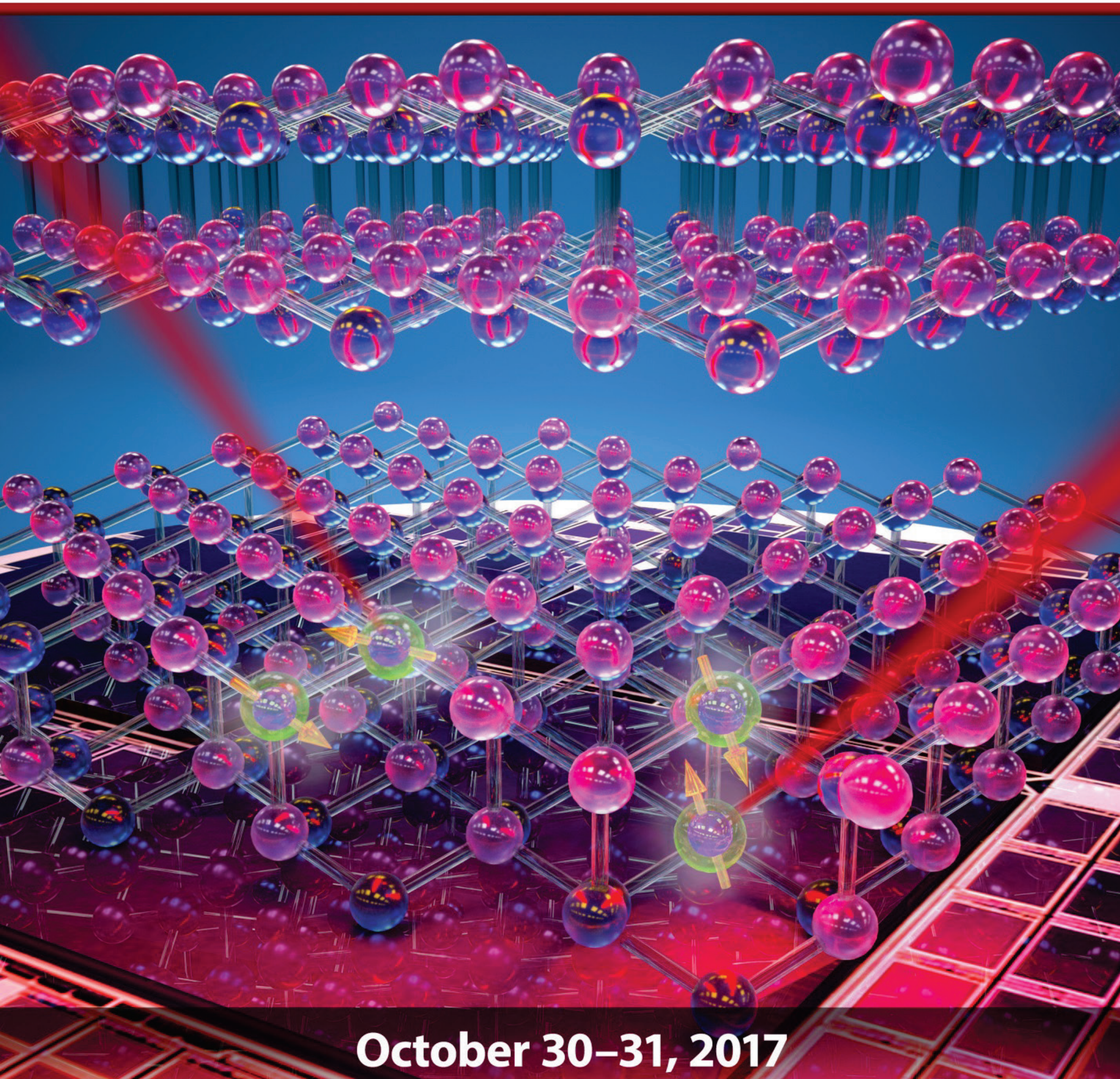
Basic Energy Sciences Roundtable

Opportunities for Basic Research for Next-Generation Quantum Systems



October 30–31, 2017

The artwork on the cover is a conceptual image of a layered two-dimensional solid state structure, to be created by computationally directed synthesis, where the quantum properties of individually-placed atomic states and their spins may be manipulated and entangled with photons, electrons, phonons, electric or magnetic fields.

Image courtesy of David Awschalom and Peter Allen, University of Chicago and Argonne National Laboratory

Report of the Basic Energy Sciences Roundtable on

Opportunities for Basic Research for Next-Generation Quantum Systems

October 30–31, 2017
Gaithersburg, Maryland

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Contents

Abbreviations, Acronyms, and Initialisms

1D	one-dimensional
2D	two-dimensional
3D	three-dimensional
BES	Office of Basic Energy Sciences
CVD	chemical vapor deposition
DOE	Department of Energy
EELS	electron energy loss spectroscopy
IFM	interaction-free measurement
MBE	molecular beam epitaxy
MZM	Majorana zero-mode
NV	nitrogen vacancy
OPTS	odd-parity topological superconductor
PRO	Priority Research Opportunity
QIP	quantum information processing
QIS	quantum information science
QS	quantum systems
SQL	standard quantum limit
STEM	scanning transmission electron microscopy
STIRAP	simulated Raman adiabatic passage
ZBP	zero bias peaks

Executive Summary

For decades, scientists have predicted that devices based on "quantum phenomena" will be able to store and manipulate information to provide radical new approaches for computing, communication, and sensing. However, only recently have quantum phenomena been incorporated into technologies for next-generation computers, sensors, and detectors that demonstrate performance characteristics rivaling those of their conventional counterparts. These devices clearly demonstrate the enormous potential for future quantum-based technologies. The novel quantum device capabilities currently envisioned include enhanced resolution in imaging, sensors, and detectors; advanced cryptography for more secure communication; and significantly larger computational capabilities at speeds far greater than those possible in classical computing. However, realizing these advances requires a detailed understanding of how quantum systems (including quantum materials or assemblies of trapped ions and electrons) behave, accurate knowledge of how to integrate the components into complex systems, and precise control of the structures. In this context, creating and controlling quantum states within molecules and materials offer exciting scientific opportunities for fundamental research, as well as for enabling next-generation quantum-based technologies. Numerous questions remain, ranging from how quantum interactions may enable innovation through the creation of novel quantum systems, to how these new quantum technologies can advance our understanding of matter and chemistry at the most fundamental levels.

To address these questions and identify priority research opportunities (PROs), the US Department of Energy (DOE) Office of Basic Energy Sciences (BES) convened a roundtable of experts in quantum materials and quantum systems encompassing the fields of physics, chemistry, materials synthesis science, device engineering, detector technology, and atomic-scale characterization techniques. This group of experimentalists and theorists met on October 30–31, 2017, to explore scientific research opportunities in this rapidly moving field, in which BES support can play a key role in advancing and utilizing quantum information science (QIS). The goals of this roundtable were to define the unique roles for BES in this active research field and to provide input on future research directions, forming the basis for a coordinated, long-term research effort that will enable major advances in quantum-based science and technology. BES is uniquely positioned to advance this field because of its long history of fundamental research support for both materials and chemical sciences, along with its construction and operation of world-class scientific user facilities. Fundamental research in this area is strongly coupled to DOE efforts in scientific computing, high-energy physics, and accelerator/detector research and related to activities in "Beyond Moore's Law" computing, next-generation semiconductor materials, and exascale computing.

The conclusions of the roundtable, highlighting the basic research challenges for both science and instrumentation, were summarized with four PROs:

Advance artificial quantum-coherent systems with unprecedented functionality for QIS

The synthesis of materials with pre-designed characteristics that are optimally suited for quantum information applications is a key requirement for the future. This PRO highlights the need for research that will lead to the development of new capabilities for real-time feedback and control of synthesis that are coupled with predictions and measurements of targeted quantum characteristics. This feedback would consist of both characterization and computation-based machine learning to optimize a material for the prescribed function. The PRO discusses opportunities in robotic synthesis of layered materials, quantum properties of hybrid (organic and inorganic) systems, the creation of topological states of matter (such as odd-parity topological superconductivity), and precise control to position atomic defects.

Enhance creation and control of coherence in quantum systems

Quantum-coherent systems have been discovered that exhibit remarkable properties and ever increasing coherence times. However, understanding of how these systems interact (for example, the complexity of entanglement) is currently limited to a small number of systems. Advances in this field require an understanding of the scaling of coherence lengths and times with system size and complexity, and the identification of new signatures of quantum states in artificial quantum-coherent systems, as described in the previous PRO. Additional research is needed to understand the mechanisms that lead to decoherence in open quantum systems, which could facilitate control of coherence beyond adiabatic limits and result in discovery and exploitation of novel entangled excitations.

Discover novel approaches for quantum-to-quantum transduction

The coherent transduction of information from one modality to another, at the single-particle or quantum level, is at the core of quantum measurement and information processing. This PRO identifies primary research needs in generating and stabilizing nonclassical states of light and matter, transferring complete wavefunctions between disparate physical systems, quantum state replication and entanglement swapping, and transferring single quanta with high fidelity. Specific challenges are identified for infrared and microwave single photon detection, light-to-electron transduction, maximization of quantum coherence, and development of theoretical approaches for understanding quantum state transfer in realistic settings.

Implement new quantum methods for advanced sensing and process control

In contrast to the first three PROs that address materials and chemical sciences issues that need to be addressed to develop quantum systems, the fourth PRO focuses on the use of quantum-based systems to enable new research capabilities. In particular, this opportunity includes the deployment of extreme sensing, detection, and control capabilities for precise measurements of time, space, and fields, as well as the development and application of these capabilities to probe material properties and chemical processes. Advances are needed in designing sensors and detectors based on correlated materials; techniques to use squeezed states for metrology; quantum systems for high-resolution and high-sensitivity imaging; quantum sensors for real-time monitoring and control of chemical reactions; and establishment of connections between entanglement and thermodynamics.

The roundtable participants concluded that successfully addressing these challenges will enable the creation of next-generation coherent quantum systems with unprecedented performance for applications in QIS. The participants also noted the importance of creating metrics and design rules for quantum-coherent materials. If successful, the proposed research will result in the ability to create novel material platforms through the rapid survey of robotically synthesized structures and the subsequent convergence toward materials with desired quantum properties. Furthermore, these studies will provide new insight into the physical sciences based on ultrasensitive quantum sensors. For both QIS and many quantum-limited sensors, it will be important to reduce the effects of decoherence to create robust quantum states.

Once a next generation of quantum-coherent materials is established, large-scale quantum manipulation, including new realizations of quantized transport (charge/spin pumps) may be realized. These advances may include spatially separating the generation and detection of entangled states (e.g., teleportation of entangled states); applications based on topological behavior (Majorana fermions, non-abelian quantum operations); and the fabrication of distributed networks incorporating high-fidelity quantum sensing, communication, and computing.

In summary, establishment of the scientific foundations for quantum systems may lead to applications such as novel electronics, efficient light harvesting and photovoltaics, and sensors with capabilities orders of magnitude beyond current standards. The ability to probe and model phenomena at the ultimate limits of detection will enable scientists to advance our understanding of fundamental physics such as emergent phenomena in strongly interacting quantum many-body systems, quantum gravity, fundamental symmetries, cosmology, and nuclear science.

1. Introduction

From the transistor to the molecular switch, quantum mechanics is at the heart of nearly all materials properties and chemical processes. Still, the subtleties of quantum behavior are often hidden from view. As a result, only a small number of scientific techniques and technological applications take advantage of the unique phenomena of quantum superposition and entanglement. Harnessing these counterintuitive properties of matter promises to yield revolutionary new approaches to computing, sensing, communication, and metrology, as well as far-reaching advances in our understanding of the world around us.

The term “quantum systems” (QS) is used in this report to describe assemblies of materials or arrangements of trapped ions or electrons in which the uniquely quantum interactions between the components are tuned to produce a specific behavior. These systems can be used to process or exchange quantum information, or to measure their environment with exquisite sensitivity. The most prominent element of such systems is quantum bits—or qubits—which are the basic units of quantum information. Qubits are the building blocks of quantum computers, which rely on both superposition and entanglement to encode and process information beyond the limitations of the 0s and 1s that are allowed in a traditional binary computer. The advent of quantum computing promises revolutionary advances in scientific calculations of quantum materials and chemical systems, advances in encryption for the secure transfer of information, and enhanced resolution in imaging and detection. The development of QS will also contribute to areas outside of computing. Control over quantum-coherent states in artificial systems may lead to enhanced transduction for novel electronics, efficient light harvesting and photovoltaics, new techniques for cosmology and nuclear science, and sensing capabilities that are orders of magnitude beyond current standards. These new capabilities will enable scientists to advance fundamental scientific goals, such as understanding emergent phenomena in strongly interacting quantum many-body systems, simulating complex chemical and biochemical reactions, probing quantum gravity, detecting dark matter and dark energy in cosmology, and understanding the fundamental symmetries of our universe.

However, implementing quantum information science (QIS) remains a significant challenge for the scientific community, on both the conceptual and practical levels. Conceptually, we need to learn how to allow QS to interact and ultimately transfer information to their classical environments without interfering with their quantum coherence—a delicate property that is needed to maintain entanglement and superposition. For sensing and detection, we need to learn how to tune QS to maximize their response to the relevant external parameters. On a practical level, we 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. This challenge requires a new understanding of what types of defects are allowed in these systems, and how these defects evolve during the synthesis and fabrication of QS.

To address these questions and identify priority research opportunities (PROs), the Department of Energy (DOE) Office of Basic Energy Sciences (BES) convened a roundtable of experts in quantum materials and QS encompassing physics, chemistry, materials synthesis science, device engineering, detector technology, and atomic-scale characterization techniques. This group of experimentalists and theorists convened on October 30–31, 2017, to explore the specific opportunities in this rapidly moving field in which BES-funded research can play a key role in advancing or utilizing QIS. The goal of this roundtable was to define the unique BES roles in this active research field and to provide input on future directions, forming the basis for a coordinated, long-term research effort that will enable advances in quantum-based science and technology. BES expertise brings unique technical diversity to this area through the materials and chemical sciences and world-class user facilities. The participants’ discussions built upon the report of a previous Basic Research Needs Workshop on Quantum Materials.[1] But they went beyond the needs of quantum materials and also focused on systems, mesoscale assemblies, and materials and chemistry for future devices. In particular, the participants were asked to address the following topics:

Opportunities to advance the scientific understanding that will enable QIS

- Use or control topological phenomena, quantum entanglement, and coherence
- Explore scientific phenomena that go beyond stand-alone quantum materials to understand and control mesoscale structures and properties
- Create theoretical and computational strategies, drawing upon perspectives from chemical and materials science, to design and integrate novel materials for QS

Opportunities to advance instrumentation for the study of QIS, and instrumentation based on QIS approaches

- Develop innovative instrumentation for the synthesis, fabrication, and characterization of quantum structures and phenomena
- Incorporate quantum phenomena into new characterization probes for materials and chemistry research, including quantum-based detectors for neutron, photon, and electron-based instruments

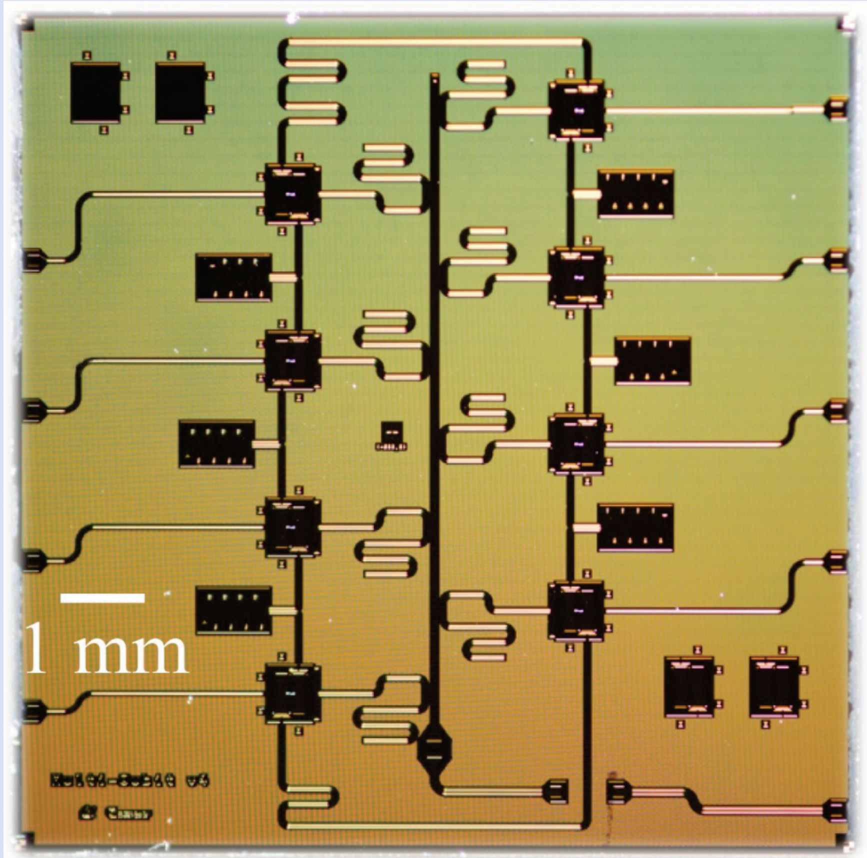
This report summarizes the basic research challenges for both science and instrumentation. The roundtable participants identified four PROs, each described in a detailed chapter of this report:

1. Advance artificial quantum-coherent systems with unprecedented functionality for QIS
2. Enhance creation and control of coherence in quantum systems
3. Discover novel approaches for quantum-to-quantum transduction
4. Implement new quantum methods for advanced sensing and process control

Successfully addressing these challenges will enable the creation of coherent QS with unprecedented performance for applications in QIS. Doing so requires creating metrics and design rules for quantum-coherent materials and novel material platforms, possibly discovered through the rapid survey of robotically synthesized structures, and it will lead to new insight into the physical sciences based on ultrasensitive custom sensors.

When a next generation of quantum-coherent materials is established, large-scale quantum manipulation—including new realizations of quantized transport (charge/spin pumps)—may be realized. This may include spatially separating the generation and detection of entangled states (e.g., teleportation of entangled states); applications based on topological behavior (Majorana fermions, non-abelian quantum operations); and the fabrication of distributed networks incorporating high-fidelity quantum sensing, communication, and computing. The creation of these systems may lead to novel electronics, efficient light harvesting and photovoltaics, advances in cosmology and nuclear science, and an ability to achieve sensing capabilities unimaginable by current methods. Such sensing capabilities will enable scientists to probe fundamental physics, such as understanding emergent phenomena in strongly interacting quantum many-body systems, quantum gravity, and fundamental physical symmetries.

Sidebar: Quantum Computers as an Example of Quantum Systems



Optical micrograph of an eight-qubit superconducting processor with a ring-type circuit topology. | Image courtesy of Quantum Nanoelectronics Laboratory, University of California–Berkeley

Quantum computers are rapidly transitioning from an intellectual curiosity to a technological reality. These machines (in which information is stored and manipulated as a superposition of different values) can already calculate the properties of simple molecules, and they will soon be capable of performing calculations that are currently unimaginable—even with the most powerful supercomputers. Such an unprecedented advance in computing would enable simulation of the exact quantum mechanical behavior of complex molecules, leading to new chemicals and medicines by untangling the complexity of molecular and chemical interactions. Quantum computing could also enable unprecedented solutions for logistics and supply chains, risk modeling, and machine learning. Superconductors are an attractive platform for quantum information processing (QIP), as they not only conduct electricity without loss but also allow electrons to be entangled "in pairs." However, a functional device needs many additional elements, including tunnel junctions, dielectric sections, and wiring. These additional materials, surfaces, and interfaces may be covered with unintentional amorphous layers and introduce microwave losses. They may also reduce the coherence of the system with excess numbers of quasiparticles, coupling to microscopic electronic defects, or spurious phonon modes. In these assemblies of superconducting qubits, developing pristine thin-film materials that mimic the bulk material is key for QIP.

2. Priority Research Opportunities

PRO 1: Advance Artificial Quantum-Coherent Systems with Unprecedented Functionality for QIS

Contributors: Amir Yacoby, Peter Denes, Danna Freedman, Giulia Galli, Stephen Jesse, Chris Palmstrom, Nitin Samarth, and Darrell Schlom

What would it take to create materials with pre-designed characteristics optimally suited for QIS? Consider, for example, a material that can host quantum bits for quantum computation. The bits created in such a material would require ultra-long coherence times suggestive of extremely weak interactions with the underlying lattice. Conversely, a material designated for quantum sensing would require extreme sensitivity to a particular physical quantity and simultaneous insensitivity to all other quantities. Beyond the active components, realizing complete integrated quantum hardware necessitates control and feedback, with specific design criteria for every class of materials that enable direct integration with peripheral components.

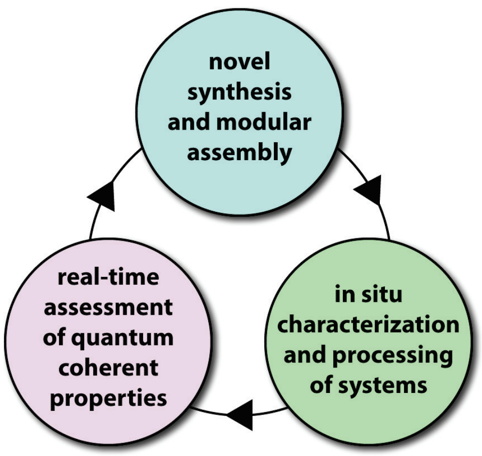


Figure 1. Creation and study of quantum systems focused into a real-time feedback cycle. | Image courtesy of Danna Freedman, Northwestern University

This PRO explores approaches to synthesize QS ideally suited for targeted applications in QIS. While many synthesis apparatuses already incorporate in situ characterization, those methods are geared toward materials properties, as opposed to QS performance. Achieving the goal of synthesizing the appropriate QS requires adding another key element within the synthesis feedback loop that provides real-time information on the specific property being optimized (Figure 1). Conceptually, at the materials level, implementing this idea requires a modular setup consisting of synthesis with in situ fabrication, as well as characterization and theoretical capabilities to determine the underlying quantum-coherent properties of the material during both synthesis and integration. On the system level, modular material components are needed that can be integrated and interfaced with the corresponding control electronics and optics. Such a cycle, executed with rapid turnaround, could generate sufficient data for integration with microscopic theoretical prediction and machine learning techniques to iteratively guide the next synthesis and fabrication steps, enabling rapid convergence.

Materials, Theory and Instrumentation, Challenges, and Proposed Approaches

The realization of frontier materials for quantum information will require a nexus between multiple innovative strategies—including the assembly of atomically precise material modules and instrumentation modules that seamlessly integrate in situ fabrication and characterization, as well as theory and computation, in a closed loop. The materials synthesis community provides a foundation to build from, with extensive expertise in integrated interdisciplinary approaches to materials synthesis. For instance, ultra–high-vacuum techniques like molecular beam epitaxy (MBE) have commonly been combined with surface science probes such as scanning tunneling microscopy and angle-resolved photoemission spectroscopy to rapidly advance the state of the art in new families of materials including topological insulators and novel superconductors.[2,3] Similarly, chemical vapor deposition (CVD) techniques have been merged with in situ optical characterization and, more recently, x-ray diffraction.[4] Despite their success, these traditional approaches have significant limitations for the development of QS. First, real-time feedback between synthesis and characterization at the nanoscale is rare, and attempts to directly incorporate theoretical input into this feedback loop are scarce. The development of innovative techniques that provide *atomic-scale characterization during synthesis* will enable the incorporation of both theoretically directed and machine learning strategies for quickly homing into the optimal window of parameter space for achieving desired materials properties. Second, the conventional approach to sophisticated materials synthesis of hybrid modular materials imposes severe constraints on the range of materials that can be explored with a given system. For example, in a given MBE or metal-organic CVD system, changing the materials being synthesized requires expensive modifications. A key challenge and opportunity thus presents itself in this context: *How can we develop a fast, iterative synthesis technology that integrates in situ fabrication and characterization and is informed and/or directed by first principles theory and machine learning, thereby enabling rapid convergence toward a desired quantum-coherent property.*

This challenge can be addressed by numerous synthetic modular approaches to create systems well suited for QIS. This section describes four research opportunities.

1. Robotic synthesis of layered materials

Layered materials, also known as van der Waals materials, offer a unique level of modularity that can be harnessed for goal-oriented synthesis, with particular advantages with regard to the metrics inherent to QIS.[5] For example, hybrid structures consisting of superconductors and semiconductors can be assembled together to host topological qubits.[6] Moreover, atomic defects in certain layered materials can serve as single photon emitters and possibly even as qubits that can be integrated and interfaced with other layers that host the relevant control electronics and optics.[7] Despite the weak interactions between layers, stacking disparate materials engenders properties distinct from those of the constituent materials. This phenomenon enables us to access a vast phase space for realizing quantum environments that are uniquely tailored for QIS.

Unlike bulk material growth, which requires deep knowledge of material compatibility chemically, structurally, and energetically, assembly of disparate layered materials offers a pathway to create any conceivable material interface. Layered materials open up exciting and rich new possibilities for material synthesis that is removed from many of the constraints that exist in traditional growth. Physics at the forefront of our understanding of matter exists within layered materials, as low-dimensional materials confer a stunning diversity of properties, including semiconducting, superconducting, magnetic, insulating, and strongly correlated properties. Some of the emergent physics displayed by layered materials include exciting examples such as high-temperature superconductors (BSCCO),[8] candidate quantum spin liquids ($RuCl_3$),[9] topological insulators (Bi_2Se_3, WTe_2),[10,11] low-dimensional ferromagnets (CrI_3),[12] and antiferromagnets ($FePS_3$).[13] Work in this area will explore new materials that can host controllable quantum-coherent degrees of freedom and optimize their performance and integration.

Similar to MBE, robotic synthesis can place one, two, or more monolayers controllably and can even control the angle between the layers. This unusually precise structural control confers profound effects on the resulting material properties. Key to integrating with QS, the inherent thinness of layered materials enables significant light/matter interactions that may be used for manipulating quantum information. Coupling these novel states of matter to one another, with extreme control over structure, will open up new possibilities for materials discovery and for realizing materials ideally suited for QIS.

Combined with rapid and automated assembly, layered materials will allow for the creation of stacks with integrated and in situ characterization, control, and possible integration with silicon microprocessor chip technology (Figure 2). These features will ultimately reduce instrumentation costs, because key components such as electronic amplifiers and sources, as well as light sources and detectors, can be easily integrated onto chips. Fast turnaround times from a theoretical material concept to an assembled and characterized quantum system will enable the accumulation of huge quantities of data related to the quantum properties of such materials and their relation to the underlying structure. For theory to inform experiments on specific pathways and desired materials properties, a framework should be developed to seamlessly integrate first principles calculations for predicting the electronic properties of 2D layered materials, with ab initio computations of coherence spectroscopic signatures. The large data sets generated will be ideal for machine learning techniques that can predict and speed up the discovery of new quantum bits and quantum sensors with optimized coherence ideally suited for QIS applications.

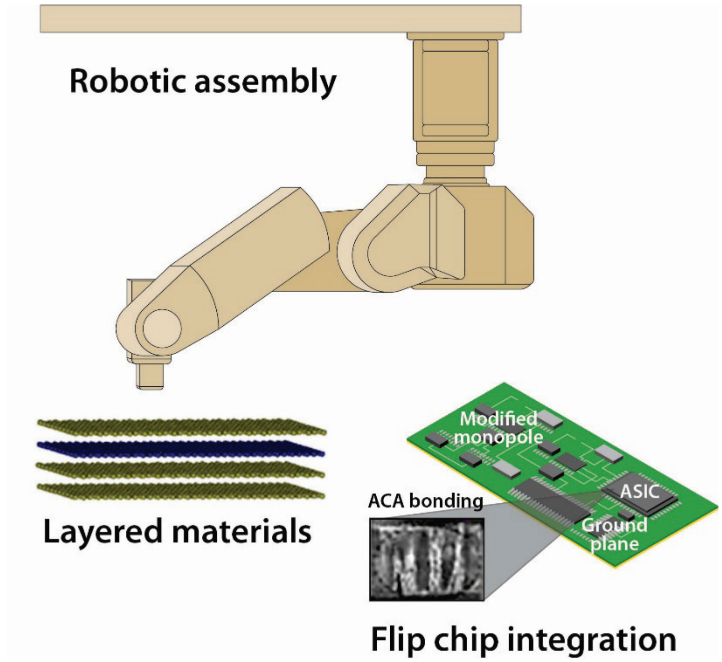


Figure 2. Design of layered materials through robotic assembly and their ultimate incorporation into complete systems. | Image courtesy of Oak Ridge National Laboratory

2. Incorporating qubits into metal-organic hybrids and interfacing them

Bottom-up assembly of QIP systems consisting of precisely spaced molecular-based qubits provides an alternate pathway to the next generation of QIP. A chemical approach to the synthesis of metal-organic hybrid qubits benefits from the combination of reproducible qubit fabrication, the extraordinary programmability and tunability of the qubits by chemical design, and the ability to order qubit monomers into large-scale arrays through the creation of coordination materials (Figure 3).[14] These capabilities enable thinking beyond traditional fabrication techniques for the creation of 3D architectures, as well as the creation of 2D arrays amenable to integration with established technologies.[15,16] Within this approach, molecular systems can be studied, assembled into multi-qubit architectures, and ultimately integrated into systems. The versatility of metal-organic hybrid materials provides two distinct, powerful approaches to creating new QIP systems. One of these approaches focuses on integrating metal-organic systems employing those approaches with the device technology detailed in the previous section. The

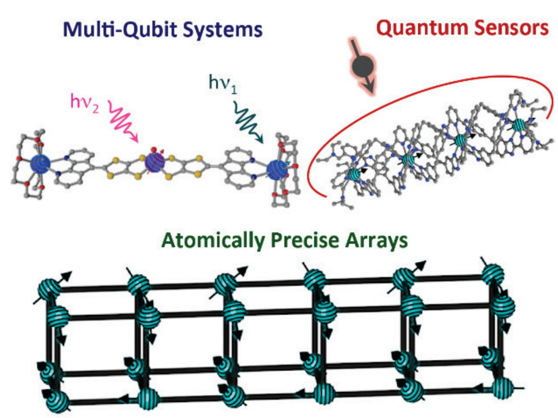


Figure 3. Coordination compounds as viable qubits. Three potential applications of coordination compound qubits, where precise synthetic control enables sensing and computing applications. | Image courtesy of Danna Freedman, Northwestern University

initial step within this approach is interfacing metal-organic hybrid systems with functionalized surfaces, as depicted in Figure 4. Integrating qubits onto surfaces will enable rapid feedback regarding qubit performance, as described above. A second, more chemically demanding pathway focuses on engendering optical addressability within electronic spin-based qubits. The distinct steps required to enable these two manifestations of QIP are outlined below.

Approaching this challenge requires not only the rational design of metal-organic hybrid qubits with long-lived coherence times[17] but also their assembly into larger architectures. There are three crucial challenges to surmount with regard to coordination chemistry–based quantum computing: (1) single molecule addressability, (2) realizing gates to control coupling between two or multiple qubits, and (3) integrating metal-organic qubits into larger systems through coupling with surfaces and/or light.

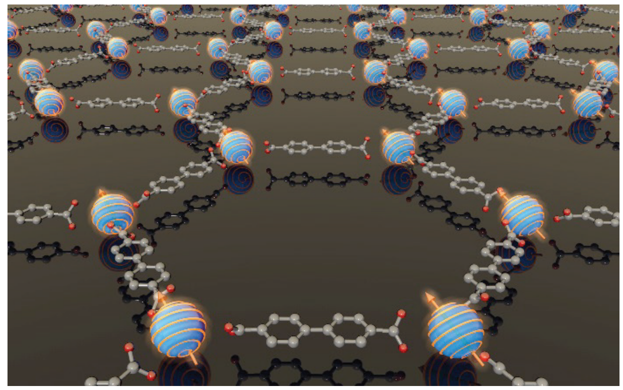


Figure 4. Schematic of metal-organic hybrid system integrated with a surface. | Image courtesy of Danna Freedman, Northwestern University

Creating systems incorporating metal-organic hybrid qubits has two prerequisites: demonstrating single-molecule control over a qubit, and establishing two-qubit and multi-qubit interactions. Careful design of molecules displaying long coherence times and their subsequent integration into devices will require an interdisciplinary effort, bridging materials synthesis, system fabrication, and read-out control.[18,19,20] Demonstrating this proof of concept will not only achieve qubit control on the atomic scale but also enable scaling of molecular systems. A second crucial challenge is demonstrating gate operations within long-lived qubits and determining the parameters required for their operation. The initial challenges in this field are the construction of a vast library of coupled qubit systems and, from these systems, designing optimal inter-qubit coupling.[21,22] Employing a mononuclear building unit paradigm for creating multi-qubit systems could lead to a dramatic increase in the coherence time of the constituent qubits.[23,24]

Once they are synthesized and characterized, the next key step is integrating 2D metal-organic hybrid materials with other low-dimensional materials to create designer QIP systems. The initial steps are assembling 2D metal-organic hybrids on surfaces and functionalizing those surfaces.[25] These steps can be performed in conjunction with the approaches described in the previous section. An alternate approach is creating optically addressable qubits from hybrid metal-organic systems. In that case, it is possible to harness the tunability of coordination compounds to engineer the ideal optical properties. Coordination compounds offer the additional advantage of precise qubit positioning, thereby enabling the synthesis of arrays of optically addressable qubits. These qubits could then be integrated into larger constructs.

3. Endowing new materials with desired topological properties

In virtually all implementations to date of QS, one of the states is an excited state that must, of necessity, decay spontaneously into its ground state. This decoherence quickly destroys the quantum calculation and is one of the most significant challenges facing QIS. A fascinating alternative form has been proposed: braiding pairs of ground-state non-abelian anyons in two dimensions.[26,27] Importantly, an anyon is *not* an excited state and so does not suffer decoherence, preserving quantum information ad infinitum. By avoiding decoherence, QIS calculations can continue for a much longer time using this approach. In principle, one of the simplest ways to create and use pairs of such anyons occurs in odd-parity superconductors; *p*-wave, *f*-wave, and so on, can be topological and, according to theory, would all support a bound $E = 0$ quasiparticle state.[28] When localized in real space, this bound $E = 0$ state is dubbed the "Majorana zero-mode" (MZM); the MZM is its own antiparticle, and the braid group of MZM is non-abelian.

Over the past decades, several promising candidates for such odd-parity topological superconductors (OPTSs) have been identified; yet clear and convincing evidence for any system remains to be established. These enabling materials are of paramount importance to the future of QIS, and if such materials can be found,[29,30] they will readily be implemented in QIS device architectures that are already worked out. Thus, research to develop OPTSs and to establish that they indeed harbor MZMs and are capable of non-abelian quantum operations is highly promising.

One strategy is to develop an OPTS that can be deposited as a 2D sheet over large-area wafers. This approach has the advantage of scalability and would provide a robust platform for the study of ground-state non-abelian anyons in two dimensions. Such wafers could be patterned into thousands of anyonic qubits and thereby lay the practical foundation for anyonic ground-state QIS. The leading single-phase OPTS is Sr_2RuO_4,[31] but compelling evidence for its odd-parity superconductivity remains elusive.[32] Superconducting thin films of Sr_2RuO_4 were recently synthesized,[33,34] and strain appears to be a promising way to significantly increase their superconducting transition temperature (T_c) from the 1.5 K of unstrained Sr_2RuO_4.[35,36,37] A higher T_c pushes the excited states of the system to higher energies, which is beneficial for ground-state quantum computing, in which it is desirable to braid ground states and operate under conditions that minimize contributions from excited states. A higher T_c also means a larger superconducting gap Δ, making it easier to establish whether a material is an OPTS. Materials-specific embodiments of OPTS at interfaces are being predicted and are an exciting area for materials discovery.[38,39]

Another strategy is to follow the proposal by Fu and Kane to create an OPTS at the interface between a topological insulator and an *s*-wave superconductor.[40] Sau et al.[41] predicted that a conventional semiconductor, in which *s*-wave superconductivity and Zeeman splitting are induced by the proximity effect, would also support MZMs. Signatures of zero bias peaks (ZBP) in differential conductance data consistent with MZM were first reported for InSb semiconducting nanowires with a NbTiN superconductor contact.[42] Replacing NbTiN with epitaxial aluminum as the superconductor, combined with recent advancements in fabrication and processing, has yielded hard superconducting gaps[43] (enduring up to $B \approx 0.9T$) and substantial improvement in the ZBP, reaching close to the theoretical predicted value of $2e^2/h$.[44] One of the key challenges of the nanowire approach is that it requires fine tuning of the chemical potential and magnetic field to reach the topological phase. Additionally, its 1D nature poses severe challenges in scalability. Recently, there have been several proposals for realizing induced topological superconductivity with MZM using 2D architectures[45] that do not require fine tuning and have the potential for scalability.[46] Such 2D approaches are also implementable using the layered approach described in the earlier section on robotic synthesis.

4. Precise positioning of atomic defects

Direct manipulation of individual atoms in matter at the atomic scale is a recent and revolutionary technology.[47,48] Scanning probe and electron microscopes are being reinvented to not only image the structure and function of materials with atomic resolution but also modify materials at the fundamental level.[49,50] These emerging capabilities open new pathways for imbuing solid-state systems with quantum functionality by enabling direct fabrication and editing of local structure and chemistry. The controlled introduction and manipulation of complex defect systems, combined with atomic-scale measurements of quantum behavior, provide a fast and tight feedback loop to accelerate research in QIS via real-time interaction with the basic building blocks of matter.[51]

The advent of capabilities to address single atomic sites, and the ability to position atomic-scale defects, offer promise for the creation and manipulation of novel atomic defect–based QS. It is notable that even for very well-known materials such as diamond or SiC, new defects with unique coherent properties continue to be discovered, suggesting that the phase space for defect-derived quantum functionality is truly vast.[52,53] In such cases, though, progress depends on natural random processes for defect creation and serendipity in their discovery. Alternatively, local manipulation and measurement of matter allows for the construction of complex defect ensembles and the ability to study these ensembles by systematically varying, for instance, bond conformation, spacing between dopants, or dopant types. The variation enables a direct understanding of the correlations between non-quantum observables, such as structure, with specific quantum behaviors. This approach is being successfully employed to realize spin qubits in silicon.[54] Note that it may also be possible to employ this approach in conjunction with the bottom-up chemical synthesis for metal-organic hybrids described earlier.

Scanning transmission electron microscopy (STEM) offers an emerging path for imaging and direct manipulation of atomic structures as well as measurement of quantum properties (Figure 5).[55] Recent years have seen a proliferation of high-resolution STEMs, and their propensity for beam-induced modifications in solids has led several groups to observe atomic-level beam-induced modifications, including sculpting,[56] crystal-amorphous phase transitions,[57] bond creation, vacancy creation,[58] directed single-atom doping,[59] and controlled dopant motion and arrangement[60] within 2D and 3D crystals. The ultimate goal of guiding transformations to yield specific final designs with desired behavior requires the development of advanced feedback and control systems based on large-scale data acquisition, and advanced machine learning–based processing, coupled with theoretical models that capture beam-matter interactions and can predict specific spectroscopic signatures and coherence times.

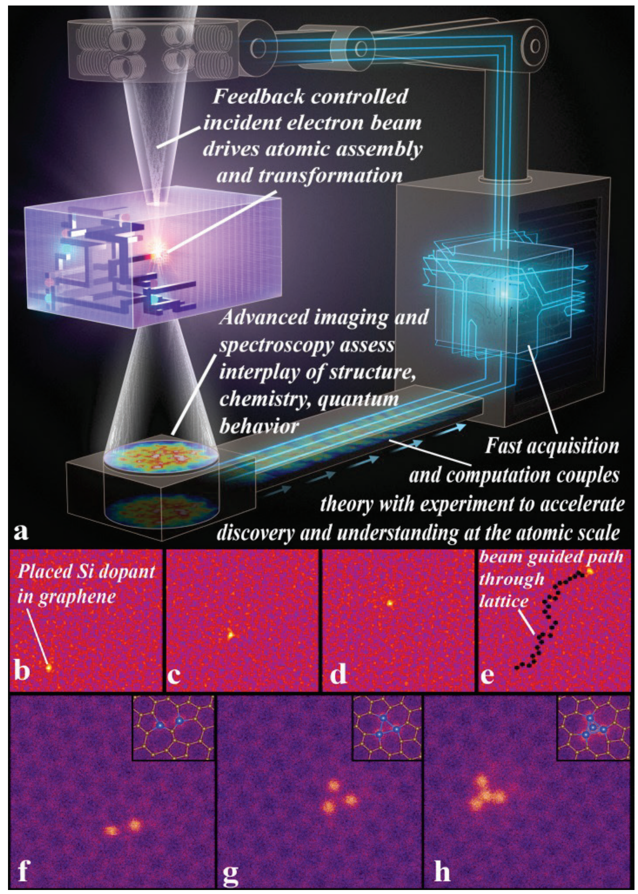


Figure 5. (a) Enhanced STEM enables building and editing of atomic assemblies and assessment of their quantum properties. (b–e) Directed doping and guided motion of dopant through graphene lattice. (f–g) Beam-directed atom-by-atom fabrication of silicon dimer, trimer, and tetramer. | Reprinted by permission from Nature Publishing Group. *Nature*, Fire up the atom forge, S. Kalinin, A. Borisevich, and S. Jesse, copyright 2016

Although final applications necessarily rely on macroscopic contacts or optoelectronic connections, of interest here is prototyping and probing quantum behaviors via microscopy-based observables to accelerate the research cycle. Further advances in electron energy loss spectroscopy (EELS) can be used to chemically identify single atoms and map local plasmon and phonon behavior. Electronic properties can be probed via cathodoluminescence to map local densities of states, emitter decoherence dynamics, and information about the quantum state of a defect with picosecond temporal resolution.[61] They can be predicted by first principles calculations based either on density functional theory or advanced many-body perturbation theory methods.[52]

Operating interactively at the fundamental length scale of materials sciences through direct observation and control will provide new insight into how and why novel phenomena emerge and will provide new pathways for creating and exploiting valuable properties for novel devices for QIS.

Potential Impact

The overall aim of this program is to create the fundamental scientific and technological understanding to develop integrated coherent QS with unprecedented performance for applications in QIS.

Real-time feedback with atomic-level control of synthesis, based on theoretical predictions and measurements of quantum characteristics, will enable rapid development of artificial quantum-coherent systems with predesigned functionality for QIS. Development of in situ lithographic processing of quantum materials down to the atomic scale will allow for unprecedented control to facilitate the fabrication of structures for QS. Integration of in situ techniques to measure quantum properties will allow immediate feedback between synthesis and functionality, providing important fundamental experimental measurement feedback to theory. Creating and measuring control structures specifically to test theoretical predictions is crucial for theory development and will aid the cycle of quantum information development. Sculpting and deposition can introduce small-scale topological changes (by cutting holes and closing loops) and can be used to locally tune confinement and strain-related properties (e.g., local bandgap). Arrays of dopant atoms, or metal-organic sites, with specified arrangements can be introduced to create highly tunable superlattices to enhance particular phonon, plasmon, or optical modes. By the use of atoms with accessible spin states, atomic-scale magnetic structures or quantum entangled arrays can be artificially created and studied. Operating interactively at the fundamental length scale of materials science through direct observation and control will provide new insight into how and why novel phenomena emerge and will provide new pathways for creating and exploiting valuable properties for novel materials and devices, such as ultrasensitive sensors, that will give insight into other fundamental areas of science.

Automation of the synthesis process, combining data-based machine learning and atomistic theory with real-time analysis, will allow rapid surveys of materials systems and convergence toward materials with desired quantum properties. The large amounts of data created will provide input for developing metrics and design rules for quantum-coherent materials and systems.

PRO 2: Enhance Creation and Control of Coherence in Quantum Systems

Contributors: Michael E. Flatté, Darrell Schlom, Irfan Siddiqi, and Toni Taylor

Quantum-coherent systems have exhibited remarkable coherent phenomena,[62–67] including the ever increasing coherence times necessary for QIS.[68–70] Even more important than the absolute time scales of coherence are the greater than ten orders of magnitude by which coherence times can exceed the intrinsic dynamical time scales of such systems.[71] This exceptional ratio of coherence times to evolution times suggests extensive regimes of coherent behavior during which complex entangled states can be established and evolve before they decay. Our understanding of the complexity of entanglement remains limited to the behavior of small numbers of quantum-coherent systems. Advancements in this field will come from new understandings of the scaling of coherence lengths and times with system size and complexity, from clarifying the distinction and interactions between the quantum-coherent system and its surrounding incoherent bath of excitations, and from identifying new signatures of quantum states in artificial quantum-coherent systems. The current focus of the field on slow changes in the parameters and features of quantum-coherent systems, in order to adiabatically change their properties, will expand to scenarios in which fast, non-adiabatic changes can be made that weakly couple to an incoherent bath, if at all. Researchers can expect to discover, during these investigations, novel entangled excitations with unexpected properties, including surprisingly long coherence times or stable behavior when manipulated. This behavior will enable advances in artificial quantum-coherent systems as described in PRO 1.

Specific Challenges and Proposed Approaches

The following four sections discuss specific challenges within this area.

1. Overcoming the tyranny of low temperature

At room temperature, the environment continually exposes QS to excitations with intrinsic dynamical time scales of less than 100 femtoseconds.[62,63] This has forced most implementations of QS to operate at low temperatures. Nonetheless, quantum states in many quantum-coherent systems overcome this tyranny of low temperature and remain impervious to this hot, incoherent background. At the same time, these quantum-coherent systems respond dramatically to other perturbations, such as the average temperature or fluctuating magnetic fields, which have characteristic time scales of microseconds or longer. Quantum-coherent systems that demonstrate this behavior include color centers in wide-gap semiconductor materials, such as the nitrogen vacancy (NV) center; triplet/singlet systems in organic molecules and complexes; and unpaired spins in insulating barriers, especially in tunneling transport.

The resilience of quantum-coherent systems against the hot bath—even as they retain their sensitivity to specific types of excitations—is connected to the enforcement of particle statistics, such as the Pauli exclusion principle, within a limited set of available states of a small discrete system. A common arrangement of states is that orbital and exchange energy scales in excess of an electron volt establish selection rules for transitions at energies of much less than 1 eV, including at room temperature (equivalent to 25 meV). Certain specific perturbations, however, break these selection rules. Thus, a perturbation with an energy scale in the micro-electron volts can dramatically influence an observable at room temperature (Figure 6). A characteristic feature of such phenomena is the “state bottleneck” in which the system attempts to make a transition, is thwarted by the selection rule, and then succeeds, aided by the perturbation. Systems far from equilibrium, such as color centers under optical pumping or orbitally incoherent transport in organic materials under large electric fields, enhance these bottleneck effects.

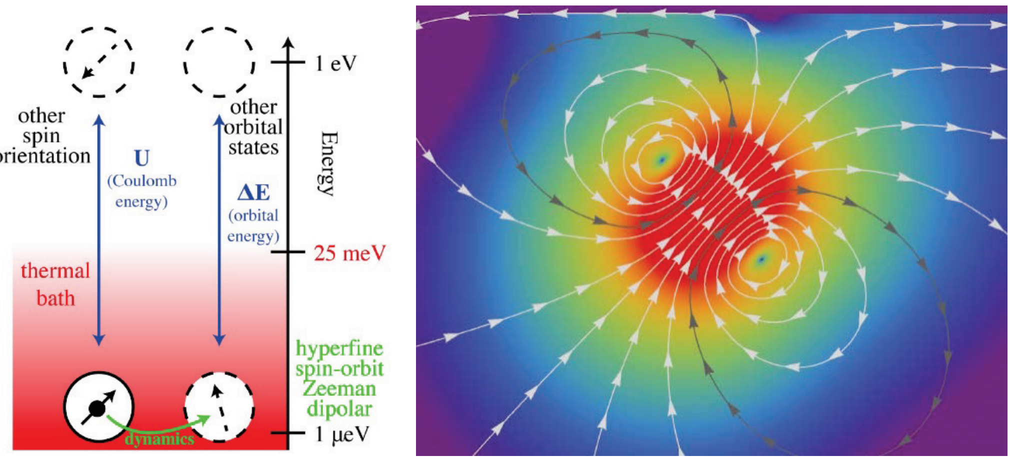


Figure 6. (Left) Schematic energy scales for spins when coherence influences dynamical transitions in transport, recombination, or reactions. Spin selection rules push other possible states far from accessible thermal energies as a result of Coulomb charging or orbital transition energies. | Image courtesy of M. Flatté, University of Iowa. Much smaller energies that break these selection rules can manipulate spin-correlated dynamics even at room temperature. (Right) Back-action of magnetic fields induced in a sample on an NV sensor.[72] | Reprinted figure with permission from J. van Bree and M. E. Flatté, Atomic-scale magnetometry of dynamic magnetization, *Phys. Rev. Lett*. 118, 087601, 2017, copyright 2017 by the American Physical Society

Challenges in understanding these situations persist. They include how to understand the coherent evolution of a superposition of quantum states on microsecond time scales, when the bath causes fluctuations on far shorter time scales that perturb the relative energy of the quantum states in the superposition by far more than the coherent evolution rate. Although a theoretical analysis based on a limited number of possible quantum states of a bath suggests that the bath fluctuations quench quantum coherence, experimentally the quantum coherence survives. Thus, a central challenge remains to understand the decoherence of open QS, which appears to be far less rapid than current theories suggest. In other scenarios, there is a bath that does couple strongly to the quantum-coherent system under exploration. An enduring problem in condensed matter physics is the so-called central spin,[73] which is a distinct spin entity that interacts with a bath of excitations with spin character. Examples include the evolution of the NV spin (here the central spin, since it is independently measurable) during interaction with a surrounding bath of electronic spins (e.g., from substitutional nitrogen dopants) and nuclear spins (e.g., from nitrogen or carbon nuclei).[74] A related and equally important challenge is to experimentally characterize the coupling of quantum-coherent systems to the bath and to better describe the behavior and dynamics of the bath. Does it consist of a collection of nearly homogeneous systems—as in a uniform spin ensemble, or a heterogeneous assembly of systems with very different coherent properties—such as a solid with electron spins of various types, some mobile and some not; nuclear spins; and possibly ferromagnetic order.

2. Toward rapid manipulation of quantum-coherent systems

Our simple current pictures of quantum coherence, which appear inadequate to understand the persistence of coherence in a hot bath, also motivate researchers to focus on slow manipulations of QS to avoid unintended transitions to other quantum states. In an adiabatic transition, to avoid Landau-Zener tunneling across the gap, the time of transition, Δt, must be sufficiently long that it exceeds $\hbar/\Delta E$, where ΔE is the energy gap in the system's spectrum to other excitations. However, under some conditions, a hot bath fails to efficiently drive transitions to other quantum states even in the complete absence of any spectral energy gap to these other quantum states. Therefore, it must be recognized that fast, nonequilibrium, nonadiabatic changes in the parameters of the quantum system should also be possible that do not substantially damage the coherence of these quantum-coherent systems.[75] A new theoretical framework for non-adiabatic manipulations of quantum-coherent systems may point the way to highly efficient changes in the quantum states of certain systems. For example, as a result of the limited set of relevant quantum states for an NV center in diamond, researchers have demonstrated extremely fast manipulation of its spin state, going beyond the rotating wave approximation for spin resonance (Figure 7). Faster manipulation may also assist in the quantum-to-quantum transduction described in PRO 3.

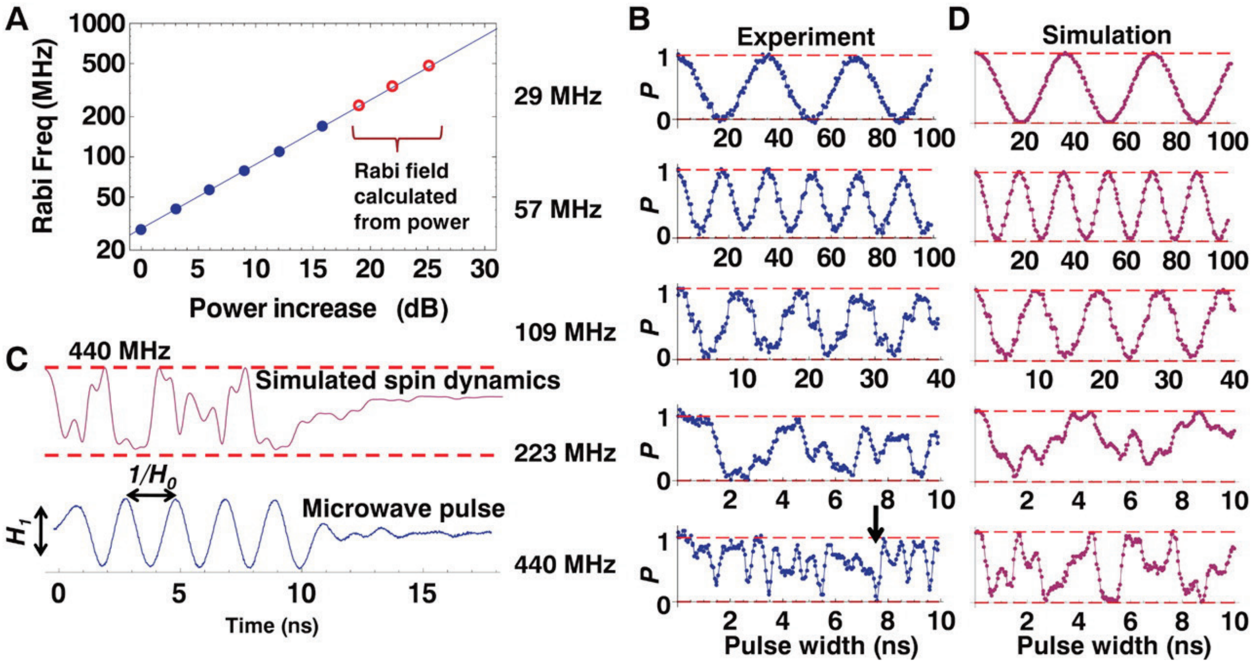


Figure 7. Highly nonadiabatic transitions for a coherent spin center in diamond, showing accurate pictures of the complex spin dynamics even though the rotating wave approximation has failed. | From G. D. Fuchs et al. Gigahertz dynamics of a strongly driven single quantum spin, Science 326(5959), 1520–1522. Reprinted with permission from AAAS. Except as provided by law, this material may not be further reproduced, distributed, transmitted, modified, adapted, performed, displayed, published, or sold in whole or in part, without prior written permission from the publisher.

3. Novel quantum states of quantum-coherent systems require novel probes and new theories

Considerable development effort has been devoted to the techniques that can measure individual quanta, including single photons, single phonons, single electrons loaded into or out of a quantum dot, or single spins. Understanding the nature of and opportunities for coherence in QS involves exploring the correlations and entanglements between individual quanta and how they persist, decohere, or otherwise evolve in time or over space. The tools available for probing such correlations and entanglements are only at an early stage of development. Typical approaches for correlated measurements such as Bell state measurements require manipulating the entangled state of the system into a product state before performing the measurement. However, the use of multiphoton entangled states as probes permits measurement of objects below the Rayleigh refraction limit. Probes producing entangled photons should also allow direct measurements of entanglement in electronic systems[76] (Figure 8); however, new methods of preparing and preserving these quantum states, and of directing them toward materials to be measured, must be developed. As the generation of entangled photons typically requires optical nonlinearities whose effects improve at high flux, facilities that produce high flux provide unique opportunities to implement these novel probes. Measurements of these quantum signatures of quantum-coherent systems require, in the end, conversion to classical information. This requirement identifies the challenge of connecting signatures of quantum phenomena to classical signatures as a critical step in quantum measurement theory and in the development of successful new probes of quantum-coherent behavior. These key features, the features required to probe new quantum-coherent behavior, and their impact on the fundamental limits to measurement, are explored further in PRO 4.

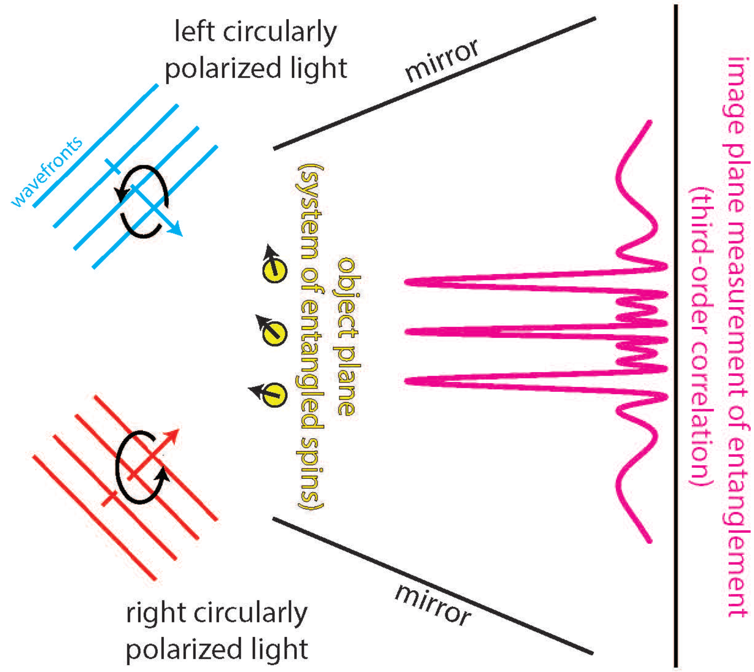


Figure 8. Schematic configuration for use of entanglement induced in photons to measure entangled electronic states, as proposed in Leuenberger et al.[73] The third-order correlation measurement with three detectors (C_3 in Leuenberger et al.) of an entangled state of the spins of three quantum dots, $(|\uparrow\downarrow\downarrow> +|\downarrow\uparrow\uparrow>)\sqrt{2}$, is shown. One detector responds to left circularly polarized light, one responds to right circularly polarized light, and one does not sense polarization. The separation between each polarized detector and the unpolarized detector is the same; the pattern is plotted as a function of that separation. | Image courtesy of the Flatté group, University of Iowa

Along with the exploration of methods to access the behavior of entangled states with outside probes, we can expect approaches to manipulate the internal coupling between entangled states of quantum-coherent systems in order to enhance or suppress those internal correlations, which can then be measured with these new probes. As advances in the theoretical understanding of quantum-coherent systems are made in constructing new correlation functions, direct probes of those correlations will provide the best test of new theoretical descriptions of coherence. To take advantage of such situations, the bath itself might be manipulated to reduce coupling to interesting quantum states in order to allow those correlations and entanglements of interest to persist for longer times.

4. Revealing the role of disorder through material control

The complex role of disorder in quantum-coherent phenomena has been anticipated since the earliest work on nuclear magnetic resonance, when disordered systems were found to have longer coherence times due to motional narrowing. A similar effect lengthens spin coherence times in semiconductor materials such as gallium arsenide, whereas disorder shortens spin coherence times in copper and silicon. These different effects originate from differing and competing influences of disorder on the spin-orbit interaction, when combined with ordinary electronic scattering events in the materials. Control of disorder can perhaps be understood, therefore, as a way of manipulating the coupling of the quantum-coherent system to the ever-present thermal bath, and of limiting or enhancing the effect of the bath on decoherence. Similar effects should occur in more complicated quantum states of quantum-coherent systems. Thus the design, simulation, and characterization of new materials with controlled disorder will offer insight into the nature of coherence in these quantum-coherent systems.[77] Included in this opportunity would be the unique design and fabrication of artificial disordered systems, including the "defect in an effective crystal" approach that has proved very powerful for photonic and magnonic crystals (Figure 9) (discussed in more detail in PRO 1).

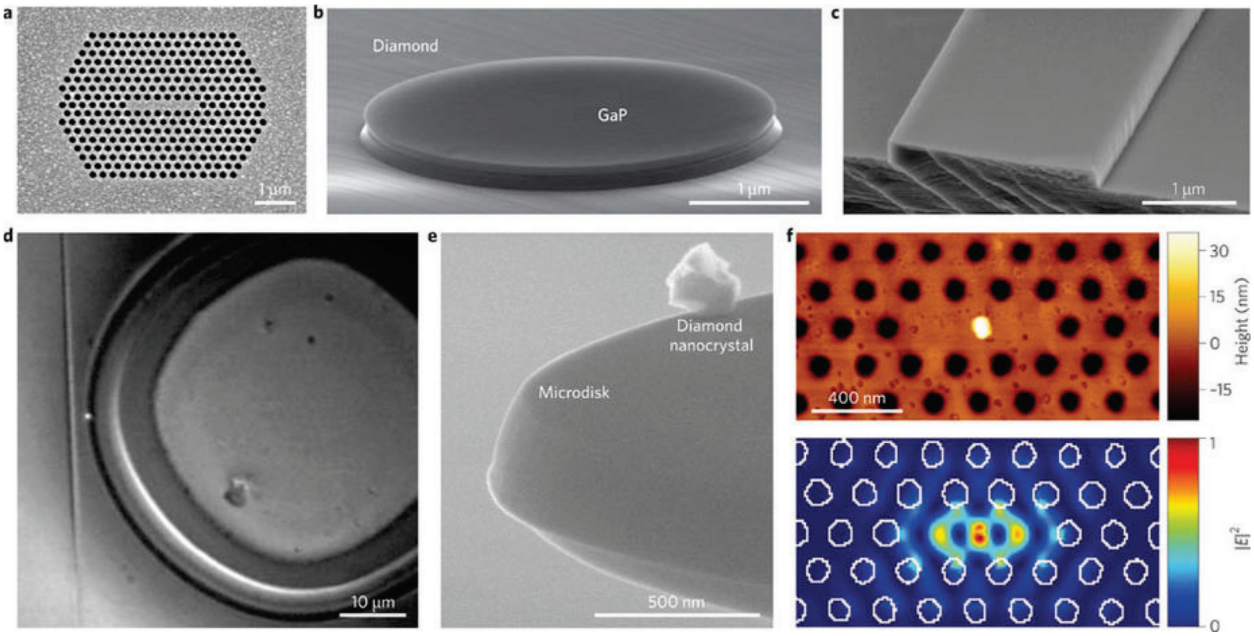


Figure 9. (a) A 2D photonic crystal cavity made from a nanodiamond film. (b) GaP microdisk and (c) GaP waveguide deposited on single-crystal diamond. (d) Manipulating a nanodiamond hosting a single emitter onto a toroidal microresonator using a fiber taper. (e) Nanodiamond hosting a single emitter on a silica microdisk. (f) Atomic force microscopy image of a diamond nanocrystal placed in a GaP photonic crystal cavity (top) and the simulated electric field profile of the cavity's fundamental mode (bottom). | Reprinted by permission from Nature Publishing Group. *Nature*, Diamond photonics, I. Aharonovich, et al. copyright 2011

Impact: Understanding Coherence in Quantum-Coherent Systems

The simplest coherent properties of quantum-coherent systems have already been enhanced to macroscopic time scales and length scales; however, the more robust these systems can be made, the more complex and revealing the coherent phenomena they demonstrate. Simple examples of quantum manipulation, such as charge and spin pumps, have been demonstrated over short times and short distances but are not practical for the precise control of transport. Advances in controlling coherence should expand the range of systems in which charge and spin pumps can be constructed, perhaps to organic molecules and even to room temperature. Teleportation of simple quantum states has been demonstrated in a wide variety of QS, including photons, spins, and atomic excitations. How far can we go in teleporting entangled states? At what degree of spatial separation can we generate and detect entangled states? Can these be used to illuminate new quantum phenomena? Or to detect very small changes in the fabric of space and time, such as those created by gravitational waves? Novel sensing modes have emerged from each advance in the control of coherence, from magnetic resonance imaging to precise, local sensing of temperature in liquids.

Novel manipulation of coherent systems is planned for QIP, which poses challenges in the size and number of the quantum-coherent systems to be connected together. Some robust proposed forms of quantum computation require manipulation of the parameters of a gapped system that has unique topological properties under parametric control. The opportunities identified here suggest that, based on the properties of some quantum-coherent systems, the nature of a system's energy gap need not be so complete, or perhaps the manipulation of parameters need not be as slow, as currently anticipated. However, when considering the behavior of these unusual excitations, and how they behave when braided together, we simply do not have a solid description yet of how that phenomenon can be observed. How can these excitations be uniquely identified? How is braiding itself to be measured? For a specific system of interest, what is the best way to characterize and quantify entanglement, as practicalities may limit access to the ideal experimental observables? Only by building a thorough understanding of creating, controlling, and transporting coherence in quantum-coherent systems can we address these fundamental questions.

PRO 3: Discover Novel Approaches for Quantum-to-Quantum Transduction

Contributors: Irfan Siddiqi, William Oliver, and Birgitta Whaley

At the core of quantum measurement and information processing is the transduction of information from one physical modality to another at the single quantum level. Such processes span the simple detection and recording of the number of quanta in an input signal, such as in a photon counter, to the full transfer of the quantum wavefunction implicit in some quantum repeaters needed for the long-distance transmission of quantum signals. Furthermore, hybrid-QS[78] that distribute detection, storage, and processor functionality into different physical architectures rely on efficient transduction between different parts of a complex material system or between constructed heterosystems with well-defined interfaces. An example of such a hybrid is a doped semiconductor in which a long-lived, isolated system, such as a nuclear spin bath, is used as a memory element in combination with more interactive electron spins suitable for gate-based logic operations. Experimental and theoretical directions in quantum transduction include developing schemes to encode and decode quantum information across different physical systems, elucidating quantum and statistical mechanical limits to sensitivity, and optimizing materials to suppress decoherence—and thereby harnessing quantum effects that include entanglement for information processing.

Scientific, Instrumentation, and Computational Challenges and Opportunities

A grand challenge in QIS is the generation and stabilization of quantum states in a variety of different materials systems. QIS holds the promise of superclassical performance in information processing and communication. To realize this promise, quantum coherent states must be realized and maintained in physical systems. Although local systems constitute a processor, it is advantageous to additionally distribute this quantum information across multiple nodes. Whereas one materials system may be well suited to a given task, it is likely that multiple coherent systems will be used to sense, process, and distribute quantum information. Examples of such objects include nonclassical states of light and matter—including Fock and squeezed states, as well as superposed and entangled combinations of electronic, magnetic, and vibrational degrees of freedom. Additionally, efficient quantum-state transduction relies on the identification of materials systems and associated control protocols that allow coupling to these quantum signals without directly inducing decoherence or resulting in an additional susceptibility to noise. Moreover, decoherence from imperfections at materials interfaces and in the bulk needs to be mitigated in conjunction with a deep understanding of noise—both in isolation and coupled to a bath—to generate the precursors for high-fidelity quantum devices. Near-term opportunities include (1) the detection of single quanta in key photon frequency bands, single magnons, individual spin dynamics and excitations in magnetic materials, and individual lattice vibrations; (2) the efficient transmission of quantum information; and (3) the development of functional interfaces for energy conversion and harvesting.

1. Quantum state replication

Quantum communication enables enhanced security against eavesdropping attacks by using nonclassical states of light—e.g., single-photon states or two-photon entangled states—to encode and decode a transmitted message.[79] There are three primary challenges to realizing practical quantum communication. First, the generation of the nonclassical states of light is generally stochastic and low in fidelity. Second, in modern optical fiber or free-space communication, there is distributed loss that limits the communication distance to on the order of 1200 km.[80] Third, the no-cloning theorem of quantum mechanics forbids the duplication of a quantum state and is a foundation for the security of these protocols. While this theorem prevents an eavesdropper from copying a message in transit without detectably altering the measurement outcomes, it also prevents the intentional reconditioning of the quantum states over large distances.

A quantum version of an optical repeater, a quantum repeater, enables long-distance quantum communication by addressing these limitations.[81] A quantum repeater is a local quantum memory (potentially with local error correction) that stores distributed entanglement at several nodes along the communication channel. Nonclassical light is generated at each node in the link and shared with adjacent nodes, whereby teleportation is used to distribute the entanglement across multiple nodes that make up the link. Because the generation is stochastic and, at least currently, of limited quantum efficiency, each node must also have a quantum memory to preserve the local entanglement while the entire link is being established. Quantum communication would benefit from the development of on-demand, high-efficiency sources of nonclassical light, the development of long-lived quantum memories, and the advent of quantum error correction to maintain the memory.

2. Microwave single photon detectors

Whereas the most advanced solid-state information processors to date all operate in the microwave regime, the ability to route and detect microwave photons on-chip is currently limited compared with similar technology operating in the optical domain.[82] Current microwave single photon detectors can broadly be divided into three categories: (1) event detectors that operate continuously in time and attempt to accurately record the arrival time of a photon, (2) time-gated devices by which a photon can be detected with high efficiency only if accurate information about the arrival time is given, and (3) frequency-selective detectors that can detect photons within a certain bandwidth. Not only are very high quantum efficiency and low dark count rate required for most applications; an efficient photon counter also requires fast measurement; large bandwidth; short dead times; low timing jitter; and, in certain applications, spectral resolution. Depending on the application, the ability to resolve photon numbers is also desirable, as well as photon detectors that are nondestructive, i.e. that do not destroy the photon in the detection process.

Although some of the theoretical proposals and proof-of-principle experiments have reported progress on some of the mentioned metrics, no proposal has been put forth yet that convincingly performs well across all specifications needed. In particular, many detectors that promise high quantum efficiency suffer from narrow bandwidth and long detection times. Others impose technical constraints not easily dealt with experimentally, such as the need for multiple cascaded circulators, which are currently bulky and lossy. The development of these supporting quantum microwave components—e.g., isolators, circulators, diplexers, mixers, and beam splitters working in the quantum domain—will have a large impact both for quantum computing and in the broader field of quantum control and measurement. Single photon detection in this domain and into the mid-infrared has many sensing applications as well, including dark matter detection in cosmology.

3. Light to electron transduction: Light harvesting in photosynthesis

The light harvesting apparatus of plants and bacteria possesses remarkable capabilities of reaching near unit efficiency for the conversion of an absorbed photon to an electron, which goes on to initiate the "dark" or chemical reactions of photosynthesis.[83,84] This is an example of transduction of excitonic energy to electron current (Figure 10) in a natural setting that is highly efficient, unusually so for a biological system, with quantum efficiencies for the conversion reaching 95–99% under weak light conditions. It is also extremely robust against changing conditions: the photosynthetic apparatus possesses a highly sophisticated chemical sensing and feedback mechanism that shuts down the critical conversion step when the plant is saturated with light, to avoid overproduction of electrons and consequent photo-damage. Recent ultrafast spectroscopy and theoretical work have revealed insight into the quantum dynamics of the energy transfer and show how the excitonic degrees of freedom interact cooperatively with phonons to ensure the optimality and robustness of the transport in the presence of disorder. This approach can provide important insights for the design of quantum-to-quantum transducers. However, the process of photon absorption in light-harvesting systems is not very efficient and renders the overall efficiency of generating electrons from incident photons much lower than the internal quantum efficiency. To enable single photon counting experiments that correlate absorbed and fluorescent photons on time scales shorter than nanoseconds, it is essential to develop robust heralded single photon sources in the 600–700 nm regime relevant to electronic absorption by chlorophylls and other photosynthetic pigments, fast (picosecond) photon detectors, and improved time resolution correlators. Such studies can play a valuable role in elucidating the spatio-temporal correlations among the multiple absorption events necessary for light-harvesting systems (e.g., for Photosystem II in green plants) to absorb the full energy equivalent of a single photon, which is required for transduction of the excitonic energy to an electron-hole pair and thus to a discrete electron.

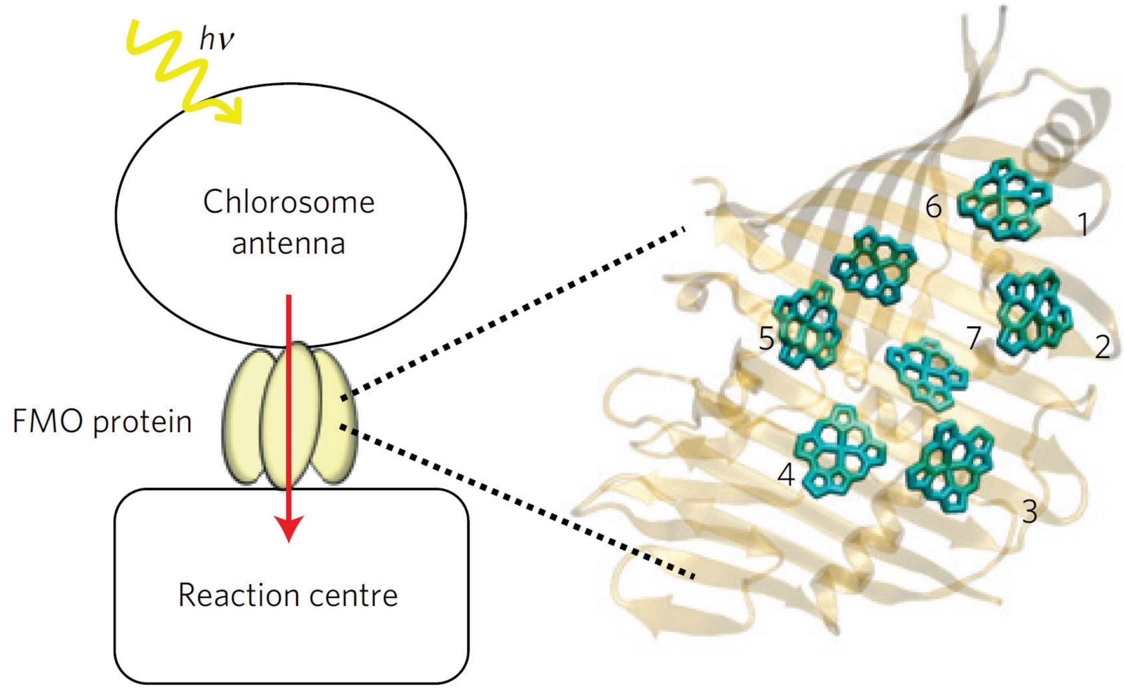


Figure 10. The light-harvesting apparatus of green sulfur bacteria and the Fenna-Matthews-Olson (FMO) protein. The schematic on the left illustrates the absorption of light by the chlorosome antenna and transport of the resulting excitation to the reaction center through the FMO protein. On the right is an image of a monomer of the FMO protein, showing also its orientation relative to the antenna and the reaction center. The multi-ring units are BChla molecules and the surrounding β sheets and α helices form the protein environment in which the BChla molecules are embedded. | Reprinted by permission from Nature Publishing Group. *Nature Physics*, Quantum entanglement in photo-synthetic light-harvest complexes, M. Sarovar, et al. copyright 2010

4. Maximizing coherence at quantum interfaces

There is a general consensus within the research community that understanding and further mitigating sources of decoherence in condensed matter systems (Figure 11) is critical to the development of more advanced applications. Coherence times should be made as long as possible, as exceeding the thresholds for quantum error correction will considerably reduce redundant resource requirements. Both energy relaxation and pure dephasing times, T_1 and T_φ, are related to the environmental noise seen by the qubit, as characterized by a spectral density, $S(f)$, and much is known about this noise.[84,85] For example, inhomogeneous dephasing arises from broadband, low-frequency (e.g., $1/f$-type) noise in the charge, spin, and critical current. However, although it is consistent with a bath of two-level fluctuators (or clusters of fluctuators), its precise microscopic origin is still being investigated.[86,87] Energy relaxation occurs as a result of noise at the qubit frequency, and design modifications can change the device sensitivity to this noise in ways that are understood. However, although several mechanisms are known to exist (e.g., coupling to microscopic defects), their origin is not well understood. Mitigating these types of decoherence mechanisms ultimately reduces to two general approaches:

1. Reducing sensitivity to a given type of noise through design modifications
2. Identifying and mitigating noise sources through materials/fabrication improvements

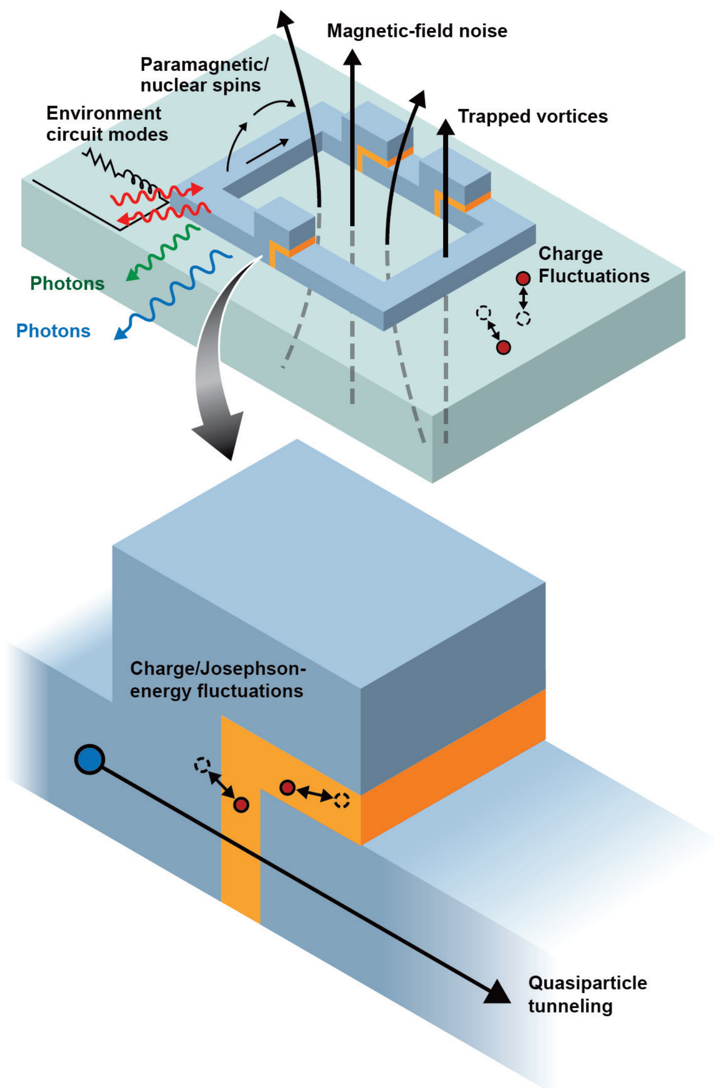


Figure 11. Illustration of various decoherence mechanisms that can affect superconducting qubits. The mechanisms include those related to materials and fabrication, as well as design and packaging considerations (environmental circuit modes and photons). | Image from W. D. Oliver and P. B. Welander, Materials in superconducting quantum bits, *MRS Bulletin* 38(10), 816–825, 2013, copyright 2013 by Cambridge Core. Reproduced with permission

In practice, the coherence improvements over the past decade were made through a combination of improved designs, improved fabrication, and improved materials.[88] From this perspective, there remains an important role for materials and fabrication research to further improve qubit coherence times, with regard to both identifying new noise mechanisms and incorporating novel materials that, for example using topological effects, can exhibit immunity to sources of imperfection.

5. Theory of quantum state transfer

A key challenge in any quantum transduction scheme is to find a quantum system that is flexible enough to couple strongly and coherently to a variety of distinct systems and is thus capable of acting as a "quantum bus." In many cases, systems that have this requisite flexibility are themselves more susceptible to loss and noise. A prime example is the use of vibrational modes of a mechanical resonator as a quantum bus, as has been recently realized in optomechanical systems attempting the coherent conversion of optical photons to microwave photons (see, e.g., Andrews et al. 2014[89]). The large laser powers used to achieve strong coupling in these systems naturally lead to heating in the mechanical mode. For standard sequential transfer protocols, this heating then corrupts any desired quantum state transfer. One ideally would like a transfer protocol that allows the effective coupling mediated by such a noisy quantum bus to be used without being affected by any associated noise or loss. Adiabatic state transfer schemes (such as STIRAP[90]) provide a potential solution but have extremely slow protocol times. A key theoretical goal is thus to find methods to accelerate such protocols in such a way that the protection of the adiabatic scheme remains without the extremely long time scales required for adiabatic evolution. A variety of approaches to this very general problem in quantum dynamics have been suggested (so-called "shortcuts to adiabaticity"[91]), but their application to quantum state transfer is only in its infancy: current approaches are limited to systems with a limited number of degrees of freedom and do not fully account for quantum dissipative effects.[92] The development of shortcuts to adiabaticity for quantum state transfer in realistic settings will have a dramatic impact on the variety of systems capable of acting as quantum buses and could also lead to new general insights into quantum dynamics.

6. Thermodynamics of quantum machines

QIS provides the tools to understand and to probe the interactions of quantum systems with their environments. In building and controlling quantum devices—whether these are computers, repeaters for communication, or sensors—issues of energy and power efficiency and heat transfer arise. They raise fundamental questions about the nature of thermodynamics in the quantum regime and at the nanoscale; i.e., how should quantum thermodynamics be analyzed and how does it help in the quest to build and operate quantum devices in an open environment where work, heat, and even particles may be exchanged?

Understanding and exploiting quantum measurements of variable strength is a key component of the opportunity to explore how thermodynamic quantities such as work and heat are affected by quantum correlations, fluctuations, and coherences.[93] Monitoring in an interaction-free limit will be a valuable and possibly essential component of validating quantum state transfer between two quantum systems—i.e., quantifying the fidelity of a quantum-to-quantum transduction process under non-ideal conditions. The practical implications of doing so are general, affecting all quantum devices that operate with some degree of coherence. Some key questions are

- How can we construct a coherent engine and optimize its efficiency and power output?[94]
- Can we construct and operate a single-atom engine?[95]
- How do we describe and probe heat management for quantum devices?
- What are the trade-offs between speed of operation and accuracy of outcome?

Classical thermodynamics says that faster processes are generally less efficient. This rule is often summarized by fluctuation theorems that relate fluctuations in response to external forces to the irreversible work. How do the corresponding quantum fluctuation relations constrain the behavior of real quantum devices—both atomic-scale, as in trapped atoms and ions, and macroscopic, as in superconducting qubits? How do nanoscale quantum devices thermalize, and how may this reaction be controlled? The design and optimization of nanoscale and mesoscale thermal devices, such as atomic-scale refrigerators for quantum simulations with atoms and ions, and artificial light harvesting devices, force us to analyze the functioning of open quantum systems in thermodynamic terms.

7. Quantum mechanical systems and transduction

Quantum coherent behavior can be supported in many distinct forms of matter and light. Such systems can be prepared in well-defined quantum states, and range from the microscopic to the macroscopic; they also bridge the traditional divides among condensed matter, quantum optics, and atomic physics. New functionalities can be achieved by combining these quantum mechanical building blocks in heterostructures involving quantum-to-quantum transduction. Examples of candidate quantum primitives include, on the microscopic side, spins in semiconductors (both nuclear and electronic), where coherent control has been used to prepare entangled states and perform basic quantum operations. These include defect spins (e.g., NV centers in diamond) as well as gate-defined quantum dot structures. Quantum control and manipulation of photonic states has also been demonstrated in a variety of systems, typically employing the use of high-Q cavities. Physical realizations in this category range from nanophotonic cavity quantum electrodynamics systems, to free-space optical cavities, to microwave photons that are manipulated in superconducting circuits. Quantum states of vibrational (i.e., phononic) degrees of freedom have also been realized; the prime example comes in the form of optomechanical systems, in which mechanical motion couples strongly to photons (optical or microwave) in a resonant cavity.

Impact and Outlook

The long-term impact of research in this basic science realm is the realization of novel quantum-coherent materials systems and the means to manipulate and probe them for information science. In particular, the ability to seamlessly shuttle quantum information between different physical systems will enable distributed quantum networks for communication, sensing, and processing. A detailed examination of the thermodynamics of quantum machines promises insight into light harvesting for clean energy production and bio-inspired detection.

PRO 4: Implement New Quantum Methods for Advanced Sensing and Process Control

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Quantum sensing, along with quantum computing and quantum communication, forms the core of QIP. Groundbreaking advances in the ability to control QS have brought dramatic improvements in measurement science. In general, large ensembles are favored to enhance measurement sensitivity. In particular, collections of noninteracting particles such as atoms, molecules, and electronic or nuclear spins can be used to maximize precision or sensitivity. Although increasing the number of particles always improves the signal-to-noise ratio, inter-particle interactions may limit the measurement performance.

The outstanding goals in the field of quantum control are thus the synthesis of large QS that can be manipulated down to the level of individual, constituent particles and the understanding of the collective properties of such systems. Achieving these goals would provide a powerful platform through which many-body interactions could be probed and then controlled. However, the long-standing challenge has been the extreme difficulty of achieving high-fidelity control of a many-particle system, and it often leads to a compromise between the system size and control capabilities. The ability to accurately quantum engineer—a key ingredient to realizing meaningful simulations and computations—has been restricted to limited system sizes. Recently, a number of technological platforms have emerged that can provide answers to the challenge of microscopic manipulation of many-body states of atomic or molecular systems.[96] These technologies emerge from microscopic control along several orthogonal axes—space, time, number, and energy—to provide new opportunities in the field of quantum many-body physics. These advances in the ability to synthesize, manipulate, and detect quantum many-body systems bring quantum control into a new exploratory paradigm. In parallel, these novel experimental capabilities stimulate new theoretical methods to benchmark and understand observations, and they guide future directions that leverage these advances. Interestingly, recent advances also suggest that by using certain states of driven quantum matter, one can turn strong interactions from a challenge into an advantage resulting in significant enhancements in terms of both sensitivity and bandwidth.

This PRO seeks to advance a long-term scientific goal: to achieve extreme sensing, detection, and control capabilities for time/space and fields using emerging quantum technologies; and to develop and apply these capabilities to probe material properties and chemical reaction processes. Achieving this goal requires developing QS that will nurture emerging quantum technologies, with capabilities including (1) producing useful correlations and achieving maximal quantum coherence and robust entanglement; (2) understanding entanglement, including classification, quantification, and separate control of quantum subsystems; and (3) demonstrating simultaneous time/frequency domain control.

Anticipating material and instrumentation challenges, we should strategize in the following areas:

- Combining single-particle coherence, multiple qubit correlations, and many-particle entanglement to maximize measurement gains
- Developing optimal measurement protocols that demonstrate the true advantage of quantum approaches and enable new breakthroughs in measurement capabilities
- Connecting quantum entanglement with specific measurement needs and goals and providing experimental verification and validation of entanglement-based measurement

As researchers apply these advanced quantum measurement capabilities to materials and chemistry, they must understand the complexity of molecules and materials if the quantum advantage is to be gainfully employed. For example, to implement high-efficiency quantum control of chemical reactions, we need to develop novel spectroscopy probes, such as frequency combs, that provide frequency and time domain information for exploration and control. We must develop tailored optical pulses for steering chemical processes, creating out-of-equilibrium states of molecules for specific reaction gains. We may use entangled light with time-frequency correlation to record excited state dynamics in complex systems with better spectral resolution. Finally, we are on the verge of developing a new type of imaging instrument that utilizes Bell-type readout of entangled electron (or photon) pairs after interacting with materials, thus achieving high detection sensitivity while preserving the material properties without strong perturbation or damage.

Specific Challenges and Proposed Approaches

The following pages discuss four research areas:

1. Quantum state preparation, measurement, and real-time control of molecular interactions and chemical reactions
2. New approaches for microscopy
3. Extreme sensing based on an emerging measurement strategy with long coherence, multiple qubit correlations, and many-particle entanglement
4. Understanding the connection of entanglement, thermal dynamics, many-body localization/diffusion

Research along these directions is expected to yield strong impact upon physical science. The aim is to achieve sensing capabilities orders of magnitude beyond current standards. These capabilities will enable researchers to probe fundamental physics such as quantum–gravity connection and fundamental symmetry, as well as facilitate the exploration and understanding of emerging phenomena in strongly interacting quantum many-body systems.

1. Quantum state preparation, measurement, and real-time control of molecular interactions and chemical reactions

Characterization and control of molecular transformations and chemical reactions are a central topic in chemical science, particularly in the areas of catalysis, combustion, and reaction kinetics. The relatively young field of quantum control for QIS—which impacts the realization of high-fidelity quantum gates, quantum simulation, and advanced metrological methods—has close intellectual and technological connections to coherent control of chemical processes ranging from dynamics of coupled spins in electron spin resonance and nuclear magnetic resonance studies of molecules, to control of branching pathways in chemical reactions. Chemical reaction dynamics was revolutionized in the 1980s by the development of molecular beam techniques that enabled the characterization and study of state-to-state molecular transformations, both inelastic and reactive.[97] More recently, the rapid development of the field of cold molecules has provided unprecedented capabilities in molecular state control for both the internal and external degrees of freedom, opening the door to studying and controlling chemical reactions in the fully quantum mechanical regime.[98] Also, coherent control techniques have been integrated into ultrafast spectroscopic studies of chemical and biological transformations, opening new paths to understanding the microscopic dynamics of complex molecular processes.[99] For example, optimal state preparations for photosynthetic energy and charge transfer in biosystems have been studied by 2D spectroscopy with pulsed laser light. Such experiments involve coherently shaping three phase-locked pulses. Analysis of energy flow along different molecular pathways is enhanced by controlled phase shifting of subpulses in structured pulse sequences. Recent advances in spectroscopic methods, such as the use of time-resolved direct frequency comb spectroscopy, allow mapping of real time kinetics and dynamics on molecular potential energy surfaces by simultaneous measurement of reactants, intermediates and products (Figure 12).[100] A new, exciting scientific field involves the exploration of coherent control methods that will couple to time-resolved spectroscopies to leverage these new capabilities for probing real-time chemical dynamics. The high level of quantum control needed for QIP has led to the development of both open loop control paradigms and closed ("feedback") paradigms. In QIS, coherent control is an enabler of high-fidelity operations. Research that builds on or combines these QIS coherent control techniques with emerging state preparation of molecules and ultrafast spectroscopic techniques will enable transformative chemical research targeting metastable molecular species at or near transition states, molecular conformational changes relevant to the functional control of biological processes, and the characterization of the temporal and energy scales of chemical reactions relevant to combustion and catalysis.

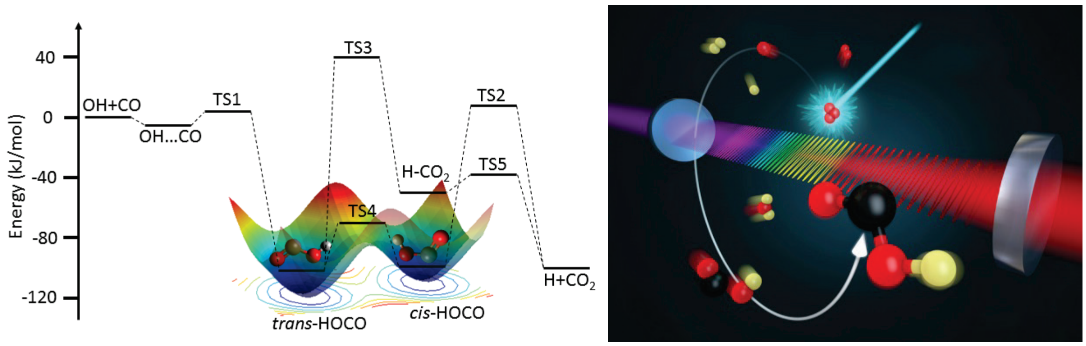

Figure 12. (Left) Potential energy surface of the OH + CO reaction showing the elusive reaction transients (see TS1 through TS5). | Reproduced from T. Q. Bui et al., Direct measurements of DOCO isomers in the kinetics of OD + CO, Science Advances 4, eaao4777, Fig. 1 (2018); copyright Bui et al., some rights reserved; exclusive licensee American Association for the Advancement of Science. Distributed under a Creative Commons Attribution Noncommercial License 4.0 (Right) An infrared frequency comb watching a reaction in real time, monitoring the transient populations of trans-HOCO and cis-HOCO produced in the ambient reaction. | Image courtesy of The Ye Group and Steve Burrows, JILA, University of Colorado

2. New approaches for microscopy

Scanning probe microscopes functionalized with individual quantum emitters like color centers and quantum dots are an ideal platform for probing material properties at the nanoscale. Because the optical properties of any two-level quantum system can be modified by interactions with the vacuum field, characterizing the optical response of quantum-emitter functionalized probes through fluorescence lifetime imaging microscopy enables the complete nanoscale description of the local density of states. In addition, quantum-emitter functionalized probes probe other fields and material properties with state-of-the art sensitivity. For instance, NV color centers in diamond nanoparticles[101] provide a particularly promising platform for high-sensitivity detection of electric and magnetic fields at the nanoscale because of the long NV spin coherence time and efficient optical spin preparation and characterization techniques. The ability to map electrical and magnetic properties of materials at nanometer length scales in ambient conditions, and with field sensitivity two orders of magnitude better than that of other scanning probe techniques, will enable fundamental advances in the understanding of the evolution of emergent properties in quantum materials. Quantum sensors have also begun to exploit noise reductions beyond the capabilities of classical devices. For example, micro-electromechanical systems such as those used in atomic force microscopes have reduced the noise levels to below the shot noise. The use of squeezed light with a specific quadrature noise below the standard quantum limit in microscopy and spectroscopy is under active investigation. With entangled optical fields, the quantum correlations can be exploited in performing differential measurements. To date, low collection efficiency has limited the benefits of squeezed light. Enhanced collection efficiency in near-field scanning microscopes, for instance, stands to enable the measurement of these enhanced statistics from squeezed excitation fields.

Electron microscopy allows the visualization of nanometer and subnanometer structures and has played a foundational role in advancing science and technology. Recently developed QIS-inspired measurement strategies appear to enable a new generation of low-damage, possibly noninvasive, electron microscopes.[102] The ultimate goal is dynamic imaging of damage-sensitive targets such as polymers and proteins, which is currently impossible with existing technology. The basic measurement principle is based on the interaction-free measurement (IFM) paradigm, which exploits counterfactual quantum measurements—i.e., values that are not directly determined—to realize a class of measurements that are damage-free for absorbing targets. In the form originally proposed by Elitzur and Vaidman,[103] the protocol is inefficient, since only a fraction of observations result in a damage-free outcome. The combination of counterfactual measurement with repeated coherent interrogation enables protocols that are near unity efficiency: the presence of an absorber can be inferred with, in principle, a vanishingly small probability of an absorbing event. This principle forms the foundation for nondestructive electron microscopy.

The quantum imaging protocols converge around common instrument architectures that achieve high-efficiency IFM through repeated interrogation of weakly phase shifting (<< 1 rad per pass), weakly absorptive (<1% per pass) imaging targets. The simplest implementation is a straightforward multi-pass protocol. The general idea is that, although the read-out/detection noise does not depend on the number of passes through the sample, the phase shift grows linearly with the number of passes. Thus, the detection signal-to-noise ratio improves with the number of passes through the sample in a phase contrast mode. The phase shift is observed using, for example, phase contrast or dark-field microscopy methods. A simple analysis shows that an efficient IFM regime can be realized with this protocol. The efficacy of this approach has recently been demonstrated in an optical microscope configuration, where noise below the single-pass photon-shot noise limit has been observed with a post-selected, pulsed interrogation configuration.[104] Previous analysis has indicated that multi-pass methods are equally effective as methods based on exotic entangled probe states and are quantum mechanically optimal for imaging applications. The potential gains associated with the use of this protocol in electron microscopy have recently been analyzed, and it has been shown to enable imaging of small proteins that cannot be imaged using conventional transmission electron microscopy methods because of beam damage.

Further improvements are expected from exploiting more complex configurations involving coupled modes. The realization of such configurations requires high-efficiency coherent electron diffraction and can be implemented with the addition of diffractive elements into a multi-pass microscope. Compact electron sources with high coherence and controlled spin states are enabled by plasmonic nanostructures, which enhance the optical driving fields in femtosecond pulsed sources. Recent demonstrations show that electron beam statistics can reach the shot noise limit. As in optical quantum sensors, the signal-to-noise ratio in such systems can be enhanced further by employing squeezed states. Such squeezed states in the electron beam would consist of reduced noise in the electron arrival time on detectors and reduced noise in a beam's amplitude or in its phase. Noise reduction in any of these variables would enable enhanced-resolution imaging with lower integration times, thereby limiting damage to the sample. The scientific payoff for low-damage or near damage-free imaging at the nanometer scale is difficult to overstate. It will enable new paths to understanding and engineering of matter and structures at the nanometer scale.

3. Extreme sensing based on an emerging measurement strategy with long coherence, multiple qubit correlations, and many-particle entanglement

Quantum-based measurements of many quantities are approaching the standard quantum limit (SQL)—a hard limit that prevents further measurement improvements using existing metrology, which relies on the quantum properties of ensembles of independent particles. The intellectual development of QIS provides an excellent opportunity to break this limit. Quantum interactions and measurement will be employed to engineer robust quantum many-body states and to create quantum correlations (entanglement) to both improve and surpass the SQL, laying the foundation for new-generation quantum sensors of acceleration, rotation, electromagnetic field, gravity, and time. These emerging tools will have transformational applications ranging from precision sensing and navigation, to quantum communication and QIS.

Control over both the internal and external quantum states of single atoms has led to today's best metrological tools for time/frequency (Figure 13), length, and magnetic fields, and to advanced capabilities for measuring electric fields, accelerations, rotations, gravity, and temperature.[105] The technology is approaching the point at which improvements in sensing capabilities based on individual-particle control have diminishing returns because of physical and practical constraints. The steady improvement in measurement precision, accuracy, and bandwidth may thus come to a halt. This situation presents a clear need for quantum sensors that operate beyond individual-particle measurement protocols.[106,107] Many-body interactions can create an energy penalty that protects quantum states against external perturbations, providing intrinsic immunity to noise.[108] Furthermore, quantum measurement noise, present with N independent atoms, provides precision and bandwidth that, as classical noise, improve as $\sqrt{N}$ (the SQL); whereas entangled atoms in a sensor can conspire to cancel each other's quantum noise in such a way that improvements can scale as N. For typical $N = 10^3$ to 10^6 particles, this affords the opportunity for orders-of-magnitude improvements in sensor precision, bandwidth, and size.

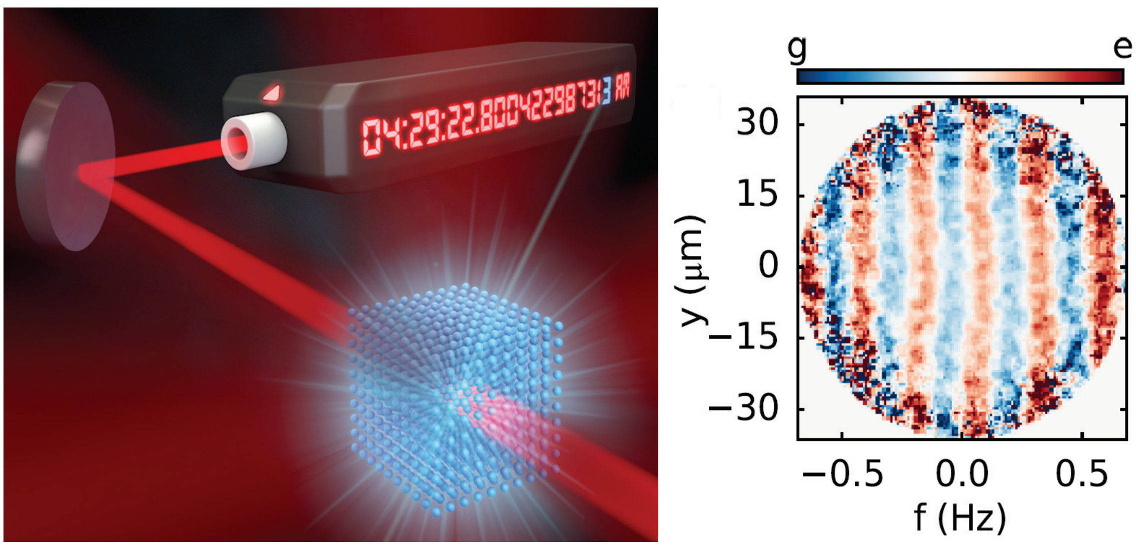

Figure 13. (Left) Optical atomic clock based on a Fermi degenerate quantum gas loaded in a 3D optical lattice. | Image courtesy of the Ye Group and Steve Burrows, JILA, University of Colorado. (Right) Imaging spectroscopy provides clock measurement precision at the 19th decimal point. Reprinted figure with permission from G. E. Marti et al., Imaging optical frequencies with 100 mHz precision and 1 mm resolution, *Phys. Rev. Lett.* 120, 103201, 2018. Copyright 2018 by the American Physical Society

Current sensing limits could be surpassed by making the leap to a new generation of quantum sensors that exploit an untapped resource for metrology: creating, controlling, and harnessing interactions to create robust (noise-resistant) many-body quantum states and entanglement between many atoms. New measurement technologies will be developed that rely on interacting many-particle states and on entanglement. Of course, this new research direction is challenging: precise control of quantum many-body states requires insights and emerging technologies, and entangled states are intrinsically fragile and difficult to create and maintain. So far, entanglement-assisted measurements have been limited to proof-of-principle experiments. To connect many-body states to robust sensing applications requires fundamental new insights and advanced technical competence to dramatically enhance measurement capabilities in prototype and world-leading sensors. To mitigate the fragility of entanglement, multiple approaches must be developed across several different physical systems for quick, robust creation of entanglement and its preservation, via interaction-energy penalties, in the presence of noise.

The rewards are great. A significant improvement in fundamental sensor efficiencies could allow technologies with reduced size, higher measurement bandwidth, greater precision, or enhanced accuracy to meet the needs of the end user. An important outcome of this research thrust will be the development of core insights and fundamental understanding to broadly guide future applications of quantum coherence, interactions, and entanglement as new and powerful tools for quantum metrology.

4. Understanding the connection of entanglement and quantum many-body dynamics

Quantum correlations are often nonintuitive. Entanglement violates either an intuitive understanding of an underlying reality to quantum states, or our notions of measurements being made in local environments. This non-local quantum correlation was referred to by Schrödinger as "the characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought."[109] Understanding of such quantum correlations has come a long way since Schrödinger's day. Currently, entanglement is used in the context of correlations and in the context of quantum information, where it has a key role in providing a valuable resource for tasks in information processing. Thus, entanglement provides insights for strongly correlated quantum materials, for understanding the complexity of many-body states, for understanding how quantum phase transitions occur, and for when and how self-thermalization occurs in closed QS. For QIS, entanglement provides a quantum communication resource for teleportation and quantum key distribution, enables quantum algorithms, and is a key component of measurement-based quantum computation. As stated in the prior section on "Extreme Sensing," entanglement will feature prominently in quantum metrology.

The quantum information perspective has shown itself to be particularly useful for understanding common features uniting very diverse dynamical phenomena, including quantum chaos, black holes, and spin systems in condensed matter. The scrambling of information in these dynamical phenomena can be measured by out-of-time–ordered correlators that give insight into the dynamics of thermalization, while the rate of growth of entanglement in many-body-localized system reveals information about the nature of the localization.

A challenge for the experimental community is to measure these quantum correlations. Although many measures of entanglement "witnesses" have been proposed, experimental measurement of these is often challenging. Alternatives to direct measurement of entanglement witnesses are indirect methods, such as a quantum gas microscope approach, in which some properties of quantum correlations are directly characterized experimentally.[110] A good challenge for quantum metrology is to go beyond characterization of state properties and ask how much information we have gained, how the information gained relates to dynamics or to a given quantum information task, and what correlations motivated by quantum information are essential for the existence of the state and its properties that were measured. An example of a specific challenge with implications for understanding quantum correlations in a wide context is how to distinguish thermal from mixed quantum states.[111] General methods of obtaining state information without performing full quantum state tomography, with its high dependence on system size, is a task for which quantum information can have critical input.

A striking development over the past five years is the emergence of protocols for the detection of entanglement in large, many-body systems that do not require full quantum state tomography. In parallel, the concept of entanglement itself has become a focus of many-body physics, as it has become increasingly evident that its properties can finely distinguish varied states of matter. Indeed, entanglement plays a key role in subjects ranging from statistical mechanics to topology. Therefore, the development of tools to quantify entanglement is central to the goal of characterizing and elucidating quantum many-body systems. These protocols for measuring entanglement rely heavily on the preparation of pure quantum states—those which are not entangled with other degrees of freedom, i.e., not coupled to a bath—and microscopic probes of particle number, position, and energy scales. These capabilities are not available in traditional condensed matter settings. Hence, ultracold atoms and molecules are a primary avenue to experimentally characterize and test the role of entanglement in many-body systems, and the continued development of a microscopic tool set is vital. For example, through quantum gas microscopy, it has become possible to extract all orders of correlation functions for a quantum many-body system. Such platforms have also allowed the microscopic tuning of Hamiltonian parameters down to lattice length scales, allowing for the tailored evolution of a quantum system. Going forward, this approach is ideally suited to tackle a variety of new challenges on the horizon, such as testing the emergence of high-T_c superconductivity in the Fermi-Hubbard model, synthesizing correlated states of topological matter, and isolating low-entropy samples of interacting spin systems of polar molecules.

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Appendix A: Workshop Participants

BES Roundtable on Opportunities for Basic Research for Next-Generation Quantum Systems

Chair: David Awschalom, University of Chicago/Argonne National Laboratory

Co-Chair: Hans Christen, Oak Ridge National Laboratory

Panel: Opportunities to Advance Scientific Understanding to Enable QIS
David Awschalom, University of Chicago/Argonne National Laboratory
Michael Flatté, University of Iowa
Danna Freedman, Northwestern University
Giulia Galli, University of Chicago
Chris Monroe, University of Maryland
William Oliver, Massachusetts Institute of Technology
Nitin Samarth, Pennsylvania State University
Birgitta Whaley, University of California–Berkeley
Amir Yacoby, Harvard University

Panel: Opportunities to Advance Instrumentation for and Based on QIS
Hans Christen, Oak Ridge National Laboratory
Peter Denes, Lawrence Berkeley National Laboratory
Stephen Jesse, Oak Ridge National Laboratory
Mark Kasevich, Stanford University
Chris Palmstrom, University of California–Santa Barbara
Darrell Schlom, Cornell University
Irfan Siddiqi, University of California–Berkeley/Lawrence Berkeley National Laboratory
Toni Taylor, Los Alamos National Laboratory
Jun Ye, JILA, University of Colorado

PRO 1: Advance Artificial Quantum Coherent Systems with Unprecedented Functionality for QIS
Amir Yacoby, Harvard University: Lead
Peter Denes, Lawrence Berkeley National Laboratory
Stephen Jesse, Oak Ridge National Laboratory
Danna Freedman, Northwestern University
Giulia Galli, University of Chicago
Darrell Schlom, Cornell University
Nitin Samarth, Pennsylvania State University
Chris Palmstrom, University of California–Santa Barbara

PRO 2: Enhance Creation and Control of Coherence in Quantum Systems
Michael Flatté, University of Iowa: Lead
Darrell Schlom, Cornell University
Irfan Siddiqi, University of California–Berkeley/ Lawrence Berkeley National Laboratory
Toni Taylor, Los Alamos National Laboratory

PRO 3: Discover Novel Approaches for Quantum-to-Quantum Transduction
Irfan Siddiqi, University of California–Berkeley/ Lawrence Berkeley National Laboratory: Lead
David Awschalom, University of Chicago/Argonne National Laboratory
William Oliver, Massachusetts Institute of Technology
Birgitta Whaley, University of California–Berkeley

PRO 4: Implement New Quantum Methods for Advanced Sensing and Process Control
Jun Ye, JILA, University of Colorado: Lead
Amir Yacoby, Harvard University: Lead
Hans Christen, Oak Ridge National Laboratory
Peter Denes, Lawrence Berkeley National Laboratory
Stephen Jesse, Oak Ridge National Laboratory
Mark Kasevich, Stanford University
Chris Monroe, University of Maryland
Toni Taylor, Los Alamos National Laboratory
Birgitta Whaley, University of California–Berkeley

Invited Participants

David Awschalom, University of Chicago/Argonne National Laboratory
Hans Christen, Oak Ridge National Laboratory
Peter Denes, Lawrence Berkeley National Laboratory
Michael Flatté, University of Iowa
Danna Freedman, Northwestern University
Giulia Galli, University of Chicago
Stephen Jesse, Oak Ridge National Laboratory
Mark Kasevich, Stanford University
Chris Monroe, University of Maryland/IonQ
William Oliver, Massachusetts Institute of Technology
Chris Palmstrøm, University of California–Santa Barbara
Nitin Samarth, Pennsylvania State University
Darrell Schlom, Cornell University
Irfan Siddiqi, University of California–Berkeley/Lawrence Berkeley National Laboratory
Toni Taylor, Los Alamos National Laboratory
Birgitta Whaley, University of California–Berkeley
Amir Yacoby, Harvard University
Jun Ye, JILA, University of Colorado

Invited Observers

Dimitri Argyriou, AMES Laboratory
Kramer Akli, DOE Office of Science, Fusion Energy Sciences
Paul Bayer, DOE Office of Science, Biological and Environmental Research
Chuck Black, Brookhaven National Laboratory
Jeff Blackburn, National Renewable Energy Laboratory
Steve Binkley, DOE Office of Science
Tof Carim, DOE Office of Science, High Energy Physics
Lali Chatterjee, DOE Office of Science, High Energy Physics
Claire Cramer, DOE Office of Science, Advanced Scientific Computing Research

David Dean, Oak Ridge National Laboratory
Jim Davenport, DOE Office of Science, Basic Energy Sciences
Tom Devereaux, SLAC National Accelerator Laboratory
Chris Fecko, DOE Office of Science, Basic Energy Sciences
Bruce Garrett, DOE Office of Science, Basic Energy Sciences
Matthias Graf, DOE Office of Science, Basic Energy Sciences
Barbara Helland, DOE Office of Science, Advanced Scientific Computing Research
Linda Horton, DOE Office of Science, Basic Energy Sciences
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Jeff Krause, DOE Office of Science, Basic Energy Sciences
Sriram Krishnamoorthy, Pacific Northwest National Laboratory
Harriet Kung, DOE Office of Science, Basic Energy Sciences
Peter Lee, DOE Office of Science, Basic Energy Sciences
Eliane Lessner, DOE Office of Science, Basic Energy Sciences
Vince Lordi, Lawrence Livermore National Laboratory
John Mandrekas, DOE Office of Science, Fusion Energy Sciences
George Maracas, DOE Office of Science, Basic Energy Sciences
Gail McLean, DOE Office of Science, Basic Energy Sciences
Raul Miranda, DOE Office of Science, Basic Energy Sciences
Shashank Misra, Sandia National Laboratories
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Jim Rhyne, DOE Office of Science, Basic Energy Sciences
Tom Russell, DOE Office of Science, Basic Energy Sciences
John Sarrao, Los Alamos National Laboratory
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Tom Settersten, DOE Office of Science, Basic Energy Sciences
Jim Siegrist, DOE Office of Science, High Energy Physics
Ceren Susut-Bennett, DOE Office of Science, Advanced Scientific Computing Research
Thiyaga Thiyagarajan, DOE Office of Science, Basic Energy Sciences
Robert Tschirhart, Fermi National Accelerator Laboratory
Jane Zhu, DOE Office of Science, Basic Energy Sciences

Appendix B: Workshop Agenda

BES Roundtable on Opportunities for Basic Research for

Next-Generation Quantum Systems

Gaithersburg Marriott Washingtonian Center • October 30–31, 2017

Monday, October 30, 2017	
7:30 – 8:30 a.m.	Registration and breakfast – Lakeside Room
Opening Session — Lakeside Room	
8:30 – 9:00 a.m.	**Welcome and Roundtable Charge** Steve Binkley, Acting Director, Office of Science Harriet Kung, Associate Director of Science for Basic Energy Sciences
9:00 – 9:45 a.m.	**Welcome, Roundtable Structure, and Summary of Homework** David Awschalom, University of Chicago/Argonne National Laboratory (Chair) Hans Christen, Oak Ridge National Laboratory (Co-Chair)
9:45 – 10:00 a.m.	Break
10:00 – 11:00 a.m.	Group Discussion
11:00 – Noon	Break and Group Discussion (continued)
12:00 – 1:00 p.m.	**Working lunch – Lakeside Room**
1:00 – 4:45 p.m.	**Parallel Panel Sessions**
	Opportunities to Advance Scientific Understanding to Enable QIS – Lakeside *David Awschalom*
	Opportunities to Advance Instrumentation for and Based on QIS – Salon G *Hans Christen*
3:00 – 4:00 p.m.	Refreshments available – Lakeside
4:45 – 5:30	**Draft Group Presentations** – Lakeside
5:30 – 7:00 p.m.	Break for dinner (location for participants TBA)
7:00 – 10:00 p.m.	**Parallel Panel Discussions** (continued) – Lakeside
Tuesday, October 31, 2017	
7:30 – 8:30 a.m.	Breakfast – Lakeside
8:00 – 10:00 a.m.	**Finalization of Group Presentations** Opportunities to Advance Scientific Understanding to Enable QIS – Lakeside *David Awschalom* Opportunities to Advance Instrumentation for and Based on QIS – Salon G *Hans Christen*
10:00 – 11:30 a.m.	**Presentation and Discussion** – Lakeside
11:30 – Noon	Roundtable adjourned

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