Quantum Information Science in BES

BERAC Meeting

Gaithersburg, MD
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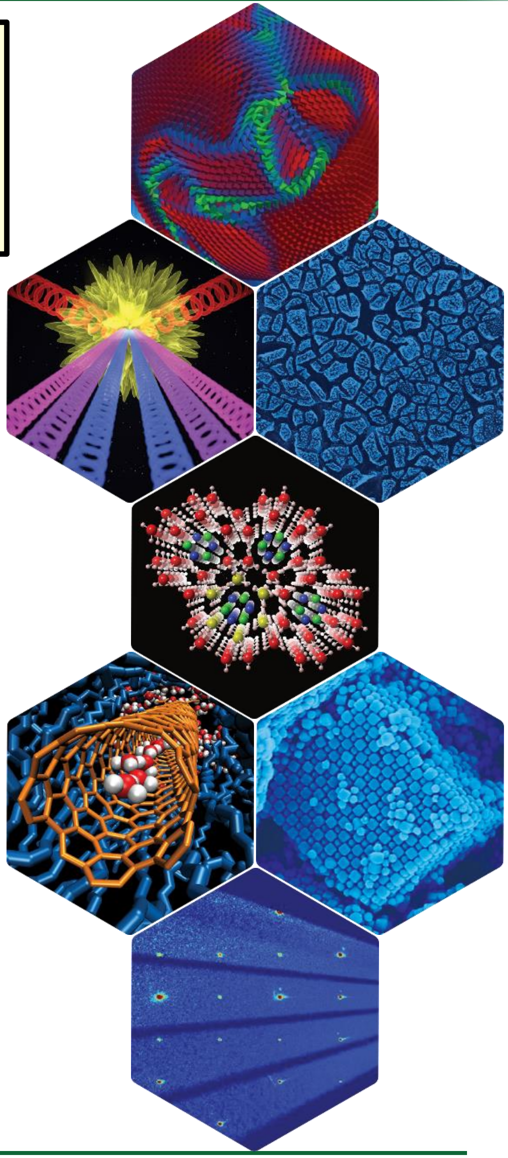
Office of Science, U.S. Department of Energy

Growing Optimism Around Quantum Information Science

- Richard Feynman (1972), *Simulating Physics with Computers*
- Two Aspects
  - Quantum Computing
    - Deals with *exponential* growth in requirements with increasing size to solve atomic and molecular scale problems
  - Sensors
    - Deals with the extreme sensitivity of QIS systems and noise levels far below classical devices
- Exploit and measure entanglement – a uniquely quantum phenomenon
  - Einstein's 'spooky action at a distance'
- Optimism
  - Physical systems approaching 'quantum supremacy'
    - i.e. faster than a classical computer
  - Large investments by IBM, Google, Intel, Microsoft……
- Emerging Opportunities throughout Office of Science

Basic Energy Sciences Mission

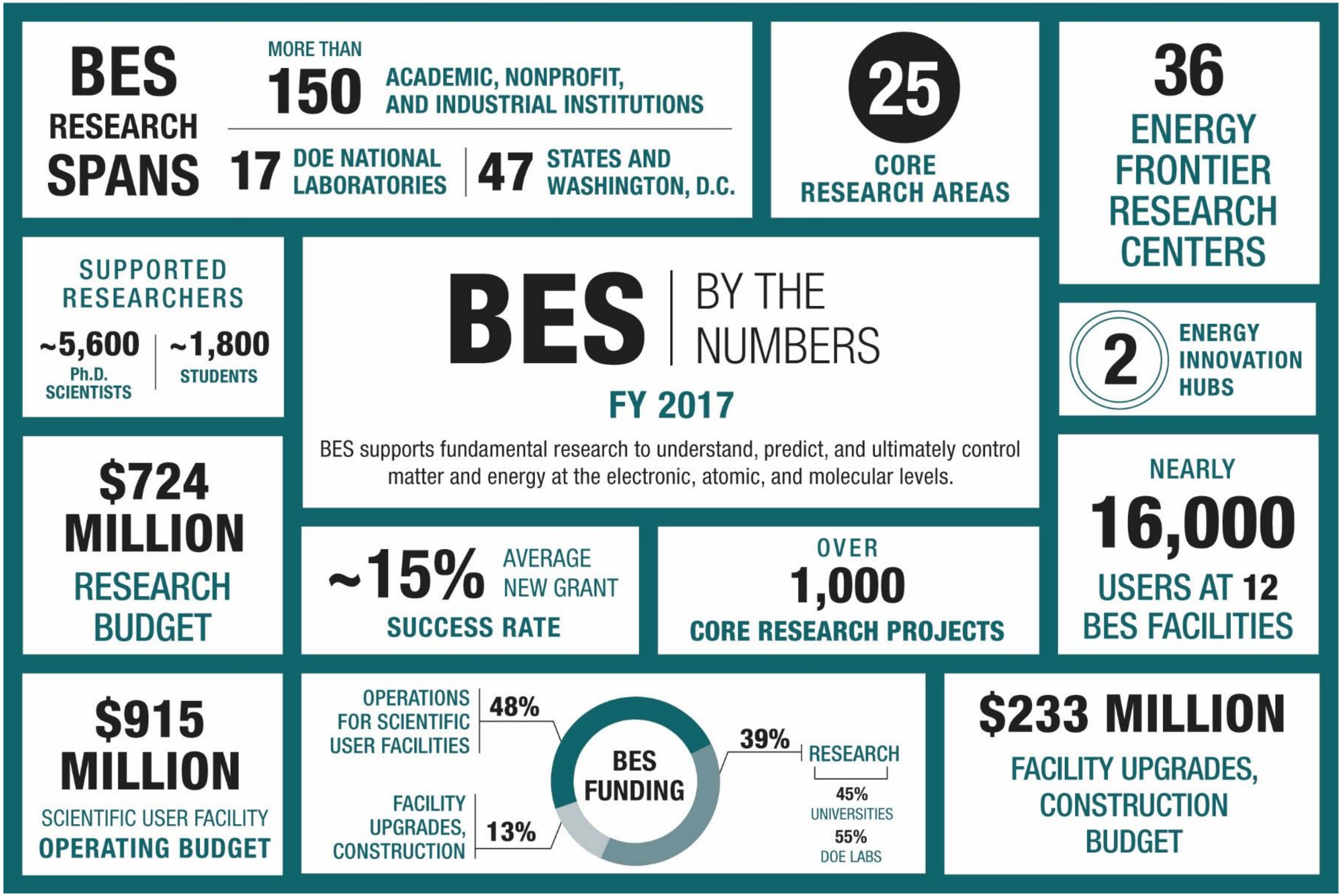
To understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels



BES fulfills its mission through:

- Supporting basic research to discover new materials and design new chemical processes that underpin a broad range of energy technologies
- Operating world-class scientific user facilities in x-ray, neutron, and electron beam scattering as well as in nanoscale research
- Managing construction and upgrade projects to maintain world-leading scientific user facilities

BES By the Numbers

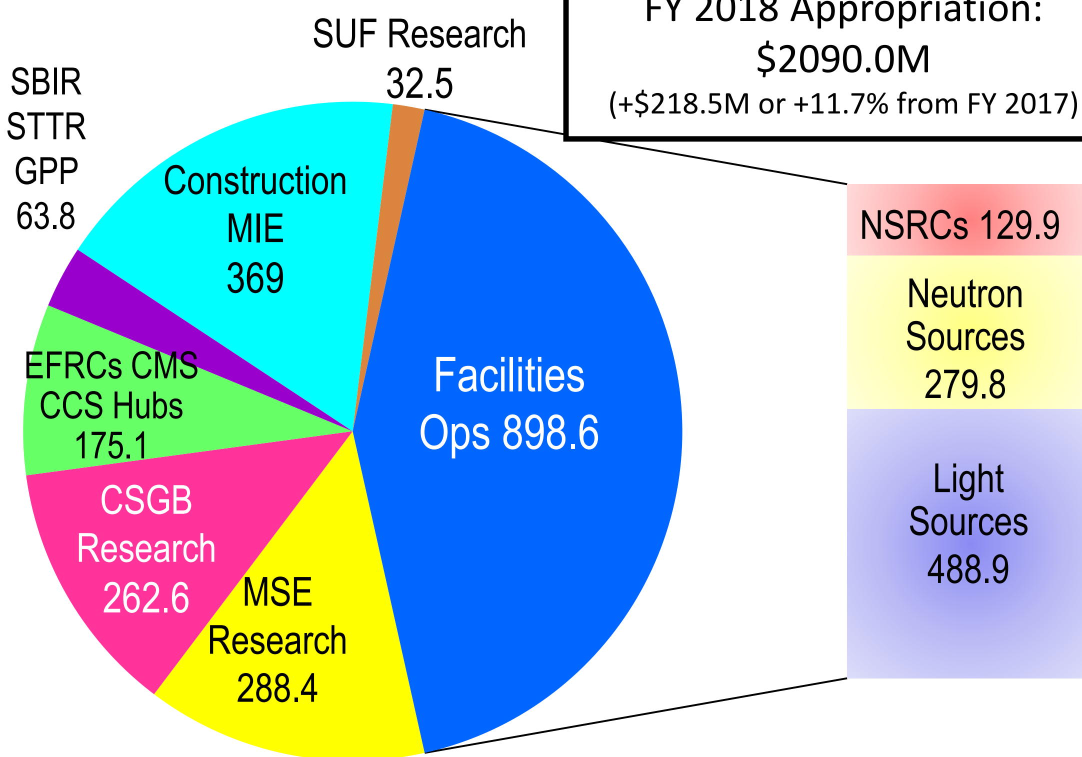


FY 2018 BES Budget

Research programs

- Core Research will emphasize quantum materials and chemistry, ultrafast science, and BRN topics ($551M; Δ=+$62.9M).
- Computational Materials and Chemical Sciences continue ($26M)
- Energy Frontier Research Centers continue ($110M)
- Funding continues for Energy Innovation Hubs (JCAP & JCESR) ($39M).

FY 2018 Appropriation:
$2090.0M
(+$218.5M or +11.7% from FY 2017)



Scientific user facilities

- Operations of 12 facilities at ≥ 95% optimal level ($898.6M; Δ=+$21.3M)
- $1M Lujan equipment disposition; $8.5M Long Term Surveillance and Maintenance

Construction/MIE* Δ=+$131.5M

- Last year of funding for LCLS-II ($200M)
- Advanced Photon Source Upgrade($93M)
- Three new starts: LCLS-II-HE ($10M) and ALS-U ($30M); PPU ($36M)

*includes OPC

FY 2018 – FY 2019 BES Research Priorities

- **Quantum Information Science (QIS)**
  - By exploiting the intricate quantum mechanical phenomena, QIS will create fundamentally new ways of obtaining and processing information and open new vistas of science discovery and technology innovation. Research priorities were identified in two QIS roundtables held in October 2017.
- **Ultrafast Science**
  - Ultrafast science remains a priority in both research divisions to position the U.S. leadership in this critical field of science and in anticipation of the completion of the LCLS-II construction project. Research priorities were identified in a roundtable held October 2017.
- **Computational Materials and Chemical Sciences**
  - Computational Materials Sciences (CMS) and Computational Chemical Sciences (CCS) are maintained in support of the Exascale Computing Initiative. CCS was funded in FY 2017 and is moved to a new budget line in the FY 2019 Request.
- **Materials and Chemical Sciences for Future Nuclear Energy**
  - Research will be supported to achieve a multi-scale spatial and temporal understanding of fundamental physical and chemical processes that govern the properties and performance of novel material systems and fuels required for advanced reactors.
- **Priorities identified by Advisory Committee and Basic Research Needs Reports**
  - Both the core research and EFRCs will emphasize emerging high priorities identified by the Basic Energy Sciences Advisory Committee and recent Basic Research Needs workshop reports.

DOE Office of Basic Energy Sciences: Scientific User Facilities

Nearly 16,000 users in FY 2017

- **Available to all researchers *at no cost* for non-proprietary research, regardless of affiliation, nationality, or source of research support**
- **Access based on external peer merit review of brief proposals**
- **Coordinated access to co-located facilities to accelerate research cycles**
- **Collaboration with facility scientists an optional potential benefit**
- **Instrument and technique workshops offered periodically**
- **A variety of on-line, on-site, and hands-on training available**
- **Proprietary research may be performed at full-cost recovery**

Light Sources

- Advanced Light Source (LBNL)
- Advanced Photon Source (ANL)
- Linac Coherent Light Source (SLAC)
- National Synchrotron Light Source-II (BNL)
- Stanford Synchrotron Radiation Laboratory (SLAC)

Neutron Sources

- High Flux Isotope Reactor (ORNL)
- Spallation Neutron Source (ORNL)

Nanoscale Science Research Centers

- Center for Functional Nanomaterials (BNL)
- Center for Integrated Nanotechnologies (SNL & LANL)
- Center for Nanophase Materials Sciences (ORNL)
- Center for Nanoscale Materials (ANL)
- Molecular Foundry (LBNL)

What does a Quantum Computer Look like?

A bit of the action

In the race to build a quantum computer, companies are pursuing many types of quantum bits, or qubits, each with its own strengths and weaknesses.

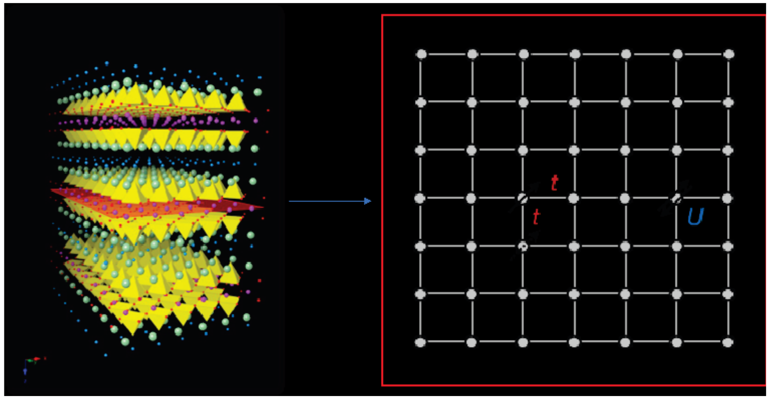
	Superconducting loops	Trapped ions	Silicon quantum dots	Topological qubits	Diamond vacancies
	A resistance-free current oscillates back and forth around a circuit loop. An injected microwave signal excites the current into super-position states.	Electrically charged atoms, or ions, have quantum energies that depend on the location of electrons. Tuned lasers cool and trap the ions, and put them in superposition states.	These "artificial atoms" are made by adding an electron to a small piece of pure silicon. Microwaves control the electron's quantum state.	Quasiparticles can be seen in the behavior of electrons channeled through semi-conductor structures. Their braided paths can encode quantum information.	A nitrogen atom and a vacancy add an electron to a diamond lattice. Its quantum spin state, along with those of nearby carbon nuclei, can be controlled with light.
Longevity (seconds)	0.00005	>1000	0.03	N/A	10
Logic success rate	99.4%	99.9%	~99%	N/A	99.2%
Number entangled	9	14	2	N/A	6
Company support	Google, IBM, Quantum Circuits	ionQ	Intel	Microsoft, Bell Labs	Quantum Diamond Technologies
Pros	Fast working. Build on existing semiconductor industry.	Very stable. Highest achieved gate fidelities.	Stable. Build on existing semiconductor industry.	Greatly reduce errors.	Can operate at room temperature.
Cons	Collapse easily and must be kept cold.	Slow operation. Many lasers are needed.	Only a few entangled. Must be kept cold.	Existence not yet confirmed.	Difficult to entangle.

Note: Longevity is the record coherence time for a single qubit superposition state, logic success rate is the highest reported gate fidelity for logic operations on two qubits, and number entangled is the maximum number of qubits entangled and capable of performing two-qubit operations.

G. Popkin, Science **354,** 1091 (2 December, 2016)

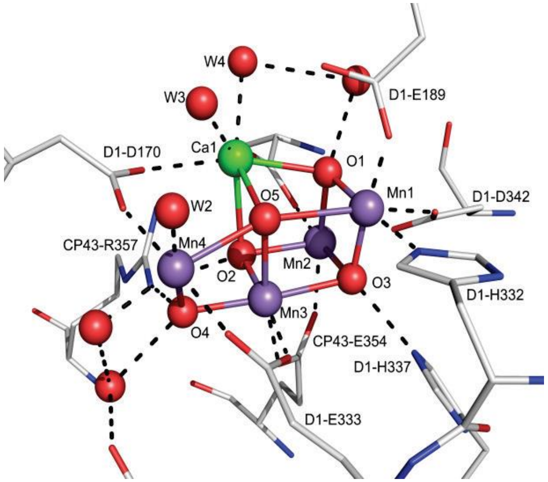
What Can You Do With QIS Systems?

- Quantum Sensors
  - Ultra-high resolution scanning probe microscopy
  - Low damage e^- microscopes for polymers and proteins
    - Nanoscale resolution on proteins
  - Particle detectors for high energy physics
- Quantum Computing
  - Quantum dynamics of non-equilibrium chemical systems
  - Physics of strongly correlated materials, superconductivity and magnetism
  - Fully quantum mechanical description of liquid water
  - Quantum Machine learning



Fermi Hubbard Model

Oxygen evolving complex of cytochrome P450

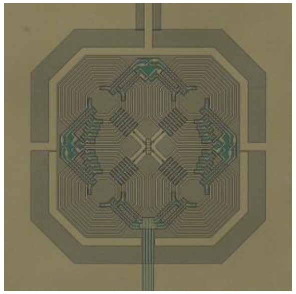


BES: Detectors for Quantum Information Systems

QIS systems use quantum properties (associated with photons, electrons, . . .) to encode, manipulate data and information:

- Requires efficient generation, transport, and entanglement
- Quantum entanglement dramatically reduces measurement noise (from $1/\sqrt{N}$ to $1/N$)
- Opens avenues for quantum sensor, detector, and imaging technology applications

Superconducting circuits used for quantum-based sensors for x-ray spectroscopy



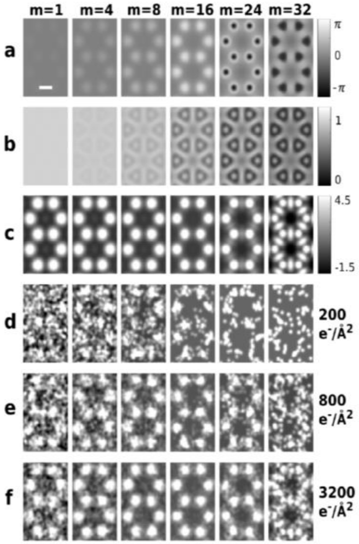
Low temperatures and dissipation-less electronic transport make a range of quantum phenomena accessible, including precise energy measurements:

- Solid-state devices based on charge, flux, phase, in patterned superconducting circuits
- Micro- and nano-fabrication provide paths to >> 10^3 solid-state devices with tunable couplings (many physics obstacles remaining)
- As sensors improve, single-photon detection with high efficiency/count rates may become possible for far-infrared and microwave wavelengths

SLAC National Laboratory, NIST

Quantum electron microscope

Current electron beam-induced damage precludes high-resolution imaging of sensitive materials – *quantum-based methods would avoid this issue*



- Probes that have little interaction with materials would lead to an order-of-magnitude reduction in damage
- Retains sub-nanometer resolution

Lawrence Berkeley National Laboratory

U.S. DEPARTMENT OF ENERGY | Office of Science

BES Roundtables on Quantum Information Sciences

- Opportunities for Basic Research for Next-Generation Quantum Systems
  - October 30-31, 2017 (1.5 days)
  - Chair – David Awschalom (U Chicago/ANL)

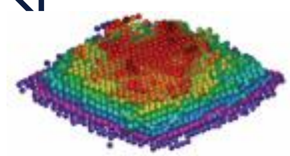
    Co-chair – Hans Christen (ORNL)
  - Identify opportunities for basic materials and chemical sciences, including nanoscale research, to enable the next-generation of quantum devices and systems.
- Opportunities for Quantum Computing in Chemical and Materials Sciences
  - October 31 – November 1 (1.5 days)
  - Chair – Joel Moore (UC-Berkeley/LBNL)

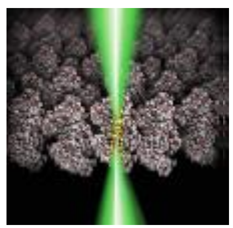
    Co-chair – Alan Aspuru-Guzik (Harvard U)
  - Identify opportunities for quantum computing (QC) to enable significant and impactful advances in understanding of important fundamental challenges in chemical and materials sciences

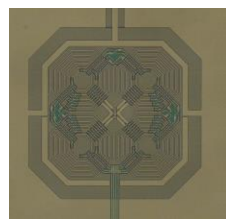
BES & Quantum Information Science

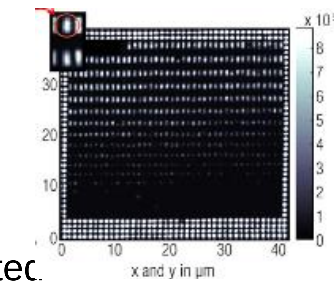
- Quantum materials and chemistry supported by BES core research and EFRCs are foundational to exploring and controlling novel quantum behaviors.
- BES Nanoscale Science Research Centers capabilities are key to nano-to-micro-scale electronic/ photonic quantum structure fabrication. Integration and testing will couple closely with theory, design and systems efforts.
- Research will enable next-generation qubit concepts, innovative quantum and classical architectures (Ion traps, quantum dots, nitrogen vacancies, donor centers, etc.)

Theory, Modeling, Synthesis, Characterization, Design, Fabrication, Prototypes

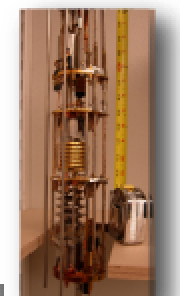

Characterization with Atomic Spatial Resolution and Ultrafast Precision


Single-nm lithography

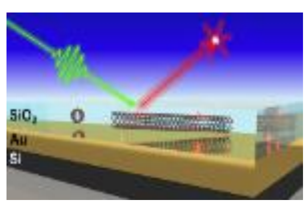

Quantum-Limited Sensors



Entangled Qubit Arrays

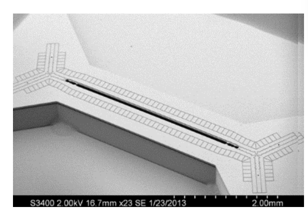

Quantum Chip Testing

Atomic Precision Fabrication



Single Photon Emitters and Detectors

Nanoscale 3D Printing


Waveguides, Cavities, Traps

BES

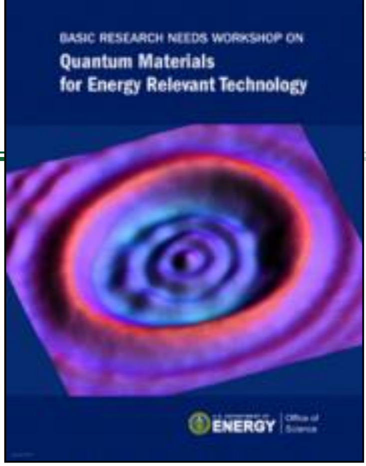
Quantum Computing

Encrypted Communi-cations

Sensors & Detectors

ASCR, HEP NP, BER

Basic Research Needs for Quantum Materials for Energy Relevant Technology



Control and exploit fluctuations in quantum matter for the design of bulk materials with novel functionality

Looking beyond the standard paradigms of simple metals and semiconductors, how do strongly-interacting electrons organize themselves in quantum materials, and how can this be controlled for energy-relevant technologies?

- **Understand and control competing, coexisting, and intertwined order**
- **Predict, realize, and probe new states of quantum magnets**

Harness topological states for groundbreaking surface properties

Building on recent advances in the field of topological insulators, what new topological states of matter can be realized, what are their signatures, and how can these be used for energy-related applications?

- **Discover new topological quantum materials**
- **Design new platforms to probe and exploit topology**

Drive and manipulate quantum effects (coherence, entanglement) in nanostructures for transformative technologies

How can the extraordinary properties of coherent quantum states be controlled and utilized for energy-related applications?

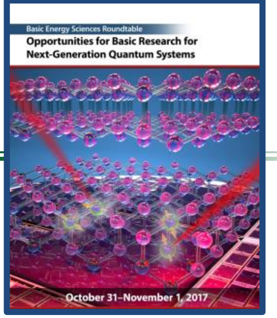
- **Employ nanoscale structuring to elucidate and exploit coherence and entanglement**
- **Understand transport in quantum materials**
- **Dynamically visualize and manipulate quantum materials**

Design revolutionary tools to accelerate discovery and technological deployment of quantum materials

What new methodologies and tools are needed to advance synthesis of quantum materials and our ability to probe and predict their properties?

- **Enhanced synthesis of quantum materials**
- **Develop new windows into quantum materials**
- **Develop efficient methods for static and dynamic states beyond 1-electron paradigms**

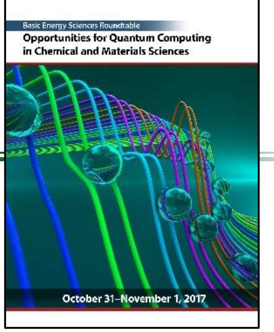
Quantum Information Science: Opportunities for Basic Research for Next Generation Quantum Systems



Roundtable in October 2017 defined a BES research agenda for quantum systems for QIS and provided input on priority research opportunities:

- **Advance artificial quantum-coherent systems with unprecedented functionality**
  - Develop new capabilities for synthesis that couple theoretical predictions and real-time measurements of targeted quantum characteristics, including coherence
  - Explore robotic synthesis of layered materials, design of quantum properties for hybrid (organic and inorganic) systems, creation of topological states of matter, and precise control to position atomic defects
- **Enhance creation and control of coherence in quantum systems**
  - Understand scaling of coherence lengths and times with system size and complexity, and identify new signatures of quantum states in artificial quantum-coherent systems
  - Investigate mechanisms to prevent decoherence, leading to discovery and exploitation of novel entangled excitations
- **Discover novel approaches for quantum-to-quantum transduction**
  - Advance new capabilites for coherent transfer of complete wavefunctions between disparate physical systems, the core of quantum measurement and information processing
  - Develop new techniques for generation and stabilization of nonclassical states of light and matter; high fidelity transfer of quantum wavefunctions; and quantum state replication and entanglement
- **Implement new quantum methods for advanced sensing and process control**
  - Design new quantum-based sensors, detectors, and imaging systems for precise measurements of time, space, and fields to probe material properties and chemical processes
  - Create novel methods to use squeezed states for metrology and understand the connections of entanglement, thermodynamics, and many-body localization/diffusion

Quantum Information Science: Quantum Computing Opportunities in Chemical and Materials Sciences



Roundtable in October 2017 defined a BES research agenda for emerging quantum computing and provided input on priority research opportunities:

- Controlling the quantum dynamics of nonequilibrium chemical and materials systems
  - Elucidate the fundamental principles underlying chemical reactions and catalytic pathways; discover dynamical phases of matter; and understand how to prepare entangled states across many quantum degrees of freedom
- Unraveling the physics and chemistry of strongly correlated electron systems
  - Enable a correct description of the quantum behavior of strongly entangled electrons to allow discovery of the principles controlling superconductivity, magnetic states and the dynamics of electronic states
- Embedding quantum hardware in classical frameworks
  - Develop efficient hybrid algorithms that embed quantum computing for strongly correlated quantum components in classical computing for more weakly correlated parts, thus enabling simulations of molecular and materials problems containing thousands of atoms
- Bridging the classical–quantum computing divide
  - Improve the efficiency of quantum computing using approximate results from classical computing as input, and improve the accuracy of classical computing using high-accuracy results from quantum computing to parameterize and optimize complex models

BES Funding Opportunity in Quantum Information Sciences

- Materials and Chemical Sciences Research for Quantum Information Science
- Issued April 10, 2018
- Letter of Intent due **May 3 Required**
- Full Proposals due **May 24**
- Proposals requested for
  - Quantum Computing in Chemical and Materials Sciences
  - Next-Generation Quantum Systems
- Must address priority Research Opportunities identified in two BES Roundtables
- Must be programmatically aligned with BES research