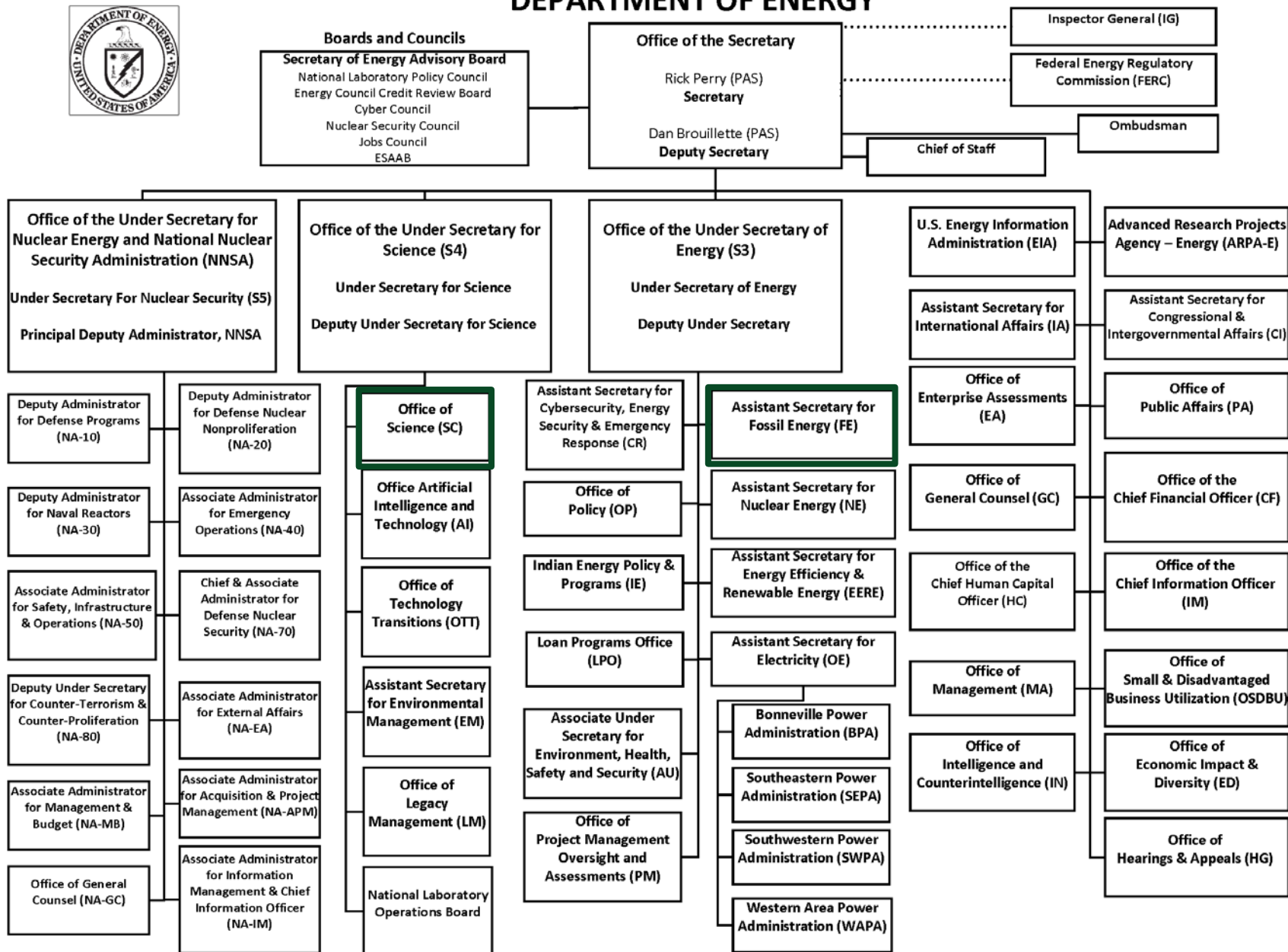# Quantum Information Science in the Department of Energy's Office of Science

Barbara Helland
Advanced Scientific Computing Research
November 19, 2019

DEPARTMENT OF ENERGY

Boards and Councils
Secretary of Energy Advisory Board
National Laboratory Policy Council
Energy Council Credit Review Board
Cyber Council
Nuclear Security Council
Jobs Council
ESAAB

Office of the Secretary

Rick Perry (PAS)
Secretary

Dan Brouillette (PAS)
Deputy Secretary

Inspector General (IG)

Federal Energy Regulatory Commission (FERC)

Ombudsman

Chief of Staff

Office of the Under Secretary for Nuclear Energy and National Nuclear Security Administration (NNSA)

Under Secretary For Nuclear Security (S5)

Principal Deputy Administrator, NNSA

Office of the Under Secretary for Science (S4)

Under Secretary for Science

Deputy Under Secretary for Science

Office of the Under Secretary of Energy (S3)

Under Secretary of Energy

Deputy Under Secretary

U.S. Energy Information Administration (EIA)

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Advanced Research Projects Agency – Energy (ARPA-E)

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Assistant Secretary for Cybersecurity, Energy Security & Emergency Response (CR)

Assistant Secretary for Fossil Energy (FE)

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Associate Administrator for Emergency Operations (NA-40)

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Office of Policy (OP)

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Office of General Counsel (GC)

Office of the Chief Financial Officer (CF)

Associate Administrator for Safety, Infrastructure & Operations (NA-50)

Chief & Associate Administrator for Defense Nuclear Security (NA-70)

Office of Technology Transitions (OTT)

Indian Energy Policy & Programs (IE)

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Associate Under Secretary for Environment, Health, Safety and Security (AU)

Bonneville Power Administration (BPA)

Office of Intelligence and Counterintelligence (IN)

Office of Economic Impact & Diversity (ED)

Southeastern Power Administration (SEPA)

Office of General Counsel (NA-GC)

Associate Administrator for Information Management & Chief Information Officer (NA-IM)

Office of Project Management Oversight and Assessments (PM)

Southwestern Power Administration (SWPA)

Office of Hearings & Appeals (HG)

National Laboratory Operations Board

Western Area Power Administration (WAPA)

Updated 10/7/2019

U.S. DEPARTMENT OF **ENERGY**

The DOE Office of Science Research Portfolio

Basic Energy Sciences (BES)	• Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels
Advanced Scientific Computing Research (ASCR)	• Delivering world leading computational and networking capabilities to extend the frontiers of science and technology
Biological and Environmental Research (BER)	• Understanding complex biological, climatic, and environmental systems
Fusion Energy Sciences (FES)	• Building the scientific foundations for a fusion energy source
High Energy Physics (HEP)	• Understanding how the universe works at its most fundamental level through research, projects, and facilities
Nuclear Physics (NP)	• Discovering, exploring, and understanding all forms of nuclear matter

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https://www.energy.gov/science/office-science

Quantum Information Science (QIS) in the DOE Office of Science (SC)

QIS is a thriving area of multidisciplinary science.

- It exploits particular quantum phenomena to measure, process, and transmit information in novel ways that greatly exceed existing capabilities.

QIS provides a basic foundation for numerous application areas.

- Potential transformative impact on SC grand challenges.

QIS is at a tipping point.

- Major companies are embracing QIS, foreign competition is expanding rapidly.

Progress in QIS is driven by basic research in physical sciences.

- DOE SC is the Nation's leading supporter of basic research in physical sciences.

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SC's QIS Strategy

- ✓ Builds on community input
- ✓ Highlights DOE/SC's unique strengths
- ✓ Leverages groundwork already established
- ✓ Focuses on cross-cutting themes among programs
- ✓ Targets impactful contributions and mission-focused applications

DOE/SC Contributions to QIS

Fundamental Science ⟷ **Tools, Equipment, Instrumentation**

DOE Community Resources

QIS Applications

Quantum Computing: Simulation, Optimization, Machine Learning

Analog Quantum Simulation

Sensing and Microscopy

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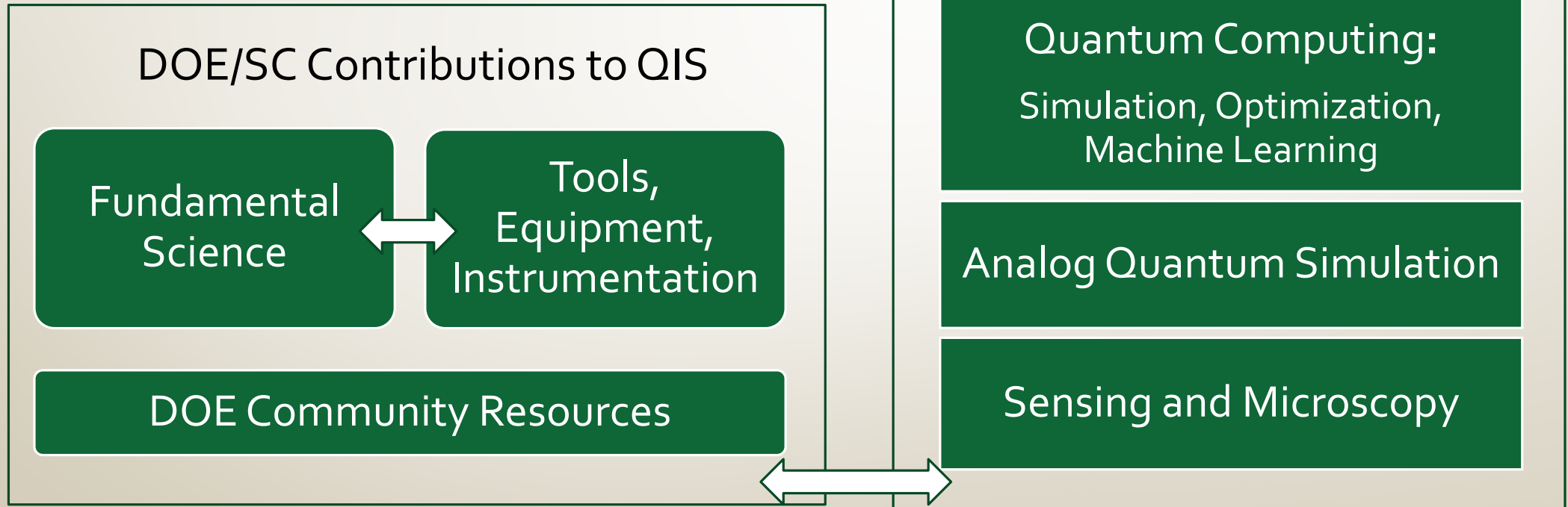
Fundamental Science That Advances QIS

ASCR	**BES**	**HEP**	**NP**
Quantum algorithms; uncertainty quantification and verification & validation methods; software stack; quantum networks	Synthesis, characterization, modeling, and instrumentation to advance quantum chemistry and materials	Black hole physics; quantum gravity and quantum error correction; fundamental aspects of entanglement	Isotopes and trapped ions for quantum devices; lattice quantum chromodynamics

◄──── Quantum Field Theory and Topology ────►

◄──── Control of Quantum Phenomena ────►

SC Unique Strengths

- Intellectual capital accumulated for more than a half-century
- Successful track record of forming interdisciplinary yet focused science teams for large-scale and long-term investments
- Demonstrated leadership in launching internationally-recognized SC-wide collaborative programs

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Tools, Equipment, Instrumentation

Quantum Computing Hardware

ASCR's Testbeds Program:
- Research into device architectures and system integration optimized for science applications
- Development of hybrid platforms and quantum/classical coprocessors
- Early access to new quantum computing hardware for the research community

Tool R&D for QIS

- Extensive nanoscience tools for quantum structure synthesis and integration
- Detectors and metrology
- Quantum sensors enabling precision measurements
- Quantum computational tools
- Superconducting RF cavities, laser cooling, neutral ion traps, spin manipulation technology, and isotope production

Key DOE-SC Contributions:

- Well-established co-design practices in computer hardware development
- Experience in collaborations with industry and core competencies in delivering major projects involving equipment, tools, and instrumentation for discovery and implementation
- Demonstrated success in generating leading scientific tools with and for the international user community

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DOE Community Resources

World-Class National Laboratory resources

- Advanced fabrication capabilities, (e.g. Microsystems & Engineering Sciences Applications (MESA) facility at SNL)
- Specialized synthesis and characterization capabilities (e.g. Enriched Stable Isotope Prototype production plant)
- Internal research computing capabilities, experimental equipment, and prototypes (e.g. D-Wave)
- Engineered physical spaces (e.g. EM-shielded rooms, low-vibration chambers, deep shafts)

Focused programs and intellectual property

- Internships and visiting programs for students and faculty
- National Laboratory technical assistance programs
- Access to intellectual property developed at National Laboratories via technology licensing agreements
- Early Career Research Program
- Small Business Innovation Research
- Computational Science Graduate Fellowship

User Facilities include:

Synchrotron and x-ray free electron laser light sources

Observational and communications networks

Nanoscale Science Research Centers
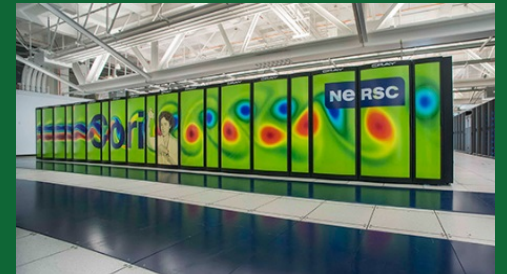
High Performance Computing and Network

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QIS Applications for DOE/SC Mission

✓ Target mission-focused grand challenge problems

✓ Application requirements guide DOE/SC contributions to QIS

✓ Take a multidisciplinary approach by forming partnership programs

DOE/SC Contributions to QIS

Fundamental Science ⟷ **Tools, Equipment, Instrumentation**

DOE Community Resources

QIS Applications

Quantum Computing:
Simulation, Optimization, Machine Learning

Analog Quantum Simulation

Sensing and Microscopy
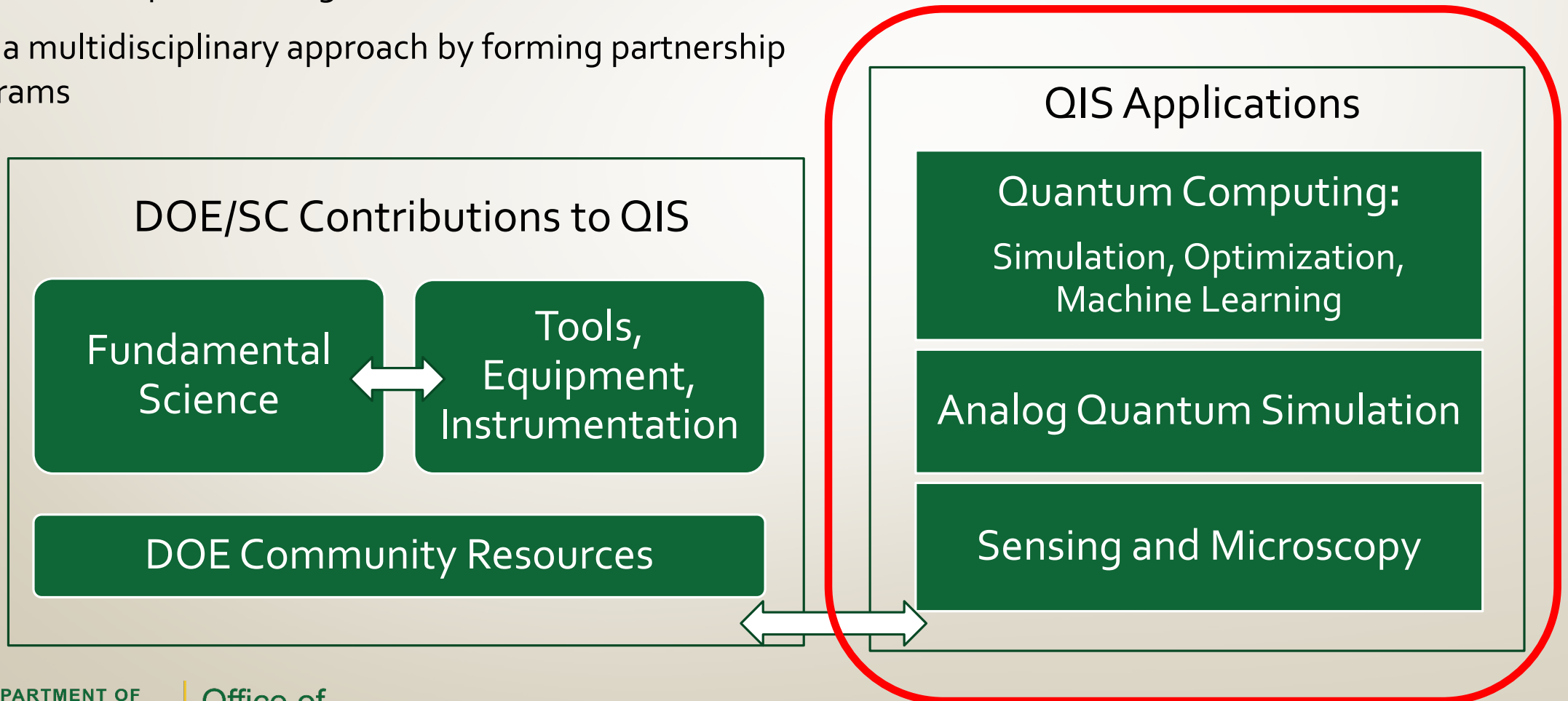
Quantum Computing Applications for SC Grand Challenges

Simulation of quantum many body systems for materials discovery, chemical processes, and nuclear matter equation of state

Simulations of quantum field theory and quantum dynamics

Machine learning for large data sets and inverse molecular design

Optimization for prediction of biological systems such as protein folding

Transformative Impact Through ASCR, BER, BES, HEP, NP Programs

Algorithms, Software Tools, and Testbeds

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Analog Quantum Simulation

Simulation of many-body systems (e.g. quantum chemistry, physics of neutron stars,...)

High Impact on Targeted Challenges Through ASCR, BES, HEP, NP Programs

Theory, Testbeds, Verification and Validation, Algorithms

Modeling an experimental system that simulates another quantum physical system

PHYSICAL SYSTEM   QUANTUM SIMULATOR

(Phenomenological) Hamiltonian   Physical Hamiltonian

Example: Hubbard model in 2D: $H = -t \sum_{<ij>,\sigma} c_{i\sigma}^+ c_{j\sigma} + h.c. + V \sum_i n_{i\uparrow} n_{i\downarrow}$
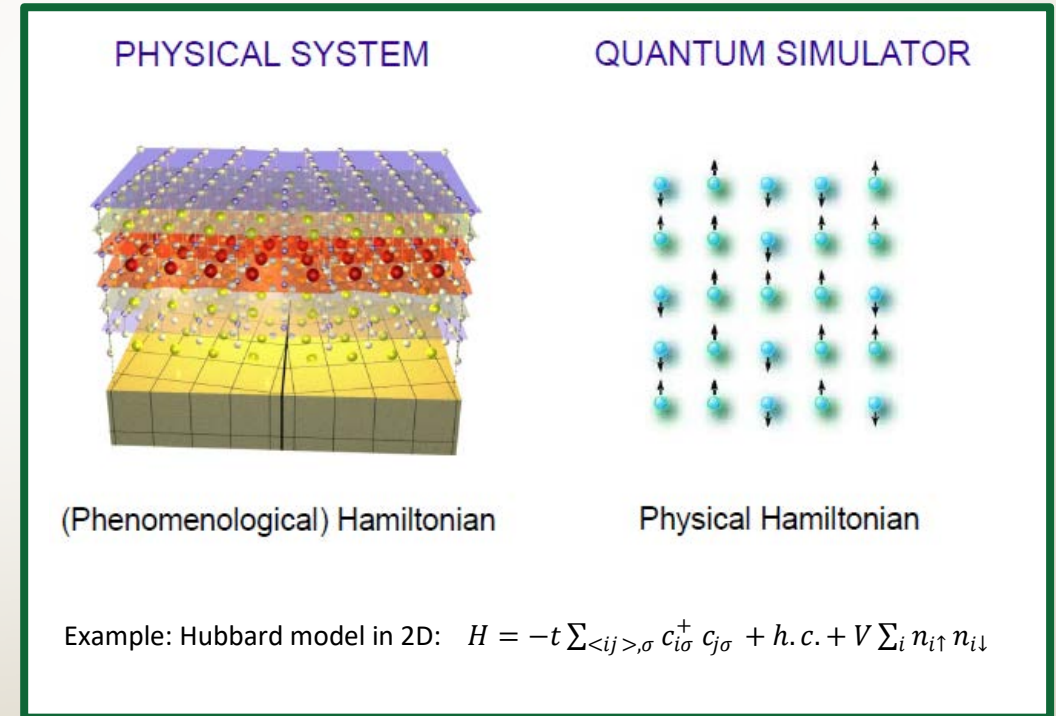
Offers an approach to problems that are not tractable via classical computing

Sensing and Microscopy
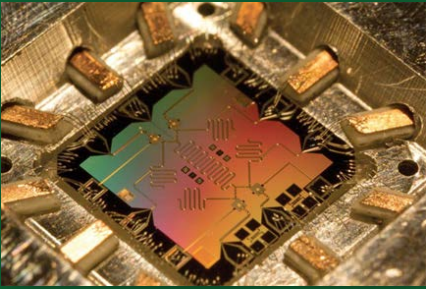
Superconducting qubit sensors for x-ray spectroscopy. As sensors improve, single-photon detection may become possible at far infrared and microwave wavelengths.

Nanostructured single photon emitters and detectors could be integrated for sensing, communications, and computing systems at room temperature.

SiO$_2$
Au
Si
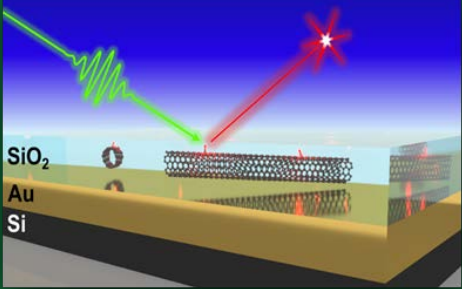
Quantum sensors to perform dynamic, non-invasive visualization of subcellular biological processes

Cross-Cutting Applications in BER, BES, HEP, NP

Quantum devices for environmental sensing in field settings for integrating multi-model and multi-scale data (e.g. quantum lidar)

200 e⁻/Å²
800 e⁻/Å²
3200 e⁻/Å²
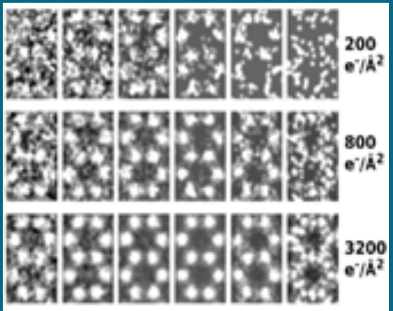
Quantum electron microscope for high resolution at very low doses for imaging of sensitive materials

Single photon detectors can expand the range of discovery for dark universe, non-Newtonian gravity, and new forces. Quantum error correction reduces noise in matter wave interferometry for such searches.
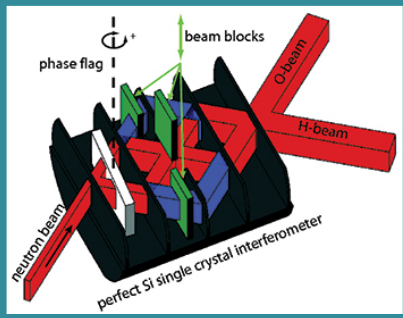
SC's QIS Strategy Builds On Community Engagement

- ASCR Quantum Computing Discussion, January 15, 2014, Germantown MD
- LANL Workshop on Materials Opportunities for Quantum Computing, October 7-8, 2014, Los Alamos NM
- ASCR-HEP Study Group: Grand Challenges at the Interface of QIS, Particle Physics, and Computing, December 11, 2014, Germantown MD
- BES-HEP Roundtable: Common Problems in Condensed Matter and High Energy Physics, February 2, 2015, Germantown MD
- ASCR Workshop on Quantum Computing in Scientific Applications, February 17-18, 2015, Bethesda MD
- BES Basic Research Needs on Quantum Materials for Energy Relevant Technology, February 8-10, 2016, Gaithersburg MD
- ASCR-HEP Quantum Sensors at the Intersections of Fundamental Science, QIS & Computing, February 25, 2016, Gaithersburg MD
- Computing Beyond 2025, August 15-16, 2016, Chicago IL
- ASCR Quantum Testbeds Study Group, August 23, 2016, Germantown MD
- The 1st International Workshop on Post-Moore Era Supercomputing (PMES), November 14, 2016, Salt Lake City UT
- LBNL Workshop on Quantum Simulations 101, January 11, 2017, Berkeley CA

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Community Engagement Continues

- ASCR Quantum Testbed Stakeholder Workshop, February 14-17, 2017, Washington DC
- ASCR Extreme Heterogeneity Summit, June 8-9, 2017, Germantown MD
- Workshop on Computational Complexity and High Energy Physics, July 31-August 2, 2017, College Park MD
- BES Roundtable Discussion on Opportunities for Basic Research for Next-Generation Quantum Systems, October 30-31, 2017, Gaithersburg MD
- BES Roundtable Discussion on Opportunities for Quantum Computing in Chemical and Materials Sciences, October 31 – November 1, 2017, Gaithersburg MD
- INT Workshop on Quantum Computing, Seattle, November 14-15, 2017
- The 2nd International Workshop on Post Moore's Era Supercomputing (PMES), November 13, 2017, Denver CO
- FNAL Workshop on Near-term Applications of Quantum Computing for High Energy Physics, December 6-7 2017, Batavia IL
- ANL Workshop on Quantum Sensors for High Energy Physics, December 12-14, 2017, Argonne IL
- NSF/DOE Quantum Science School, 2017-2020
- ASCR Quantum Communications Networks Roundtable, December 4, 2017, Germantown MD
- SC Quantum PI meeting January 31 – February 1, 2018

ASCR: Quantum Computing and Networking

- ASCR is supporting investments in Quantum Computing Hardware & Testbeds to
  - Provide decision support for future investments in QC hardware
  - Provide the research community with novel, early-stage QC resources
- ASCR is supporting projects to
  - Advance basic research in quantum algorithms, quantum computer science & networks
  - Form interdisciplinary teams of QIS experts, applied mathematicians and computer scientists that adopt a methodical approach to fill in the missing elements in order to connect SC grand challenges to quantum computing hardware.
- ASCR is supporting research projects to develop and deploy a transparent optical quantum internetworking ecosystem capable of supporting diverse types of geographically distributed quantum information science applications.

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BES: Materials and Chemistry Research for Next Generation QIS Systems and Quantum Computing Applications

- **BES is supporting research projects to discover and advance the implementation of next generation quantum systems and quantum computing applications**

  - Focus on control of entanglement; novel approaches for synthesis including automation and control of defects; in situ characterization and metrology; coherent coupling of spins, phonons, and photons; theory for materials discovery, simulation platform; manipulation of Majorana modes

  - 2D materials, NV centers, trapped ions, superconducting qubits, molecular systems

  - Applications in quantum sensing, computing, and instrumentation
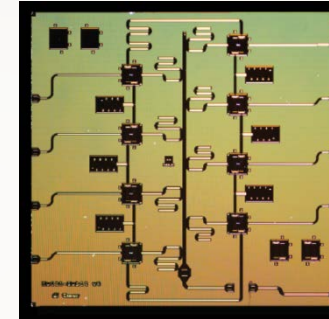
Optical micrograph of an eight-qubit superconducting processor with a ring-type circuit topology
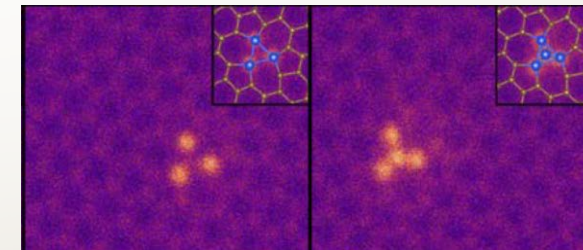
Beam-directed atom-by-atom fabrication of silicon trimer and tetramer
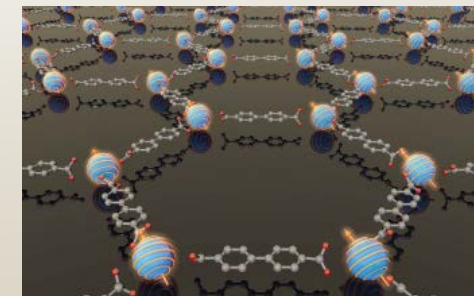
Schematic of metal-organic hybrid system integrated with a surface.

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BES Nanoscale Science Research Centers Advances QIS

Quantum Integration Across Scales

- BES Nanoscale Science Research Centers user facilities, at ANL, BNL, LBNL, ORNL and SNL/LANL, are key to the synthesis and characterization of materials and structures from nano-components to prototype-scale quantum systems.
  - Integration and testing couple closely to theory, design, and systems efforts
  - Development and testing of physical models of behavior of quantum devices
  - Co-located with National Lab x-ray, neutron, computing, and microfabrication facilities for understanding and scale-up of quantum structures
  - Next-generation qubits and sensors
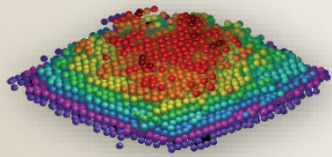
Sub-atomic Spatial Precision
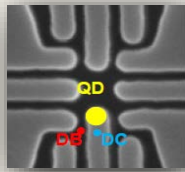
Solid State Artificial Atoms
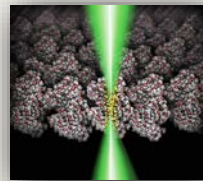
Single-nm lithography
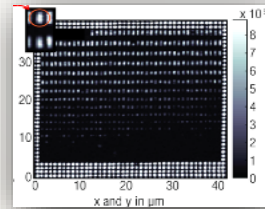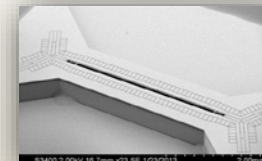
Entangled Qubit Arrays
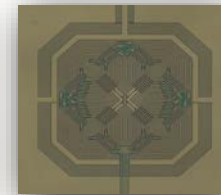
Quantum-Limited Sensors

Quantum Chip Testing
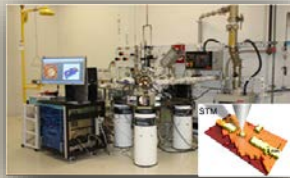
Atomic Precision Fabrication
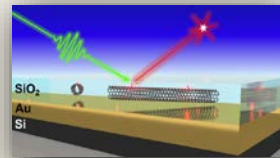
Single Photon Emitters and Detectors

Nanoscale 3D Printing

Waveguides, Cavities, Traps

Nano — Meso — Micro

FES and QIS

- FES is supporting QIS projects to

  - Explore the static and dynamical properties of beryllium hydride systems on quantum computing (QC) hardware and emulators by extending existing methods to include excitations, extended basis sets, time-dependent Hamiltonians, and hybrid quantum-classical methods.

  - To compute the complex dynamics in systems of interest to FES such as wave-particle interactions in plasmas. The team plans to implement their algorithms on the LANL quantum testbed hardware platform and compare performance to alternative quantum computing platforms.

New Quantum Materials with Lasers and XFELs

Extreme pressures could be key to unlocking hidden secrets of quantum matter

- Potential for varying atomic distances with laser pressure
- Potential for tuning material properties (energy levels)
- Potential for discovery of new phenomena (electrides, novel superconductors, metallic superfluids)
- Potential for new materials (kinetic stabilization of metastable phases and novel synthetic routes)

Could HED facilities open a new window into Quantum Materials?

Carbon phase stronger than diamond
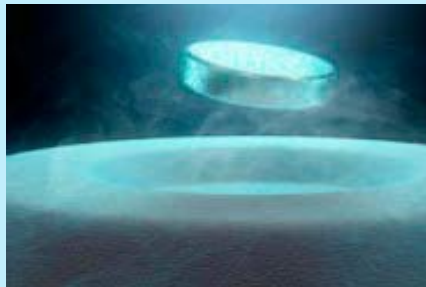
Hot superconductors

Transparent aluminum

High-energy-density (HED) facilities capable of conducting this research

- MEC at the Linac Coherent Light Source (SLAC)

- HED instrument at the European XFEL

ENERGY | Science

HEP: Quantum Information Science Enabled Discovery for High Energy Physics

- HEP is funding projects to conduct research on early stage quantum technologies for science includes:

  - Quantum Sensors that open new horizons for discovery and detection of dark matter and/or understanding of dark energy, new physics, and new interactions.

  - Quantum communication techniques that advance the state of the art and address fundamental physics questions via simulating cosmic physics including worm hole traversal;

  - Applying HEP developed technology and expertise in the areas of SRF (superconducting radio frequency) cavities for stabilizing superconducting qubit devices;

  - Applying HEP developed technology and expertise in controls, readouts and cold electronics for use in qubit systems and technology.

- HEP also sponsors an innovative QIS foundational research portfolio at the same labs that includes:

  - exploring connections between the cosmos and protocols and scrambling in qubit systems;

  - foundational development and formulations of particle physics phenomena and particle interactions that can be simulated and computed on quantum emulators and computers;

  - quantum machine learning and quantum computing for particle physics experiments including first principle developments of entropy entanglement in particle production;

  - QIS based experiments probing the science drivers like dark matter, dark energy, new particle and interactions, and physics beyond the Standard model.

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NP and QIS

- NP is supporting research projects to
  - Develop the expertise and knowledge that builds toward a Quantum Chromo Dynamics (QCD) simulations on Quantum Computers and Analog Quantum Simulators
  - Develop superconducting nanowire detectors capable of working in strong magnetic fields.
  - Measure and quantify the impact of background radioactivity on qubit coherence times

- Special materials are required to implement next-generation Quantum Information Systems. DOE/NP's Isotope Program is developing enriched stable isotope production capabilities in the U.S. for isotopes of interest for QIS with a near-term focus on gas centrifuge development.

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National Quantum Strategy and SC

DOE SC is well aligned with the national quantum strategy which provides a framework and a strategic vector for DOE and the labs to pursue their strategic objectives.

- **Science:** Research in quantum sensors, computing, and will advance QIS techniques and tools, while foundational studies (e.g., chemistry, cosmology, materials, nuclear and particle physics) together with quantum information theory will advance fundamental science and enable the design and discovery of novel quantum information systems

- **Workforce:** Postdocs and graduate students are supported at national laboratories. Early Career awards support promising scientists to pursue research careers in QIS and related areas. Programs such as SC-GSR and CSGF allow students to leverage DOE lab resources during their graduate training.

- **Industry:** Laboratories are partnering with the quantum computing vendors such as IBM, Ion-Q and D-wave to explore current NISQ technologies. User facilities at laboratories are available to industry.

- **Infrastructure:** DOE user facilities, including x-ray light sources and supercomputers, are already being used for QIS-related research. Development of specific technologies such as SRF cavities for qubits, imaging tools, etc. will provide infrastructure for others. Investments in NSRC user facilities provide advanced capabilities for QIS.

- **Economic and Security:** Foundational research at national labs will provide a base for future technologies. Exploration of technology at the precompetitive level (e.g. at ASCR's Quantum Testbeds) mitigates risk for industry.

- **International:** The national laboratories have partnership that include the international QIS community.

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National Quantum Initiative Act

- The National Quantum Initiative Act (NQIA) directs DOE to carry out a basic research program on quantum information science; leverage knowledge from existing QIS research and providing QIS training for additional undergraduate and graduate students; and coordinate research efforts with currently funded programs such as the Nanoscale Science Research Centers.

- The NQIA also directs the Office of Science establish with at least 2 but nor more than 5 National Quantum Information Science Research Centers. The DOE National labs are eligible Center applicants and are actively establishing multi-institutional partnerships.

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National Science and Technology Council Subcommittee on QIS

- Subcommittee on QIS
  - Co Chairs: Steve Binkley, DOE; Anne Kinney NSF; Carl Williams, NIST and Jacob Taylor, OSTP.
  - Members: Barbara Helland, DOE/SC and Mark Anderson, NNSA

- Subcommittee on Economic and Security Implications and Quantum Science (ESIX)
  - Co-Chairs: Steve Binkley, DOE: Deb Frincke, NSA; Paul Lopata, DOD and Jacob Taylor, OSTP
  - Members: Barbara Helland, DOE/SC and Mark Anderson, NNSA

- DOE is coordinating QIS activities with other Federal Agencies
  - NIST through the Quantum Economic Development-Consortium (QED-C), Bill Vanderlinde, DOE/SC serving on Board
  - NSF through coordination of NSF research activities and institutes with DOE research activities and institutes. A MOU is in progress.

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