in molecular aggregates to gain insights into designing molecular systems with longer coherence lifetime or greater exciton and charge-transfer rate. **The proposed research will focus to achieve three goals:** (1) Develop quantum-computing algorithms for open quantum systems, (2) Create and characterize molecules and materials with strong correlation and entanglement and (3) Manipulate, control, and protect coherent quantum states and excitons.

[1] Purdue University
[2] University of Chicago

Parametrically Induced Quantum Engineering (PIQUE)

Archana Kamal,[1] Leonardo Ranzani,[2] Diego Ristè,[2] José Aumentado,[3] Raymond W. Simmonds,[3]

Efficient creation of robust, long-lived entangled states is one of the main challenges in all physical implementations for quantum information processing. This challenge is rendered particularly compelling given that entangled states underpin almost every quantum information application. Besides being of critical importance for implementing universal quantum computation, Bell or EPR-like states are a necessary resource for quantum communication applications, such as teleportation and super-dense coding, and quantum-enhanced metrology. Conventional protocols for entanglement generation, however, are susceptible to decoherence and require complex controls and tightly-matched system parameters.

Our proposal introduces a new paradigm for overcoming these limitations, using a new and powerful framework, which we refer to as PIQUE (Parametrically-Induced QUantum Engineering). The proposed approach employs continuous-wave tunable parametric interactions to implement multi-qubit entanglement stabilization, and joint qubit measurement. Besides being inherently robust to dissipation, PIQUE schemes allow new functionalities, such as tunable and phase-sensitive interactions, significantly advancing the interface of parametric quantum control with dissipative quantum engineering. The experimental platform for implementation of proposed ideas will be superconducting quantum circuit-based few-qubit systems. Our team combines theoretical and experimental expertise in parametric systems and superconducting qubit technology of the PIs at University of Massachusetts Lowell and Raytheon-BBN, along with fabrication and measurement expertise available at National Institute of Standards and Technology (NIST).

We will present theoretical results on new generation of fast stabilization protocols employing strong parametric interactions which can achieve robust entanglement generation with fidelities in excess of 99% within a few 100 ns. Unlike conventional schemes that achieve low error by driving the system slower than the effective linewidth of the dressed states to maintain resonant driving, these protocols exhibit no tradeoff between fidelity and stabilization rate. We will discuss the prospects for scalable extensions of PIQUE schemes to generate multipartite entangled states in large qubit systems. We will also discuss experimental results on our first generation of devices, demonstrating fast qubit-qubit and qubit-cavity parametric interactions, and progress toward the stabilization of 2-qubit entangled states in our circuit.

[1] University of Massachusetts Lowell, Lowell, MA 01854
[2] Raytheon-BBN Technologies, Cambridge, Massachusetts 02138, USA
[3] National Institute of Standards and Technology, 325 Broadway, Boulder, CO 80305, USA

Frontiers in Quantum Metrology and Transduction

Mark Kasevich,[1] Jason Hogan[1], Benjamin Lev[1], Amir Safavi-Naeini[1], Monika Schleier-Smith[1], Jelena Vuckovic[1]

Quantum mechanics places fundamental constraints on the precision, speed, and spatial resolution with which we can measure forces and fields. Advancing towards these limits will offer new opportunities in areas ranging from characterization of strongly correlated materials to tests of fundamental physics. A challenge, however, is the requirement of having an exquisitely well controlled quantum system as a probe. While no single technology will answer to all applications, we are rapidly making progress in assembling an array of complementary options, from ultracold atoms to solid-state spins to nano-mechanical transducers.

Common to all of these physical platforms is a broad set of challenges and questions. How can we engineer highly non-classical states of matter enabling us to access the extreme limits of quantum sensing? Can we proceed beyond proof-of-principle demonstrations to incorporate quantum sensing into technologically relevant settings? In addressing these challenges, a recurring theme is the need to transfer quantum information between disparate physical systems, e.g., atomic or solid-state spins, photons, and phonons. Hybrid interfaces between these systems provide a means of generating metrologically useful entanglement, and can furthermore enable applications beyond sensing, notably in quantum communications.

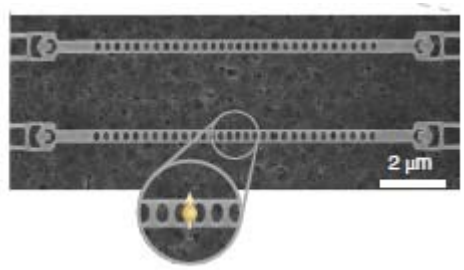


Fig. 1. SEM image of a suspended nanobeam array used to investigate light-matter interactions with a single color center.

This research project will advance methods to create, manipulate and observe entangled states of matter and light for quantum sensing and transduction applications. The PIs will exploit these methods to demonstrate sensors for magnetic, electric and gravitational fields, including next generation magnetometers, gravity gradiometers, electron microscopes and clocks. The research team will apply them to couple acoustic, solid-state, atomic spin and super-conducting qubits relevant to future quantum computing platforms. The research will advance the state-of-knowledge for superconducting, solid-state (diamond and SiC), acoustic, atomic, free-electron and photonic entangled quantum systems.

As an example of recent work in these directions, Fig. 1 shows an integrated photonic nanobeam resonator which has been used to investigate light-matter interactions with a single color center.

[1] 1.Lukin, D. M. et al. 4H-silicon-carbide-on-insulator for integrated quantum and nonlinear photonics. Nat. Photonics 1–5 (2019) doi:10.1038/s41566-019-0556-6.

Designing Quantum Algorithms and Hardware for Chemistry and Materials

Christopher Monroe,[1] Jungsang Kim,[2] Kenneth Brown,[2] Jianfeng Lu,[2] Thomas Barthel,[2] Vladimir Manucharyan,[1] Alexey Gorshkov,[1] Maxim Vavilov,[3] and Ivar Martin[4]

The goal of the project is to design, develop, and execute new computational methods on practical quantum computing platforms to simulate hard problems in chemical and materials science. The project tasks are categorized into three parts: (1) developing new computational methods to study the various physical properties of molecules and materials with strong quantum correlations using quantum computers, such as molecular structure, quantum chemistry, quantum magnetism and correlated electronic materials, (2) adopting quantum computer hardware within the team, both based on trapped ion qubits and superconducting circuits, to find paths to implementing simple versions of these computational methods, and (3) continue the co-design process for the methods and the quantum computer hardware, with a focus on the optimization of algorithm execution. We report on some progress made in the first year of our project. On the computational methods front, we report (1) theoretical result where circuit complexity, representing the difficulty of preparing a given quantum state from another, can be used to detect topological phase transitions, using one-dimensional Kitaev model. (2) Computational and memory-efficient numerical algorithm for computing full configuration interaction method in quantum chemistry, which we refer to as the coordinate descent full configuration interaction (CDFCI) method. Here, the huge-scale eigenvalue problem in full configuration interaction is reformulated as unconstrained optimization problem, and a solution is sought using various methods such as greedy coordinate pick, line search and data compression. (3) Optimized Lie-Trotter-Suzuki (LTS) decomposition method, where the errors are reduced by an order of magnitude compared to conventional decomposition methods. In this method the leading error term is expanded in nested commutators and the 1-norm of the coefficients are minimized. (4) New tensor network states were explored for variational quantum eigensolver (VQE) methods, and worked out the scaling of entanglement entropies in excited states of condensed matter systems to derive universal scaling functions that describe the crossover from ground state area-laws to volume laws as the energies and subsystem sizes grow. (5) We developed a set of tests problems that can be simulated on both trapped ion and superconducting qubit hardware, related to the thermalization and weak ergodicity breaking problems. On the hardware development front, we report (1) a theoretical study for the response of a disordered system of interacting spins to a local microwave drive, which can be used to study the localization phenomena in systems of highly coherent interacting qubit systems such as the trapped ions or chains of fluxonium qubits. (2) Improved the fidelity of entangling gates between pairs of ions in a moderate-length chain (5 ions or less) to better than 99%, by understanding and correcting for the various control errors introduced in the gate implementation. (3) Experimentally implemented quantum approximate optimization algorithm (QAOA) using an analog trapped ion quantum simulator with up to 40 qubits, to estimate the ground state energy of the transverse field Ising model with tunable long-range interactions. This is the first demonstration of practically useful material simulation problem at scales that are challenging for classical methods. (4) Continued fabrication and testing of fluxonium qubits in a cascaded chain, that will allow us to simulate the interaction of a linear chain of interacting spins with high fidelity qubit gates and tunable interactions.

[1] University of Maryland, College Park, MD
[2] Duke University, Durham, NC
[3] University of Wisconsin, Madison, WI
[4] Argonne National Laboratory, Lemont, IL

Quantum probes of the materials origins of decoherence

S. Kolkowitz,[1] V. Brar,[1] J. Choy,[1] J. DuBois,[2] M. Eriksson,[1] L. Faoro,[1] M. Friesen,[1] A. Levchenko,[1] V. Lordi, [2] R. McDermott,[1] K. Ray,[2] and Y. Rosen[2]

Motivated by the potential for transformative applications such as simulation of quantum phenomena, exponential speedup of certain difficult computations, and ultra-precise sensing, research into engineered quantum systems has given rise to a diverse set of solid-state quantum sensors and qubits based on superconducting Josephson junctions, quantum dots, and atomic-scale defects in wide-bandgap semiconductors. Unfortunately, in solid-state environments decoherence due to noise emanating from surfaces and the bulk degrades sensing performance and limits the fidelity of quantum gates in qubits. We are undertaking an ambitious but realistic path to the realization of high-fidelity, scalable quantum systems by utilizing powerful quantum probes along with detailed theory and modelling to determine the microscopic origins of decoherence in solid-state qubit platforms.

By focusing on the materials origins of decoherence, this project has the potential to transform qubit and quantum sensor design. The successful outcome we seek, improved materials to reduce the environmental sources of decoherence, will enable qubit and sensor designs that focus less on protection from a sub-optimal environment. This will open the door to quantum sensors with higher spatial resolutions and greater sensitivities, and will free qubit design to focus much more strongly on qubit-qubit interaction, enhancing the scalability of future solid-state quantum processors.

We will use complementary quantum metrology tools including single spin magnetometry, spin-polarized scanning tunneling microscopy, Kelvin probe force microscopy, and qubit spectroscopy to probe the microscopic sources of decoherence in qubit systems, including superconducting qubits, semiconductor quantum dots, and defects in crystals. In parallel we will use theoretical modeling tools including DFT, Monte Carlo simulations, and other first-principles methods to simulate and predict the effect of microscopically observed defects on quantum devices. This cycle of measurement, growth, and theory will allow for systematic improvements in the materials used to fabricate solid state quantum systems.

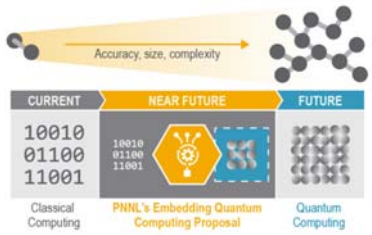
The deeper understanding of materials-induced decoherence developed through our project will enable a next generation of quantum devices. These devices will realize useful quantum error correction and significantly reduce the physical qubit overhead required for fault tolerant quantum computation. These material improvements will also open up a much wider range of parameters and geometries for viable qubits and quantum sensors, improving the prospects for scaling-up quantum computation and enhancing the spatial resolution and sensitivity of quantum sensors.

[1] University of Wisconsin - Madison
[2] Lawrence Livermore National Laboratory

Embedding Quantum Computing into Many-body Frameworks for Strongly Correlated Molecular and Materials Systems

Karol Kowalski,[1] Wibe A. de Jong,[2] Travis Humble, [3] Nathan Wiebe,[1] Dominika Zgid[4]

Recently, the U.S. Department of Energy (DOE) Basic Energy Sciences (BES) has reiterated the transformative character of emerging quantum information technologies. Quantum computers have a hardware advantage over conventional machines in simulating quantum systems and will enable more accurate simulations of complex chemical transformations. Of special importance are problems characterized by strong entanglement of electrons that elude the description provided by most many-body formalisms and therefore remain inaccessible even when using the most powerful classical computers that exist or are likely to ever exist. Although quantum computing (QC) can reshape the landscape of molecular/materials simulations, many issues of QC related to the decoherence time or quantum gate depth of existing algorithms preclude purely quantum algorithms from being applied to realistic-size systems. The main focus of the "Embedding Quantum Computing into Many-body Frameworks for Strongly Correlated Molecular and Materials Systems" project is on the development of computational infrastructure that combines the maturity of conventional computing with the power of emerging quantum hardware to address outstanding problems in catalysis, photochemistry, actinide chemistry, and other fields important to DOE-BES that are currently intractable on classical computers. To this end, the project's team combines recent advances in many-body theory, high-performance computing, and quantum information sciences to develop novel dimensionality reduction algorithms, coupled cluster formulations, and quantum algorithms for fermionic systems [1]. It has already been demonstrated that various downfolding techniques can be successfully applied to describe ground and excited electronic states in strongly correlated molecular systems using quantum algorithms [2]. This hybrid quantum and classical approach will enable the use of today's quantum computers and those available in the near (10 year) term to address some of the most pressing problems in the BES scientific portfolio.



The proposed hybrid classical and quantum computing approach will enable researchers to combine the powers of classical and quantum computing in studies of complex chemical processes.

[1] N.P. Bauman, E.J. Bylaska, S. Krishnamoorthy, G.H. Low, N. Wiebe, C.E. Granade, M. Roetteler, M. Troyer, K. Kowalski, *"Downfolding of many-body Hamiltonians using active-space models: Extension of the sub-system embedding sub-algebras approach to unitary coupled cluster formalism,"* J. Chem. Phys. 151, 014107 (2019).

[2] N.P. Bauman, G.H. Low, K. Kowalski, *"Quantum simulations of excited states with active-space downfolded Hamiltonians,"* J. Chem. Phys. (in press, 2020).

[1] Pacific Northwest National Laboratory
[2] Lawrence Berkley National Laboratory
[3] Oak Ridge National Laboratory
[4] University of Michigan

Nanoscale quantum and classical sensing for superconducting and topological quantum information

Ben Lawrie[1], Eugene Dumitrescu[1], Gabor Halasz[1], Matt Brahlek[1], Peter Maksymovych[1], Chengyun Hua[1]

Superconducting materials are vital to state-of-the-art single photon detectors and qubits that have become increasingly viable solutions for quantum sensing and quantum computing over the past decade. Photonic interactions with quasiparticles, two-level systems and vortices define the limiting behavior of these devices. Fundamental understanding and control of such interactions are essential to further development of these platforms for optical and superconducting quantum information science. Control of these interactions will likely also be critical to proposed topological quantum computers that rely on the spatial manipulation of Majorana zero modes supported by vortices in topological superconductors. Thus, the overarching goal of this project is to reveal and control fundamental nanoscale processes that constrain the behavior of qubits and quantum sensors based on topological and superconducting materials. The specific aims include: (1) Develop nanoscale understanding of photon-induced vortex and quasiparticle interactions in superconducting nanowire single photon detectors, (2) Reveal fundamental materials limitations of superconducting qubits and resonators by understanding nanoscale interactions of quasiparticles and two-level systems, and (3) Manipulate the spatial distribution of vortex-pinned Majorana fermions in topological superconductors to enable braiding operations for topological quantum computing.

Initial research efforts currently underway include:

- Tests of the fundamental limits of quantum sensors based on quantum noise reduction and spin coherence measurements in diamond defect centers at mK temperatures.
- Characterization of single- and multi-photon interactions with superconducting nanowire single photon detectors as a function of position, wavelength, and photon number.
- Synthesis and characterization of candidate topological superconductors.
- Modeling of photonic interactions with Majorana zero modes in topological superconductors.

New quantum and classical sensors in milliKelvin environments allow us to probe photonic interactions with quasiparticles, two-level systems, and vortices in current and emerging superconducting and topological devices for quantum information science. This research will help enable fundamentally new experiments in quantum photonics as well as guide future progress needed to transcend the noisy intermediate-scale quantum computing era.

[1] Oak Ridge National Laboratory

Quantum Sensed Nuclear Magnetic Resonance Discovery Platform

Michael Lilly,[1] Edward Bielejec,[1] and Andrew Mounce[1]

Our project objective is to use a qubit's extreme sensitivity to magnetic fields to create a unique, first-of-its-kind Quantum Sensed Nuclear Magnetic Resonance (QSNMR) Discovery Platform™ for magnetometry and nuclear magnetic resonance (NMR) spectroscopy at the smallest scale possible. The QSNMR Discovery Platform consists of two components: precisely placed nitrogen-vacancy (NV) centers in diamond substrates to serve as a quantum sensor and an NV-NMR spectrometer composed of precisely timed optical, microwave, and radio frequency pulsing. This QSNMR Discovery Platform will provide a scale and resolution for measuring magnetic properties of nanoparticles, topological materials, 2D atomic materials, polymers, single molecules and biological materials, unavailable by other means.

The development, calibration, and demonstration of the QSNMR Discovery Platform will be achieved through three thrusts. Thrust 1: Develop a high-resolution, low-energy nitrogen implantation capability to consistently implant NV centers in diamond at precise depths and locations for use as nanoscale magnetometers. Thrust 2: Construct a custom NV-NMR spectrometer, which is then used to measure the depth of implanted NV centers, and calibrate our QSNMR Discovery Platform by measuring an NV-NMR standard. Thrust 3: Test the prototype's efficacy as an NV-NMR spectrometer on two exemplar systems, (1) by achieving separate measurements of surface and bulk nanoparticles, thus determining the spectroscopic limit of our ability to examine these nanoparticles, and (2) exploring the phase diagram of various densities of interacting donors in semiconductors thus demonstrating our capability to perform NV-NMR on 2D material films.

The primary tool planned for creating color centers is the Raith Velion focused ion implantation system. While delivery is anticipated in early 2020, we already making progress on developing new sources for implantation and working with a wide range of users to implant various elements in diamond and silicon carbide for QIS experiments. For the quantum sensing community, one important goal of this project is developing a nitrogen implant capability for focused beam ion systems. We will report on progress using liquid metal sources with nitrogen such as InN and ionic liquid sources for creating NV centers.

The NMR spectroscopy component of the Discovery Platform is also under development. We are currently determining NV locations and coherence times through coherent microwave control of the NV centers. Using an ensemble of NVs in diamond, we have measured NMR of 13C in diamond and 1H on the surface. We are currently studying how to integrate nanoparticles on surface of diamond for close proximity to NV sensor. Finally, we have built a wide field NV magnetometer allowing for extremely sensitive magnetic imaging.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

[1] Center for Integrated Nanotechnologies, Sandia National Laboratories, New Mexico

Materials for Ultra-Coherent, Mobile, Electron-Spin Qubits

Stephen Lyon,[1] Mark Dykman,[2] M. David Henry,[3] Eric Shaner[3]

Since early in the 20th century quantum mechanics has been recognized as the theory which best describes most physical phenomena. However, only recently has it become possible to directly control the interactions within small quantum systems and to engineer them to perform useful functions. Great strides have been made in the operation of small-scale quantum information processors in recent years, though no technology has yet demonstrated a clear superiority. One important approach is to use very simple quantum systems as the fundamental building blocks – as the quantum bits, or qubits. We plan to develop a new technology utilizing individual electrons, a leading candidate for future quantum information processors, in which the qubit consists of the electron's magnetic moment (or spin).

A key property of a qubit is its coherence time, which is roughly the time before quantum errors appear. Usually researchers study electron-spin qubits inside a semiconductor host, owing to their long coherence, fast quantum gates, and extremely compact devices. However, the electron spin coherence time becomes very short if the electrons are moved through the host semiconductor. While a quantum processor can be constructed without moving the qubits, mobile qubits can simplify the processor architecture and far fewer are required for the same complexity and speed. Mobile qubits may be particularly advantageous for near-term quantum simulators, where the additional flexibility will expand the range of a given processor.

This new research program is aimed at exploring electron-spin qubits in a different materials system, in which electrons are bound to the surface of superfluid helium. There is indirect evidence that mobile electrons will have exceptionally long coherence in this system, along with the other advantages of spin qubits. However, there is neither a full theory of electron spin coherence for these electrons, nor direct experimental measurements of these spins. The key goals of this program are (1) to develop a theory of the details of the interaction between the electrons' spins and the helium, and in particular how high perpendicular electric fields as might be found in future quantum devices will modify these interactions and affect the spin relaxation and decoherence rates; and (2) to develop experimental approaches for measuring ensemble electron spin coherence for these mobile qubits, and understand how control electrodes can be optimized for preserving the ultra-long spin coherence of the electrons while enabling the efficient control of their motion. Time permitting, this program will also work towards extending the experimental spin measurement and control to the single-electron level.

[1] Princeton University
[2] Michigan State University
[3] Sandia National Laboratories

Photon Qubit Entanglement and Transduction

Xuedan Ma,[1*] Xufeng Zhang,[1*] Stephen Gray,[1] David Czaplewski,[1] Axel Hoffman,[2] Daniel Rosenmann[1]

In recent years, there has been an increasing interest in developing distributed quantum networks that combine the advantages of different quantum systems to complete complicated tasks in quantum information processing. Distributed quantum networks require the development of individual quantum systems both in the microwave and optical domains, as well as their interconnection. Despite the rapid development in microwave qubits based on superconducting technologies, deterministic optical single-photon sources are still underdeveloped. High-efficiency quantum interconnections between these systems are also missing because of the incompatibility of the superconducting technique with optical photons and their huge frequency difference. Most importantly, comprehensive facilities that simultaneously host a variety of different quantum systems and enable their transduction are still lacking.

In the Center for Nanoscale Materials, we are developing key technologies that address the two grand challenges facing the distributed quantum network community (Fig. 1). In the first scientific thrust, we are developing non-classical optical photon sources based on semiconductor nanomaterials.[1] To optimize the emission properties of the nanomaterials, we are integrating them with photonic structures to reduce undesirable charge carrier recombination processes.[2] In the second scientific thrust, we are developing integrated opto-magnonic quantum transduction systems to convert quantum information between the microwave and the optical domains. Using advanced material fabrication, we are able to demonstrate exceptional point in magnon-based microwave cavities, thus opening up opportunities for multi-dimensional control of quantum transduction systems.[3]

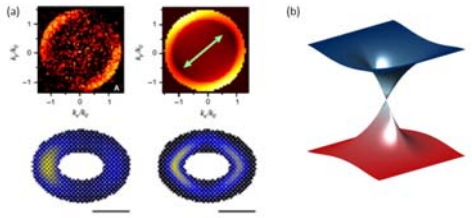


Figure 1. (a) Abnormal optical transition dipoles in semiconductor single photon sources for QIS applications. (b) Exceptional point in magnon-microwave cavities.

We are also developing a centralized user lab, the *Quantum Entanglement and Transduction (QET) Lab*, which addresses the major tool requirements for advancing hybrid quantum network technologies (Fig. 2). The QET Lab is being equipped with design, fabrication, and characterization capabilities that cover microwave, THz, and optical domains. It will offer quantum optics and transduction characterization tools that enable a broad range of user science including the development and measurement of optical and spin qubits, as well as quantum transduction systems. New tools developed in the first project year include a photo-correlation microscope and a magneto-electro-spectrometer. With these new tools, we are witnessing a rapidly growing user base for the QET lab.

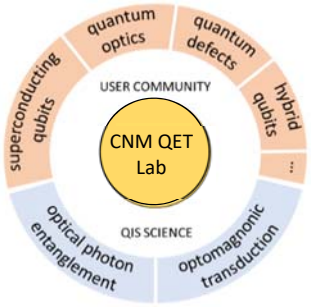


Figure 2. Outline of the project objectives.

This work was performed at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility, and supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357.

References:

1. X. Ma *et al. Nano Lett*. 2018, **18**, 4647; N. F. Hartmann *et al. Nat. Commun*. 2019, **10**, 3253.
2. C. Husko *et al. Nano Lett*. 2018, **18**, 6515; L. Peng *et al. Adv. Funct. Mater*. 2019, in press.
3. X. Zhang *et al. Phys. Rev. Lett.* in press.

[1] Center for Nanoscale Materials, Argonne National Laboratory; xuedan.ma@anl.gov; xufeng.zhang@anl.gov
[2] Material Science Division, Argonne National Laboratory. Current Address: Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign

Direct Observation of Fractional Quantum Hall Quasiparticle Braiding Statistics via Interferometry

Michael Manfra[1]

Utilizing a novel design of AlGaAs/GaAs heterostructures we have recently demonstrated Aharonov-Bohm (AB) interference of fractional quantum Hall effect edge modes. Clear demonstration of AB interference of fractional edge modes is a vital step towards demonstration Abelian and non-Abelian braiding statistics. We propose a series of interferometry experiments aimed at answering the most important questions surrounding quantum coherence and braiding statistics in quantum Hall systems. Fine control of device parameters in this new system facilitates systematic investigation of quantum coherence, edge state reconstruction, and braiding statistics. The objectives of this project are:

- Measurement of Abelian phase for the fractional quantum Hall state at ν=1/3
- Exploration of the limit of interferometer size reduction while maintaining operation in Aharonov-Bohm regime
- Quantification of quantum coherency of fractional edge modes via measurement of the temperature dependence of AB oscillation amplitude and dependence on interferometer size
- Design of heterostructures and measurement of interferometers to probe non-Abelian braiding statistics at ν=5/2
- Measurement of interferometers in which the edge potential prolife is systematically modified through variation of screening well-quantum well separation to study impact on edge mode reconstruction

Using a combination of heterostructure growth, mesoscopic device fabrication, and low temperature electronic transport measurements, this project aims to provide the first direct measurement of Abelian and non-Abelian braiding statistics. Information learned during this work will be crucial to determination if quantum Hall systems are capable of hosting topological qubits. Our work will also inform investigations of other topological material systems where systematic control of epitaxial growth, device fabrication and operation are currently in more nascent stages. We hope our work may serve as a blueprint for interrogation of other topological phases needed to support next generation quantum systems.

[1] Department of Physics and Astronomy, Purdue University

Hybrid Quantum/Classical Algorithms for Photochemistry and Nonadiabatic Dynamics

Todd J. Martinez,[1] Edward Hohenstein,[1] Dmitry Liakh,[2] Alexander McCaskey,[2] Abraham Nitzan,[3] Robert Parrish, [4] David Reichman,[5] and Joseph Subotnik[3]

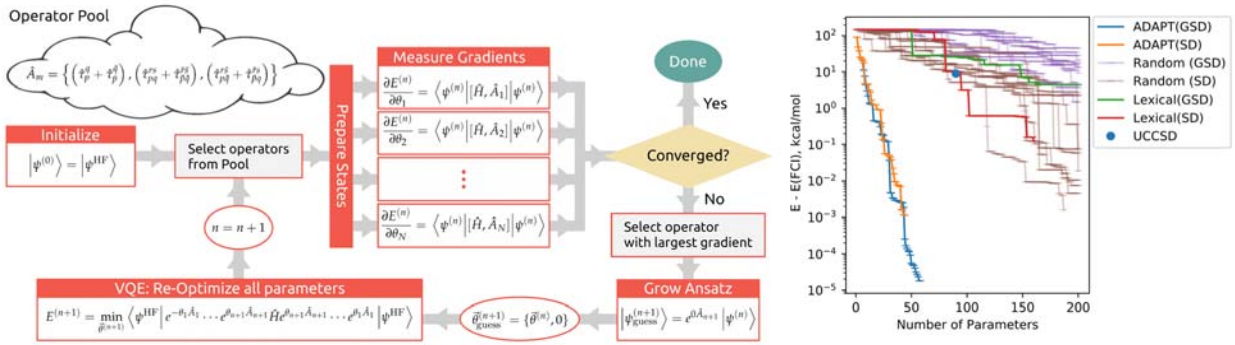
Many problems, including the simulation of quantum mechanical phenomena for light-harvesting and solar energy applications, are difficult or impossible to solve using classical computers but could become feasible or even simple using quantum computers. Even though tremendous progress is being made towards the development of quantum computers, the earliest hardware implementations will be noisy and error-prone, leading to serious limitations on circuit complexity. This research project will develop new mixed classical/quantum approaches for the simulation of natural and artificial light-harvesting systems. Using both quantum and classical computers leverages the advantages of both and suppresses noise-induced errors in the quantum computer. The outcomes of this project will be 1) development, implementation, and application of algorithms that can exploit early stage implementations of quantum computers to simulate the interactions of molecular materials with light and subsequent charge and energy transport, 2) demonstration of these algorithms on existing, noisy quantum computing hardware, and 3) development of new frameworks to simplify the use of quantum computers in hybrid classical/quantum algorithms. These advances will lay the foundation for computer-aided design of new, efficient molecular materials to convert solar energy to fuels and/or electricity and the routine use of quantum computers in molecular simulation.

[1] SLAC National Accelerator Laboratory
[2] Oak Ridge National Laboratory
[3] University of Pennsylvania
[4] QC-Ware Corporation
[5] Columbia University

Simulating strongly correlated molecules with a superconducting quantum processor

Nicholas J. Mayhall,[1] Edwin Barnes,[1] Sophia E. Economou,[1] David Pappas[2]

Many of the biggest challenges in expanding the nation's access to clean and low-cost energy resources are fundamentally chemistry or materials challenges. An important case is the development of new catalysts for the up-conversion of cheap and readily available materials such as methane or water into materials suitable for use as a fuel such as methanol or oxygen. To understand and exploit such processes, computer simulations of chemical reactions provide a natural complement to experimental studies. Unfortunately, most catalytic reactions involve so-called "strongly correlated" molecules which are notoriously difficult to study with simulation algorithms that can be executed on existing (classical) computers. The recent growth in quantum information science offers an alternative potential route for simulating these difficult systems. As a result, an increasing number of computational chemists are becoming interested in quantum computing. At the same time, quantum information scientists have identified chemistry simulation as a possible first demonstration of a quantum computer providing a useful improvement over a classical computer. The objective of this project is to accurately simulate strongly correlated molecules on a quantum processor. To meet the high challenges of this objective, new hybrid quantum/classical algorithms are currently being co-designed with advanced quantum gate developments and computed on customized quantum hardware. The first major breakthrough in our project has been the development of a novel variational quantum algorithm for computing molecular ground state energies. This algorithm adaptively determines a quantum circuit which converges to exact energies with a drastically reduced parameter count. The figure below gives an illustration of the algorithm:



This approach has also been extended in a variety of directions, which will be discussed in this presentation. Additional techniques are also being designed to directly couple the theoretical simulation techniques with custom chips fabricated by the Pappas group.

[1] Virginia Tech
[2] NIST/CU Boulder

Center for Novel Pathways to Quantum Coherence in Materials
Energy Research Frontiers Center (EFRC)

Joel E. Moore (Director),[1] James Analytis,[1] Stefano Cabrini,[1] Michael Crommie,[1] Peter Ercius,[1] Naomi Ginsberg,[1] Alessandra Lanzara,[1] Jeffrey Neaton,[1] Joseph Orenstein,[1] Ramamoorthy Ramesh,[1] Eli Rotenberg,[1] Feng Wang,[1] Chao Yang,[1] Norman Yao,[1]
David Awschalom (Deputy Director),[2] Aashish Clerk,[2] Giulia Galli,[2] Supratik Guha,[2] F. Joseph Heremans,[2] Martin Holt,[2] Jiwoong Park,[2] Xufeng Zhang,[2] Dmitri Basov,[3] Ania Bleszynski Jayich[4]

This Energy Frontier Research Center for Novel Pathways to Quantum Coherence in Materials will dramatically expand our understanding and ability to control coherence in solids by building on recent discoveries in quantum materials along with advances in experimental and computational techniques. Common threads are the need to understand defects in complex material environments, the use of high-resolution optical techniques and other cutting-edge experimental tools, and the role of inhomogeneity in various types of quantum materials. The first thrust of research involves point defects in simple and complex insulators and the improvement of their coherence properties for potential uses such as quantum sensing of temperature, magnetic fields, and local strain and electric fields. The second thrust builds on recent discoveries in interfaces and boundaries of two-dimensional materials, in order to understand coherent one-dimensional conduction with the potential to avoid dissipation and heating. These unique "quantum wires" can serve as interconnects for quantum information.

The third thrust aims to understand and enhance linear and nonlinear electrodynamic responses in topological, magnetic, and other highly correlated quantum materials, using advanced coherent methods to elucidate the role of static and dynamic fluctuations at short length scales. In addition to possibly providing alternatives for solid-state quantum computation, strongly correlated materials such as these are one of the key science drivers that the first quantum computers will be used to attack. Progress in these thrusts will enable new solid-state approaches to quantum sensing, communication, and computation. Improved understanding of the quantum materials under study will also impact more conventional electronic and optical applications by demonstrating new materials for switchable and nearly dissipation less transport, single-pass frequency doubling, and efficient terahertz detection.

Research is being carried out at four institutions (LBNL, ANL, Columbia, and UCSB) by an integrated team of experimentalists and theorists, taking advantage of unique facilities available at the national laboratories. Important QIS-related results from the first year include advances in NV sensing of quantum materials and the discovery of superconductivity in trilayer graphene.

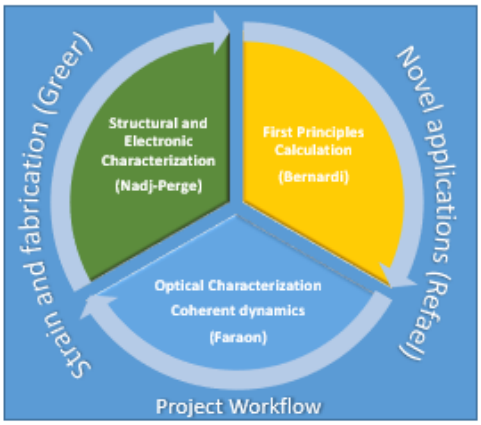
[1] Lawrence Berkeley National Laboratory (LBNL)
[2] Argonne National Laboratory (ANL)
[3] Columbia University
[4] University of California, Santa Barbara

Quantum States in Layered Heterostructures Controlled by Electrostatic Fields and Strain

Stevan Nadj-Perge (PI),[1] Andrei Faraon (Co-Pi),[1] Marco Bernardi (Co-PI),[1]
Julia Greer (Co-I),[1] Gil Refael (Co-I)[2]

This project aims to advance understanding of defects in a novel family of materials, known as two-dimensional (2D) transition metal dichalcogenides (TMDs), for the development of quantum information devices. This materials class exhibits a range of fascinating electronic and optical properties and, because of their sub-nanometer thickness, are particularly well suited for confining electronic quantum states in atomic size structures. The main goal of this work is to identify and characterize point and line defects in two-dimensional transition metal dichalcogenides with the focus on defects that host quantum states that can be coherently manipulated by electrical or optical means. The project is a collaborative effort of five Caltech investigators (Bernardi, Faraon, Greer, Refael, Nadj-Perge) who carry out different aspects of this synergistic project with the three specific goals: **(i)** Identifying novel point and line defects embedded in 2D materials for quantum optoelectronic applications; **(ii)** Establishing their structural, electronic and coherent properties, and exploring ways of controlling their properties with strain and electrostatic gating; (iii) Identifying new platforms for studying dynamics of driven quantum systems that are based on 2D materials.

The outlined goals are supported by the range of new ab initio numerical calculations and theoretical approaches developed within this project. These include: advanced first principles methods for calculating spin lifetimes without using any empirical or fitting parameters; new algorithms for extracting radiative lifetimes based on the GW-BSE approach; and innovative theoretical schemes for investigating Floquet quantum states that emerge from continuous time-periodic driving. Experimentally, point and line defects in mono- and few-layer TMD are created by strain engineering using advanced nanofabrication of vertical pillars and piezo-active nanowires. Optical properties of such defects are investigated using optical spectroscopy and their electronic structure studied through scanning tunneling microscopy.



The figure on the left illustrates the project workflow. Bernardi develops first principles calculations predicting radiative and spin lifetimes of defects in TMDs while Nadj-Perge and Faraon perform electronic and optical characterization. Experimental results will be compared to theoretical predictions to advance understanding of such defects. Advanced nanofabrication protocols needed for their creation are developed in Greer's group. Rafael investigates innovative schemes for coherent control of quantum states hosted in TMD defects and novel applications in quantum science.

[1] Department of Applied Physics and Materials Science, California Institute of Technology, Pasadena, USA.
[2] Department of Physics, California Institute of Technology, Pasadena USA.

Enhancing Entanglement: Non-Markovian and Floquet Reservoir Engineering in Many-Qubit Superconducting Quantum Circuits

Oskar Painter[1] and Aash Clerk[2]

Quantum information science is by now a diverse field, with many different systems of interest, and a variety of target applications. There is a common theme however to almost all work in this area: one needs robust methods for both preparing and stabilizing non-trivial, entangled quantum states. An extremely attractive approach to this general problem is dissipation engineering: through driving and system design, tailor the dissipative evolution of a quantum system so that this dynamics relaxes it to the state (or state space) of interest. Such methods are inherently robust, and have been successfully implemented in a variety of physical platforms. Despite these successes, the full power of dissipation engineering has not been explored theoretically or experimentally. First, previous work has almost exclusively focused on regimes where the dissipative dynamics is Markovian, or local in time. Second, the use of explicitly time-dependent dissipative couplings and modulated dissipation (i.e.~akin to Floquet engineering) has not been explored in the context of dissipation engineering. Our broad vision is that extending reservoir engineering to incorporate these non-trivial elements will enable a transformative new class of dissipative quantum state stabilization protocols. This will allow us to transcend the limitations of current approaches. These extensions represent a fundamentally new theoretical paradigm; moreover, they are regimes that can be directly probed in the superconducting quantum circuit (SQC) architecture we will develop and study in this proposed program.

Our team, consisting of lead PI Painter on the experimental side and PI Clerk on the theoretical side, will explore new theoretical tools and methodologies to describe non-Markovian and time-dependent engineered dissipation, and devise new entanglement generation and stabilization protocols in many-qubit quantum systems. We propose to experimentally implement these ideas in a many-qubit waveguide circuit QED platform.

General scientific questions of interest include: (i) How do non-local temporal and spatial correlations in the external reservoir manifest themselves in the system dynamics? How can we use system degrees of freedom as a quantum probe of these correlations? (ii) How are the concepts of information flow, entanglement production and propagation impacted by non-Markovianity? Can these be harnessed as resources? (iii) What are optimal methods of external control that enable the reservoir to steer the quantum dynamics of the target system and ultimately stabilize non-trivial states? (iv) Are there effective (approximate), simple methods for describing the system dynamics, or dynamics within a sub-manifold of the system?

[1] California Institute of Technology
[2] University of Chicago

Integrated Development of Scalable Materials Platforms for Topological Quantum Information Devices

Vlad Pribiag,[1] Paul Crowell,[1] Sergey Frolov,[2] Noa Marom,[3] Chris Palmstrøm[4]

Topological excitations such as Majorana modes provide unique pathways to fault-tolerant quantum computing. Recent progress in this direction has been enabled by proximity effects between non-superconducting materials and superconductors; however, further breakthroughs leading to topological quantum computation require developing new material systems that integrate semiconductors not only with superconductors, but also with epitaxial ferromagnets or antiferromagnets. Currently, Majorana devices based on semiconductors require application of an external magnetic field to induce spin splitting and open a helical gap – necessary to realize an odd-parity topological superconductor. However, the presence of this magnetic field limits the robustness of topological properties (by weakening the induced superconductivity). Moreover, the stringent requirements on its orientation with respect to the device greatly restrict the scalability of Majorana-based quantum information systems. A promising path forward is to realize Majorana modes without an applied magnetic field by closely integrating epitaxially-grown ferromagnets or antiferromagnets with semiconductors and superconductors (Fig. 1). Our inter-disciplinary effort combines materials synthesis with in-situ characterization and device fabrication, integrated with a computational approach based on lattice matching, genetic algorithm (GA) optimization, and machine learning. We are developing novel one- and two-dimensional materials platforms, and work to leverage them to discover novel topological excitations and to demonstrate topological quantum systems with novel functionality. Ultimately, we aim to use these new materials platforms to demonstrate robust topological properties of Majorana modes. Importantly, our approach will be compatible with large-area scalability to form two-dimensional arrays of non-Abelian qubits. We report our recent progress (Fig. 1), including: the realization of quantum devices based on InSb nanowires with magnetic contacts; growth of MgO-InSb VLS nanowire structures with partial shells of Fe (or perpendicularly-magnetized Fe/Ru multi-layers) and varying thicknesses of MgO tunnel barriers; investigations of the static and dynamic magnetic properties of epitaxial Fe on InAs (100) and InSb (100); the development of a new DFT method based on a Hubbard U correction optimized with machine learning, that enables simulations of large interface models with high efficiency.

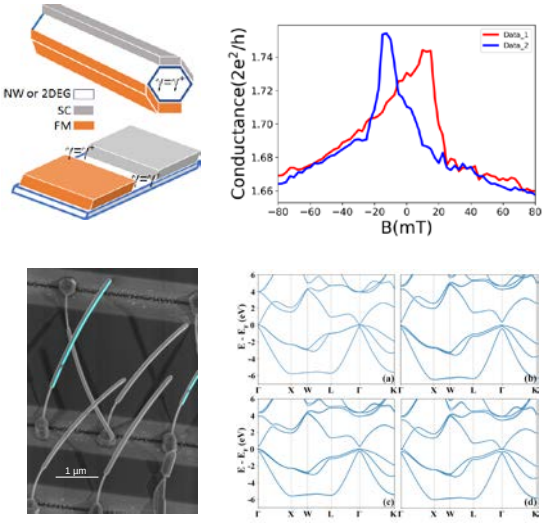


Fig. 1: (top-left) Schematic of devices integrating a ferromagnet (FM), semiconductor and superconductor (SC) for realizing MZMs. **(top-right)** Magneto-resistance from an InSb quantum device with Fe contacts. **(bottom-left)** InSb nanowires with MgO barrier and partial shells of Fe. **(bottom-right)** Comparison of band structure of InAs calculated using different functionals that include correlation effects.

[1] University of Minnesota
[2] University of Pittsburgh
[3] Carnegie Mellon University
[4] U. C. Santa Barbara

An Ion-Trap Quantum Simulator for Exotic 2D Materials

Philip Richerme,[1] Gerardo Ortiz,[1] Babak Seradjeh[1]

This joint experimental and theoretical effort seeks to develop a flexible platform for the atom-by-atom synthesis and characterization of exotic two-dimensional (2D) quantum materials. The objectives of this research will be to implement a fully-controllable 2D quantum simulation system, which (1) can be periodically driven out-of-equilibrium to create quantum topological matter, and (2) can simulate the dynamics of frustrated quantum spin systems. The experimental platform is comprised of trapped atomic ions, which will encode an ensemble of effective spin-1/2 particles and will be controllably coupled together to form a pristine quantum material. This 2D ion trap quantum simulator, which would be the first of its kind, would offer unprecedented opportunities to address open questions in quantum many-body physics associated with geometric frustration, exotic phases of matter (such as topological materials, valence-bond states, and spin glasses/liquids), and the relationship between entanglement, frustration, and high-temperature superconductivity. Understanding the full phase diagrams and dynamical behavior for these various quantum spin systems is of strong and widespread interest, but has so far proven elusive due to the lack of clean and controllable experimental test systems. The results of this work will therefore guide future theoretical efforts to understand highly complex 2D systems, for which no reliable analytic or numeric descriptions are currently possible.

[1] Indiana University, Bloomington IN

Thin film platform for rapid prototyping of novel materials with entangled states for quantum information science

Christopher Rouleau (PI),[1] Gyula Eres,[1] Rama Vasudevan,[1] David Geohegan,[1] Alexander Puratzky,[1] Kai Xiao,[1] and An-Ping Li[1]

The Basic Energy Sciences Roundtable Report titled, *"Opportunities for Basic Research for Next-Generation Quantum Systems,"* identifies the need to learn how to "create the necessary materials, devices, and chemical systems with the exquisite precision needed to achieve long coherence times and entanglement." Rapid feedback between synthesis and the identification of quantum states as well as characterization of their lifetime and entanglement is critical to achieving this goal. Generating feedback requires an ability to connect characterization of defects and dopants with quantum properties and the measurement of entanglement in materials, which is not generally straightforward. For example, tomographic characterization - i.e., imaging by sections using penetrating optical waves - of the quantum state of light emitted by defects or excitons can be used to characterize the quantum state of the emitter in some cases, but the characterization of entanglement states are, in general, more complicated than are pair of coupled spin states or any other coupled pair in a two level systems. Similarly, spin systems supporting ground states with many-body entanglement critical to the development of elementary excitations such as the Majorana fermion for topological quantum computing are still not well-understood, and the signature of the state still remains unknown. To address these challenges, the overarching goal of this project is to develop a rapid exploration platform for the synthesis and characterization of quantum systems with entangled states in space and time domains for quantum information science (QIS), as follows:

1. Establish an agile artificial intelligence (AI)-guided synthesis platform coupling reactive pulsed laser deposition with quick decision-making diagnostics to enable the rapid exploration of a wide spectrum of candidate thin-film materials for QIS.

2. Understand the dynamics of photonic states with required sub-picosecond temporal resolution, such as single photon emitters localized at specific defect sites, by combining a novel SEM platform that couples ultra-fast electron microscopy and cathodoluminescence at low temperature, with existing Center for Nanophase Materials Sciences femtosecond pump-probe laser spectroscopy capabilities.

3. Enable understanding of entangled spin states for topological quantum computing by developing a novel STM platform capable of injecting electrons with controllable angular momentum and probing spatially resolved spin entanglements with atomic resolution at ultra-low temperature and with variable vector magnetic fields essential to QIS.

[1] Oak Ridge National Laboratory (ORNL)

Developing Molecular f-Element Quantum Materials with Strong Electron Correlations

Eric J. Schelter,[1] Corwin Booth,[2] and Jochen Autschbach[3]

Materials that display high temperature emergent quantum phenomena are a grand challenge of chemistry and physics. f-Element materials are uniquely poised to express quantum phenomena because of their electronic characteristics. Core-like, f-electron atomic orbitals confer protection against decoherence and underpin 'heavy electron' behavior and unconventional superconductivity. There is a clear need to develop materials chemistry that allows for study of local strong electron correlations in a small enough system that exact theoretical and spectroscopic methods can be applied, and for elaboration of such correlations into an emergent, heavy electron quantum lattice. The long-term goal of this project is to synthesize heavy electron coordination polymers and/or molecular solids for the first time, whose properties can be tuned systematically using molecular design principles, and ultimately, to achieve superconductivity in a molecular material. The team is synthesizing metal complexes and extended coordination polymers using linkages known to promote strong electron correlations. They will characterize the heavy electron behavior of molecular solids using magnetism, transport properties, spectroscopy studies and computational chemistry. This approach is expected to result in isolation of the first f-element, molecular heavy electron materials, providing new families of quantum materials.

[1] Department of Chemistry, University of Pennsylvania
[2] Lawrence Berkeley National Laboratory
[3] Department of Chemistry, University at Buffalo, State University of New York Buffalo

QUINTESSENCE: Quantum Instrumentation for Novel Techniques Applying Entanglement and Spin-polarization for Studies with Low Energy Coherent Electrons

Andreas Schmid,[1] Alexander Stibor,[1] D. Frank Ogletree,[1] Alex Weber-Bargioni,[1] Andy Minor,[1] Colin Ophus,[1] Jim Ciston[1]

Creating, measuring and controlling coherence in quantum systems forms the foundation of quantum information science (QIS). We are building novel quantum instruments based on spin polarized and spin-entangled low-energy electron beams at the Molecular Foundry, one of the five DoE Nanoscale Science Research Centers (NSRCs). We are creating a platform of worldwide unique techniques to provide QIS user communities with new means to study quantum decoherence and entanglement. We will extend spin-polarized low-energy electron microscopy (SPLEEM) to the cryogenic regime, enabling nanoscale imaging of spin textures and phase transitions in quantum materials such as superconductors and fragile nanosystems incorporating molecular components.

The cryo-SPLEEM, the centerpiece of QUINTESSENCE, will combine a Foundry-developed helium-temperature sample manipulator with a customized commercial LEEM instrument. Implementation of the spin-gun and spin-manipulator for the SPLEEM will draw on over a decade of experience running the highly-productive Foundry/NCEM user-program built around it's first-generation SPLEEM. The new instrument will incorporate in-situ molecular beam epitaxy capabilities, developed in the existing program, for the fabrication and optimization of quantum structures. The new SPLEEM will be able to perform 3D vector-magnetometry with nanometer spatial resolution; mapping of occupied electronic states below the Fermi energy (by angle resolved photoemission) as well as unoccupied structure above the vacuum level (by angle resolved electron reflection); and damage-free "mirror imaging" of surface potentials and ordered domains.

The second QUINTESSENCE component is a highly-coherent electron bi-prism interferometer capable of producing electron interference fringes on an imaging detector. When the superposed electron waves pass near a sample surface, electron coherence is degraded. The imaging detector records the attenuation of the interference fringes as a function of distance from the conducting sample surface, creating a new tool to investigate the scaling of quantum decoherence processes. This new tool will allow users to study Coulomb-induced decoherence in various materials and structures as a function of temperature, material composition and the presence of surface adsorbates, research that will support efforts to create robust quantum states.

Finally, we are exploring field emission from a superconducting Nb field emission tip as a source of highly coherent electrons. Previous work on Nb field emission found a sharp peak in the electron energy distribution at the Fermi edge that scaled with the superconducting order parameter, and theoretical predictions and solid-state experiments suggest that Cooper pairs can be emitted as entangled electrons with anti-parallel spin. We will attempt to confirm this experimentally, and explore applications of an entangled electron source in SPLEEM and interferometry experiments.

[1] Molecular Foundry, Lawrence Berkeley National Lab, Berkeley, CA

Planar Systems for Quantum Information

Jie Shan,[1] James Hone,[2] Allan H. MacDonald,[3] Kin Fai Mak,[4] Tony F. Heinz [5]

Many solids have distinct, but degenerate valleys and the valley degree of freedom has been the subject of interest as a possible internal degree of freedom for quantum information. Until recently, however, there have been few approaches to accessing, much less controlling this degree of freedom in solids. One of the distinguishing features of the transition metal dichacogenide (TMD) family of 2D semiconductors such as MoS2, MoSe2, WS2, and WSe2 is the direct access to the valley degree of freedom by means of optical excitation. These materials exhibit strong valley circular dichroism, i.e. each handedness of light couples only to one of the two independent valleys in the Brillouin zone of the material. In addition, the spin-valley coupling in both valence and conduction bands provides a method of correlating the valley and spin excitations, as well as the possibility of stabilizing excitations within the valley degree of freedom. These recently revealed possibilities for access to a largely unexploited and unstudied quantum degree of freedom in solids have prompted efforts to develop methods to exert active control over the valley degree of freedom, and also to understand and eliminate the factors limiting coherence.

This integrated team of six investigators aims to investigate the valley pseudospin degree of freedom in 2D TMDs as a candidate for the construction of quantum bits. In particular, we will develop approaches including stimulated Raman adiabatic passage and dynamic exchange magnetic field for full control of valley pseudospin. We will seek to determine the factors controlling decoherence and develop approaches for enhancing coherence times using approaches including spin-forbidden excitons, valley polarized carriers, and arrays of localized excitons and carriers.

The research relies on advanced methods for material synthesis and 2D assembly developed by the team and others. These extend from bulk crystal growth using a flux synthesis method and the creation of tailored 2D heterostructures with on demand control of the rotation angle using dry transfer techniques to novel approaches of creating localized excitons and carriers in 2D materials. The properties of the resulting heterostructures of 2D materials will be probed using a wide variety of electrical and optical methods, including optical pump-probe spectroscopies. The experimental research will be pursued in a close feedback loop with predictions and modeling using ab-initio and analytical calculations.

The research will provide fundamental understanding of how tailored 2D quantum systems can be harnessed and developed for quantum information science. The goals of the project, to develop understanding and approaches for the creation of qubits with long coherence times, precise tunability, and novel functionality, are strongly aligned with priorities identified in the Basic Energy Sciences Roundtable on Opportunities for Basic Research for Next-Generation Quantum Systems.

[1] Cornell University, Ithaca, NY
[2] Columbia University, New York, NY
[3] University of Texas at Austin, Austin, TX
[4] SLAC National Accelerator Laboratory, Menlo Park, CA
[5] Stanford University, Stanford, CA

Optical Generation and Manipulation of Spin Qubits

David A. Shultz[1] and Martin L. Kirk[2]

This project aims to produce polarized molecular electron spins using visible light. It examines multispin molecular systems that are important to molecular and nanoscale optical-thermal energy transformation, new magnetic exchange-modulated photoprocesses, and in particular quantum information science (QIS). The research will advance our understanding of how photogenerated quantum (spin) bits (qubits) can be used to develop large ground state spin polarizations on an ultrafast timescale, photoentangle multiple ground-state qubits, employ antenna effects to enhance the spin polarization signal response, and markedly decrease excited state lifetimes to increase the timescale for qubit manipulation in the ground state. Our long-term goal is to develop novel molecular systems that can be optically initiated to enable magnetic exchange-mediated multi-qubit entanglement, and by virtue of designed short-lived excited states, facilitate large spin qubit polarizations in recovered ground states. This will allow us to develop spatial and temporal control of spin qubits, as well as promote spin coherence lifetimes that are markedly longer than the spin initiation process.

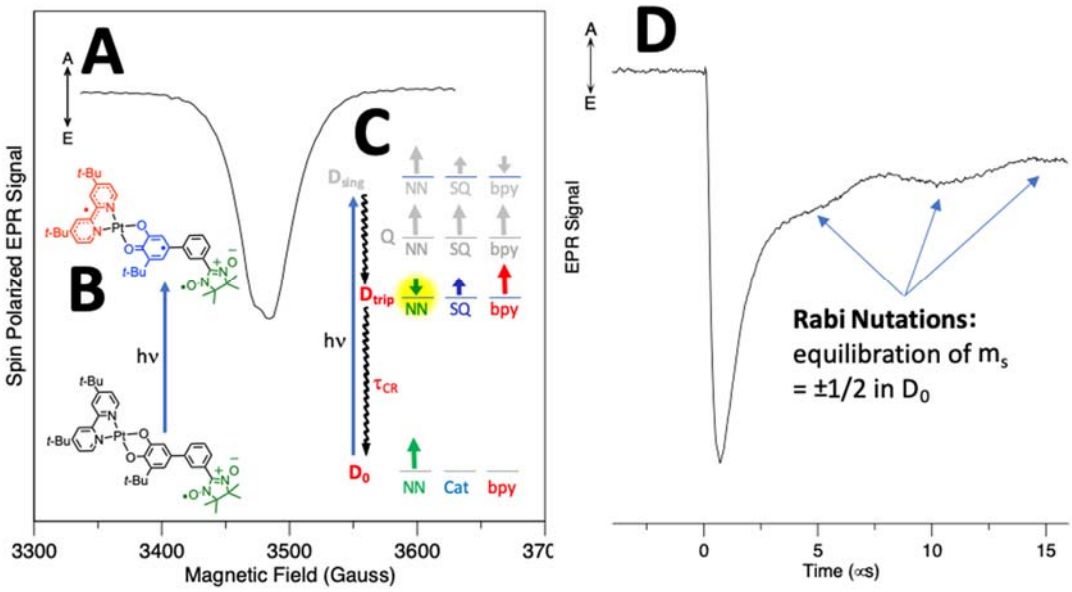


Figure 1. Example of spin-polarized recovered ground-state EPR spectrum (**A**) for compound and photoprocess shown in **B**. Excited doublet (D_{sing}-D_{trip}, **C**) mixing and therefore spin density on the NN radical are dependent on the structure of the complex (specifically, the *meta*-phenylene bridge in this case).

[1] Department of Chemistry, North Carolina State University
[2] Department of Chemistry and Chemical Biology, The University of New Mexico

High-Coherence Multilayer Superconducting Structures for Large Scale Qubit Integration and Photonic Transduction

Irfan Siddiqi,[1] Stefano Cabrini,[1] D. Frank Ogletree,[1] Alex Weber-Bargioni,[1] Andrew Minor,[1] Norman Yao,[1] William Oliver[2]

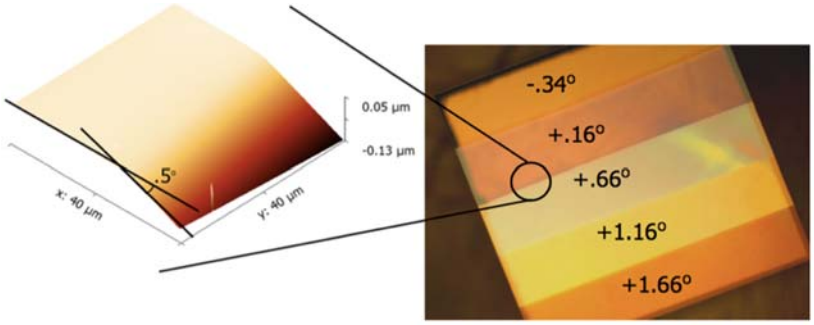
We propose a joint experiment/theory collaboration to develop next-generation quantum systems, targeting new paradigms for the creation and control of coherent phenomena in superconducting materials with an emphasis on elucidating and enhancing entanglement generation and characterization, as well as the transduction of quantum information between disparate modalities, specifically microwave photons and solid matter. We will focus on the tool set afforded by thin films and tunneling junctions as a laboratory to (i) control decoherence channels within novel 3D material architectures, varying material type and defect/doping density, (ii) apply advanced imaging, spectroscopy, and noise-sensing techniques to characterize static structural disorder as well as dynamic fluctuations in metallic and dielectric layers, (iii) develop functional quantum interfaces based on linear and nonlinear waveguides to efficiently transmit and receive coherent quantum information, and (iv) develop new theoretical and computational tools to efficiently characterize large-scale entanglement in such systems.

In the last year, we performed characterization both electrically using standard qubit coherence benchmarks and structurally using a suite of multi-modal imaging techniques. These techniques included transmission electron, scanning tunneling, and atomic force microscopy in combination with spectroscopic probes such as Auger, FTIR, and XPS with depth profiling our quantum processors' metal/dielectric/substrate landscape and topography. We have also started to develop and fabricate initial prototypes for 3D-integrated qubit chip-control/readout stack using atomic layer deposition (ALD) and to fabricate initial prototypes of flip-chip architectures 3D-integrated bonded chips. We began resonator, quantum processing chip and Josephson junction (JJ) characterization via the foundry's suite of structural characterization tools. We also began to design and model airbridge crossover structures for suppression of lossy electromagnetic modes. We designed, optimized, and fabricated a narrowband photodetector. We also designed and fabricated an array of single-photon source chips with varying source-detector input coupling to optimize efficiency. We developed JJ processes to produce less junction variation. We performed a 3000-junction uniformity study with automated probe station. We demonstrated better than SOA junction uniformity: relative standard deviation (RSD) of 2.7 percent across a wafer and 1 percent within 1 cm2 patches. We designed and fabricated three tunable transmon qubits capacitively coupled to transmission line and used it to demonstrate non-classical photon state production on-demand. Finally, on the theory front we investigated magnetic and dielectric properties of Nb oxides that plague our qubit processors.

[1] Lawrence Berkeley National Laboratory
[2] Massachusetts Institute of Technology

Topological phases of quantum matter and decoherence

Nikolai Sinitsyn (PI),[1] W. Zurek,[1] S. Lin,[1] V. Zapf,[1] D. Yarotksi,[1] L. Cincio,[1] and P. Coles,[1] V. Chernyak,[2] A. Bleszynski Jayich[3]



Decoherence in quantum systems is ordinarily viewed as a barrier to revealing purely quantum effects. The objective of our project is to explore, detect, and characterize decoherence-induced phases in real quantum systems under strong time-dependent driving conditions using the insight from emerging quantum computers. Here, we present the main results that our team has already achieved:

(i) Our study of many-body entanglement and its control by time-dependent fields revealed an unusual quantum echo phenomenon that reverses decoherence effects even after a qubit is fully entangled with a bath. Interestingly, this effect was demonstrated by IBM's 5-qubit quantum processor, which has natural decoherence. We can partly unwind the entanglement by our control protocol. We also describe the experimental research that should detect this effect using NV-centers in diamond. The figure shows AFM image (Left) of (100)-oriented diamond substrate with varying miscut across the sample as a template for CVD-diamond growth with Nitrogen delta-doping for generating dense, interacting spin ensembles to study decoherence and our spin echo phenomenon. On the Right, figure shows the optical image of a diamond sample polished with five different mis-cut angles.

(ii) During our search for a proper quantum material, we found that the 1D chain compound Sr3NiIrO6 has one of the largest coercive magnetic fields, which is thought to be a result of quantum spin-orbit-lattice coupled states on the Ir ions. We will describe our studies of the Ir quantum state and its spin flipping properties. We will also describe a topological phase transition that we predicted in mechanically driven graphene.

(iii) On theoretical side, we designed a method to solve explicitly time-dependent equations for evolution of many-body systems. Recent developments of this method predicted new phenomena, including advanced quantum annealing strategies and novel micro-laser design.

(iv) Finally, we will describe our techniques to optimize quantum-information circuits and achieve higher depth for quantum simulations of physical processes.

We will also discuss our plans to combine these theoretical predictions, quantum simulations, and experimental techniques in order to achieve the ultimate project goal: to demonstrate quantum computer assisted studies of decoherence and phase transitions in materials at nonequilibrium conditions.

[1] Los Alamos National Laboratory
[2] Wayne State University
[3] University of California, Santa Barbara

Intrinsic Topological Superconductors for Next-Generation Quantum Systems

Susanne Stemmer,[1] Leon Balents,[1] Stephen Wilson,[1] Andrea Young[1]

The drive to create robust, next generation quantum computing systems relies on the discovery and development of new materials capable of both hosting entangled electronic states and protecting them from rapid decoherence. Topological superconductor are an exciting frontier for realizing such protected states, but are exceedingly rare and many details remain controversial. Progress in topological band theory, recent advances in the synthesis of quantum materials and novel in-situ techniques that can detect the signatures of topological superconductors promise to accelerate the discovery of new candidate materials.

Towards this objective, this project undertakes a coupled theoretical and experimental search for materials hosting topological superconductivity. Efforts focus on the prediction, growth, and characterization of topological superconductor candidates as well as the study of their exotic electronic properties. Promising new classes of materials are explored theoretically, complemented by high purity bulk crystal and tunable thin film synthesis of candidate materials and explored via novel, in-situ imaging techniques. Ultimately, the project looks to demonstrate new intrinsic topological superconductors as components for next-generation quantum devices.

At this meeting, we will present results of experimental investigations of single crystals and thin films of the antiperovskites Dirac materials as well as families of strongly spin-orbit coupled, noncentrosymmetric superconductors. We will present scattering experiments and transport studies that reveal the symmetries and phase behaviors of these materials. Theoretical investigations focus on the response to magnetic fields and to thermal gradients, and how these may be used to prove their topological nature. We will also discuss our development of techniques that can elucidate the experimental signatures of topological edge states in candidate unconventional superconductors including FeSeTe. Such measurements are sensitive to the local temperature, resolving small thermal gradients on the micron scale. Gapless thermally conductive topological edge states are expected to manifest as temperature spikes on the boundary of the gapped, thermally insulating superconducting bulk.

[1] University of California, Santa Barbara

Hybrid quantum systems: spins, photons and superconducting qubits

Hong Tang,[1] Steve Girvin,[1] Peter Rakich,[1] Robert Shoelkopf,[1] Liang Jiang,[2] Rufus Cone [3], Charles Thiel[3]

We propose experimental and theoretical efforts to develop a hybrid quantum platform of spins, photons and superconducting qubits. The aim is to marry two quantum technologies: superconducting qubits and spin-systems, based on the thin film Lithium Niobate (LN). In addition to having strong piezoelectric and Pockels responses and superb optical properties, LN crystals are a particularly promising host for rare-earth-ion (REI) spin centers; spin centers in LN crystals have exhibited remarkably long spin coherence and strong optical and microwave transition strengths. In this three-year program, our goal is to exploit the inherent piezoelectric and Pockels effect in LN to achieve coherent coupling between spins, photons and superconducting qubits, and ultimately realize quantum state transfer from superconducting qubits into rare-earth ion spin states acting as quantum memories.

The team have progressed so far on two fronts: the study of spin-qubits and the study of phonon coupling to transmon qubits. The Yale team have successfully fabricated Er-implanted LN microresonators that reach quality factor over a million after post-annealing which recovers the processing damages to the LN crystals. Fluorescence spectroscopy records long optical T1 time of 3.5 ms in Er3+:LN waveguides. Purcell enhanced ion-cavity coupling is observed. We also developed very high Q superconducting resonators for addressing the spin states of the Er ions at dilution refrigerator temperatures. Work at MSU has focused on fabricating and charactering indiffusion and ion-exchange doping of Er3+ into LN wafers. Initial measurements reveal ion lifetime and coherence properties comparable to bulk-doped crystals. In parallel, our work on bulk-doped LN crystals indicates nuclear hyperfine lifetimes of 300 ms under a very weak bias magnetic field which is critical for building on-chip multifunctional photonic and microwave hybrid circuits.

The Yale team also works to understand and manipulate both intentional and unintentional coupling between transmon qubits and acoustic phonons. Using linear piezoelectric coupling between transmon qubits and bulk acoustic phonons we have previously demonstrated the ability to create nonclassical states of sound in new hybrid quantum acoustic systems. With efficient coupling to long lived phonon modes offered by lithium noibate, we seek to push these interactions in to the strong dispersive coupling regime. To date, we have developed new techniques for LN device fabrication and co-integration with transmon qubits. However, studies of phonon coherence in these patterned substrates has revealed that subtle forms of material damage can devastate the phonon coherence times in pristine crystalline media. To address this problem, we have developed new procedures for passivation of material surfaces which greatly extend phonon lifetimes. Through complementary studies, we have also discovered that imperfections in centro-symmetric media also result in unwanted coupling between microwaves and phonons that could represent a dominant decoherence pathway for superconducting transmon qubits. Hence, we believe that understanding of defect-induced decoherence pathways offer a path towards both improved superconducting qubits and high-performance hybrid quantum systems.

[1] Departments of Electrical Engineering, Physics and Applied Physics, Yale University
[2] Institute of Molecular Engineering, University of Chicago
[3] Department of Physics, Montana State University

ECRP: Coherent Control of Strongly Interacting Spins in the Solid-State

Jeff Thompson[1]

Harnessing quantum coherence in many-body systems provides diverse opportunities ranging from understanding quantum materials to applications in quantum information processing or quantum-enhanced metrology. A central challenge in this field is maintaining full control at the single-particle level while increasing the system complexity. We have developed an experimental platform for studying strongly interacting spin systems in the solid state. The central experimental tool is a technique that we have recently developed, which allows the spins of single Erbium (Er^{3+}) ion impurities in a crystal host to be optically initialized and measured through a nanophotonic cavity. Importantly, the addressing of individual ions is achieved in the frequency domain, instead of spatially, allowing for control of individual spins with sub-10 nm separation, and therefore strong interactions.

We have recently demonstrated high fidelity (95%) single-shot readout of a single spin within a dense ensemble, as well as simultaneous initialization, measurement and single-spin rotations on two spins separated by much less than the diffraction limit, in both cases using the spectral addressing approach. We will present these results, as well as ongoing efforts to extend these techniques to strongly interacting systems by tailoring the density profile of the spins to realize sub-10 nm separation. We will also discuss recent results on novel hosts for rare earth ions with less magnetic noise, in particular rutile TiO_2.

[1] Department of Electrical Engineering, Princeton University

Controlled synthesis of solid-state quantum emitter arrays for quantum computing and simulation

Jelena Vuckovic,[1] Dirk Englund,[2] Tony Heinz,[1] Mikhail Lukin,[3] Nicholas Melosh,[1] Hongkun Park,[3] Susanne Yelin[3]

Quantum emitters in solids are at the core of a wide range of quantum technologies, from nanoscale quantum sensors to quantum networks. This program aims to realize dramatic performance leaps by developing quantum emitters and quantum emitter arrays in diamond, silicon carbide (SiC) and two-dimensional (2D) van der Waals (vdW) materials, with precise control of their spatial position and uniformity, long electron spin coherence time, excellent optical properties, and small inhomogeneity, and with access to external tuning.

We have developed a new method of introducing of SnV color centers in diamond which combines shallow ion implantation at low energies combined with subsequent diamond overgrowth. The use of low implantation energies prevents to degradation of the materials properties of diamond and color centers [1].

We have also made significant progress in the development of ion implantation into diamond through gold apertures. In addition, we are setting up a new tool that combines annealing and electron irradiation in one tool, with the intention of sharing access to this tool to our DOE collaborators -- for example, through shuttle runs.

In SiC, we are collaborating with SLAC researchers on optimizing the condition for electron irradiation in order to produce the highest quality silicon vacancy (VSi) color centers.

We have developed methods to apply highly localized strain distributions in 2D semiconductors. The resulting localization of excitons was revealed through a dramatic decrease in the exciton line width, as well as by explicit demonstration of single-photon emission behavior through intensity correlation measurements.

References

1. "Generation of Tin-Vacancy Centers in Diamond via Shallow Ion Implantation and Subsequent Diamond Overgrowth," Alison E. Rugar, Haiyu Lu, Constantin Dory, Shuo Sun, Patrick J. McQuade, Zhi-Xun Shen, Nicholas A. Melosh, and Jelena Vuckovic, arXiv:1910.1416 (2019)

[1] Stanford University
[2] Massachusetts Institute of Technology
[3] Harvard University

Systems for Transducing Entanglement between Photons and Electron Spins

Michael R. Wasielewski (PI),[1] Emily A. Weiss,[1] Theodore Goodson III,[2] and Shaul Mukamel [3]

The scientific community is on the verge of a revolution in which Quantum Information Science (QIS) will change the way we live, work, and understand our world. Indeed, QIS may have the opportunity to transform industries, create jobs, and yield great benefits for the world's population. Transferring information between stationary (spin) qubits, the fundamental units of quantum information typical involved in quantum computation, and propagating (photon) qubits, typically involved in quantum communications, is a critical step in realizing these transformative technologies. The transfer of quantum properties and entanglement between photons and matter (transduction) is a major challenge in QIS because transduction is essential for networking quantum information processors. In order to overcome this challenge, it is important to know how non-classical light (single or entangled photons) interacts with matter. This project specifically addresses fundamental questions about how single and entangled photons interact with molecules and nanostructures to produce entangled electron spin qubits, thus resulting in transduction.

Toward these goals, two new molecules that upon photoexcitation produce 2-qubit entangled electron spin pairs (spin qubit pairs, SQPs) have been prepared. These molecules are being examined using an entangled photon source. We are also in the process of incorporating optical detection into a time-resolved EPR spectrometer to achieve the sensitivity levels needed to probe the interaction of entangled photons with the photogenerated SQPs. We are also synthesizing and characterizing colloidal quantum dots and nanoplatelets for use as quantum emitters, and measuring coherence lifetimes and emitted photon antibunching through fluorescence correlation spectroscopy. Theoretical work is focused on extending the two-state Bloch model for exciton coherence to multiple states necessary to describe the exciton fine structure of the nanocrystals, on calculating two photon absorption spectra of molecules and model systems with entangled photons, and on exploring the advantages offered by quantum light. These advantages include improved spectral resolution and better scaling with light intensity.

[1] Department of Chemistry, Northwestern University, Evanston, IL 60208
[2] Department of Chemistry, University of Michigan, Ann Arbor, MI, 48109
[3] Department of Chemistry, University of California, Irvine, Irvine, CA 92697

QPress: Quantum Press for Next-Generation Quantum Information Platforms

Amir Yacoby,[1] Philip Kim[1], Pablo Jarillo-Herrero[2], Joe Checkelsky[2], Efthimios Kaxiras[1], Alan Aspuru-Guzik[3], Willian Wilson[1,4]

Quantum information science (QIS) holds promise for revolutionizing computation, communication, and sensing. Of course, realizing this promise requires material platforms that can host quantum bits with pre-assigned characteristics that are uniquely attuned to such functionalities. While tremendous advances in QIS have been achieved in recent years, the underlying properties of the materials that host these quantum bits remains one of the key limitations in their performance.

The advent of layered materials opens up exciting and rich new possibilities for material synthesis that is removed from many of the constraints limiting bulk growth and that can be targeted towards specific applications in QIS. Here we propose to explore the basic science required to develop an automated quantum layered materials press (QPress) and use such assembly methods to create new material platforms for QIS. Such an automated printing machine will create stacks of layered materials, with integrated and in-situ characterization, fabrication and possible integration with silicon microprocessor chip technology. The fast turnaround time of the QPress, from a theoretical material concept to an assembled and characterized structure, including their quantum coherent properties, will allow generating large data sets of material properties and their relation to the underlying structure and target application. Such large data sets will be ideal for machine learning techniques that will be used to predict and speed up discovery of novel new materials and phenomena that are ideally suited for QIS.

Our effort will be divided into two main tasks. The first consists of developing the underlying building blocks composing the QPress. Here we will explore new characterization tools and adapt existing ones for integration with an automated process. We will investigate which materials are amenable for exfoliation and use first principle techniques such as density functional theory to predict properties of assembled stacks. Together with the accumulated data sets from characterized stacks we will develop machine learning protocols to make predictions for new stacks that are better suited for target applications. Our second main thrust will be to make use of the constructed methodology to improve two material platforms that are of interest for QIS. The first will be to enhance topological superconductivity for topological quantum computations and the second will be to develop electron arrays based on twisted layers for quantum simulations. Our proposed research addresses directly the needs described in “Opportunities for Basic Research for Next-Generation Quantum Systems” PRO1 sections 1, A3, and 4.

[1] Harvard University
[2] MIT
[3] University of Toronto
[4] Center for Nanoscale Systems

Quantum Computing Enhanced Gutzwiller Variational Embedding Approach for Correlated Multi-Orbital Materials

Yongxin Yao,[1,2] Feng Zhang,[1] Noah Berthusen,[1,3] Niladri Gomes,[1] Cai-Zhuang Wang,[1,2] Kai-Ming Ho,[1,2] and Peter P. Orth[1,2]

Accurately predicting properties of strongly correlated quantum materials from a microscopic *ab initio* description of the electronic degrees of freedom is one of the grand challenges in materials research. Major workhorse methods for correlated materials simulations include density functional theory combined with dynamical mean-field theory, or a Gutzwiller embedding approach. Despite recent progress, severe numerical challenges for complex materials persist, in particular for multi-orbital materials with strong spin-orbit coupling. The complexity is intrinsic and arises from the exponential growth of the complexity of the general many-body wave function.

To overcome these limitations, this project aims to leverage existing noisy intermediate-scale quantum computers technology to achieve highly accurate total energy calculations and to simulate quantum dynamics in correlated multi-orbital quantum materials. Specifically, we will implement a hybrid quantum-classical computational framework combining a Gutzwiller variational embedding approach with quantum variational eigensolver techniques that run on state-of-the-art quantum hardware. Gutzwiller variational wave functions with larger correlation projectors will yield quantum embedding Hamiltonians of higher dimension, which will be solved more efficiently using quantum computers, systematically improving accuracies while reducing overall computational time.

The capability of this new approach will first be established by benchmarking it to advanced classical algorithms. This methodology will then be used to investigate a series of rare-earth based strongly interacting multi-orbital materials to discover their complex phase diagrams and coherent quantum dynamics. On a broader level, this work will facilitate the discovery and design of correlated functional materials by building an efficient hybrid quantum-classical computational framework for simulating equilibrium and out-of-equilibrium behavior of correlated materials. The codes that are being developed during this project will be open source and made freely available to other researchers.

[1] Ames Laboratory, U.S. Department of Energy, Ames, Iowa 50011
[2] Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011
[3] Department of Electrical and Computer Engineering, Iowa State University, Ames, Iowa 50011

ECRP: The emergent photophysics and photochemistry of molecular polaritons: a theoretical and computational investigation

Joel Yuen-Zhou[1]

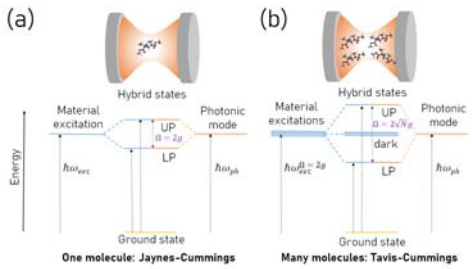


Fig. 1. The various flavors of strong light-matter coupling. A tightly confined electromagnetic mode can couple to a (a) single ($N = 1$) or (b) many ($N \gg 1$) molecular transitions. In both cases, hybrid light-matter states called upper and lower polaritons (UP, LP) are formed, which are separated in energy by a collectively enhanced Rabi splitting $\Omega = 2\sqrt{N}g$. Having $N \gg 1$ yields a large number ($N - 1$) of dark states which do not couple to light and which are crucial in the description of incoherent dynamics of molecular polaritons. Most experiments at present belong to the (b) case. Adapted from [1].

Program scope. This project started in September 2018 and aims to develop a theoretical and computational framework to address emergent room-temperature photophysical and photochemical processes afforded by molecular polaritons (MPs), hybrid states arising from the strong coupling of organic dye electronic/vibronic excitations and confined electromagnetic modes (Fig. 1). Recent experimental progress on MPs prompts for the development of robust theoretical tools that can describe the novel phenomenology afforded by these systems under realistic dissipative conditions. Our project aims to fill this gap. The molecular or photonic components of MPs can be tuned to rationally modify the physicochemical properties of molecular matter. In this work, we will pioneer formalisms based on open-quantum systems theory to address the low-energy dynamics of MPs in the presence of room-temperature realistic conditions such as in the presence of static and dynamic molecular disorder as well as absorptive losses in the electromagnetic environment. This framework will allow us to harness MPs to design control strategies to harvest dark molecular populations (work in progress) or even exotic paradigms for the remote control of chemical reactions (Fig. 2) in condensed phases. Our research aims to investigate "quantum-optically-mediated" chemical processes, where the new tools of quantum optics and quantum information can serve chemical purpose.

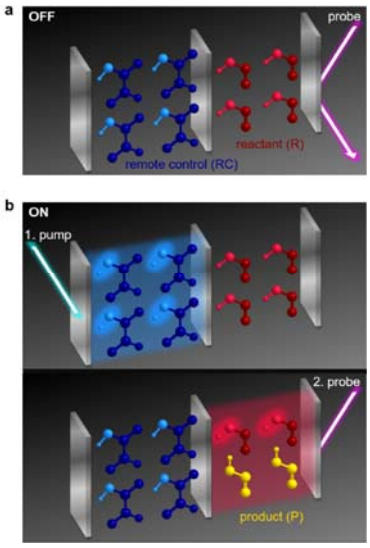


Fig. 2. Schematic of remote control of infrared-induced conformational isomerization of HONO. a, Without excitation of 'remote catalyst' (RC, blue) Tc-glyoxylic acid, the 'probe' laser pulse impinging on the mirror of the cavity containing reactant (R, red) *cis*-HONO is reflected; the reaction does not occur. **b**, First, a pump laser pulse impinging on the mirror of the RC cavity excites a polariton whose character is predominantly this cavity and the strongly coupled OH (light blue) stretch of RC. Within <100 ps, coupling between this vibration and solvent modes induces relaxation from the eigenstate to optically uncoupled (dark) RC states. Next, the 'probe' pulse efficiently excites a polariton whose character is predominantly the impinged cavity and the strongly coupled OH (light red) stretch of R; R is subsequently converted into the product (P, gold) *trans*-HONO. Adapted from [2]

[1] J. Yuen-Zhou and V. M. Menon, Polariton chemistry: thinking inside the (photon) box, Proc. Nat. Acad. Sci., 116 (12) 5214 (2019).

[2] M. Du, R. F. Ribeiro, L. A. Martínez-Martínez, and J. Yuen-Zhou, Remote control of chemistry in optical cavities, Chem 5, 5, 1167 (2019).

[1] University of California San Diego, Department of Chemistry and Biochemistry, La Jolla, CA 92093.