BES Quantum Information Science NSRC Awards FY 2018

PI Name	Title	Institution	City, State
Black, Charles	Building the Quantum Material Press: An Enabling Nanoscience Facility for Quantum Information Science	Brookhaven National Laboratory (BNL)	Upton, NY
Rouleau, Christopher	Thin film platform for rapid prototyping novel materials with entangled states for quantum information science	Oak Ridge National Laboratory (ORNL)	Oak Ridge, TN
Ma, Xuedan	Photon Qubit Entanglement and Transduction	Argonne National Laboratory (ANL)	Lemont, IL
Schmid, Andreas	Quantum Instrument for Novel Techniques Applying Entanglement and Spin-polarization for Studies with Low Energy Coherent Electrons (QUINTESSENCE)	Lawrence Berkeley National Laboratory (LBNL)	Berkeley, CA
Cabrini, Stefano	Nanofabrication Toolset for Correlating Coherence and Structure in Quantum Information Systems	Lawrence Berkeley National Laboratory (LBNL)	Berkeley, CA
Lilly, Michael	Quantum Sensed Nuclear Magnetic Resonance Discovery Platform	Sandia National Laboratories, New Mexico (SNL-NM)	Albuquerque, NM
Htoon, Han	Deterministic Placement and Integration of Quantum Defects	Los Alamos National Laboratory (LANL), Los Alamos, NM	Los Alamos, NM

Nanoscale Science Research Centers

Quantum Information Science Awards Abstracts

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Thin Film Platform for Rapid Prototyping of Novel Materials with Entangled States for QIS
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Quantum Instrument for Novel Techniques Applying Entanglement and Spin-polarization for Studies with Low Energy Coherent Electrons (QUINTESSENCE)
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Building the Quantum Material Press:
An Enabling Nanoscience Facility for Quantum Information Science

Kevin G. Yager, Greg Doerk, Aaron Stein, Jerzy T. Sadowski, and Charles T. Black
Center for Functional Nanomaterials, Brookhaven National Laboratory (BNL)

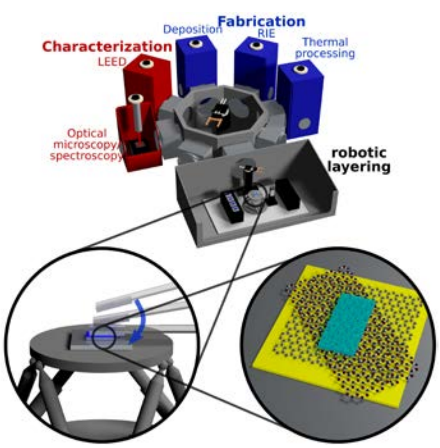
The Quantum Material Press (QPress) will be a first-of-its-kind facility for automated synthesis of layered heterostructure materials by assembly of atomically-thin, two-dimensional (2D) components. With integrated capabilities for *in-situ* characterization and fabrication, the QPress will accelerate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

We are strongly collaborating with colleagues at Harvard and MIT, who in parallel are investigating the underlying QPress basic science, including: synthesis of new van der Waals materials, machine learning for heterostructure discovery, *in-situ* characterization methods, and applying the QPress to topological superconductivity and quantum simulation.

The primary goal of this project is to develop a unique user facility for automated synthesis of stacked heterostructures from 2D components. The QPress will be supported at the Center for Functional Nanomaterials at BNL and be a valuable resource for the QIS research community.

The QPress will:

- Controllably exfoliate 2D layers from parent van der Waals crystals by automated, robotic motion profiles. Machine learning will direct the QPress toward optimized motion profiles providing highest yields for different van der Waals materials.
- Automatically catalog exfoliated 2D flakes, capturing their physical dimensions and properties and indexing them in a searchable materials library.
- Combine the materials database with predictive materials modeling to study the influence of synthesis and processing conditions on ultimate material quantum properties.
- Systematize automated assembly of layered heterostructures by sequential stacking of 2D flakes, optimizing the process for speed and accuracy. Deliver improved methods for handling 2D materials, such as use of thermal/electric field gradients, and photo-initiated flake transfer.
- Integrate automated modules for *in-situ* property characterization, and fabrication/processing to prepare heterostructures for detailed studies.



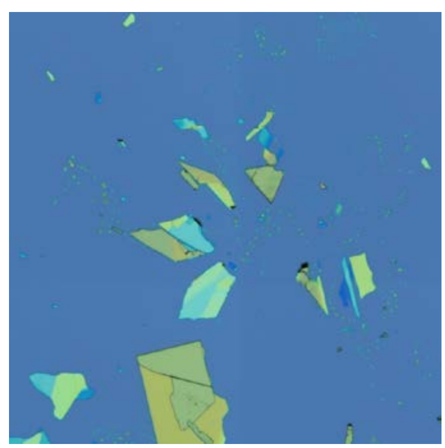
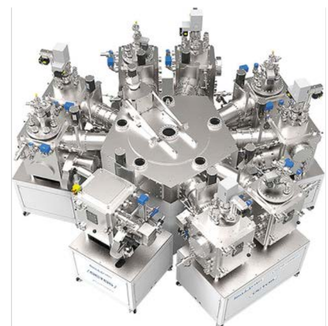


Figure. (Left) The QPress will be a cluster tool, organizing modules for characterization (red) and fabrication (blue) around a robotic exfoliation/stacking module for creating QIS heterostructure materials. (Right) The QPress will acquire and analyze optical images of 2D flakes (e.g., graphene), identifying those best-suited for heterostructures and indexing them in a searchable materials library.

Nanofabrication Toolset for Correlating Coherence to Structure in Quantum Information Systems

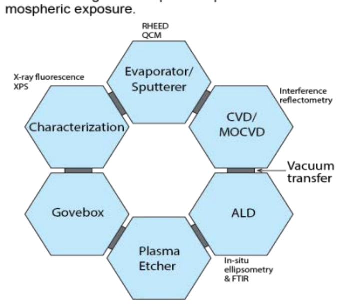
Stefano Cabrini, D.Frank Ogletree, Adam Schwartzberg, Shaul Aloni,
Alexander Weber Bargioni, David Prendergast, Andrew Minor
Molecular Foundry, National Center for Electron Microscopy
Lawrence Berkeley National Laboratory

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



Above: Example cluster tool with multiple deposition and characterization platforms coupled through a vacuum transfer system

Below: Schematic of proposed cluster system containing multiple material growth/deposition systems with advanced in-situ characterization and a glovebox for loading and sample manipulation without atmospheric exposure.



1. A robotic fabrication cluster system with materials deposition, including atomic layer and physical vapor depositions, ion etching, and analytical characterization instrumentation, all automated by and contained within a vacuum sample handling robot (see figure).

2. A high resolution electron beam writing system will allow quantum device patterning with complete flexibility in feature shape, density and size, enabling nanoscale feature control.

3. A low temperature transport measurement system will allow for the investigation of novel materials for superconductors and dielectrics and “close the loop” between design and fabrication, proxy measurements such as interface characterization, and actual performance of quantum computation and sensing elements.

Combined with the existing fabrication and characterization capabilities at Molecular Foundry, the new instrumentation suite will enable the elucidation of chemical composition, structure, location, and size of all microscopic noise sources in a superconducting quantum system, understanding the fabrication steps that may affect the energy relaxation time (T1) and the dephasing time (T2) as well as different resonance frequencies. This understanding and the defect control will enable the community to create larger arrays of coherent qbits, improved their integration and fabrication yield and moreover will allow to develop 3D integration architectures of nanoscale superconducting qubits, enabling the integration of a much larger number of qubits on a single chip.

Deterministic Placement and Integration of Quantum Defects

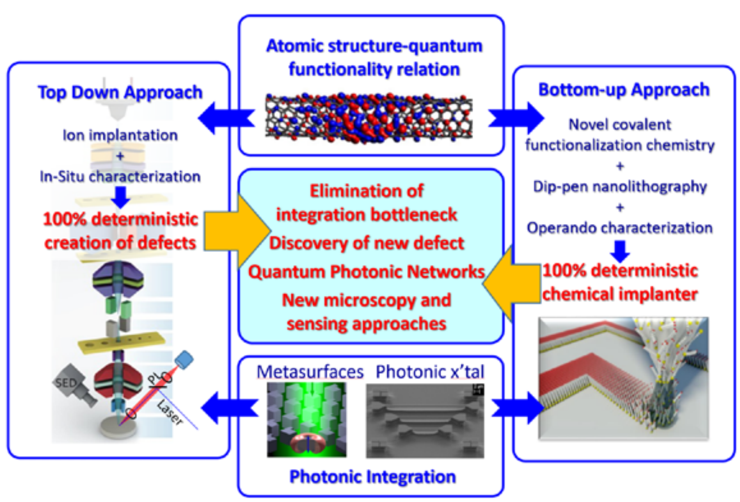
Han Htoon[1], Edward Bielejec[2], Jennifer A. Hollingsworth[1], Yongqiang Wang[1],
Sergei Tretiak[1], Stephen K. Doorn[1], Igal Brener[2]
Center for Integrated Nanotechnologies
Los Alamos National Laboratory
Sandia National Laboratories

Solitary defects with quantum mechanical states mimicking those of trapped ions have been delivering many breakthroughs in quantum information science and technologies. Recent works report discoveries of multiple new defects in a wide range of materials, including single-walled carbon nanotubes and GaN defects capable of room temperature quantum light emission in telecommunication wavelength regime; and defects of two dimensional van der Waals materials, which bring opportunities to exploit robotic synthesis of layered materials for the fabrication of quantum photonic networks. Together, these discoveries clearly demonstrate that the phase space for defect-derived quantum functionality is truly vast.

However, to date, quantum defect research has primarily relied on serendipitously discovered, naturally formed defects that not only distribute randomly in host materials but also exhibit diverse optical and quantum coherence properties. As a result, integration of defects into electronic/photonic nanodevices – an essential step for realizing most QIS technologies – can only be achieved by very complex, costly, and time consuming approaches that place a bottleneck on the progress of QIS research. *DOE report "Opportunities for Basic Research for Next-Generation Quantum System" directly calls for deterministic creation of defects capable of surviving room temperature and then coupling of these defects to photonic/plasmonic cavities in PRO 1.4, "Precise positioning of atomic defects;" PRO 2.1, "Overcoming the tyranny of low temperature" and PRO 2.4, "Revealing the role of disorder through material control".*

In direct response to these PROs, we propose to establish new CINT-based infrastructures capable of addressing the needs for: (1) Deterministic creation of atomic defects capable of mimicking trapped ions in a wide variety of host materials; (2) Understanding the correlation between the atomic structure of defects and their quantum functionalities; and (3) Integration of these defects into photonic/electronic devices. We propose to achieve Aim (1) via two complementary strategies based upon top-down, ion implantation technologies and bottom-up, scanning probe based, chemical quantum defect implantation. Novel in-situ/operando single defect optical characterization capabilities will be integrated with these ion and chemical defect implantation capabilities to achieve an unprecedented, one functional defect per one site, 100% deterministic defect creation capability. The fundamental understanding attained in Aim (2) will further enhance the capabilities of Aim (1) by revealing a path toward tailoring quantum behaviors of the defects. Finally in Aim (3), we will implant functional quantum defects into the prefabricated electronic/photonic devices with nanometer scale precision by using both top-down and bottom up strategies. Through these experiments we will establish our deterministic defect creation strategies as the perfect tool set for eliminating the integration bottle neck *impeding defect-driven QIS research.*

This set of unique capabilities will enable our Nanoscale Science Research Center user community to perform novel QIS experiments that were not possible before. They will also allow users to explore the vast phase space in search of new defects with novel quantum functionalities. This, in turn, could inspire the development of new microscopy and sensing approaches identified in *PRO 4: Implement new quantum methods*. Ultimately, through these user services, we aim to address our nation's needs to maintain its lead in QIS research that has the capacity to fundamentally change our daily life.



Quantum Sensed Nuclear Magnetic Resonance Discovery Platform

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

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

Photon Qubit Entanglement and Transduction

Xuedan Ma,[1*] Xufeng Zhang,[1*] Stephen Gray,[1] David Czaplewski,[1] Axel Hoffman,[2] Daniel Rosenmann[1]
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In recent years, there has been an increasing interest in developing distributed quantum networks that combine the advantages of different quantum systems to complete complicated tasks in quantum information processing. Distributed quantum networks require the development of individual quantum systems both in the microwave and optical domains, as well as their interconnection. Despite the rapid development in microwave qubits based on superconducting technologies, deterministic optical single-photon sources are still underdeveloped. High-efficiency quantum interconnections between these systems are also missing because of the incompatibility of the superconducting technique with optical photons and their huge frequency difference. Most importantly, comprehensive facilities that simultaneously host a variety of different quantum systems and enable their transduction are still lacking as of today.

We are developing a centralized user facility, the *Quantum Entanglement and Transduction (QET) User Facility*, which addresses the major tool requirements for advancing hybrid quantum network technologies (Fig. 1). The QET User Facility will be equipped with design, fabrication, and characterization capabilities that cover microwave, THz, and optical domains. It will offer quantum optics and transduction characterization tools that enable a broad range of user science including the development and measurement of optical and spin qubits, as well as quantum transduction systems. Computational modeling environments will be part of the facility.

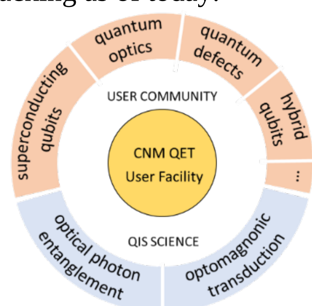

Figure 1. Outline of the project objectives.

Leveraging the QET user facility, we will develop key technologies that address the two grand challenges facing the distributed quantum network community (Fig. 2). In the first scientific thrust, we will develop chip-scale, single- and entangled-photon sources based on semiconductor nanomaterials. To optimize the emission properties of the nanomaterials, we will integrate them with photonic structures to reduce undesirable charge carrier recombination processes. Quantum information, including the polarization states of optical photons and the local spin states of charge carriers, will be encoded into the photons to generate optical qubits that interact with the quantum transducers.

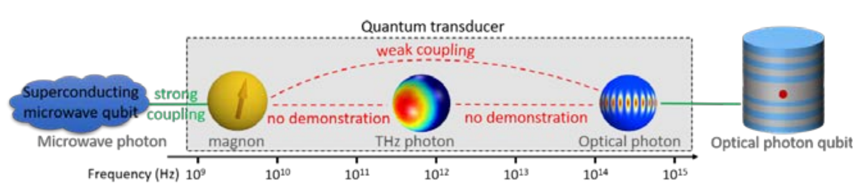

Figure 2. Schematics of a hybrid quantum network.

In the second scientific thrust, we will develop integrated opto-magnonic quantum transduction platforms. Opto-magnonic systems use magnons to convert quantum information between the microwave and the optical domains. Although magnons can strongly couple with microwave quantum systems, the bottleneck of magnon-assisted microwave-optical transduction lies in the weak interaction between magnons and optical photons. We will address this challenge by lifting the limitation in material fabrication as well as seeking THz-intermediated transduction stages. We will prototype opto-magnonic transduction systems and study their interactions with microwave and optical qubits in the quantum regime.

Thin Film Platform for Rapid Prototyping of Novel Materials with Entangled States for Quantum Information Science (QIS)

Christopher Rouleau, Eres Gyula, Rama Vasudevan, David Geohegan
Ben Lawrie, Alexander Puretsky, Kai Xiaon An-Ping Li
Center for Nanophase Materials Sciences
Oak Ridge National Laboratory (ORNL)

The Basic Energy Sciences Roundtable Report titled, *"Opportunities for Basic Research for Next-Generation Quantum Systems,"* identifies the need to learn how to "create the necessary materials, devices, and chemical systems with the exquisite precision needed to achieve long coherence times and entanglement." Rapid feedback between synthesis and the identification of quantum states as well as characterization of their lifetime and entanglement is critical to achieving this goal, and to address this challenge the projects aims to:

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

2. Understand the dynamics of photonic states with required sub-picosecond temporal resolution by combining existing Center for Nanophase Materials Sciences (CNMS) femtosecond pump-probe laser spectroscopy capabilities with a novel low temperature scanning electron microscopy platform that couples ultra-fast electron microscopy and cathodoluminescence.

3. Enable understanding of entangled spin states for topological quantum computing by combining existing CNMS spin polarized probe expertise with a novel scanning tunneling microscope platform that is capable of injecting electrons with controllable angular momentum and probing spatially resolved spin entanglements with atomic resolution at ultra-low temperature and with variable vector magnetic fields.

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

Andreas Schmid, Alexander Stibor, D. Frank Ogletree, Alex Weber-Bargioni, Andy Minor, Colin Ophus, Jim Ciston, Alessandra Lanzara*

*Molecular Foundry and *Materials Sciences Division, Lawrence Berkeley National Lab, Berkeley, CA*

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

The cryo-SPLEEM, the centerpiece of QUINTESSENCE, will combine a Foundry-developed helium-temperature sample manipulator with a customized commercial LEEM instrument. Implementation of the “spin-gun” and spin-manipulator for the SPLEEM will draw on over a decade of experience running the highly-productive Foundry/NCEM user-program [1,2] built around it’s first-generation SPLEEM. The new instrument will incorporate in-situ molecular beam epitaxy capabilities, developed in the existing program, for the fabrication and optimization of quantum structures. The new SPLEEM will be able to perform 3D vector-magnetometry with nanometer spatial resolution; mapping of occupied electronic states below the Fermi energy (by angle resolved photoemission) as well as unoccupied structure above the vacuum level (by angle resolved electron reflection); and damage-free “mirror imaging” of surface potentials and ordered domains.

The second QUINTESSENCE component is a highly-coherent electron bi-prism interferometer capable of producing electron interference fringes on an imaging detector. When the superposed electron waves pass near a sample surface, electron coherence is degraded [3]. The imaging detector records the attenuation of the interference fringes as a function of distance from the conducting sample surface, creating a new tool to investigate the scaling of quantum decoherence processes. This new tool will allow users to study Coulomb-induced decoherence in various materials and structures as a function of temperature, material composition and the presence of surface adsorbates, research that will support efforts to create robust quantum states.

Finally, we are exploring field emission from a superconducting Nb field emission tip as a source of highly coherent electrons. Oshima’s group investigated Nb field emission and found a sharp peak in the electron energy distribution at the Fermi edge that scaled with the superconducting order parameter [4]. Theoretical predictions and solid-state experiments suggest that Cooper pairs can be emitted as entangled electrons with anti-parallel spin. We will attempt to confirm this experimentally, and explore applications of an entangled electron source in SPLEEM and interferometry experiments.

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