

Department of Energy Announces \$37 Million for Materials and Chemistry Research in Quantum Information Science

Both Universities and National Laboratories Will Lead Projects

WASHINGTON, D.C. – Today, the U.S. Department of Energy (DOE) announced \$37 million in funding for targeted research in materials and chemistry to advance the important emerging field of Quantum Information Science (QIS).

QIS seeks to exploit intricate quantum mechanical phenomena to create fundamentally new ways of obtaining and processing information. It is expected to play an increasingly important role in the information technology of the future, with the promise of potentially powerful new capabilities in computing, networking, and sensing.

The current initiative includes projects aimed at synthesizing and observing material and chemical systems with exotic quantum properties as well as efforts to use quantum computing to better understand complex material and chemical systems. The goal is both to lay the groundwork for the development of new quantum information systems and to use current quantum information capabilities to advance research in material and chemical sciences.

Details of awards selected for negotiation are shown below:

PI	Institution	City, State	Proposal Title
Ashoori, Raymond	Massachusetts Institute of Technology	Cambridge, MA	Creating and Probing Large Gap 2D Topological Insulators for Quantum Computing
Clark, Bryan	University of Illinois	Champaign, IL	Porting classical approaches for quantum simulations to quantum computers
Coker, David	Boston University	Boston, MA	Control of Energy Transport and Transduction in Photosynthetic Down-Conversion
Fu, Kai-Mei	University of Washington	Seattle, WA	Quantum Entanglement between a Solid-State Spin and Trapped Ion via a Photonic Link
Hen, Itay	University of Southern California	Marina del Rey, CA	Resource-Efficient Quantum Simulations on NISQ Devices: Advancing the State-of-the-Art
Hill, Stephen	Florida State University	Tallahassee, FL	A Route to Molecular Quantum Technologies Using Endohedral Metallofullerenes
Hoffman, Jennifer	Harvard University	Cambridge, MA	Design & Assembly of Atomically-Precise Quantum Materials & Devices
Kolkowitz, Shimon	University of Wisconsin	Madison, WI	Quantum Probes of the Materials Origins of Decoherence
National Laboratory Subaward	Lawrence Livermore National Laboratory	Livermore, CA	Quantum Probes of the Materials Origins of Decoherence

PI	Institution	City, State	Proposal Title
Lawrie, Benjamin	Oak Ridge National Laboratory	Oak Ridge, TN	Nanoscale Quantum and Classical Sensing for Superconducting and Topological Quantum Information
Lyon, Stephen	Princeton University	Princeton, NJ	Materials for Ultra-Coherent, Mobile, Electron-Spin Qubits
National Laboratory Subaward	Sandia National Laboratories	Albuquerque, NM	Materials for Ultra-Coherent, Mobile, Electron-Spin Qubits
Manfra, Michael	Purdue University	West Lafayette, IN	Direct Observation of Fractional Quantum Hall Quasiparticle Braiding Statistics via Interferometry
Martinez, Todd	SLAC National Accelerator Laboratory	Menlo Park, CA	Hybrid Quantum/Classical Algorithms for Photochemistry and Nonadiabatic Dynamics
National Laboratory Subaward	Oak Ridge National Laboratory	Oak Ridge, TN	Hybrid Quantum/Classical Algorithms for Photochemistry and Nonadiabatic Dynamics
Painter, Oskar	California Institute of Technology	Pasadena, CA	Enhancing Entanglement: Non-Markovian and Floquet Reservoir Engineering in Many-Qubit Superconducting Quantum Circuits
Richerme, Philip	Indiana University	Bloomington, IN	An Ion-Trap Quantum Simulator for Exotic 2D Materials
Schelter, Eric	University of Pennsylvania	Philadelphia, PA	Expressing Tunable Emergent Quantum Phenomena in Molecular Materials with Strong Electron Corrections
National Laboratory Subaward	Lawrence Berkeley National Laboratory	Berkeley, CA	Expressing Tunable Emergent Quantum Phenomena in Molecular Materials with Strong Electron Corrections
Shultz, David	North Carolina State University	Raleigh, NC	Optical Generation and Manipulation of Spin Qubits
Stemmer, Susanne	University of California, Santa Barbara	Santa Barbara, CA	Intrinsic Topological Superconductors for Next-Generation Quantum Systems
Vuckovic, Jelena	Stanford University	Stanford, CA	Controlled Synthesis of Solid-State Quantum Emitter Arrays for Quantum Computing and Simulation
Wasielewski, Michael	Northwestern University	Evanston, IL	Systems for Transducing Entanglement between Photons and Electron Spins
Yao, Yongxin	Ames Laboratory	Ames, IA	Quantum Computing Enhanced Gutzwiller Variational Embedding Method for Correlated Multi-Orbital Materials

Basic Energy Sciences

Quantum Information Science Awards Abstracts

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

PI: Raymond Ashoori, Massachusetts Institute of Technology

Co-PIs: Joseph Checkelsky (MIT), Liang Fu (MIT), Nuh Gedik (MIT), Pablo Jarillo-Herrero (MIT)

Porting classical approaches for quantum simulations to quantum computers

PI: Bryan Clark, University of Illinois

Control of Energy Transport and Transduction in Photosynthetic Down-Conversion

PI: David Coker, Boston University

Co-PIs: Ksenia Bravaya (Boston University), Gregory Scholes (Princeton),
Sahar Sharifzadeh (Boston University)

Quantum Entanglement between a Solid-State Spin and Trapped Ion via a Photonic Link

PI: Kai-Mei Fu, University of Washington

Co-PI: Boris Blinov (U Washington)

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

PI: Itay Hen, University of Southern California

Co-PI: Amir Kalev (Maryland)

A Route to Molecular Quantum Technologies Using Endohedral Metallofullerenes

PI: Stephen Hill, Florida State University

Co-PI: Jianyuan Zhang (Rutgers)

Design & Assembly of Atomically-Precise Quantum Materials & Devices

PI: Jennifer Hoffman, Harvard University

Co-PIs: Taylor Hughes (University of Illinois), Boris Kozinsky (Harvard), Julia Mundy (Harvard)

Quantum Probes of the Materials Origins of Decoherence

PI: Shimon Kolkowitz, University of Wisconsin

Co-PIs: Victor Brar (Wisconsin), Jennifer Choy (Wisconsin), Jonathan DuBois (LLNL),
Mark Eriksson (Wisconsin), Lara Faoro (Wisconsin), Mark Friesen (Wisconsin),
Alex Levchenko (Wisconsin), Vince Lordi (LLNL), Robert McDermott (Wisconsin), Keith Ray (LLNL),
Yaniv Rosen (LLNL)

Nanoscale Quantum and Classical Sensing for Superconducting and Topological Quantum Information

PI: Benjamin Lawrie, Oak Ridge National Laboratory

Co-PIs: Matthew Brahlek (ORNL), Eugene Dumitrescu (ORNL), Gabor Halasz (ORNL),
Peter Maksymovych (ORNL)

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

PI: Stephen Lyon, Princeton University

Co-PI: Mark Dykman (Michigan State), Eric Shaner (SNL), M. David Henry (SNL)

Direct Observation of Fractional Quantum Hall Quasiparticle Braiding Statistics via Interferometry

PI: Michael Manfra, Purdue University

Hybrid Quantum/Classical Algorithms for Photochemistry and Nonadiabatic Dynamics

PI: Todd Martinez, SLAC National Accelerator Laboratory

Co-PI: Edward Hohenstein (SLAC), Dmitry Liakh (ORNL), Alexander McCaskey, (ORNL), Abraham Nitzan (U Pennsylvania), Robert Parrish (QC Ware Corporation), David Reichman (Columbia), Joseph Subotnik (U Pennsylvania)

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

PI: Oskar Painter, California Institute of Technology

Co-PI: Aashish Clerk (University of Chicago)

An Ion-Trap Quantum Simulator for Exotic 2D Materials

PI: Philip Richerme, Indiana University

Co-PIs: Gerardo Ortiz (Indiana), Babak Seradjeh (Indiana)

Expressing Tunable Emergent Quantum Phenomena in Molecular Materials with Strong Electron Corrections

PI: Eric Schelter, University of Pennsylvania

Co-PIs: Corwin Booth (LBNL), Jochen Autschbach (University at Buffalo)

Optical Generation and Manipulation of Spin Qubits

PI: David Shultz, North Carolina State University

Co-PI: Martin L. Kirk (University of New Mexico)

Intrinsic Topological Superconductors for Next-Generation Quantum Systems

PI: Susanne Stemmer, University of California, Santa Barbara

Co-PIs: Leon Balents (UC Santa Barbara), Stephen Wilson (UC Santa Barbara),

Andrea Young (UC Santa Barbara)

Controlled Synthesis of Solid-State Quantum Emitter Arrays for Quantum Computing and Simulation

PI: Jelena Vuckovic, Stanford University

Co-PIs: Dirk Englund (MIT), Tony Heinz (Stanford), Mikhail Lukin (Harvard), Melosh Nicholas (Stanford), Hongkun Park (Harvard), Susanne Yelin (Harvard)

Collaborator: Adam Gali (Hungarian Academy of Sciences)

Systems for Transducing Entanglement between Photons and Electron Spins

PI: Michael Wasielewski, Northwestern University

Co-PIs: Theodore Goodson (Michigan), Shaul Mukamel (UC Irvine), Emily Weiss (Northwestern)

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

PI: Yongxin Yao, Ames Laboratory

Co-PIs: Kai-Ming Ho (Ames), Peter Orth (Ames), Cai-Zhuang Wang (Ames)

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

PI: Raymond Ashoori, Massachusetts Institute of Technology

Co-PIs: Joseph Checkelsky (MIT), Liang Fu (MIT), Nuh Gedik (MIT), Pablo Jarillo-Herrero (MIT)

Quantum computers store information not as ordinary bits, but instead as qubits that become quantum mechanically entangled with one another during a computation. This can lead to a massive potential speed-up of computations compared with traditional computers. However, qubits tend to lose their information over time to the environment, causing severe limitations on the implementation of quantum computers. Recently physicists have developed concepts for qubits based on newly understood “topological insulator” materials. Remarkably, qubits made from topological insulators and superconductivity can have “topological protection” that prevents information loss to the environment because doing so would require an unlikely change of topology of the entire electronic system.

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 can produce atomically thin flakes of topological insulator materials and place and stack them with other materials to create larger electronic structures. Theorists have proposed using such structures to create topological qubits, with the information processing elements existing 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 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 material flake size or their destruction in exposure to air in transporting these materials to characterization facilities.

This project will focus on the synthesis of candidate topological insulators and characterization of their electrical properties without direct electrical contact. The measurements include (1) A novel pulsed quantum tunneling method that permits very high resolution electronic structure; (2) A capacitance method that precisely measures the thermodynamic properties of the electronic system; 3) Methods for laser-based angle resolved photoemission spectroscopy that determine the electronic bands in the material; and (4) A THz technique that determines the topological properties of the material.

This award 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 offers complementary 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.

Porting classical approaches for quantum simulations to quantum computers

PI: Bryan Clark, University of Illinois

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. 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; new quantum algorithms are needed. 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.

Control of Energy Transport and Transduction in Photosynthetic Down-Conversion

PI: David Coker, Boston University

Co-PIs: Ksenia Bravaya (Boston U), Gregory Scholes (Princeton), Sahar Sharifzadeh (Boston U)

The project will combine theoretical and computational methods with ultrafast spectroscopy to enable accurate, first-principles modeling of excitation energy flow through light harvesting proteins of natural photosynthesis. The models will sample thermally accessible conformations of the photosynthetic pigment molecules and their protein environment. Electronic structure calculations will provide pigment excitation energies and electronic couplings. Their dependence on nuclear geometry will reveal the coupling of electronic transitions to excitation transfer between pigments, which may also excite local vibrations to dissipate excess energy at each transfer. Photosynthetic light harvesting proteins function as excitation energy funnels in which inter-pigment electronic coupling and local energy dissipation guide excitation energy flow. Our studies will provide fundamental understanding of how chemical structures regulate that flow at the nanoscale.

Energy flow in light harvesting proteins will be monitored using ultrafast two-dimensional electronic spectroscopy (2DES) to observe the time-evolving vibrational and electronic (vibronic) quantum wave packets. 2DES can provide detailed maps of how excitation moves through light harvesting proteins but many 2DES features of these samples overlap so theoretical modeling is needed to disentangle mechanistic details. To this end, 2DES signal calculations will use the first principles models as input. New methods for open system quantum dynamics of many coupled electronic and vibrational degrees of freedom that include directed energy dissipation and relaxation mechanisms will be iteratively compared with experimental results to refine the models.

Next, quantum optimal control theory combined with the dissipative quantum system dynamics methods will be used to study the use of adaptive feedback controlled laser pulse shaping to prepare specific initial excited states with two goals: (1) understanding their influence on subsequent dynamics as probed in the 2DES signals and (2) understanding how control is realized in the adaptive feedback control experiments. These studies explore the possibility of reducing quantum decoherence by using model Hamiltonian-inspired shaped laser pulses to prepare initial coherent superposition states that entangle the system and environment in such a way that the composite system state can sustain long-lived quantum coherent dynamics. The over-arching goal is to understand mechanisms of quantum control and initial state preparation in noisy complex systems.

Coherent/incoherent mechanistic control will also be studied by manipulating chromophore vibronic and environmental couplings. Subunits of light harvesting proteins from cryptophyte algae can be dissociated and refolded into functioning hybrids to manipulate these parameters. Similarly, the down-conversion mechanism in the peridinin - chlorophyll-a protein complex of dinoflagellate algae, where internal conversion, excited state nuclear rearrangement, and intramolecular charge transfer state mixing have been implicated from indirect experiments, will be studied with 2DES and theoretical protocols enabling direct mechanistic interpretation.

Photosynthetic light harvesting proteins are of both practical and fundamental interest. This project combines theory, computation and experiment to explore the feasibility of quantum state preparation in highly complex molecular systems. The information gained can also guide design of excitonic circuit elements for high efficiency, high fidelity control of excitation energy in light harvesting applications.

Quantum Entanglement between a Solid-State Spin and Trapped Ion via a Photonic Link

*PI: Kai-Mei Fu, University of Washington
Co-PI: Boris Blinov (University of Washington)*

Quantum mechanics, the theory that describes the microscopic world, allows objects to be at several places at the same time, a property called quantum superposition. If several objects are in such a superposition state, then their individual properties may become “entangled” in such a way that detecting one of the objects would affect the others even though there is no direct physical connection between them. Termed “spooky action at a distance” by Albert Einstein, this property has no classical physics analog, and its study is essential for our understanding of quantum mechanics. Entanglement also has important practical applications and implications for the rapidly developing fields of quantum computing and quantum communication. Quantum computers may soon be able to break computational speed records for some very important and useful algorithms; their very existence requires quantum entanglement between the quantum bits, or “qubits”, that they operate. Quantum communication channels can transmit data extremely securely; the reliability and range of this transmission depend crucially on the ability to generate the entanglement.

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.

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

PI: Itay Hen, University of Southern California

Co-PI: Amir Kalev (Maryland)

Simulating quantum many-body systems is a central challenge in Physics, Chemistry and Material Sciences as well as in other areas of science and technology, aiming to advance our understanding of phenomena associated with controlling the quantum dynamics of non-equilibrium chemical and materials systems, unraveling the physics and chemistry of strongly correlated electron systems and so much more. While no classical algorithms are known to efficiently simulate quantum many-body systems, still, a significant fraction of the world's computing power is spent on solving instances of this problem. 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, as well as for other potential applications, it is paramount to devise quantum algorithms whose resource efficiency is tightly optimized to run on small noisy circuits. In this effort, we theoretically develop and experimentally benchmark a novel algorithmic approach for resource-efficient Hamiltonian simulation that aims to supersede the current state-of-the-art.

To further reduce the resource cost of the simulation, 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. The utilization of this additional information allows us to tailor the digitization of the quantum time-evolution operator to the initial state on which it acts through the use of the recently developed 'off-diagonal series expansion' technique. This in turn yields a more resource-lean Hamiltonian simulation algorithm as compared to the existing state-of-the-art. In addition to the theoretical thrust, the proposed technique will be benchmarked on currently available quantum hardware by studying a range of physical models via which the capabilities of noisy intermediate-scale quantum (NISQ) hardware will be determined, as well as their limitations.

A Route to Molecular Quantum Technologies Using Endohedral Metallofullerenes

PI: Stephen Hill, Florida State University

Co-PI: Jianyuan Zhang (Rutgers)

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 ¹²C 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. Gd³⁺) 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.

Design & Assembly of Atomically-Precise Quantum Materials & Devices

PI: Jennifer Hoffman, Harvard University

Co-PIs: Taylor Hughes (University of Illinois), Boris Kozinsky (Harvard), Julia Mundy (Harvard)

The investigators of this award plan to develop a platform of new materials to be used in quantum information devices. The efforts will 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”.

Quantum Probes of the Materials Origins of Decoherence

PI: Shimon Kolkowitz, University of Wisconsin

*Co-PIs: Victor Brar (Wisconsin), Jennifer Choy (Wisconsin), Jonathan DuBois (LLNL),
Mark Eriksson (Wisconsin), Lara Faoro (Wisconsin), Mark Friesen (Wisconsin),
Alex Levchenko (Wisconsin), Vince Lordi (LLNL), Robert McDermott (Wisconsin), Keith Ray (LLNL),
Yaniv Rosen (LLNL)*

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. Here we propose 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 origins of decoherence, the proposed work 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.

This proposal brings together leaders in experimental qubit and quantum sensor platforms with experts in state-of-the-art predictive materials modelling in collaborative, tightly- integrated team. We will develop the understanding and control over sources of materials-induced decoherence required to realize more than an order-of- magnitude improvement in solid-state qubit and quantum sensor coherence times.

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.

Nanoscale Quantum and Classical Sensing for Superconducting and Topological Quantum Information

PI: Benjamin Lawrie, Oak Ridge National Laboratory

*Co-PIs: Matthew Brahlek (ORNL), Eugene Dumitrescu (ORNL), Gabor Halasz (ORNL),
Peter Maksymovych (ORNL)*

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. However, nanoscale interactions between photons, vortices, unpaired electrons, and magnetic defects constrain their performance. Fundamental understanding and control of such interactions are essential to further development of these platforms for photonic and superconducting quantum information. The overarching goal of this work 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. The fundamental material science that will be explored is tightly intertwined between these three specific aims. The photon induced vortex formation explored in aim one will be critical to the optical control of vortex-pinned Majorana fermions in aim three, and the exploration of two-level systems and quasiparticle interactions with superconducting qubits and resonators in aim two will be critical to the control of Majorana fermions in aim three and to the improved understanding of photon-superconductor interactions in aim one. 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. While a growing body of research has modeled the microscopic origins of 1/f noise in superconducting devices for quantum information science, there have been very limited nanoscale *in situ* measurements of quasiparticle, two-level system, and vortex interactions in these prototypical quantum devices. At the same time, the detection and spatial manipulation of superconducting vortices paves a path towards the elusive task of Majorana braiding in topological superconductors. Optical and scanning probe microscopies using classical and quantum sensing modalities at millikelvin temperatures will be employed to characterize and control nanoscale magnetic effects in superconducting qubits and nanowire single photon detectors. Overall, 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.

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

PI: Stephen Lyon, Princeton University

Co-PI: Mark Dykman (Michigan State), Eric Shaner (SNL), M. David Henry (SNL)

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.

Direct Observation of Fractional Quantum Hall Quasiparticle Braiding Statistics via Interferometry

PI: Michael Manfra, Purdue University

Utilizing a recent breakthrough in AlGaAs/GaAs heterostructure design that allows for operation of electronic Fabry-Perot interferometers with reduction of quantum dot-like charging effects while simultaneously generating sharper edge potential profiles, 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 $v=1/3$
- 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 $v=5/2$
- Measurement of interferometers in which the edge potential profile 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.

Hybrid Quantum/Classical Algorithms for Photochemistry and Nonadiabatic Dynamics

PI: Todd Martinez, SLAC National Accelerator Laboratory

*Co-PI: Edward Hohenstein (SLAC), Dmitry Liakh (ORNL), Alexander McCaskey, (ORNL),
Abraham Nitzan (U Pennsylvania), Robert Parrish (QC Ware Corporation), David Reichman (Columbia),
Joseph Subotnik (U Pennsylvania)*

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.

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

PI: Oskar Painter, California Institute of Technology

Co-PI: Aashish Clerk (University of Chicago)

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, has extensive experience working together. Specific research goals of the team will be to develop new theoretical tools and methodologies to describe non-Markovian and time-dependent engineered dissipation, and to use these to 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 recently developed by PI Painter.

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? In addition to fundamental science inquiry and exploration, our proposed research activities will also lead to new, more powerful theoretical techniques and hardware for quantum simulation and quantum information processing. *The work proposed here will lead to new methods for entanglement creation and control, and thus specifically addresses PRO 2 (Enhance Creation and Control of Coherence) in the BES Roundtable report; it also addresses topic 4 of PRO 4 (entanglement and many-body physics).*

An Ion-Trap Quantum Simulator for Exotic 2D Materials

PI: Philip Richerme, Indiana University

Co-PIs: Gerardo Ortiz (Indiana), Babak Seradjeh (Indiana)

This joint experimental and theoretical effort seeks to develop a flexible platform for the atom-by-atom synthesis and characterization of exotic 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.

Expressing Tunable Emergent Quantum Phenomena in Molecular Materials with Strong Electron Corrections

*PI: Eric Schelter, University of Pennsylvania
Co-PIs: Corwin Booth (LBNL), Jochen Autschbach (University at Buffalo)*

High-temperature, emergent quantum phenomena is a grand challenge of chemistry and physics. Molecular assemblies comprising f-elements, such as the lanthanides, are uniquely poised to express quantum phenomena because of their electronic characteristics. The f-electrons reside in core-like atomic orbitals that confer protection against quantum decoherence and underpin quantum ‘heavy electron’ behavior and unconventional superconductivity. To expand the study of quantum effects involving f-elements, there is a clear need to develop 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, superconducting lattice. Molecular assemblies provide an important venue for the development of new examples because the critical local interactions can be tuned using coordination chemistry at appropriate energy scales. The long term goal of this project is to synthesize heavy electron coordination polymers and molecular solids with properties that can be tuned systematically using molecular design principles, and ultimately, to achieve superconductivity. The central hypothesis of this proposal is that emergent quantum phenomena can be elaborated from molecular precursors of redox active lanthanide elements that possess both magnetic moments and strong electron correlations. This approach is expected to result in isolation of the first f-element molecular heavy electron materials and the first f-element molecular superconductor, providing new families of quantum materials. Results from this work are expected to provide new knowledge and information on materials that exhibit strong electron correlations, such as high temperature superconductors, which are expected to find use in quantum information processing.

Optical Generation and Manipulation of Spin Qubits

PI: David Shultz, North Carolina State University

Co-PI: Martin L. Kirk (University of New Mexico)

This project focuses on a novel approach to producing polarized molecular electron spins using visible light. Investigations of multi-spin molecular systems are important to molecular and nanoscale optical-thermal energy conversion, magnetic exchange-modulated photoprocesses, and in particular, quantum information science (QIS). The research will advance 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. The 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 may allow the development of spatial and temporal control of spin qubits, as well as promote spin coherence lifetimes that are markedly longer than the spin initiation process.

Intrinsic Topological Superconductors for Next-Generation Quantum Systems

PI: Susanne Stemmer, University of California, Santa Barbara

Co-PIs: Leon Balents (UC Santa Barbara), Stephen Wilson (UC Santa Barbara),

Andrea Young (UC Santa Barbara)

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 superconducting states are an exciting frontier for realizing such protected states, but are exceedingly rare and many details remain controversial. This project envisions chemically homogenous, intrinsic topological superconductors as an important leap forward. 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, the project will undertake a coupled theoretical and experimental search for manifestations of topological superconductivity. Efforts will focus on the prediction, growth, and characterization of topological superconductor candidates as well as the study of their exotic electronic properties. The focus of this project will be on families of materials that are known to have topologically non-trivial nodal structures and have superconductivity in some of their family members. Promising new classes of materials will be 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.

Controlled Synthesis of Solid-State Quantum Emitter Arrays for Quantum Computing and Simulation

PI: Jelena Vuckovic, Stanford University

*Co-PIs: Dirk Englund (MIT), Tony Heinz (Stanford), Mikhail Lukin (Harvard), Melosh Nicholas (Stanford),
Hongkun Park (Harvard), Susanne Yelin (Harvard)*

Collaborator: Adam Gali (Hungarian Academy of Sciences)

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 (QE) 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 will combine the developed quantum emitter arrays with optimized nanophotonic structures to make a platform for complex quantum state generation and for controlling quantum states of light.

The program is structured in three interacting research thrusts (T1-T3). T1 and T2 are devoted to the creation and study of QE arrays in diamond, SiC, and vdW materials with precisely defined positions, tunable spectral properties, and long coherence times. T3 extends the use of tunable, position-controlled emitters from T1 and T2 to demonstrate new light-matter interactions in interacting arrays of QEs, for applications in cluster state generation, quantum simulators, and quantum gates. The ambitious program proposed here requires bringing together deep expertise in diverse fields and the ability to work effectively as a team. Our researchers have already collaborated extensively and provide the necessary experimental and theoretical capabilities: 2D material electronic and optical properties and assembly (TH, HP), quantum optics and spin-photon interfaces in diamond and SiC (JV, ML, DE), advanced materials growth, characterization, and defect control (NM), electronic structure theory for spin/optical properties and the study of localized defects in solids (AG), and quantum optics theory (SY).

The proposed program directly addresses all of the major priority research opportunities (PROs) for next generation quantum systems identified in the DOE QIS Roundtable Report. In particular, the tailored arrays of interacting QEs will enable the exploration of foundational aspects of quantum mechanics, the simulation of complex quantum behavior, and quantum error correction.

Systems for Transducing Entanglement between Photons and Electron Spins

PI: Michael Wasielewski, Northwestern University

Co-PIs: Theodore Goodson (Michigan), Shaul Mukamel (UC Irvine), Emily Weiss (Northwestern)

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.

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

*PI: Yongxin Yao, Ames Laboratory
Co-PIs: Kai-Ming Ho (Ames), Peter Orth (Ames), Cai-Zhuang Wang (Ames)*

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.