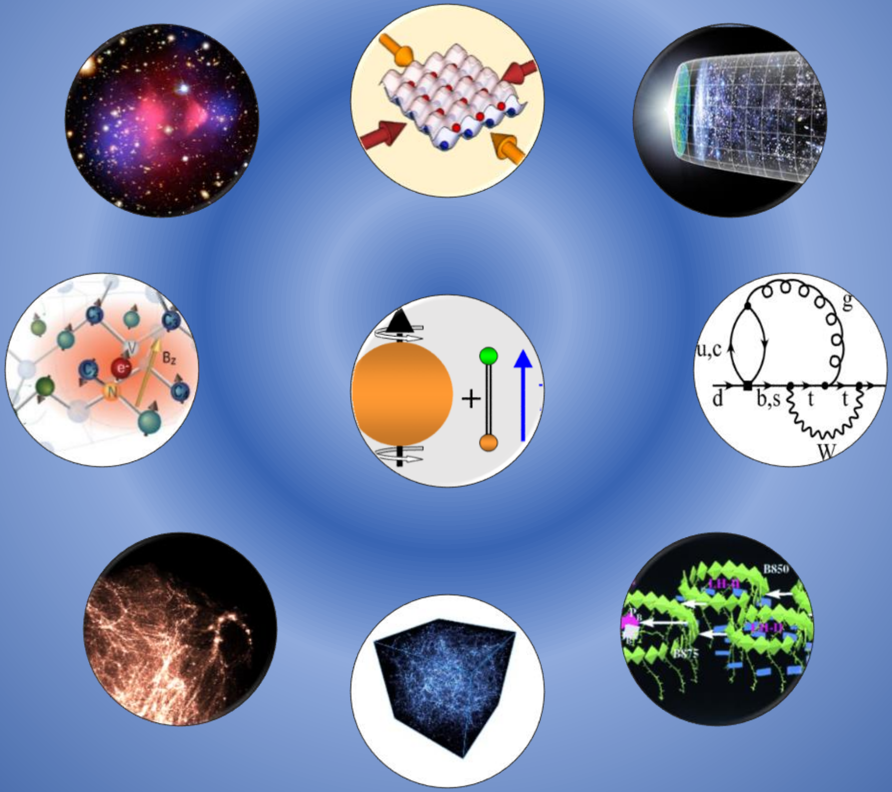
Quantum Sensors at the Intersections of Fundamental Science, Quantum Information Science & Computing

Co-Chairs: Swapan Chattopadhyay, Roger Falcone, and Ronald Walsworth

Report of the DOE Roundtable held February 25, 2016



U.S. DEPARTMENT OF
ENERGY
Office of Science

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This is a report of a Roundtable that was held on February 25, 2016, at the Hilton Gaithersburg, MD. The Roundtable was approved by the DOE Office of Science Associate Directors Jim Siegrist, High Energy Physics (HEP) and Steve Binkley, Advanced Scientific Computation Research (ASCR). The Co-Chairs Ronald Walsworth (Harvard University), Swapan Chattopadhyay (FNAL), and Roger Falcone (LBNL) invited the participants and organized the meeting in response to the DOE charge.

Federal Agency officials Altaf Carim (OSTP), Steve Binkley (DOE ASCR), Jim Siegrist (DOE HEP), Carl J Williams (NIST), and Denise Caldwell (NSF) attended and presented perspectives from their agencies. Other Federal Agency representatives in attendance: Laura Biven and Ben Brown (DOE Office of Science); Barbara Helland, Claire Cramer, Carolyn Lauzon, Robinson Pino, and Ceren Susut (DOE ASCR); Tom Russel and George Maracas (DOE BES); Eric Colby and Lali Chatterjee (DOE HEP); Michael Cavagnero (NSF). The DOE POC for the meeting was Lali Chatterjee (DOE HEP).

The Report is organized as follows:

Executive Summary, Report, List of Participants with Affiliation, Agenda, Charge Letter

Image Credits:

Top row left NASA/WMAP Science Team; top row center Trey Porto, JQI/NIST; top row right NASA/CXC/CfA/M. Markevitch *et al.*; middle row left Paola Cappellaro, MIT; middle row center and right David DeMille, Yale University; lower row left and center simulations under the INCITE program at ALCF and OLCF by the DOE funded Argonne HACC team; lower row right Klaus Schulten, University of Illinois

Cover Design: Michael Cooke (DOE HEP)

Executive Summary

An invited group of leading US quantum scientists, joined by interested officials from Department of Energy (DOE) Office of Science (SC) and other Federal science agencies, met in the DC area for an all-day 'Roundtable' discussion on February 25, 2016. Agency representatives from Office of Science and Technology Policy (OSTP), DOE, National Institute of Standards and Technology (NIST), and National Science Foundation (NSF) shared introductory remarks from Agency perspectives, followed by scientific presentations from Roundtable participants about opportunities & challenges at the 'Quantum Frontier' — i.e., the rapidly growing and interdisciplinary field of quantum science and technology. Supporting materials were also provided by experts who were invited but could not attend the Roundtable. Participants represented specialized expertise within the intersecting fields of quantum information science (QIS), quantum sensors, fundamental science, computing, materials science, and a wide range of applications. Scientific and technical topics discussed included the use of high-precision quantum techniques, many realized in 'table-top' experiments, to probe physics at very high energy (beyond tera-electron-volts) scales; the possibility of engineering/building useful 'quantum machines' (e.g., quantum computers and communication networks); advancing quantum sensors to enable atomic-scale sensing, imaging, and control for diverse applications in both the physical and life sciences; developing networks of quantum sensors to provide unique capabilities to probe dark matter, gravitational waves, and other 'weak' physical phenomena; quantum simulators for chemistry and other fields; and synthesizing, probing, understanding, and controlling quantum materials using diverse methods. There was then a productive discussion focused on: (i) identifying the most promising scientific directions at the Quantum Frontier; (ii) detailing what is needed to advance progress in the US most effectively; and (iii) suggesting key roles that DOE could play in this effort, consistent with its mission.

Roundtable participants felt that the most promising areas for advancement in quantum science include continued development and interdisciplinary application of the diverse portfolio of quantum sensors (e.g., solid-state, optical, atomic, microwave, hybrid); use of high-precision quantum technologies, including quantum networks, for high-energy and dark sector physics; build-up of a research and educational base in quantum engineering to enable useful quantum machines beyond sensors (e.g., quantum computers); and progress in advanced materials and theory coupled to the scientific opportunities and needs of quantum science. The participants recognized the growing impact of quantum science and technology on a wide range of both the physical and life sciences, and hence the importance of maintaining national leadership while fostering international collaboration and keeping in mind competitive aspects (e.g., commercial and security issues). To this end, the Roundtable identified a complementary set of mechanisms to maintain US leadership in quantum science, including implementing intermediate- and larger-scale project models, specialized facilities at government laboratories, and re-optimization of existing research portfolios and programs. In particular, Roundtable participants felt that DOE SC could effectively advance the Quantum Frontier via a portfolio of mechanisms: (a) to provide external research funding across a variety of scales of time, project and team size, institution type, career status, and idea maturity, all of which are essential for optimal progress; and (b) to enable effective integration of DOE lab capabilities (both DOE scientists and facilities) with the external quantum science community, e.g., supporting collaborations between DOE scientists and peers at universities and elsewhere through both financial and administrative mechanisms. Following the Roundtable, the Co-Chairs constructed the present report, in consultation with all Roundtable participants and agency representatives. The remainder of the report, below, summarizes the background, opportunities, and challenges at the Quantum Frontier, provides suggestions for maximizing DOE impact in this field, and concludes with several 'Case study' reports of highlights from the Quantum Frontier.

Quantum Frontier — Background

Over the last twenty years, there has been a boom in *quantum science* — i.e., the development and exploitation of quantum systems to enable qualitatively and quantitatively new capabilities, with high-impact applications and fundamental insights that can range across all areas of science and technology. R&D at this 'Quantum Frontier' is now one of the most productive areas of the physical sciences: producing a disproportionate fraction of the papers in top journals (*Science*, *Nature, Physical Review Letters* et al.), attracting many of the best students, and recently enjoying large-scale investment from governments outside the US, as well as increasing commercialization interest including from major tech companies (e.g., Google & Microsoft). Interest in modern quantum science — including what is referred to as 'quantum information science' or QIS — was driven initially, in the 1970s and 1980s, by theoretical work on using quantum entanglement as a resource for computing and cryptography. By the early 1990s the first experimental efforts had begun on basic quantum logic realizations using single quantum bits ('qubits'). Importantly, these pioneering experiments were mostly performed in the US — in government labs, universities, and industry — with key support from the US government (mostly NIST, DOD, NSF and the intelligence agencies). Later, interest and activity grew in quantum simulation and communication — including research at the intersection of QIS, quantum field theory, and black hole physics — and most recently in quantum sensing, metrology, and imaging. Throughout this several decade period, the quantum science community expanded and diversified with the discovery of emergent quantum phenomena in condensed matter systems (e.g., the Quantum Hall effect, topological insulators), the realization of new states of matter (such as Bose-Einstein condensates and degenerate Fermi gases), continued advances in theory such as topological quantum computing, and the thrust to harness quantum degrees of freedom for practical applications (e.g., spintronics).

A key feature of quantum science is the close, cross-disciplinary interaction with more 'traditional' research areas in atomic, molecular, and optical (AMO) physics, condensed matter physics, and high energy physics, primarily because many of the scientists come from these communities and are interested both in what their communities can do for quantum science, and vice versa. In particular, there has been effective synergy between developments in quantum science and the drive for better precision measurement tools for metrology, sensing, imaging, and control, with applications ranging from fundamental physics (e.g., gravitational waves, beyond-Standard-Model physics, the 'dark universe') to materials science (e.g., topological insulators, quantum defects in solids) to biology (e.g., single protein NMR, brain science) and beyond. As just one example, David Wineland of NIST shared the 2012 Nobel Prize in Physics for his work in experimental quantum science using trapped ions, with which he and his team demonstrated the first quantum logic gate, made major advances in atomic clocks, and performed pioneering tests of fundamental physical laws and symmetries. Several other 'Case studies' of successful and ongoing translations of knowledge and technology at the Quantum Frontier are provided below in the section *Reports from the Quantum Frontier*.

Quantum Frontier — Opportunity

Everything is quantum. That is, the universe is described at its most fundamental level by quantum physics, and thus the ultimate solutions to scientific and technical problems are eventually found at the Quantum Frontier. This claim is not a trivial observation or a far-off dream — it is a great opportunity. Twentieth-century quantum science provided many of humanity's best tools, such as atomic clocks for GPS navigation; lasers for high-speed communication, fabrication, and imaging; semiconductors for modern computing; and NMR/MRI, enabled by superconducting magnets, for drug development and medical imaging. As summarized above and detailed in the 'Case studies' below, progress in quantum science has greatly accelerated in the twenty-first century, with remarkable advances in diverse fields and the promise of much more on the horizon. In addition, the cross-disciplinary nature of work at the Quantum Frontier has forged ever-stronger connections between almost every area of science of relevance to the DOE: high energy physics, chemical sciences, materials science, applied math, computer science, and even parts of the life sciences and geosciences.

What is harder? Unifying the Standard Model and General Relativity? Understanding the origin of the universe? Building a useful quantum computer? Understanding the brain and consciousness? Curing cancer? Providing cheap green energy and addressing climate change? Many of these grand challenges are central to the DOE mission. All will require breakthroughs at the Quantum Frontier, to allow us to measure and control matter and energy with ultimate efficiency and optimal result.

For example, dramatic recent improvements in optical atomic clocks allow the effects of General Relativity (curved spacetime) to be sensed in a small, table-top experiment. Similarly, by exploiting quantum effects in atoms and molecules, precision searches for a permanent electric dipole moment (EDM) of the electron in table-top experiments provide some of the most sensitive probes of supersymmetry. Over the next decade or so, quantum techniques should provide further multi-order-of-magnitude improvements in sensitivity for these and many other quantum sensor experiments addressing forefront high energy physics problems. A particularly promising approach is to create distributed networks of quantum sensors to detect gravitational waves, dark matter, and other new physics. In addition, further development of high Q microwave cavities, coupled with Quantum Non-Demolition (QND) single qubit techniques, could provide ultra-sensitive probes of dark matter; and experimental techniques exploiting entanglement may allow us to probe the intersection of black hole physics and QIS. Over the last decade, quantum sensors have also been integrated with nanoscience to yield a transformative set of new tools based on quantum defects in solids like diamond, enabling imaging, sensing, and control at the atomic scale, such as the recent demonstrations of room-temperature MRI with single proton resolution and NMR of a single protein molecule. There is tremendous potential for such quantum sensors across many fields of science — biology, chemistry, materials science, geoscience — and also to facilitate high-impact applications in the near term, e.g., to aid the development of advanced materials to address challenges in green energy and beyond Moore's Law computing. The original motivation for modern quantum science — using entanglement as a resource for computing and cryptography — has also experienced rapid recent progress, such that useful quantum computers are now a realistic grand challenge rather than a far-off aspiration, with intense interest and investment from major technology companies and foreign governments.

Quantum Frontier — Challenges

There are both technical and cultural challenges to progress at the Quantum Frontier, since it is a manifestly cross-disciplinary activity that operates across a wide range of scientific disciplines and 'scales' — e.g., the timescale for projects, size of teams, and need for resources. Therefore, leadership in the US is needed at the institutional and national level to lower cultural barriers, facilitate technical leaps forward, and provide the kind of support needed for continued rapid advances in quantum science and effective translation between disciplines and into applications.

Technical challenges include: (i) improve the performance (sensitivity, fidelity, dynamic range, control, robustness) of single qubit and semiclassical qubit ensemble technologies (e.g., atomic clocks and interferometers, solid-state sensors, microwave cavities, superconducting sensors, optics); (ii) develop, optimize, and scale up qubit networks — both spatially distributed semiclassical networks and entangled networks; (iii) develop and optimize new advanced materials, including solid-state hosts for atom-like qubits (e.g., diamond and other semiconductors), materials with emergent properties (analogous to graphene and topological insulators), and materials developed by learning lessons from evolved (natural) biological and chemical materials; (iv) develop hybrid quantum technologies for optimized, multi-modal function (e.g., to sense, process, store, and communicate quantum information and also control the environment); and (v) develop new theoretical approaches to utilize quantum technologies, connect with fundamental problems in quantum field theory and beyond Standard Model physics, and motivate new directions.

In the US, one cultural challenge to progress at the Quantum Frontier is that at most universities and major laboratories, quantum science is not recognized as a distinct discipline. Thus existing mechanisms for hiring, promoting, and allocating institutional resources are often not optimally matched to the rapid rate of progress and needs of the field. For example, at many top US universities, leading researchers in quantum science are spread thinly across multiple departments — physics, applied physics and math, engineering, chemistry, computer science et al. Though the total effort may be strong, and many of these researchers work closely together, they are small minorities in their individual departments, and hence struggle for resources, advancement, and the hiring of additional quantum science colleagues. Similarly, at government labs and other large scientific institutions, work at the Quantum Frontier crosses disciplinary barriers and thus can face many roadblocks, such as needing approval from multiple divisional chiefs, not being simultaneously aligned with strategic plans in multiple divisions, etc.

A second cultural challenge in the US is for sponsoring agencies to respond optimally to the great scientific opportunities presented by the Quantum Frontier and its rapid progress. In particular, existing funding 'silos' (usually aligned with traditional disciplinary boundaries) and program types are often not well matched to the reality of making progress in quantum science: e.g., the need to support cross-disciplinary teams addressing problems outside of any discipline; the need for long-term awards (5+ years) and multi-PI team awards to address grand challenges; the need for funding coordinated efforts at universities, government labs, and industry to allow effective translation of quantum technologies into practical application; and the great benefit provided by modest-sized seed grants to allow pursuit of high-risk/high-reward ideas. For example, one of the recent quantum science success stories is the development of nanoscale sensors for electromagnetic fields and temperature using nitrogen-vacancy (NV) quantum defect complexes in diamond. US researchers originated this field and have realized most of the high-impact applications to date (see Case study #1 below). However, it has been a struggle to get Federal funding for many in the growing community of US researchers who want to pursue diamond quantum sensing, as it sits between disciplinary boundaries. In addition, there is no reliable US source of 'quantum grade' diamond— Japan and the UK are leaders in this materials area — which impedes and endangers continued US progress.

It is useful to compare the present status of work at the Quantum Frontier in the US and elsewhere. Clearly, the US has many strengths: the largest and most diverse scientific community; the strongest track-record of path-breaking advances; and the most vital entrepreneurial culture. However, many other leading nations (and groups of nations) are well ahead of the US in overcoming the cultural issues listed above. Simply put, other major nations (UK, Germany, China, Japan, Australia, Canada, Russia, Austria, Denmark, Netherlands, Spain, others) are making major investments in quantum science and technology. They are also working intentionally to remove the other cultural barriers that impede progress and to recruit leading scientists from other countries, often targeting US scientists. In particular, many leading experts in quantum science have left the US in recent years for foreign institutions, including native-born US citizens (a 'reverse brain drain') — primarily due to struggles with the cultural issues described above. [Roundtable participants are also aware of many more US leaders in quantum science who are being actively wooed to leave the US, for similar reasons.]

Quantum Frontier — Suggested Role for DOE Office of Science

> ***"The mission of the DOE Office of Science (SC) is the delivery of scientific discoveries and major scientific tools to transform our understanding of nature and to advance the energy, economic, and national security of the United States."*** — official DOE SC mission statement.

As emphasized above and in the 'Case studies' below, this ongoing DOE SC mission necessitates continued progress at the Quantum Frontier. The US is currently a leader in quantum science and technology, and has frequently been the pioneer in quantum science breakthroughs and in translating quantum technologies into applications. However, whereas most other developed nations have already recognized the importance of the Quantum Frontier and are making large, long-term investments, a focused, consistent program of support in the US needs to be developed and maintained.

Roundtable participants envision a coherent and evolving portfolio of mechanisms by which the DOE SC can support and be closely involved with the inter/cross/multi-disciplinary activities at the Quantum Frontier, in order to optimize the return on investment and in service of the DOE mission. Such a dynamic portfolio may be preferable to a new 'silo' — i.e., a new program on quantum science and technology that appears on the DOE SC org chart parallel to or within HEP, ASCR, BES et al — and could be aided by consultation with an external advisory group to stay abreast of the latest developments in quantum science. A possible outline for such a portfolio, which builds on other successful efforts, is suggested here:

- Multi-PI, 5-year research program
  An external funding program to support multi-PI teams (typically 5-10 PIs per team) over 5 years to address 'key challenges' in DOE-relevant quantum science and technology, in loose analogy with the DOD MURI program. [MURI stands for Multidisciplinary University Research Initiative.] It would be ideal for this program to address the diversity of opportunities in quantum science, as well as the benefit provided by healthy competition on state-of-the-art problems. Thus, the optimal program could feature several new topics (i.e., key challenges) per year, with more than one team awarded per topic, ideally allowing support of participants from universities, government labs (DOE and non-DOE), nonprofit research centers, and industry, as needed to best address the key challenge. Note that some key challenges may merit continued support over more than one 5-year cycle.
- Long-term, mid-scale programs to address grand challenges
  An external funding program to address 'grand challenges' in DOE-relevant quantum science and technology that require both support over a decadal timescale as well as larger, multidisciplinary teams (~50 people). Example challenges could include developing, implementing, and operating a large-scale network of quantum sensors for probing beyond Standard Model physics; or realizing a prototype, fully functioning quantum machine with transformative capability (e.g., in information processing).
- Program to support collaboration between DOE-supported labs & non-DOE quantum scientists
  A flexible program to facilitate productive partnerships between DOE scientists and researchers in universities, other government labs, nonprofit research centers, and industry. The program could provide a wide variety of resources as needed to engage DOE-supported labs with external collaborators and advance DOE-relevant quantum science and technology: e.g., funding for DOE and non-DOE personnel to perform collaborative projects, where some key aspect of the work (not necessarily all) requires DOE facilities and/or personnel; shared space or equipment at DOE labs; funding for the collaborative development of new instrumentation either for eventual use at a DOE lab or non-DOE facility. To address the diversity of opportunities in quantum science, it would be ideal for there to be many new awards per year, i.e., several for each DOE lab involved with quantum science.

- Young investigator program
  An external funding program to support new PIs across all areas of DOE-relevant quantum science and technology, with the selection of the most promising young scientists taking precedence over near-term-DOE-relevance of the proposed projects, in order to attract the best young minds to the field.
- High-risk/high-reward program
  An external funding program to support high-risk/high-reward new ideas across all areas of DOE-relevant quantum science and technology, with the selection of the most exciting new ideas from people with a track record of success taking precedence over the risk of the idea. Again, to address the diversity of opportunities in quantum science and optimally encourage innovation, it would be ideal for there to be several new awards per year.
- DOE SBIR/STTR program for quantum science & technology
  As part of the existing DOE SBIR/STTR program, a modest fraction of awards (perhaps 10 per year) could be targeted at the translation of DOE-relevant quantum science and technology into commercialization via small-scale technology start-up companies. The experience of many Roundtable participants is that such modest-scale awards can be critical for early-stage commercialization in quantum science and technology.

Reports from the Quantum Frontier

The Roundtable identified many promising areas of opportunity in quantum science and technology. Here, a few selected examples are provided, in the form of 'Case studies'. These examples are illustrative, and not meant to be exclusive.

Case study #1 — Solid-state quantum sensors with broad application in the physical & life sciences

Recently, there has been great progress in the development and application of atomic-scale defects in solids as robust, nanoscale quantum sensors of a wide variety of phenomena across the physical and life sciences. Typically formed by introducing selected dopants in solid crystals, these quantum defects feature tightly localized electronic states that behave much like single atoms frozen inside and largely isolated from the solid lattice. Similar to atoms and ions, their quantum states can be prepared, manipulated, and measured using light, often under ambient conditions, and they can also be very sensitive to electric and magnetic fields, temperature, and other phenomena of relevance to many applications. In addition, such solid-state systems can be fabricated and integrated into a wide range of devices, including at the nanoscale, enabling a new class of quantum sensing and imaging technologies.

To date, the most well-known and widely applied of these solid-state quantum sensors is the nitrogen-vacancy (NV) color center in diamond. In particular, NV centers provide a unique combination of excellent magnetic field sensitivity and nanoscale spatial resolution while operating over a wide range of temperatures from cryogenic to well above room temperature. Because NV centers are atomic-sized defects and can be created close to the diamond surface, they can be brought within a few nanometers of a sample, greatly enhancing the sample's effect on the NV sensor and enabling nanometer resolution. For magnetic field sensing, one optically detects the Zeeman shift of the NV electronic spin levels. Similar techniques can be used for nanoscale electric field and temperature sensing. In addition, NV-diamond has other enabling properties:

fluorescence that typically does not bleach or blink; a wide range of device geometries, from nanodiamonds to high NV density bulk samples; and compatibility with most materials, including metals, semiconductors, liquids, polymers, and biological tissues.

Applications of NV-diamond quantum sensors are rapidly advancing and diversifying, with translation of the technology into other fields accelerating and commercialization beginning. Some highlights since 2014 (all from US groups) include: (a) NMR detection of a single protein and MRI of a single proton with Angstrom resolution, which may lead to structure determination of individual proteins and other materials of interest with atomic-scale resolution; (b) noninvasive sensing and imaging of biomagnetism in living cells and whole animals with submicron resolution, e.g., the pulsed magnetic field from the action potential of individual neurons, which provides a powerful new platform for studies in cell biology, genetics, brain function and disease, as well as lab-on-a-chip bioassays; (c) *in vivo* nanodiamonds used to map temperature and chemical changes in living human cells, which may be applied in the near term to guide thermoablative therapy for tumors and other lesions, and in the longer term to monitor and even repair *in vivo* damage at the cellular and molecular level; (d) mapping of heterogeneous magnetic materials within primitive meteorites and early Earth rocks (>4 billion years old) with submicron resolution, which is providing breakthrough advances in the understanding of the formation of the solar system and Earth, and may be deployed more generally to probe multi-phase magnetic solids that could be used for beyond-Moore's-law information processing; (e) imaging patterns of magnetic fields present in advanced materials (e.g., skyrmions, multiferroics) at the nanoscale, which can fill a critical technical need in the exploration and targeted development of smart materials for challenges in energy, the environment, electronics, and more; and (f) robust bulk diamond and nanodiamond sensors for extreme environments (underground, underwater, extreme heat, radiation, pressure, etc.). A MURI-like program at DOE (as outlined above) would be well-suited to support such interdisciplinary applications of solid-state quantum sensors.

Case study #2 — Quantum sensors to probe physics beyond the Standard Model

Ultra-precise measurements of quantum phenomena can be used as extremely powerful probes of new physics at very high energy scales, e.g., by testing fundamental physical symmetries and laws, and by searching for new phenomena such as that associated with the 'dark sector'. For example, one of the most exciting opportunities at the Quantum Frontier is searches for an electric dipole moment (EDM) of the electron, as well as related quantities in atomic nuclei, which arise at a measurable level only from charge-parity (CP) violation beyond that in the Standard Model. Since additional CP violation is found in nearly every theoretical model that includes new physics at higher energy scales, precision EDM searches are one of the most attractive approaches to discover new physics or constrain leading theories. Recent EDM measurements (e.g., by the ACME collaboration at Harvard and Yale) are already sensitive to new physics at the TeV scale: in some models (e.g., the simplest supersymmetric models) the experimental reach is already approaching 10 TeV. Conversely, should new particles be found at the Large Hadron Collider (LHC) at CERN, EDM experiments will provide important information about the CP-violating interactions associated with these particles, complementary to that directly accessible with collider data or from intensity-frontier projects.

Current EDM experiments exploit methods closely related to those developed for quantum sensor technologies such as magnetometers and atomic clocks. Recent advances have led to 10x improvements in the sensitivity of these experiments. Anticipated near-future developments in quantum science are opening the prospect for further, rapid improvement — likely by several orders of magnitude over the next 10-20 years. These developments include new methods for cooling and trapping polar molecules (which are used to amplify the EDM through quantum interference effects), motivated largely by the utility of molecules for quantum simulation; and new methods for spin squeezing, controlling spin decoherence, and exploiting entanglement, which are currently being actively pursued because of their applications to quantum sensors.

In addition to EDM experiments, ultra-precise quantum sensors offer many other promising approaches for probing beyond Standard Model physics. In particular, the Roundtable participants expressed great enthusiasm for the development of networks of quantum sensors optimized to search, e.g., for classes of non-WIMP dark matter (topological defects, ultra-low-mass models); violations of Lorentz and CPT symmetry; temporal variations or oscillations of fundamental physical constants; anomalous spatial variations or oscillations of physical interactions (e.g., sourced by new couplings to mass); long-distance breakdowns in standard quantum mechanics interpretations of entanglement; and many other phenomena. See also Case study #5 below.

The recent progress and opportunities highlighted here also illustrate the need for increased and optimized support for Quantum Frontier experiments. In particular, most experiments in this field have historically been performed by a single PI university group and funded by modest 3-year grants through the NSF. This approach seeded great innovation, but has become inadequate at providing the resources needed to push increasingly complex and difficult experiments to completion. For example, the best electron EDM experiment to date by the ACME collaboration — which sets the tightest limits on supersymmetric theories of any class of experiment — required the combined efforts and expertise of 3 PI groups. However, this recent success was possible only due to one-time ARRA stimulus funds from the NSF for a special 5-year duration. In many ways, this subfield has reached a position similar to that of accelerator-based high-energy physics about 50 years ago, when it became clear that an increase in the size of collaborations and facilities was needed to make continued progress. DOE is uniquely positioned to play a key role in facilitating this type of progress and thus have a transformative impact in very-high-energy-scale physics.

Case study #3 — Quantum information processing gets real

Quantum computers are able to solve tasks that are intractable using non-quantum devices, owing to the exponential storage capacity of qubits — e.g., the full representation of 300 qubits using classical means would consume every particle in the universe. While some applications such as factoring and database search seem to require millions of coherent quantum gate operations over thousands or more entangled qubits, there are now more specialized applications that are gathering attention. For example, quantum simulators using of order 100 qubits can tackle certain problems involving condensed matter systems such as magnetic phenomena or high-temperature superconductivity, as well as provide key insights on quantum field theories. By programming qubits to represent the couplings between electronic-bound molecular systems, such special-purpose quantum computers could also attack longstanding problems in quantum chemistry and materials science. Furthermore, by manipulating and 'cooling' a set of qubits with programmable interactions, it may be possible to optimize/minimize certain many-dimensional nonlinear functions whose global properties cannot easily be extracted. Such a quantum optimizer could provide enormous payoffs in the areas of operations research, pattern recognition, and machine vision.

In the laboratory, researchers are now programming and manipulating dozens of entangled qubits, mainly in the areas of atomic and solid-state physics. In particular, trapped atomic ions can be laser-cooled to be nearly at rest in electromagnetic traps; and further, laser fields can coherently manipulate and entangle the atoms and also readout the atomic qubits with very high fidelities. Superconducting Josephson junctions can now be integrated on a chip and coupled with microwave fields for the generation of simple 2D quantum circuits. Other promising examples include the use of trapped neutral atoms and crystal defects in the solid-state. These quantum technologies are complementary in use, owing to their differing gate speeds and natural connectivity, and are poised to push through soon to 100-qubit machines.

These experimental platforms are also confronting the technical limits of somewhat exotic hardware: narrow-band stable lasers, ultra-high vacuum, cryogenic devices, and integrated microwave circuitry. Such experiments are fast approaching the boundaries of conventional university research, with a much-needed focus on engineering efforts that could parallel the evolution from the first germanium transistor in 1947 to the VLSI chips of today. Quantum computers, like any computer, must ultimately be operated by people that do not know (or care) about the physical platform inside. While a few US companies have begun efforts to fabricate small superconducting quantum computers (Google, IBM, Intel) and trapped atomic ions (Honeywell, Lockheed), they lack a substantial qualified workforce to execute these plans.

It is likely that in the next 5 years, quantum research devices will finally be able to solve problems that are intractable with classical devices. To maintain its leadership, the US must establish a research base in quantum engineering that currently does not exist. The linking of DOE laboratories with DOE programs that fund the broader research community may be an optimal vehicle for the US to acquire such quantum engineering capability.

Case study #4 — Advanced materials for enhanced quantum sensors

The discovery, development, and application of new quantum sensors has an inextricable relationship to and dependence upon the discovery and development of the concomitant 'advanced materials' — whether those materials be lattices of atoms, solid-state quantum defects, hybrid quantum systems, or new classes of topological materials with emergent quantum properties such as exceptional robustness in information transfer. Given the exquisite sensitivity of quantum sensors to their environment, the full understanding and implementation of advanced materials for key DOE SC challenges has a much broader reach and requirement than one commonly invokes for materials development. Thus, the requirements for their further development are similarly broad.

In particular, the requirements go substantially beyond those of simulation and modelling alone, although these capabilities certainly play important roles in both prediction and description. For example, the groundwork of theory for topological insulators was established well before the first experimental demonstrations over the last decade. Similarly, the wealth of high-precision applications that continue to be generated from NV-diamond quantum sensors have stimulated questions about the possible existence of additional quantum defects in solid state materials, where exceptional spin coherence, coupled to distinctive photon states might generate a broad array of new quantum sensors. Currently, Density Functional Theory (DFT) calculations are being used to suggest possible new candidate materials; and some of the experimental ramifications of those calculations and predictions are being actively pursued today.

Similarly, continued development and optimization of advanced materials for quantum sensing will provide substantial challenges in the way that one places and activates the critical components of the material, and in the ways that these materials are processed and shaped into sensor structures. This lesson has already been learned well with NV-diamond (see Case study #1 above), where considerable challenges remain not only in the means by which one introduces the centers into the diamond material, but even in the delicacy of the way in which one can clean and prepare diamond structures without degradation of the critical sensing element. Materials properties are also often a key challenge for the rapidly diversifying class of hybrid quantum sensors and other devices, which commonly integrate multiple types of quantum systems (solid-state, photonic, etc.) to tailor and optimize overall system performance. Examples include superconducting materials, optimizing interfaces for high-Q microwave cavities, nano-optics materials for high-fidelity readout of

QIS or sensor signals, and controlling dissipation in active mechanical elements for force microscopy. Thus, there is a need in the US to invest in a set of tools for fabrication and analysis of quantum sensor materials, which may well necessitate new, shared facilities, including at DOE labs. In contrast to fabrication foundries that can perform rather routine processes and analysis, however sophisticated, these quantum sensor facilities must be accessible to knowledgeable users in the broader quantum science community, who can rapidly evaluate the feedback between process, analysis, and sensor performance.

Importantly, the effectiveness of new quantum sensors depends not only on the quality of the single reporter (e.g., the NV center), but also on the integrated device structure that can provide both the necessary passivation of the material structure as well as the means for robust transfer of the signal over distances much longer than the sensor-sample distances. An important advantage for NV centers in diamond is the rather natural coupling between particular spin states and photon signals. Thus, an integrated structure that guides and perhaps amplifies that photon signal can become a natural component of a quantum sensor structure. This is one reason for emphasizing continued investigation of quantum materials such as topological insulators: beyond the host of important sensing capabilities they may exhibit, their natural immunity to disorder in electron transport makes them an important complement to quantum sensing systems. For example, topological insulators with robust electronic transport have recently given rise to analogs for photon and phonon propagation. It is expected that these kinds of advanced materials will be engineered through further strategic integration of materials synthesis and processing.

Finally, there has been increasing evidence of quantum coherence in biological structures: this nascent field potentially offers vast new possibilities for advanced materials for quantum sensing. Important advances have been recently made in quantum sensors that are biocompatible. This largely untapped area of investigation could provide advanced materials for quantum sensing of biological structures (e.g., proteins) that would truly be biocompatible. As well, one could benefit enormously from understanding the role and robustness of quantum coherence in systems in aqueous environments, at room temperature and higher.

In summary, the successful development, optimization, and application of quantum sensors depends critically on the continued discovery and utilization of advanced materials. A DOE SC investment in advanced materials for quantum sensors has much broader ramifications and needs than the more conventional notions of 'materials development': it will require a closely-integrated effort of simulation, theory, synthesis, analysis, and processing. In particular, a DOE SC facilities and support program to develop advanced quantum sensor materials and translate them to the wider community could be transformative in its impact.

Case study #5 — Quantum sensors for dark sector physics

Answers to the many profound puzzles confronting fundamental high energy physics may emerge from new 'dark sectors' that contain light degrees of freedom but have ultra-weak couplings with the Standard Model. Examples include axions, relaxions, and hidden photons that are known to emerge in a variety of theories. These particles can naturally be dark matter or be identified with the field responsible for dark energy. Recent theoretical advances have also shown that the interactions of these particles with the Higgs boson can potentially explain the hierarchy problem through dynamical evolution. Similarly, it has long been recognized that it would be difficult to solve the cosmological constant (or dark energy) problem with new physics that has Standard Model interaction cross-sections. Thus, dynamical mechanisms involving light, ultra weakly coupled particles may hold the key to understanding this puzzle as well.

Due to their low mass and ultra-weak interactions, dark sector particles rarely interact with conventional detectors; and even when they do, the energy deposited in the interactions is too small to be observed. However, these particles can potentially be observed through their subtle quantum mechanical effects. In addition, quantum sensors may probe the underlying physics of cosmic acceleration, either through the detection of fields that contribute to dark energy or direct observation of cosmic inflation through primordial ripples in space-time sourced during inflation. In recent years there has been rapid progress in the technical performance of quantum sensors for dark sector physics, as well as a growing appreciation of the potential for discovery at the Quantum Frontier.

The required performance of a particular quantum sensor depends on the application. Signals that oscillate significantly in both space and time can be produced in controlled laboratory conditions or originate from disturbances propagating in space-time. For example, hidden photons can be sourced in high Q RF or microwave cavities and subsequently detected in a low noise, high Q receiver employing SQUID amplifiers. Alternatively, signals that predominantly vary in space can be produced by new fundamental forces that are sourced or screened by test masses. These forces can be subsequently detected using quantum probes such as atom interferometers and micro/nano-mechanical harmonic oscillators that can be controlled in the quantum regime. In particular, the low matter density of atom interferometers can greatly increase the sensitivity to some classes of dark sector physics relative to bulk-matter experiments. If these forces are spin-dependent, they can be detected using precision magnetometry. Signals that vary predominantly in time can arise from cosmic sources. For example, dark matter candidates such as axions can interact with a large DC laboratory magnetic field to create a free space AC current that pumps power into a high Q microwave or RF cavity; or can induce nuclear spin precessions that can be observed through precision magnetometry. In contrast, relaxions cause time dependent correlations and a cosmic gravitational wave background from the end of inflating cosmic era that may be detected using optical and atom interferometers, such as the SURF facility being developed with DOE support. Transient effects in detectors can also arise if localized clumps of energy (such as domain walls) occasionally pass through the Earth, leading to rapid excitation and de-excitation of quantum sensors. All together, progress in quantum sensors — such as breakthroughs in high Q microwave/RF cavity technology developed at DOE accelerator laboratories — have made experimentally accessible a large parameter space of well-motivated ultra-light dark matter (mass ~10^{-22} eV - 10^{-3} eV). Therefore, a DOE investment in this area is especially timely.

Case study #6 — Precision space-time sensors based on atom interferometry and optical atomic clocks

How did the universe begin? What laws govern extreme astrophysical objects such as black holes? How did mass aggregate from the nearly uniform distribution of energy following the inflationary epoch? What is driving the accelerated expansion of the universe? Are there new, yet unknown, laws of physics that govern the universe at either cosmological or sub-atomic scales? These are the types of questions that may be answered by direct observation of gravitational waves. The recent spectacular success of the LIGO observatory has shown the observational power of these space-time signals.

Direct detection of gravitational radiation is challenging. Sensors must be capable of measuring fractional changes in distances or velocities below one part in 10^{21} over time scales ranging from about 1 msec to 1000 seconds and longer, corresponding, for example, to displacements on the scale of one atomic nucleus over distances of the Earth's radius. Remarkably, modern laser and optical technology has reached a point where at the shortest time scales (about 1 msec to 30 msec), such measurements are feasible using the ground-based LIGO and Advanced LIGO detectors. However, at longer intervals, relevant to detection of gravitational waves of cosmological origin, new approaches are needed. Space-based optical interferometers (such as the proposed eLISA program) may allow gravitational wave observations on timescales of about 10 to 1000 seconds, which would still leave a large 'gap' in the monitoring of scientifically important timescales. Fortunately, recent developments in quantum science, including atom de Broglie wave interferometry and optical atomic clocks, may fill this gap by enabling gravitational wave detectors across a very wide range of timescales, from about 10 msec to 1000 seconds.

Advances in atomic and optical physics have provided tools that enable new classes of precision measurements. These tools include atom interferometry, where quantum mechanical interference of atomic de Broglie waves enables precise force measurements, and ultra-stable lasers, which have led to multi-order-of-magnitude advances in the performance of atomic clocks operating in the optical wavelength regime. Together, these methods will result in a next generation of ultra-precise inertial sensors superbly suited to gravitational wave detection and precision geodesy. Recent advances demonstrating the efficacy of quantum entanglement (“squeezing”) and quantum control (“dynamic decoupling”) for precision sensing offer a path to further enhanced sensitivities.

For example, in the atom interferometric approach, gravitational radiation is sensed through the gravitational wave-induced phase shifts on the propagation of laser beams between two spatially separated, inertially isolated, laser-cooled atomic ensembles. Momentum recoil associated with the interactions between the laser and atomic ensembles results in the concomitant interference of atomic wavepackets. Functionally, the atomic ensembles serve as precision clocks which measure the flight time of light between the atom ensembles. In the optical atomic clock approach, two spatially separated, drag-free satellites share ultra-stable laser light. Each satellite contains an optical lattice atomic clock, which serves as a sensitive, narrowband detector of the effective Doppler shifts induced by incident gravitational waves on the shared laser light. Both types of sensors may also be operated in modes which search for new forces, for example due to coupling with dark matter, or for time-variation of fundamental constants.

For atom interferometers, large baseline (km-scale) ground-based detectors, perhaps located in underground facilities such as SURF, provide a near-term path towards scientifically significant sensitivity levels. Such detectors benefit from recent demonstrations of picoKelvin-temperature atomic ensembles, meter-scale wavepacket separation atom interferometers, high power (>10 W) ultra-stable (< 1 kHz linewidth) lasers, and high flux atomic sources.

DOE Office of Science HEP-ASCR Roundtable on February 25th 2016 - Attendees

Participants

Swapan Chattopadhyay, Fermilab and Northern Illinois University; **Chair**
Roger Falcone, Lawrence Berkeley National Laboratory; **Chair**
Ronald Walsworth, Harvard University; **Chair**
Misha Lukin, Harvard University
David Schuster, University of Chicago
Holger Mueller, UC Berkeley
Alex Shuskov, Boston University
Peter Graham, Stanford University
Chris Stubbs, Harvard University
Mike Romalis, Princeton University
Surjeet Rajendran, UC Berkeley
Cindy Regal. JILA, University of Colorado
David DeMille, Yale University
Chris Monroe, University of Maryland (UMD)
Kartik Srinivasan, NIST, UMD
Irfan Siddiqui, Lawrence Berkeley National Lab

Participants who provided input but were unable to attend:

Evelyn Hu (Harvard University), Mark Kasevich (Stanford University), Jun Ye (NIST/JILA), Nergis Mavalvala (MIT),

DOE Lab Observer

Joseph Lykken, Fermilab

Agency Attendees/Observers

Altaf Carim, OSTP; Laura Biven, Ben Brown (DOE SC-2); Steve Binkley, Barbara Helland, Carolyn Lauzon, Robinson Pino, Ceren Susut, (DOE ASCR); Tom Russel, George Maracas, DOE (BES); Jim Siegrist, Eric Colby, Lali Chatterjee (DOE HEP); Carl Williams, Claire Cramer (NIST); Denise Caldwell, Michael Cavagnero (NSF);

DOE POC: Lali Chatterjee

HEP-ASCR Round Table Agenda

Quantum Sensors at the Intersections of Fundamental Science, QIS and Computing

Date: Feb 25th, 2016

Venue: Hilton Hotel, 620 Perry Parkway, Gaithersburg, MD (Darnestown/Gaithersburg Rooms)

8:15 AM - 8:45 AM	Assemble and sign in
8:45 AM - 9:00 AM	Opening remarks & going round the room - DOE POC *Lali Chatterjee*
9:00 AM - 10:30 AM	Introduction and Overview Session

- Roundtable Background and DOE Perspectives- *S. Binkley and J. Siegrist*
- View from OSTP – *Altaf Carim, OSTP*
- QIS International Status and NIST Perspectives - *Carl Williams, NIST*
- NSF Perspectives – *Denise Caldwell, NSF* (on phone)
- Goals, Expectations and Possible Grand Challenges – Round Table Chairs
  (S. Chattopadhyay, R. Falcone and R. Walsworth)

10:30 AM - 10:40 AM	Discussion Break
10:40 AM - 12: 30 PM	Presentations by Participants and Open Discussions

[Ten- minute presentations. The Study Group Chairs will lead the Session and associated Open Discussions. This session may creep into lunch schedule, and includes one remote presentation via phone.]

12:30 AM -1:45 PM	Working lunch — Brainstorm towards identifying Grand Challenges
1:45 PM -3:15 PM	Continue discussions/formulate grand challenges/draft report
3:15 PM – 3:25 PM	Discussion Break
3:25 PM – 4:15 PM	Summarize Plans and present Close-out Bullets to DOE
4:15 - 5:00 PM	DOE Comments and Open Discussions-Led by SC ADS
5:00 PM	Adjourn

Department of Energy Charge Letter for Round Table on:

Quantum Sensors at the Intersections of Fundamental Science, Advanced Computing, and Quantum Information Science (QIS)

To
Swapan Chattopadhyay, Fermilab/NIU
Roger Falcone, Director ALS, LBNL/UC Berkeley
Ronald Walsworth, Harvard University

Dear Swapan, Roger, and Ron,

Thank you very much for agreeing to lead a roundtable discussion on Quantum Sensors and other Quantum Information Science (QIS) technologies to advance the basic science and computational goals of the DOE Office of Science (SC) as well as near-term applications across the broad range of DOE-relevant fields.

The scope of the roundtable is to identify Grand Challenges for Quantum Sensors and other QIS technologies that could have transformative impact on the mission and interests of the DOE SC and thereby contribute to national priorities in science, computing, and technology. The scope includes but is not limited to the following research directions:

- QIS technologies that may make major advances in the performance of 'traditional' DOE SC approaches to basic science and advanced computing, including at national laboratories and DOE-supported research centers. Examples could include advancing and exploiting the limits of precision cavity electrodynamics, high magnetic fields, and quantum sensors (including atom interferometer and atomic clock networks) for scientific research in the mission areas of DOE SC.

- Complementary QIS-based methods to address key questions in basic science and advanced computing, which could establish at DOE SC a new interdisciplinary scientific approach — the 'quantum frontier'. Examples could include quantum entanglement and qubit technology that enables new insight into the dark universe, coherence in light and matter, fundamental symmetries in nature, and other breakthrough physical phenomena; quantum sensors that can serve as new probes for materials science, chemical science, geoscience, bioscience, and engineering problems; and the development of new QIS technologies for advanced computing.

- Experimental testbeds for exploring and optimizing QIS algorithms; performing precision tests of quantum realism; and also for probing new theories at the intersection of beyond Standard Model and QIS theories.

- Synergistic with the above activities, development of quantum sensors and other QIS technologies that could have 'near-term' applications in a wide range of basic and applied science and thereby accelerate development and adoption of such technologies.

- Supporting efforts for the above activities, including the development of new materials.

- Status of the national and international scene relevant to the scope of the round table along with suggestions of flexible and realistic mechanisms for programmatic support for the activities –that could impact advances in the field

We request that you convene a team of about 15 experts (including yourselves), spanning the research and technology aspects as outlined above, and work with them in advance to formulate some of the prospective Grand Challenges. These should be developed and sharpened during the roundtable discussions, culminating in a short report to be submitted to us in draft form within a month of the roundtable.

Please send me a list of proposed participants for the Round Table, as well as topic headlines for discussion and a draft Agenda.

The Associate Directors in the Office of Science, Steve Binkley for Advanced Scientific and Computing Research (ASCR) and James Siegrist for High Energy Physics (HEP), have approved this meeting and we are planning for a one day meeting to take place in the Washington DC area in February, 2016. We will provide travel expenses for those who are not Federal or DOE Lab employees.

Sincerely
Lali Chatterjee,
Program Manager,
High Energy Physics,
Office of Science, Department of Energy

CC Steve Binkley, Associate Director, Office of Advanced Scientific and Computing Research (ASCR)
CC James Siegrist Associate Director, Office of High Energy Physics (HEP),