PI	Institution	City, State	Proposal Title
Awschalom, David	Argonne National Laboratory (ANL)	Lemont, IL	Generation and Remote Distribution of Quantum Entanglement in Solids
Bansil, Arun	Northeastern University	Boston, MA	Design, Control and Application of Next-Generation Qubits
Campbell, Wesley	University of California, Los Angeles	Los Angeles, CA	Molecules Functionalized with Cycling Centers for Quantum Information Science
Chin, Cheng	University of Chicago	Chicago, IL	Two-dimensional quantum gas with real time control of complete Hamiltonian
Di Felice, Rosa	University of Southern California	Los Angeles, CA	Q4Q: Quantum Computation for Quantum Prediction of Materials and Molecular Properties
Evangelista, Francesco	Emory University	Atlanta, GA	Quantum Chemistry for Quantum Computers
Freedman, Danna	Northwestern University	Evanston, IL	Creating and Interfacing Designer Chemical Qubits
Freericks, James	Georgetown University	Washington, DC	Simulating long-time evolution of driven many-body systems with next generation quantum computers
Fuchs, Gregory	Cornell University	Ithaca, NY	Coherent spin-magnon coupling for quantum-to-quantum transduction
Haeffner, Hartmut	University of California, Berkeley	Berkeley, CA	Studying light-matter interactions and energy transfer at the nanoscale with a trapped-ion quantum computer
Ho, Wilson	University of California, Irvine	Irvine, CA	Space-Time Quantum Information from the Entangled States of Magnetic Molecule
Jayich, Ania	University of California, Santa Barbara	Santa Barbara, CA	Atom-defect Hybrid Quantum Systems
Jesse, Stephen	Oak Ridge National Laboratory (ORNL)	Oak Ridge, TN	Understanding and Controlling Entangled and Correlated Quantum States in Confined Solid-state Systems Created via Atomic Scale Manipulation
Johnson, Justin	National Renewable Energy Laboratory (NREL)	Golden, CO	Molecular Control of Spin-Entangled Triplet Excitons from Singlet Fission
Kais, Sabre	Purdue University	West Lafayette, IN	Quantum Computing Algorithms and Applications for Coherent and Strongly Correlated Chemical Systems
Kamal, Archana	University of Massachusetts Lowell	Lowell, MA	Parametrically-Induced Quantum Engineering (PIQUE)
Kasevich, Mark	Stanford University	Palo Alto, CA	Frontiers in Quantum Metrology and Transduction
Kim, Jungsang	Duke University	Durham, NC	Quantum Computing in Chemical and Material Sciences
Kowalski, Karol	Pacific Northwest National Laboratory (PNNL)	Richland, WA	Embedding quantum computing into many-body frameworks for strongly correlated molecular and materials systems.
Mayhall, Nicholas	Virginia Polytechnic Institute and State University	Blacksburg, VA	Simulating strongly correlated molecules with a superconducting quantum processor
Nadj-Perge, Stevan	California Institute of Technology	Pasadena, CA	Quantum States in Layered Heterostructures Controlled by Electrostatic Fields and Strain
Pribiag, Vlad	University of Minnesota	Minneapolis, MN	Integrated Materials Platform for Topological Quantum Computing Devices
Shan, Jie	Cornell University	Ithaca, NY	Planar Systems for Quantum Information
Siddiqi, Irfan	Lawrence Berkeley National Laboratory (LBNL)	Berkeley, CA	High-Coherence Multilayer Superconducting Structures for Large Scale Qubit Integration and Photonic Transduction
Sinitsyn, Nikolai	Los Alamos National Laboratory (LANL)	Los Alamos, NM	Topological phases of quantum matter and decoherence
Tang, Hongxing	Yale University	New Haven, CT	Hybrid quantum systems: spins, photons and superconducting qubits
Yacoby, Amir	Harvard College	Cambridge, MA	QPress: Quantum Press for Next-Generation Quantum Information Platforms

Basic Energy Sciences

Quantum Information Science Awards Abstracts

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Co-PIs: Claudio Chamon (Boston), Adrian Feiguin (Northeastern), Liang Fu (MIT), Eduardo Mucciolo (Central Florida), Qimin Yan (Temple)

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Co-PI: Alexander Kemper (North Carolina State)

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Studying light-matter interactions and energy transfer at the nanoscale with a trapped-ion quantum computer
PIs: Hartmut Haeffner and Birgitta Whaley, University of California, Berkeley
Co-PI: Mohan Sarovar, SNL

Space-Time Quantum Information from the Entangled States of Magnetic Molecules
PI: Wilson Ho, University of California, Irvine

Atom-defect Hybrid Quantum Systems
PI: Ania Jayich, University of California, Santa Barbara

Understanding and Controlling Entangled and Correlated Quantum States in Confined Solid-state Systems Created via Atomic Scale Manipulation
PI: Stephen Jesse, Oak Ridge National Laboratory
Co-PIs: A. Lupini, M. Yoon;Strategic Participants: Prineha Narang (Harvard), Dirk Englund (MIT)

Molecular Control of Spin-Entangled Triplet Excitons from Singlet Fission
PI: Justin Johnson (NREL)
Co-PIs: Obadiah Reid (NREL & UC Boulder), Matt Beard (NREL), Elisa Miller-Link (NREL), Chris Chang (NREL), Brian Fluegel (NREL), Natalie Pace (NREL & UC Boulder), Niels Damrauer (UC Boulder) Joel Eaves (UC Boulder), John Anthony (Kentucky)

Quantum Computing Algorithms and Applications for Coherent and Strongly Correlated Chemical Systems
PI: Sabre Kais, Purdue University

Parametrically Induced Quantum Engineering (PIQUE)
PI: Archana Kamal, University of Massachusetts

Frontiers in Quantum Metrology and Transduction
PI: Mark Kasevich, Stanford University

Developing and Running Quantum Algorithms for Chemistry and Materials
PIs: Jungsang Kim (Duke University) and Christopher Monroe (University of Maryland)
Co-PIs: Kenneth Brown, Jianfeng Lu, Thomas Barthel (Duke), Vladimir Manucharyan, Alexey Gorshkov (Maryland), Maxim Vavilov (Wisconsin), and Ivar Martin (ANL)

Embedding Quantum Computing into Many-body Frameworks for Strongly Correlated Molecular and Materials Systems
PI: Karol Kowalski, Pacific Northwest National Laboratory (PNNL)

Simulating strongly correlated molecules with a superconducting quantum processor
PI: Nick Mayhall, Virginia Polytechnic Institute and State University

Quantum States in Layered Heterostructures Controlled by Electrostatic Fields and Strain
PI: Stevan Nadj-Perge, California Institute of Technology
Co-PIs: Andrei Faraon, Marco Bernardi, Julia Greer, Gil Refael (Cal Tech)

Integrated Development of Scalable Materials Platforms for Topological Quantum Information Devices
PI: Vlad Pribiag, University of Minnesota
Co-PIs: Paul Crowell (Minn.), Sergey Frolov (Pittsburgh.), Noa Marom (Carnegie Mellon), Chris Palmstrom (UC Santa Barbara)

Planar Systems for Quantum Information
PI: Jie Shan, Cornell University
Co-PIs: Kin Fai Mak (Cornell), Cory R. Dean, James Hone (Columbia), Tony F. Heinz (SLAC/Stanford), Allan H. MacDonald (Texas-Austin)

High-Coherence Multilayer Superconducting Structures for Large Scale Qubit Integration and Photonic Transduction
PI: Irfan Siddiqi, Lawrence Berkeley National Laboratory (LBNL)

Topological phases of quantum matter and decoherence
PI: Nikolai Sinitsyn
Co-PIs: Wojciech Zurek, Vivien Zapf, Dmitry Yarotski, Shizeng Lin, Lukasz Cincio, Patrick Coles (LANL), Vladimir Chernyak (WSU), Ania Jayich (UCSB)

Hybrid quantum systems: spins, photons and superconducting qubits
PI: Hong Tang, Yale University
Co-PIs: Steve Girvin, Liang Jiang, Peter Rakich, Robert Schoelkopf (Yale); Rufus Cone, Charles Thiel (Montana)

QPress: Quantum Press for Next-Generation Quantum Information Platforms
PI: Amir Yacoby, Harvard University
Co-PIs: Philip Kim (Harvard), Pablo Jarillo-Herrero (MIT), Joe Checkelsky (MIT), Efthimios Kaxiras (Harvard), Alan Aspuru-Guzik (Toronto), William Wilson (Harvard/Center for Nanoscale Systems)

Generation and Remote Distribution of Quantum Entanglement in Solids

David Awschalom, Argonne National Laboratory

Rapid advancements in photonic and solid-state quantum technologies have enabled distributed quantum systems at the chip- and laboratory-scale in which entanglement between physically separated subsystems is generated and harnessed for quantum information and metrological applications. The expansion of distributed entanglement beyond controlled laboratory settings will advance quantum science by opening new physical realms and moving quantum technologies towards a global scale. For instance, it has been proposed that distributed entanglement can be utilized to precisely synchronize atomic clocks across the globe, with significant impacts in the field of metrology. Current state-of-the-art has allowed limited exploration of this regime, and fundamental questions remain: what are the underlying physical processes that drive decoherence and loss of information when entangled quantum systems are separated by large physical distances? What are the fundamental limits on the capacity and fidelity of remote entanglement achievable given realistic channel constraints? What is the minimum coherence in solids required to establish certifiable entanglement across a distance? Using entanglement-assisted metrology, how does the entanglement quality impact the precision of clock synchronization via a network of entangled spins?

We assemble a team of theorists and experimentalists to interrogate these questions by developing new platforms for generating and controlling remote entanglement in solids. We will construct a long-distance quantum testbed to enable scientific explorations based on long-distance distributed entanglement while realizing “real-world” operating conditions for new quantum technologies. A unique component of this collaboration is an existing 30-mile-long single mode fiber-optic link between Argonne National Laboratory and Fermi National Accelerator Laboratory. We construct quantum nodes at each end of the fiber, realizing a long-range quantum testbed for use in exploring entanglement distribution, distillation and control protocols. The nodes will have a flexible design that allows different quantum platforms to be swapped in and out, with a vision of a plug-and-play testbed for long-distance quantum entanglement.

At each quantum node, basic research focusing on quantum material design, synthesis, and coherent control will be carried out using a bottom-up approach to achieve the desired quantum characteristics. The team capitalizes on the leading material science expertise at Argonne to develop high quality material platforms including optically active spins and defects for quantum information transfer and communication applications. The material synthesis and optimization will be aided by comprehensive modeling and computations. Heterogeneous integration across multiple platforms will be sought to form complex systems that possess large scale entanglement and tailorable coherent interactions between constituent subsystems. New theoretical schemes for preparing and stabilizing remote entanglement will both be developed and implemented. We will explore schemes that exploit multiplexing between subsystems (e.g. spins, atomic ensembles, spin-waves) for enhancing the entanglement generation throughput.

We will leverage knowledge gained from Fermi National Accelerator Laboratory within their onsite quantum teleportation project. The laboratory offers additional science drivers that will attract a growing community to experiment with the quantum link as it matures. The research efforts will take place under the collaborative umbrella of the Chicago Quantum Exchange, established specifically for the purpose of enabling integrative activities of this nature through the exchange of information between students, faculty, and laboratory scientists.

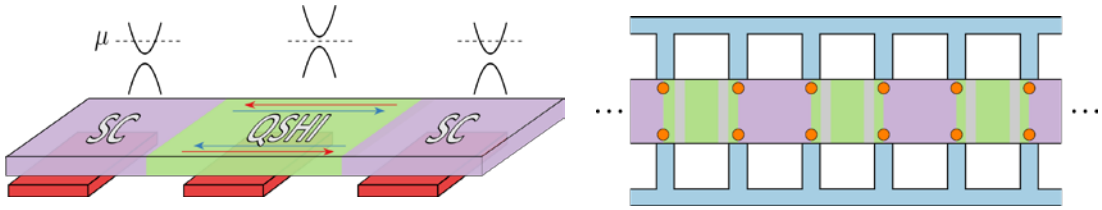
Design, Control and Application of Next Generation Qubits

Arun Bansil, Northeastern University **(Lead-PI)**
Claudio Chamon, Boston University **(Co-PI)**
Adrian Feiguin, Northeastern University **(Co-PI)**
Liang Fu, MIT **(Co-PI)**
Eduardo Mucciolo, Univ. of Central Florida **(Co-PI)**
Qimin Yan, Temple University **(Co-PI)**

The quest for developing technologies for manipulating and storing information quantum mechanically, based currently 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.

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



<u>Left</u>: A setup for realizing 4π-periodic Josephson effect with a junction in a single flake of WTe_2 with electron density controlled with gates below to allow tuning between SC and QSHI regimes. <u>Right:</u> A quantum information processing architecture based on a monolayer of WTe_2 with periodic arrangement of SC (violet) and QSHI (green) regions. Blue leads are normal metal with a long phase coherence length, which can be gated to form loops connecting different Majorana states across the system. Measuring the current in the loop will enable projective measurements of Majorana bilinears.

Molecules Functionalized with Cycling Centers for Quantum Information Science

Wesley Campbell
University of California, Los Angeles

When a molecule in a gas absorbs energy in the form of light, it will typically release this energy by emitting light of a different color than that it absorbed. Recently, a special class of molecules was discovered that will only emit light of the exact same color as they absorb, a unique property that allows the repetition of this cycle many times. This project will develop new molecules of this type and use their optical cycling property to perform quantum information storage, processing, and retrieval from individual molecules. Three operating environments have been identified where this capability will allow quantum information transport and processing that is beyond the current state of the art. The development of these new quantum systems has the potential to accelerate the move beyond classical information processing to the practical harnessing of quantum effects for secure communication and extreme high speed computation.

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

Cheng Chin and Kathryn Levin
University of Chicago

This project will develop a novel experimental and theoretical quantum platform to gain full control of individual atoms and their mutual interactions in a two-dimensional system in real time. The system, called the “quantum matter synthesizer” (QMS), is an ultimate dream for quantum physicists where the kinetic energy, potential energy, and interactions of every single atom can be independently controlled: the potential energy is holographically formed based on a digital micromirror device, the interactions between neighboring atoms is tuned by optical Feshbach resonance, and finally, each atom can be located to an accuracy of few nm based on super-resolution imaging. The QMS platform offers unprecedented opportunities to investigate quantum phenomena that are relevant to fundamental research, as well as to test innovative ideas to store and process quantum information. In the former category, the project will address the reversibility of many-body dynamics, which is at the heart of the discrepancy between quantum mechanics and thermodynamics. In the latter category, the project will explore the quantum limit of information storage by preparing each atom as a qubit, and show that no information is lost during the coherent evolution of the system.

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

Rosa Di Felice
University of Southern California

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". This effort builds upon data sets and learning techniques that arose from the materials genome initiative. 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. AQO on D-Wave will be used to implement data driven research for materials optimization toward manufacturing. GMQC on IBM and Rigetti devices will be used to solve quantum Hamiltonians for strongly correlated systems. Developed tools will be distributed as open-source software. New states of matter, inaccessible with classical computers, will be simulated.

Two specific objectives, organized in various tasks, will be pursued. Objective 1: D-Wave chips will be applied to process data within the AFLOW repository to explore if and how optimal or new properties emerge for desired applications of interest to the DoE. Two test cases have been devised: (i) extracting information on finite temperature properties by using data computed at zero temperature, (ii) providing synthesis and doping parameters for materials growth and deposition. Objective 2: Extending and adapting existing software tools to map many-body Hamiltonians of strongly correlated systems into model Hamiltonians that are solvable on gate-model quantum hardware and simulators. Specifically, the package Q-Chem will be added as a plugin to the quantum software OpenFermion. Through hybrid classical-quantum computations, correlated electron states for small molecules, single-molecule magnets and classes of materials enclosed in AFLOW will be computed.

The project will run at the University of Southern California (Rosa Di Felice and Anna I. Krylov), the University of North Texas Denton (Marco Buongiorno Nardelli) and Central Michigan University (Marco Fornari).

Quantum Chemistry for Quantum Computers

Francesco A. Evangelista[1], Alán Aspuru-Guzik[2], Garnet K.-L. Chan[3],
Gustavo E. Scuseria[4], Toru Shiozaki[5], James D. Whitfield[6], Dominika Zgid[7]

[1]Emory University, [2]University of Toronto, [3]California Institute of Technology, [4]Rice University,
[5]Northwestern University, [6]Dartmouth College, [7]University of Michigan

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: the development of efficient theories of electronic structure and 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 algorithms, there is a realistic expectation that quantum computers will outperform their classical counterparts within the next decade. However, the first generation of quantum computers is unlikely to have a transformative impact on chemistry and materials science unless their power is leveraged by combining them with new algorithms specifically designed to take advantage of quantum hardware and hybrid classical-quantum strategies.

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 of qubits (see Figure 1 for a summary of the four project thrusts). This project will result in the creation of new methods and quantum algorithms and their efficient implementation in open-source software. This research will also develop standard benchmarks for testing the accuracy and computing power of new quantum hardware and will validate prototypes of quantum computers in collaborations with industry partners. More generally, this project paves the way to applications of quantum computers to study challenging 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.

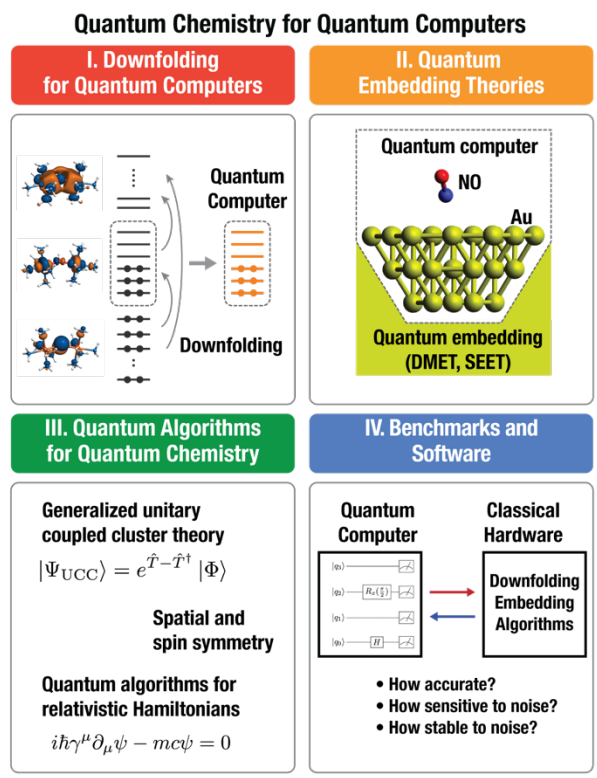
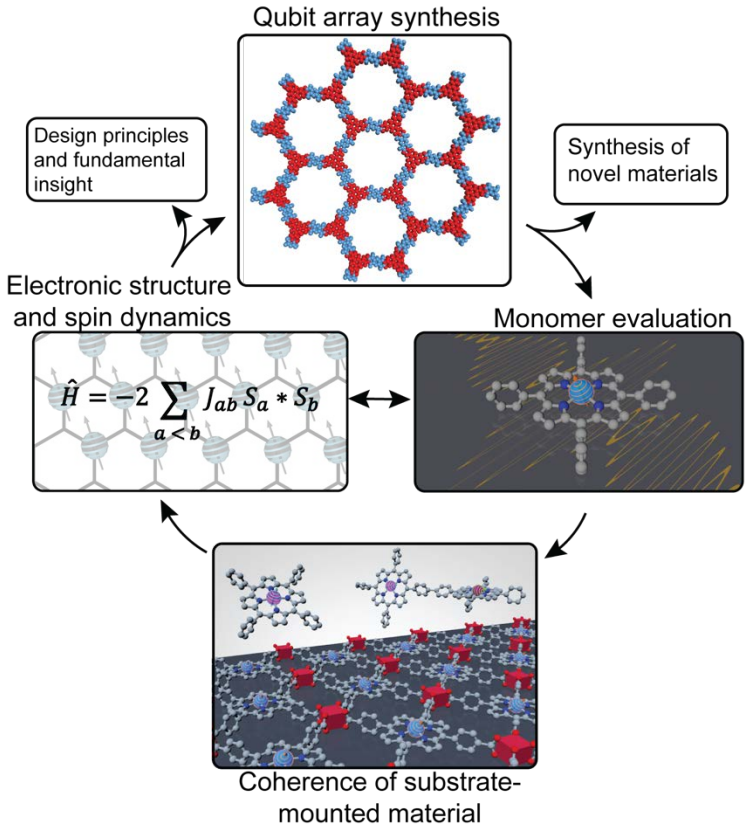


Figure 1. The four project thrusts.

Title: Creating and Interfacing Designer Chemical Qubits
Sponsoring Institution: Northwestern University
Principal Investigator: Danna Freedman | Northwestern University
Co-Investigators: William Dichtel | Northwestern; T. David Harris, Northwestern; Mark Hersam | Northwestern; James Rondinelli | Northwestern; Michael Wasielewski | Northwestern

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.



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

James Freericks (PI) **Alexander Kemper (co-PI)**
Georgetown University **North Carolina State University**

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 that are very long. 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.

We focus on three main scientific goals for doing this: (i) describing the behavior of driven-dissipative quantum systems; (ii) creating low-energy states of frustrated quantum magnets; and (iii) generating highly entangled spin states that can be employed for improved measurements. In the first problem, we will create quantum systems in artificial electric fields that will drive current through them, but will have energy removed from them at a fixed rate. They will usually end up in a complex quantum steady state, which we will explore with the quantum computer. In the second problem, we will examine a range of different strategies to create low-energy states, of magnets that are frustrated, in the sense that they cannot point their north and south poles where they would like to, to make the lowest-energy arrangement. These systems are some of the most fascinating, but most difficult to study systems in the quantum world. We will devise quantum algorithms to explore their properties. In the third problem, we will create highly entangled states which have at their core, the "spookiness" of quantum mechanics. They are difficult to make and fragile, but we will employ techniques that protect them from being destroyed as we work on making them.

Our approach is a combined classical-quantum computer hybrid approach, which uses the quantum computers primarily to calculate the strongest quantum effects, which are then post-processed by a classical computer to determine the final results. Our methodology is to develop robust algorithms that are resistant to errors and noise, and have a higher chance for successful operation with currently available quantum computers. We have collaborations with IBM, Intel, and the University of Maryland to ensure the ability to run these codes on real quantum hardware.

The impact of this project will be to set the stage for ushering in the era of quantum-computer-assisted scientific discovery. As quantum computers become more robust, we will be able to use them to tackle problems that will lead to exciting new applications of energy science.

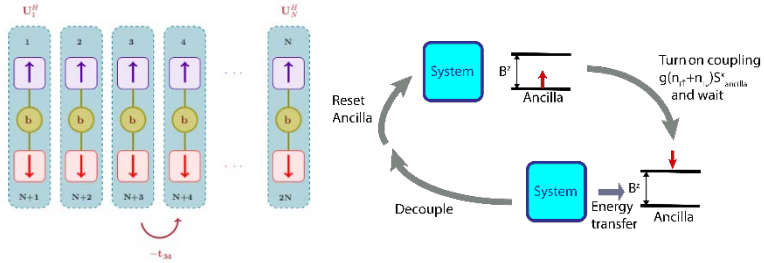


Fig. 1: Cooling algorithm to be employed in describing driven-dissipative systems on near-term quantum computers for project one.

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

Gregory Fuchs
Cornell University

This project addresses a fundamental challenge in solid-state quantum information processing – that although there has been rapid development in quantum information processing based on superconducting qubits in the microwave regime, these qubits do not possess the natural ability to emit an optical photon to form quantum networks over long distances. The development of quantum optical links between local, solid-state qubits is a key challenge for the field. The research team is studying the physics and materials science necessary to take a new approach to solving this problem: quantum coupling between isolated diamond nitrogen-vacancy (NV) center spins and magnons (quantum spin excitations of a magnet) at very low temperature. Through their coherent optical transitions, NV centers can be entangled with optical photons. Therefore, by coupling a nitrogen-vacancy center qubit to magnons in the quantum limit, this research provides a path toward establishing magnons as the critical bridge between microwave-frequency quantum processors and quantum optical networks.

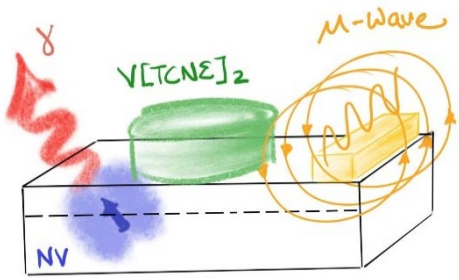


Figure 1. Schematic image of the coupling between a microwave circuit, a V[TCNE]$_{x\sim2}$ magnetic element, and a nitrogen-vacancy center spin, which is then out-coupled in the form of a photon.

In addition to theoretical predictions that nitrogen vacancy center qubits can transfer quantum information to and from a magnon mode, there is also preliminary experimental evidence that supports this approach. In this project, the research team will move these interactions to the quantum regime using a unique optical microscope and a laser-driven qubit control approach that enables the samples to be studied at temperatures that are much less than one Kelvin. At these temperatures, coherent quantum processes in the magnetic material become possible.

One critical challenge that the research team will tackle is to keep the quantum information in the magnetic system (the magnons) from decaying for as long as possible. In this project the research team is taking a new materials approach: using the hybrid organic magnetic material vanadium tetracyanoethylene (V[TCNE]$_{x\sim2}$), which now exhibits extremely low magnetic damping. Furthermore, unlike the standard crystalline alternative, this material can be grown on any substrate, which is ideal for integration with sophisticated diamond-based quantum devices.

This project seeks to understand and combine all of the necessary elements to convert quantum states from local quantum processors to an optical photon using the combination of diamond NV centers and very high quality magnons. If successful, the team will reveal new properties of quantum magnetic states at low temperature, their coupling to diamond qubits, and ultimately the conversion of those quantum states into quantum states of light. Along the way, the team will tackle relevant theory, materials development, and experimental measurement challenges to enable quantum information networking.

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

Hartmut Haeffner and Birgitta Whaley
University of California, Berkeley
Mohan Sarovar
Sandia National Laboratories

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.

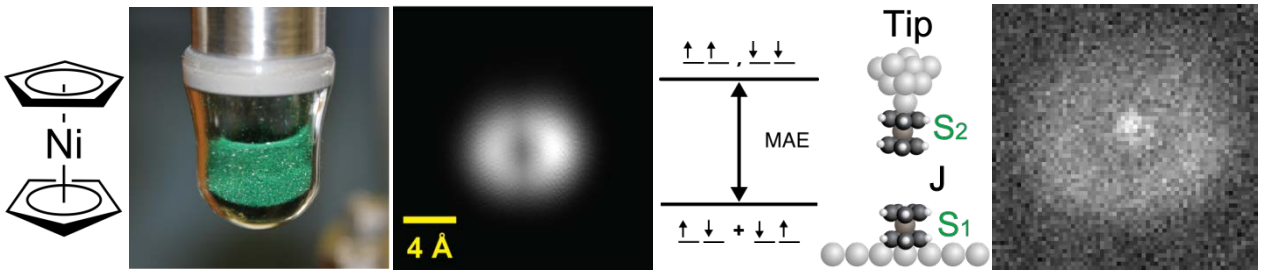
A quantum simulator, capable of implementing a realistic model of the system of interest, could provide insights into these processes in regimes where numerical treatments fail. We plan to model such transfer processes using an ion-trap quantum simulator. Sites within molecular complexes will be encoded 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 also may be 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 will be 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.

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

Wilson Ho
University of California, Irvine

The speed and capacity for information storage and processing can be greatly enhanced by tapping into the quantum properties of the system. This collaborative project combines synthesis, measurement, and theory of magnetic molecules as qubits by studying the energies of quantized excitations, the length of time the quantum states remain superposed and entangled, and the different factors that degrade their quantum behavior. Unlike the discrete and deterministic states in the classical binary 0 or 1 bit, the superposition of the two-level spin states of magnetic molecules and their quantum correlation give rise to a vast number of probabilistic states that can be tapped for quantum information processing. In this research, the magnetic excitations in molecular systems, from a single molecule to molecular lattices, are measured by inelastic electron tunneling spectroscopy with the scanning tunneling microscope (STM). The superposition and entanglement of the magnetic states are created and tracked in time by terahertz (THz) laser pulses of femtosecond duration 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 qubits. 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 qubits for quantum computing and information storage through the combined efforts of chemical synthesis, space-time measurement, and ab-initio theory.



An example of a magnetic molecule nickelocene (NiCp2), showing the schematic structure, greenish bulk solid and STM topographic image, as a qubit of the superposition of the m=0 and m=±1 states separated by the magnetic anisotropy energy (MAE); two qubits (one on the STM tip and another on the surface) and the spatial distribution of the exchange energy J(x,y).

Atom-defect Hybrid Quantum Systems

Ania Jayich
University of California, Santa Barbara

It has been known since the early twentieth century that quantum mechanics provides a truer description of the world than classical physics, albeit a nonintuitive one. This first quantum revolution revealed that objects can exist in a superposition of many places at once, and that entangled elements separated by thousands of miles can be inextricably linked. A second quantum revolution is now brewing which promises to usher in fundamental changes in the way humans obtain, manipulate, and store information by exploiting the quirky, but delicate, phenomena unique to quantum mechanics.

Individual atoms, both in isolation and as pointlike crystal defects, lie at the heart of many emerging quantum technologies powering this revolution. Isolated atoms are among the most perfect quantum systems; they can retain quantum information coherently for long periods of time, and exhibit spectra guaranteed to be identical to that of other atoms of the same species. Solid-state point defects benefit both practically and quantitatively from the strong trapping provided by their crystal host, while still exhibiting appreciable quantum coherence times even at room temperature (millisecond scale for the nitrogen-vacancy (NV) center in diamond, for example). As in a classical information processor, in which several disparate technologies (e.g. charge-based logic elements and magnetic memory elements) are combined in a single device, it has become clear that future quantum technologies will benefit from incorporating multiple quantum elements, each serving the purpose to which it is best suited.

We propose to develop 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 will be coherently coupled to subsurface NV centers, enabling creation and 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.

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

PI: S. Jesse
Co-PIs: A. Lupini, M. Yoon
Strategic Participants: Prineha Narang (Harvard), Dirk Englund (MIT)

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 to build quantum systems from the bottom up. The experimental efforts will be integrated with multifaceted predictive theory to help interpret measurements and guide materials choices and atomic scale design. Our working hypothesis is that *atomic-scale confinement can be exploited to yield unprecedented and robust correlated phenomena and revolutionize energy-efficient information technologies.* We therefore 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 the conditions under which *topological* effects emerge to form protected quantum states that can potentially persist at elevated temperatures.

A key enabling aspect of the proposed work leverages recent ORNL success in enhancing scanning transmission electron microscopy (STEM) as a platform for atomic scale manipulation that can be scaled up to allow fabrication of an array of defects with designed patterns. We will apply these novel capabilities to control the insertion and motion of multiple dopants in low dimensional materials to form arrays that can act as of quantum centers or, according to recent theoretical predictions, can transform the material locally to imbue it with robust and topologically isolated edge-states. At a slightly larger scale, we will create and position vacancies and extended defects to shape local electronic wavefunctions (in a manner similar to quantum corrals) and localize selected phonon modes near quantum centers. At a larger scale still, we will sculpt single and multilayer structures to gain understanding of how strain and heterogeneity provide critical symmetry breaking that allows otherwise forbidden states to emerge. We will combine our fine control of structure with advanced assessment of function and extend and specialize measurement capabilities of STEM for quantum systems. We will use orbital angular encoded vortex beams to probe topological states of matter and ptychography to reveal local electron wave phase. By coupling *in-situ* optical measurements within the STEM column, we will probe quantum coherence of our designed structures with near atomic resolution.

We will closely integrate theory efforts to interpret measurements and guide experiments. Currently, there is no single, standalone tool capable of capturing the needed quantum-mechanical, electro-dynamical, and quantum computational features. We will expand theory capabilities to address electronic structure modeling for many thousands of atoms, ab initio dynamics to capture thermal motion effects on decoherence, time-dependent quantum mechanical treatment of electronic structure for gating fields and electronic excitations, first principles calculations based on effective Hamiltonians to develop strategies towards room temperature topological quantum systems (e.g. anomalous Hall insulators and quantum spin Hall insulators), and coupling with quantum simulation for efficient modeling of these strongly correlated systems.

In summary, we will directly address open questions in the materials physics of atomic scale solid-state quantum systems by eliciting direct control of matter at the atomic scale. We will create and study real-world, unique quantum structures that are currently only addressable by modelling, and through a close interplay of theory and experiment, manipulate and modify these structures to form a deep understanding of the parameters that govern their behavior. By drawing on established strengths at ORNL, Harvard, and MIT in microscopy, computation, theory, and QIS, we will establish unique and world-leading capabilities and insight for qubits, sensors, and future applications that capitalize on entanglement and correlation to achieve novel material functionality.

Molecular Control of Spin-Entangled Triplet Excitons from Singlet Fission

Justin Johnson,[1] Obadiah Reid,[1,2] Matt Beard,[1] Elisa Miller-Link,[1] Chris Chang,[1] Brian Fluegel,[1] Natalie Pace,[1,2] Niels Damrauer,[2] Joel Eaves,[2] John Anthony[3]

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

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. Through systematic variation of molecular structure in dimers, oligomers, crystals and hybrid organic-inorganic structures, the sources of dephasing of the triplet pair will be thoroughly investigated. Control over the relative positions and dynamics of spin-entangled excitations can be accomplished through directed synthesis of molecules from design principles based on known routes of intermolecular coupling. Theoretical models will provide insight into the intrinsic and environmental sources of dephasing and the persistence of both spin and spatial entanglement in crystals. Production of triplet pairs near controlled nanoscale interfaces introduces energy and charge transfer pathways between dissimilar materials. Time-resolved spectroscopic measurements of the evolving spin state of excitations in both partners will reveal how the entanglement is influenced by exciton motion, interactions at the interface, and ultimately how it might influence electrical conduction (i.e., spin valves). 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.

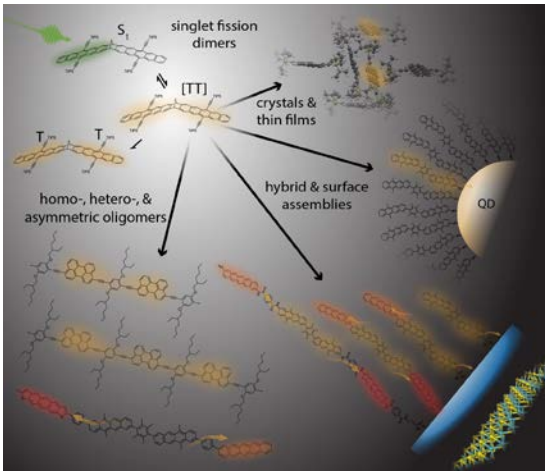


Figure 1. Schematic representation of key components and architectures for triplet pair production and manipulation.

Our initial activities have included determining the influence of substitution on electron paramagnetic resonance (EPR) spectra of triplet excitons in perylene and polyacene-based compounds (see Fig. 1). The information gained from time-resolved EPR experiments and theoretical simulations will guide our design of hetero-oligomers to both undergo SF and to drive triplets to distinct sites where they can be independently detected and manipulated. We have also created and studied guest/host matrices of SF molecules and triplet acceptors to isolate and/or separate correlated triplet pairs in well-defined positions and orientations. Other work has involved investigating novel pentadithiophene compounds cast into thin films that undergo fast SF and possess distinct spectroscopic signatures of triplet pairs of varying degrees of coupling.

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

Sabre Kais
Purdue University

The past decades have seen tremendous progress in the study and control of diverse types of quantum materials and systems, leading to the coming of the second “quantum revolution” with many new emerging “quantum technologies” poised to significantly change our life in the decades to come. A central challenge of science is the design and synthesis of “efficient” 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. The planned research will achieve three goals: a) Develop quantum-computing algorithms for open quantum systems, b) Create and characterize molecules and materials with strong correlation and entanglement, and c) Manipulate, control, and protect coherent quantum states and excitons. The development and use of quantum computers for chemical applications has potentially revolutionary impact on the way computing is done in the future.

Parametrically Induced Quantum Engineering (PIQUE)

Archana Kamal
University of Massachusetts

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 entanglement underpins almost any quantum information application. Besides being critical importance for implementing universal quantum computation, Bell or EPR-like states are a necessary resource for communication protocols, such as teleportation and super-dense coding, and quantum-enhanced metrology.

Conventional protocols for entanglement generation 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 chiral 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 expertise available at National Institute of Standards and Technology (NIST). We will discuss our recent theoretical results on new dissipative protocols that achieve correlated scaling between fidelity and speed of stabilization, and present progress towards the first generation devices that can realize desired parametric coupling strengths.

Frontiers in Quantum Metrology and Transduction

Mark Kasevich
Stanford University

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.

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.

Developing and Running Quantum Algorithms for Chemistry and Materials

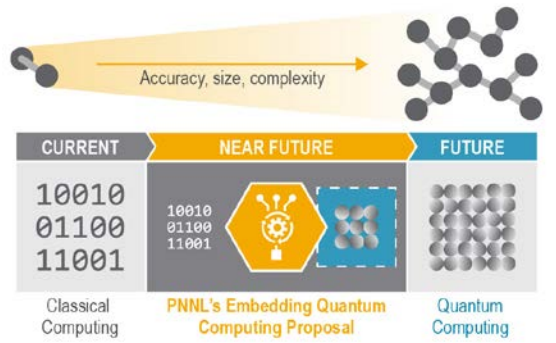
PIs: Jungsang Kim (Duke University) and Christopher Monroe (University of Maryland)
Co-PIs: Kenneth Brown, Jianfeng Lu, Thomas Barthel (Duke University),
Vladimir Manucharyan, Alexey Gorshkov (University of Maryland),
Maxim Vavilov (U. Wisconsin), and Ivar Martin (Argonne National Lab)

The recent progress made in quantum computing technology puts the prospect of practical applications of such technology within reach. One of the most promising near-term applications is the simulation of quantum properties of molecular structure, quantum chemistry, quantum magnetism, and correlated electronic materials. Traditional methods to accurately describe these inherently quantum systems on conventional, classical computers are fundamentally inefficient, forcing the studies to either be constrained to small-scale problems, or subject to approximations at the expense of accuracy in the description. Quantum computers provide the promise of accurate description of these systems that scale to larger sizes, but effective and practical methodologies have not been developed yet due to the lack of corresponding quantum computer hardware. This ambitious research project will bring together a leading team of experimentalists and theorists in the development and implementation of useful quantum algorithms for studying chemistry and materials with strong quantum correlations. On the hardware front, trapped atomic ions and superconductors are currently the two leading physical candidates to represent qubits and operate entangling quantum gates for quantum computation and simulation. Trapped atomic ions possess very long coherence times and large gate depths, while superconducting systems boast high clock speed and a natural two-dimensional topology. By exploiting the state-of-the-art experimental systems on both physical platforms with a focus on the ultimate application, practical reach of quantum simulations can be substantially broadened. The theoretical methodologies the team plans to develop will tap into both types of hardware in order to optimize for particular algorithms or applications. On the software front, various techniques to map systems of interacting electrons in molecules and solid-state lattice systems to qubit representations exists, and their effective equilibrium and dynamical properties will be explored in the context of concrete hardware platforms accessible to the team. First, conventional quantum simulation techniques such as quantum phase estimation (QPE), adiabatic ground state preparation (AGSP), and variational quantum eigensolvers (VQE) will be employed to study many-body ground states of strongly correlated systems. Hybrid quantum-classical algorithms combining AGSP and VQE with embedding techniques will then be explored to address larger systems. Finally, more advanced and widely applicable methodologies such as quantum approximate optimization algorithms (QAOA) on pure spin systems will be implemented to simulate exotic forms of magnetism, and relate such qubit optimization techniques to their parent electronic wavefunction properties. Through these activities, the project will design and test several families of algorithmic approaches to quantum simulations that will inform the future use of larger scale quantum computers. The research activities will guide the early applications of quantum computers in the current era which lacks fault-tolerant error-correction, and pave a roadmap in the quantum simulation from simple to complex molecules and electronic lattice structures that are ultimately intractable via classical means. Successful completion of this project could lead to the future development and the discovery of new chemical processes and material functions.

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

Karol Kowalski
Pacific Northwest National Laboratory (PNNL)

Many aspects of the DOE-BES scientific portfolio cannot function without support from predictive many-body models that can provide valid information relevant to various types of chemical transformations, spectroscopies, and materials properties. Novel and predictive modeling tools capable of overcoming exponential computational barriers of conventional computing are needed to describe chemical transformations that involve quasi-degenerate electronic states and corresponding potential energy surfaces that are relevant for comprehensive understanding of challenges in the areas of catalysis, actinide chemistry and nuclear-waste storage, nitrogen fixation, and storage materials. The "Embedding Quantum Computing into Many-body Frameworks for Strongly Correlated Molecular and Materials Systems" project will focus on accurate many-body methods that seamlessly integrate quantum and classical computations to describe complex electron correlation effects for strongly correlated molecular and materials systems. 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 and currently intractable challenges in the BES scientific portfolio. This multi-institutional effort involving PNNL, LBNL, ORNL, and University of Michigan, will take advantage of the team's existing strengths in adopting new computational technologies to develop advanced theoretical/computational models.



The proposed hybrid classical and quantum computing approach will enable researchers to use combined power of classical and quantum computing in studies of complex chemical processes.

Simulating strongly correlated molecules with a superconducting quantum processor

PI: Nick Mayhall
Virginia Polytechnic Institute and State University

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 a promising alternative 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 an improvement over a classical computer. The objective of this project is to accurately simulate strongly correlated molecules on a superconducting quantum processor. To meet the high challenges of this objective, new hybrid quantum/classical algorithms will be co-designed with advanced quantum gate developments and implemented on customized quantum hardware. The developed techniques will have broad applicability to other molecular systems and other quantum hardware, while the project as a whole will help define better strategies for advancing the quantum simulation of matter more generally.

Quantum States in Layered Heterostructures Controlled by Electrostatic Fields and Strain

PI Stevan Nadj-Perge, Assistant Professor; Co-PI Andrei Faraon, Professor; Co-PI Marco Bernardi, Assistant Professor; Co-Investigator Julia Greer, Professor, Department of Applied Physics and Materials Science; Co-Investigator Gil Refael, Professor, Department of Physics
California Institute of Technology, Pasadena, CA 91125

This project will investigate a novel family of materials, known as two-dimensional (2D) transition metal dichalcogenides, for the development of quantum information devices. These materials exhibit a range of fascinating electronic and optical properties and, due to 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 2D transition metal dichalcogenides with the focus on defects hosting 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 will carry out different aspects of this synergistic project with the two specific goals: (i) Identifying novel point and line defects embedded in 2D materials for quantum opto-electronic applications; (ii) Establishing their structural, electronic and coherent properties, and exploring ways of controlling their properties with strain and electrostatic gating (Fig. 1). A wide range of experimental techniques including advanced nanofabrication, scanning tunneling microscopy, electronic transport and optical spectroscopy will be employed to create and control such defects using electrostatic fields and strain and to study their quantum states and coherent dynamics. Theory and advanced numerical calculations will guide and support these research efforts. The results of this project will enable novel experimental protocols for processing and storing quantum information and for discovering dynamical topological phases in transition metal dichalcogenides.

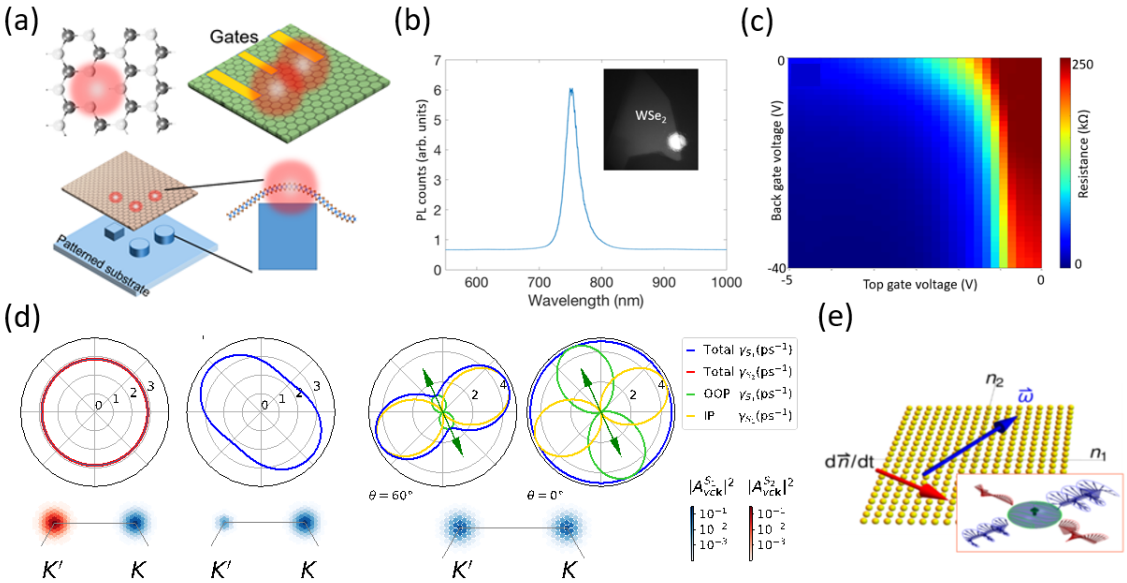


Figure 1. Project goals and team expertise. (a) Creating point defects in 2D materials and tuning their properties using electrostatic gating and strain. Line defects can be created in a similar way. Co-Investigator Greer has extensive expertise in advance nanofabrication and in understanding strain related effects. (b) Photoluminescence measurements performed in the co-PI Faraon's lab on monolayer of Tungsten Selenide (WSe_2). (c) Gate control of charge carriers and electrostatic field in WSe_2 two terminal devices in the PI Nadj-Perge's lab. (d) Light emission in monolayer WSe_2, computed with an approach recently developed by co-PI Bernardi showing the radiative rates and the corresponding exciton wavefunctions, for several excitation scenarios. (e) Proposal by co-Investigator Refael for coherent frequency converter that could be realized by coherently driving quantum states of point defects in 2D materials.

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

Topological excitations such as Majorana fermions 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). We propose an inter-disciplinary effort that will combine 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. Having developed novel one- and two-dimensional materials platforms, we will then 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. This includes detection of the non-local nature of Majorana modes, and more ambitiously, measurement-based braiding. Importantly, our approach will be compatible with large-area scalability to form two-dimensional arrays of non-Abelian qubits. Thus, if successful, the proposed research has the potential to greatly advance topologically-protected quantum information processing.

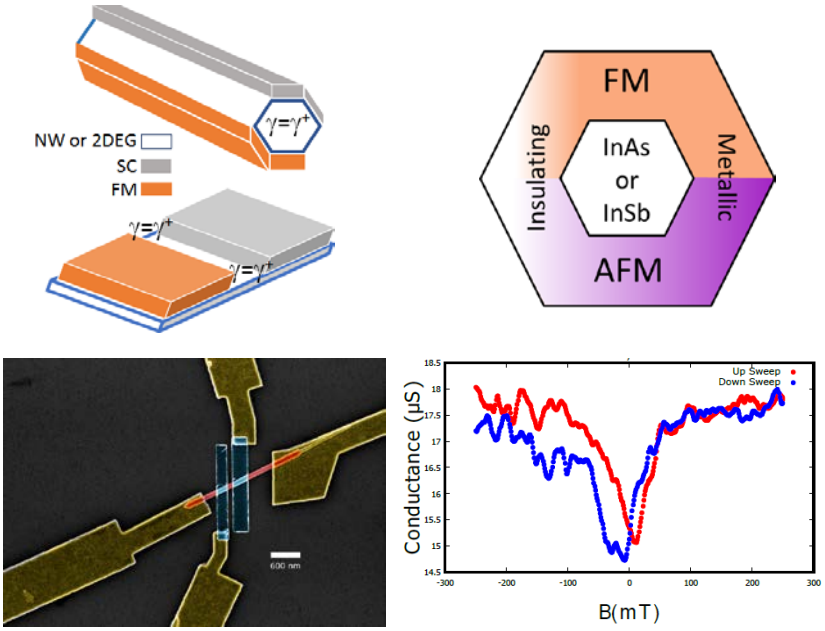


Fig. 1: (top-left) Schematic of devices integrating a ferromagnet (FM), semiconductor and superconductor (SC) for realizing Majorana zero modes. We will explore both 1D platforms based on semiconductor nanowires (NW) (top) and platforms based on two-dimensional electron gases (2DEG) (bottom). **(top-right)** Conceptual representation of materials phase space to be considered for magnetic materials coupled to InAs and InSb nanowires. **(bottom)** Example of a device consisting of an InSb nanowire with FM and normal contacts, and measured hysteretic resistance from a similar device.

Planar Systems for Quantum Information

PI: Jie Shan (Cornell University)
Co-PIs: Kin Fai Mak (Cornell University)
Cory R. Dean, James Hone (Columbia University)
Tony F. Heinz (SLAC National Accelerator Laboratory/Stanford University)
Allan H. MacDonald (University of Texas at Austin)

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 dichalcogenide (TMD) family of 2D semiconductors such as MoS_2, $MoSe_2$, WS_2, and WSe_2 is direct access to the valley degree of freedom by 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 addition, the spin-valley coupling provides a method of correlating 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 degree of freedom in 2D TMDs as a candidate for the construction of quantum bits. In particular, we will develop approaches such as stimulated Raman adiabatic passage and dynamic exchange magnetic fields for full control of valley pseudospin. The research team seeks to determine the factors controlling decoherence and to develop approaches for enhancing coherence times such as 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 with close coupling to predictions and modeling based on ab-initio and analytical calculations.

The research aims to 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.

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

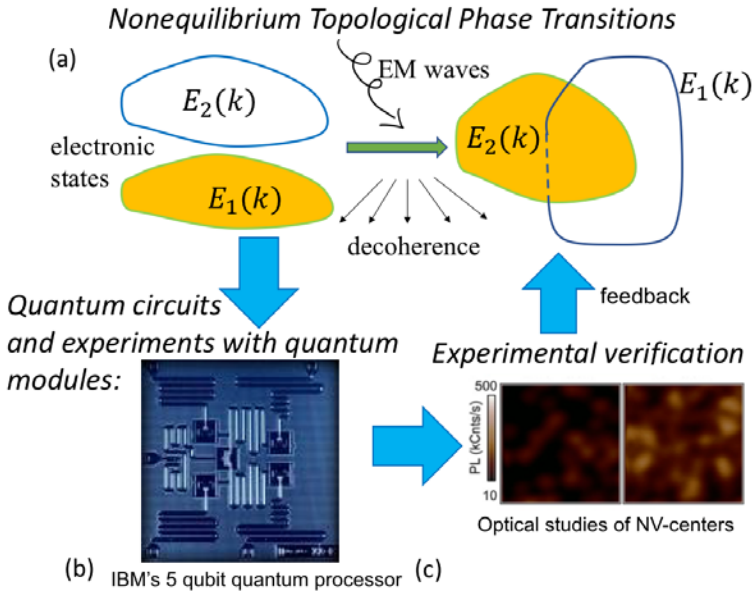
Irfan Siddiqi
Lawrence Berkeley National Laboratory (LBNL)

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. Our proposed research addresses the key basic materials challenges that need to be overcome to produce, visualize, and validate the performance of functionalized quantum materials capable of supporting quantum coherent phenomena for near term applications.

Topological phases of quantum matter and decoherence

Nikolai Sinitsyn, Wojciech Zurek, Vivien Zapf, Dmitry Yarotski, Shizeng Lin, Lukasz Cincio, Patrick Coles, *Los Alamos National Laboratory (LANL);* ***Vladimir Chernyak,*** *Wayne State University (WSU);* ***Ania Jayich,*** *University of California at Santa-Barbara (UCSB)*

Decoherence in quantum systems, due to contact with the environment, is ordinarily viewed as a barrier to revealing purely quantum effects. However, recent theoretical advances show that decoherence that competes with strong driven periodic potentials in fact creates new topological phases that can be used to design novel materials functionalities, such as fast transitions between insulating and conducting states, topologically protected quantum states, and spontaneous symmetry breaking in time domain. Our understanding of such new phases is very poor because of the difficulty to model nonequilibrium quantum matter.



The **objective of this project** is to explore, detect, and characterize decoherence-induced topological phases in real quantum systems under strong time-periodic driving conditions *using the insight from emerging quantum computers*. Our theory will lead to classification of emerging topologically nontrivial states and provide their physical interpretation. It will guide our experimental search for nontrivial topological states.

Figure illustrates the strategy for our research. Theoretical studies are done to identify potentially interesting and sufficiently simple models of topological phase transitions in electronic and spin systems. The focus is on effects that never emerge in equilibrium quantum mechanics, for example, appearance of braid and knot patterns in electronic Bloch bands (stage (a) in the figure). Next, we program our models as quantum circuits that are implemented with a small-scale gate-based quantum computer (stage (b)). Application of the new generation of quantum computers to assist in the theoretical modeling, including of laboratory experiments, is a special feature of our project. Decoherence of qubit quantum states is induced by nature, so the already available and emerging quantum computers advance our theoretical understanding of realistic decoherence effects. The insight from quantum modeling is then used to design experiments at LANL and UCSB to search for topological phase transitions that we predict (stage (c)).

By the end of the project, we will achieve the ultimate goal: to demonstrate the feasibility of a completely novel research direction: quantum computer assisted studies of quantum topological phase transitions in materials at nonequilibrium conditions.

Hybrid quantum systems: spins, photons and superconducting qubits

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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) and Lithium Tantalate (LT). In addition to having famously strong piezoelectric and Pockels responses and superb optical properties, LN & LT crystals are a particularly promising host for rare-earth-ion (REI) spin centers; spin centers in LN & LT 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.

Through this program, we leverage our team's world-class expertise in circuit QED (Yale) and spin systems (Montana State) to tackle the non-trivial task of harnessing and controlling disparate superconducting, spin, and photonic degrees of freedom on the same chip. Because these systems have ostensibly orthogonal environmental requirements, creative new strategies are needed to marry and control these systems. For example, magnetic fields—typically used to control spin systems—can be detrimental to the superconducting state. Moreover, piezoelectricity—which couples microwave photons to acoustic phonons—can cause the microwaves to radiate as acoustic energy, reducing the coherence time of a superconducting qubit. In this program, we will apply new phonon, microwave and optical spectroscopic tools—unique to the Yale/MSU teams—to pinpoint the material origins of both transmon- and spin-qubit decoherence over a range of energy scales (micro eV-eV). Using different methods to perturb the material matrix and tune spin ensembles, we devise strategies to preserved coherence of these disparate quantum systems when brought together at millikelvin temperatures.

This hybrid quantum system, if realized, will enable ground-breaking advances in quantum information processing: it will empower superconducting circuit QED systems with long-lived quantum memory for achieving advanced quantum computing capabilities, and for the first time will allow high-fidelity optical readout of circuit QED systems through spin qubits. This scalable platform therefore enables critical functionalities of quantum transceivers and will likely play an important role in future distributed quantum computation and secure quantum networks.

QPress: Quantum Press for Next-Generation Quantum Information Platforms

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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.