Basic Energy Sciences Update

BES Advisory Committee Meeting

March 7, 2019

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Associate Director of Science
Basic Energy Sciences

Outline

- Budget Update
- Program Highlights and Solicitation Update
- Upcoming BESAC Charges

Basic Energy Sciences

The Program:

Materials sciences & engineering—exploring macroscopic and microscopic material behaviors and their connections to various energy technologies

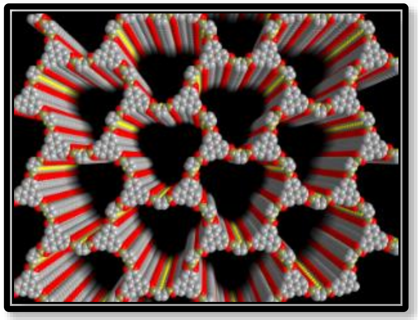
Chemical sciences, geosciences, and biosciences—exploring the fundamental aspects of chemical reactivity and energy transduction over wide ranges of scale and complexity and their applications to energy technologies

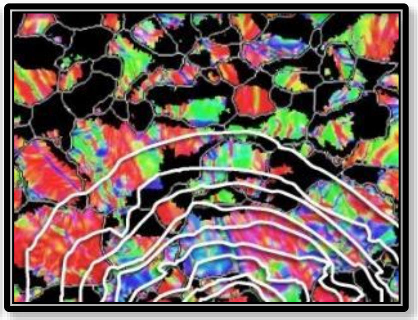
Scientific User Facilities
The largest collection of facilities for x-ray and neutron scattering and nanoscience tools in the world

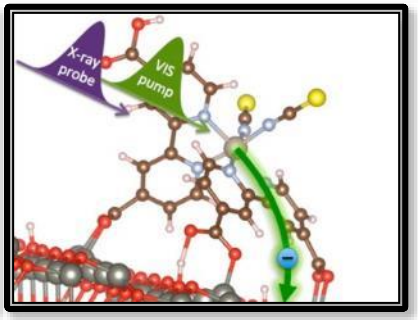
The Scientific Challenges:

- Synthesize, atom by atom, new forms of matter with tailored properties, including nano-scale objects with capabilities rivaling those of living things
- Direct and control matter and energy flow in materials and chemical assemblies over multiple length and time scales
- Explore materials & chemical functionalities and their connections to atomic, molecular, and electronic structures
- Explore basic research to achieve transformational discoveries for energy technologies

Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels







FY 2017 – FY 2019 BES Budget

FY 2017 Enacted: $1.871B

FY 2018 Enacted: $2.09B

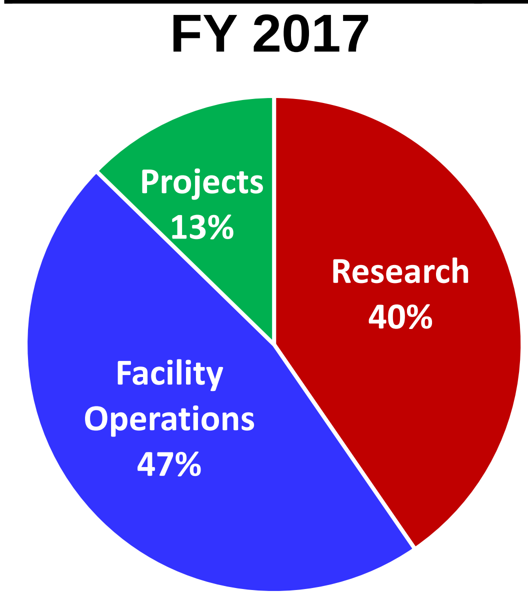
FY 2019 Enacted: $2.166B

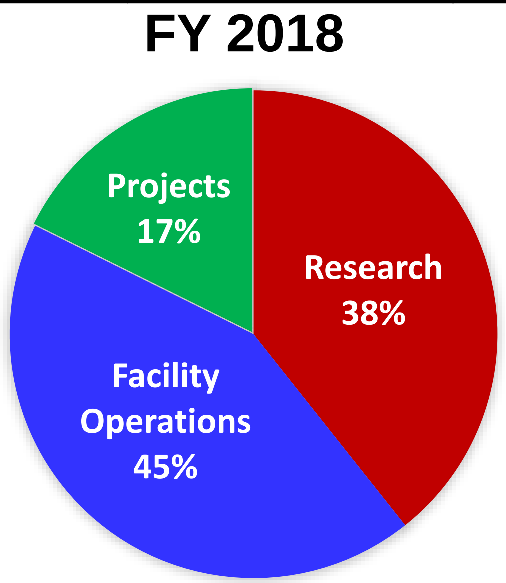
Priorities:

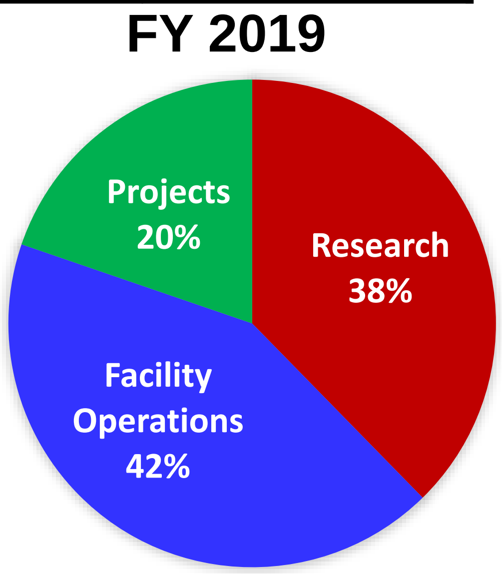
- Continue support of core research areas, EFRCs, Hubs, and CMS/CCS
- Continue support of 12 scientific user facilities at near optimal operation level
- Expand quantum information science (an SC-wide initiative) and other research priorities following strategic planning reports
- Support facility upgrades per 2016 BESAC prioritization study

BES Budget by Budget Element: 2017 - 2019

	FY 2017	FY 2018	FY 2019	
	Enacted	Enacted	President's Request	Enacted
Research	755,669	821,403	746,269	815,600
Facility Operations	877,331	898,597	878,331	922,000
Projects (Construction + MIE)	237,500	369,000	224,400	427,400
Other	1,000	1,000	1,000	1,000
Total	**1,871,500**	**2,090,000**	**1,850,000**	**2,166,000**



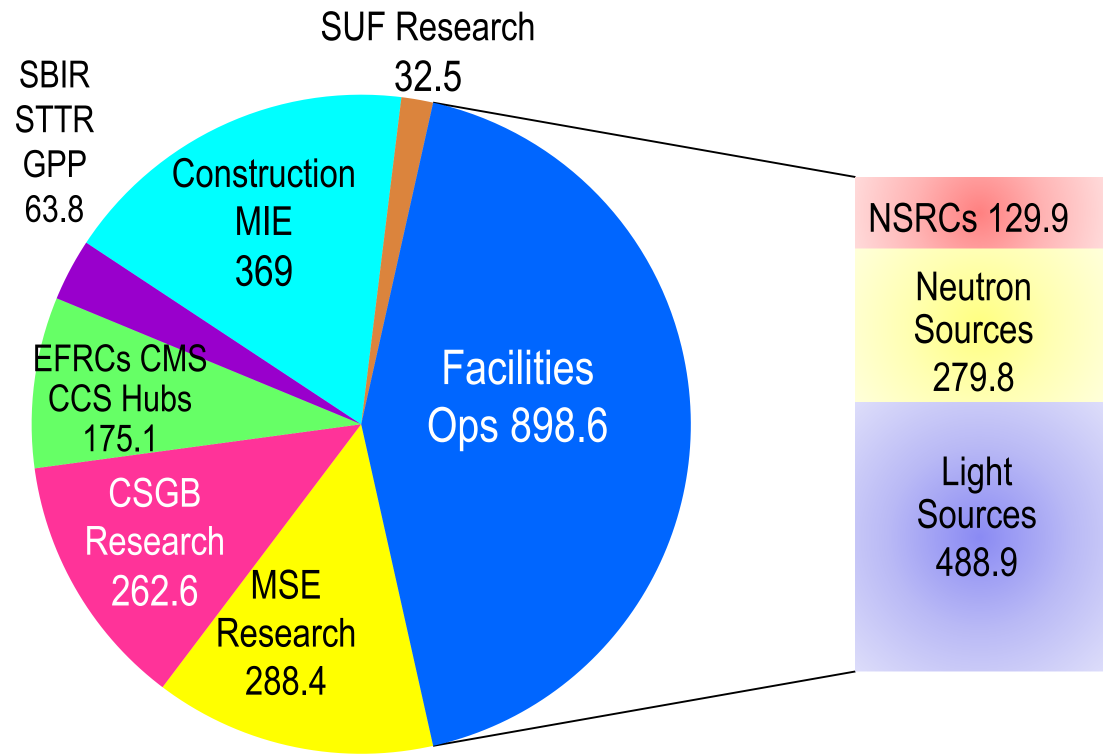




FY 2018 BES Budget:
$2090.0M (+$218.5M or +11.7% from FY 2017)

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).



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**

- Next to 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)

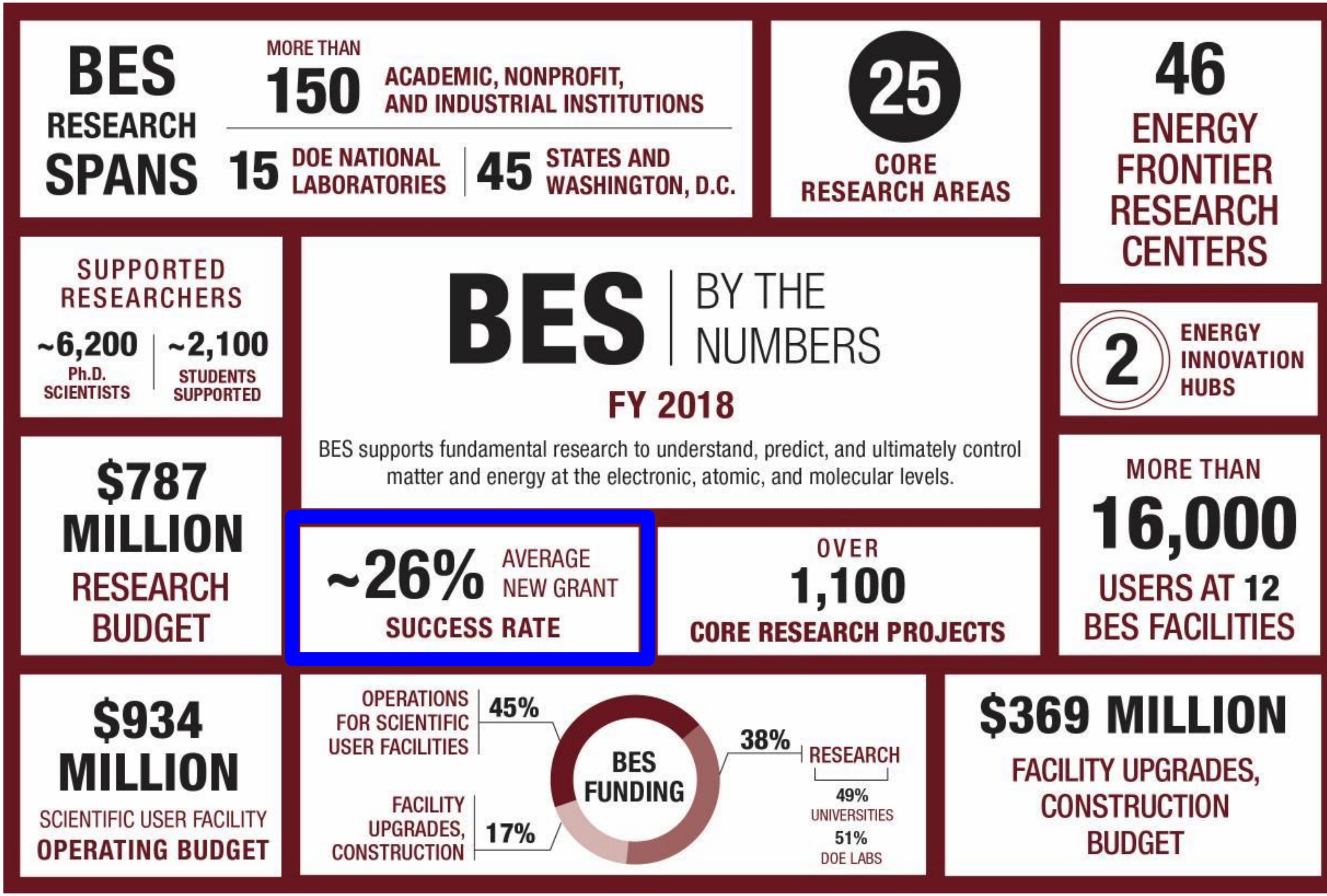
*includes OPC

Basic Energy Sciences - Research

FY 2018 Highlights

- FY 2018 appropriation provided new funds for FOAs in key topical areas:
  - **Quantum computing and quantum systems research** ($28M in FY 2018, 27 awards for 3 years)
  - **Ultrafast Chemical and Materials Sciences** ($10M in FY 2018, 10 awards for 3 years)
  - **Computational Chemical Sciences** ($5M in FY 2018, 10 awards for 3 years)
- **Energy Frontier Research Centers** were recompeted ($100M in FY 2018, 42 awards for 2 or 4 years).
- **The Batteries and Energy Storage Hub, JCESR**, was renewed for 5 years ($24M/year for 5 years).
- BES supported **40 Early Career awards** ($26M in FY 2018), up from 21 awards in FY 2017 (5-year awards).
- 82 **supplemental funds to DOE National Laboratories** ($21M) to add inflationary increases to projects and equipment awards to enhance specific capabilities.

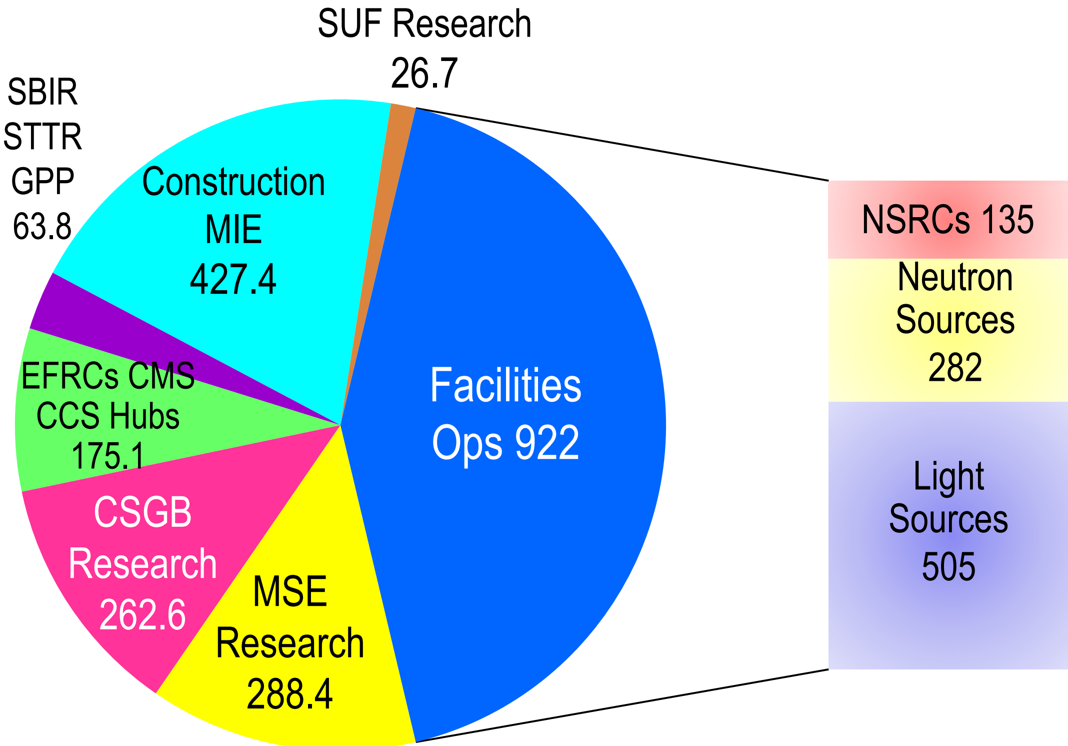
Basic Energy Sciences At a Glance (2018)



FY 2019 BES Budget:
$2166.0M (+$76M or +3.6% from FY 2018)

Research programs

- Core Research will emphasize quantum information science, data science for discovery, and BRN topics ($551M).
- Computational Materials and Chemical Sciences continue ($26M)
- Energy Frontier Research Centers continue ($110M)
- Funding continues for Energy Innovation Hubs (JCAP & JCESR) ($39M).



Scientific user facilities

- Operations of 12 facilities at nearly 100% optimal level ($922M; **Δ=+$23.4M**)

Construction/MIE* **Δ=+$58.4M**

- Last year of funding, LCLS-II ($135.4M)
- APS-U ($130M), LCLS-II-HE ($34M), ALS-U ($62M), PPU ($60M)
- One new start: STS ($6M)

*includes OPC

FY 2019 Funding Opportunity Announcements

Materials and Chemical Sciences Research for Quantum Information Science ($15M/year for 3 years)

- Focus on experiment and theory for the discovery and characterization of quantum phenomena to enable design and discovery of novel materials and chemistries for quantum information systems and the use of quantum computing to solve problems in chemical and materials science research.

Computational Materials Sciences ($8M/year for 4 years)

- Focus on the creation of computational codes and associated experimental/ computational databases for the design of functional materials that take advantage of DOE's supercomputing capabilities, including current pre-exascale and upcoming exascale systems.

Data Science for Discovery in Chemical and Materials Sciences ($10M/year for 3 years)

- Focus on development and application of data sciences approaches and tools to complex energy-relevant chemical and materials systems to develop new and more accurate understanding of emergent behavior, processes, and mechanisms.

Established Program to Stimulate Competitive Research (DOE EPSCoR) Implementation Grants ($20M in FY 2019 funds)

- Improve early-stage research capability through the support of a group of scientists and engineers working on a common scientific theme in one or more EPSCoR jurisdictions.

TITLE IV—DEPARTMENT OF ENERGY QUANTUM ACTIVITIES

SEC. 401. QUANTUM INFORMATION SCIENCE RESEARCH PROGRAM.

(a) In General.—The Secretary of Energy shall **carry out a basic research program on quantum information science**.

(b) Program Components.—In carrying out the program under subsection (a), the Secretary of Energy shall—

(1) formulate goals for quantum information science research to be supported by the Department of Energy;

(2) leverage the collective body of knowledge from existing quantum information science research;

(3) provide research experiences and training for additional undergraduate and graduate students in quantum information science, including in the fields of—

- (A) **quantum information theory**;
- (B) **quantum physics**;
- (C) **quantum computational science**;
- (D) applied mathematics and algorithm development;
- (E) quantum networking;
- (F) **quantum sensing and detection; and**
- (G) **materials science and engineering**;

(4) **coordinate research efforts funded through existing programs** across the Department of Energy, including—

- (A) the Nanoscale Science Research Centers;
- (B) the Energy Frontier Research Centers;
- (C) the Energy Innovation Hubs;
- (D) the National Laboratories;
- (E) the Advanced Research Projects Agency; and
- (F) the National Quantum Information Science Research Centers; and

(5) **coordinate with other** Federal departments and agencies, research communities, and potential users of information produced under this section.

The bill directs the President to implement a 10-year National Quantum Initiative Program.

The bill defines QIS as the storage, transmission, manipulation, or measurement of information that is encoded in systems that can only be described by the laws of quantum physics.

National Quantum Initiative Act

H.R. 6227 passed by Congress on 12/13/2018 and signed into law on 12/21/2018

Department of Energy

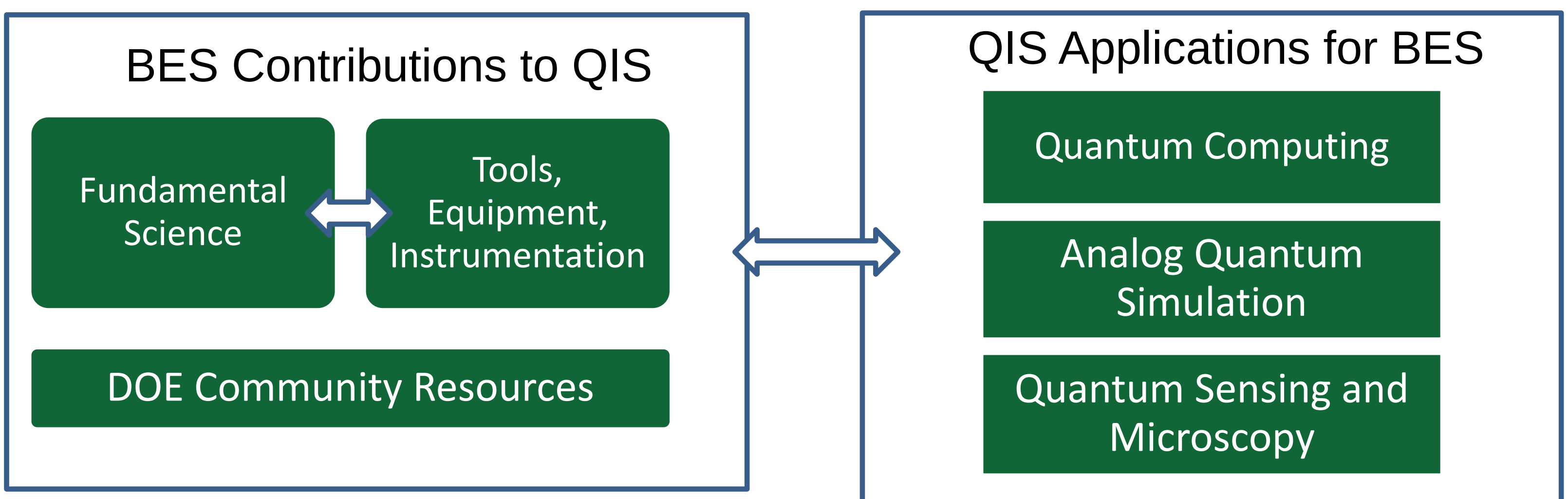
The Committee recognizes **DOE's capabilities, research infrastructure, and expertise in materials science, physics, applied mathematics, and computer science provide a foundation** for significant advances in QIS research and technological development. In particular, the **DOE National Laboratories,** which **operate world class, open-access user facilities** around the country, provide access to the supercomputers, x-ray light sources, photon sources, and neutron sources that are necessary to conduct ground-breaking quantum research. … **The Committee supports DOE's current efforts to increase investment in QIS across the Office of Science**, including for proposed programs in Biological and Environmental Research, High Energy Physics, Nuclear Physics, Basic Energy Sciences, and Advanced Scientific Computing Research (ASCR), as requested in the President's fiscal year 2019 Budget.

Sec. 402. National Quantum Information Science Research Centers

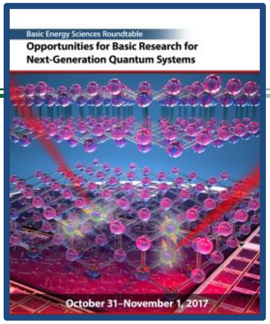
This section directs the DOE Office of Science to establish and operate **up to five National Quantum Information Science Research Centers to conduct basic research to accelerate scientific breakthroughs in quantum information science and technology**. This section also outlines criteria for establishment, collaborations, and other requirements. The Centers are directed to carry out activities for a period of five years. This section authorizes appropriations of $625,000,000 over five years for the Office of Science to carry out this section, which shall include $125,000,000 for each fiscal years 2019 through 2023.

Quantum Information Science Activities in BES

- **Next Generation Quantum Systems**: Develop understanding leading to control of quantum phenomena in chemical and materials systems to advance quantum-based science and technology.
- **Quantum Computing**: Develop quantum computing algorithms and utilize emerging quantum computing capabilities to address major scientific problems in chemical and materials sciences.
- **User Capabilities:** Research and infrastructure at the Nanoscale Science Research Centers, enabling next-generation qubit concepts, innovative quantum and classical architectures.

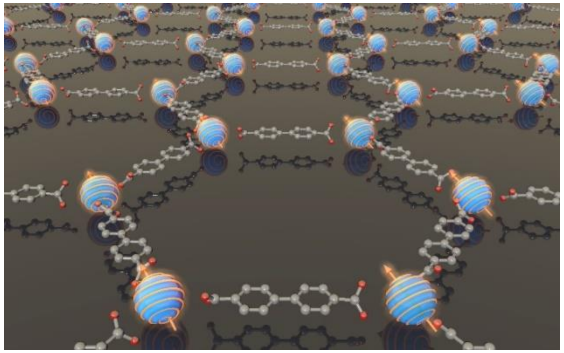


Quantum Information Science Activities in BES
Science-First Approach

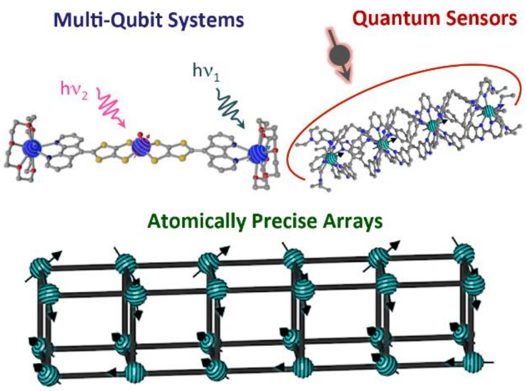


Next Generation Quantum Systems:

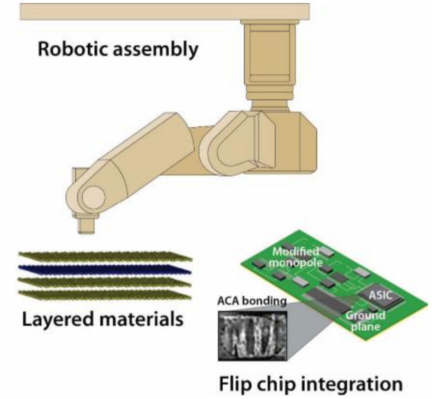
- **Design, Synthesis and Characterization – synthesize artificial quantum systems and real-time feedback with atomic-level control**
- **Coherence and Transduction – generate, entangle, stabilize and transmit coherent quantum states and mitigate decoherence**
- **Entanglement and Sensing – demonstrate many-particle entanglement and control to achieve extreme sensing and detection**



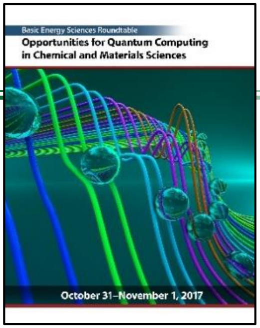
Metal-organic hybrid systems interfaced with functionalized surfaces



Coordination compounds as qubits

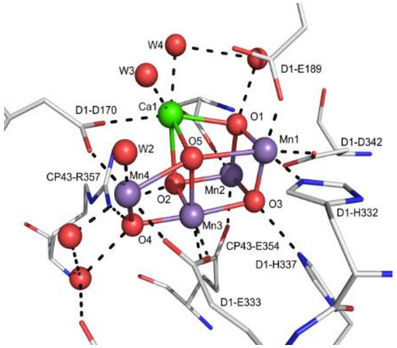


Automated assembly of layered materials

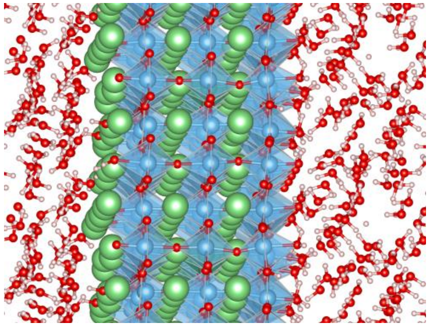


Quantum Computing:

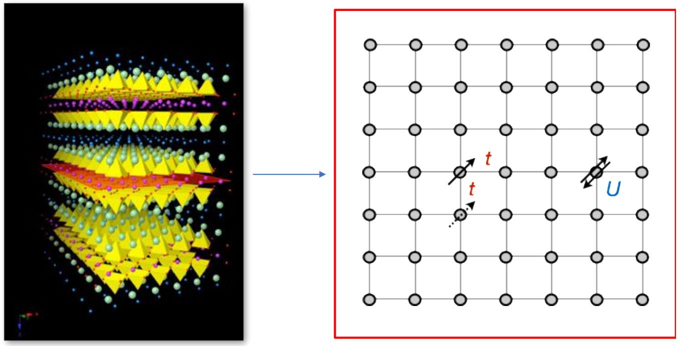
- **Quantum Dynamics – understand and explore out-of-equilibrium dynamics in driven systems, catalytic pathways, and chemical reactions**
- **Simulation of Strongly Correlated Electrons – understand strong electronic correlations and their complex many-body dynamics**
- **Classic-Quantum Hybrid Approaches – embed quantum hardware and algorithms to pass information back and forth between quantum and classical platforms in real time**



Oxygen evolving complex of Photosystem II



Catalytic properties at liquid-solid interfaces of $SrTiO_3$

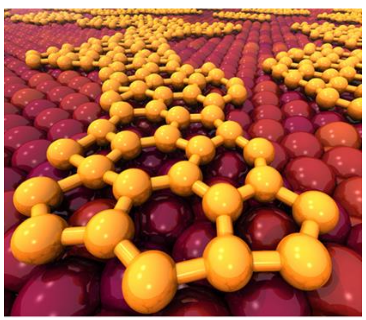


Fermi-Hubbard model of layered high-temperature copper-oxide superconductors

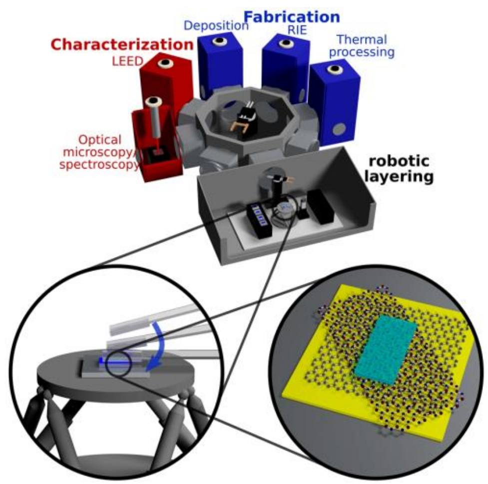
User Capabilities at Nanoscale Research Science Centers:

Understand the limits of coherence and entanglement in quantum information systems

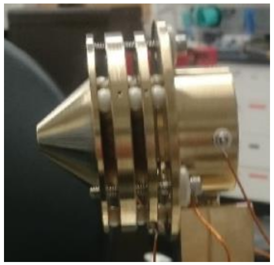
- Synthesis of quantum materials and structures with atomic precision
- Fabrication and integration of photon and spin qubit systems
- Advanced instrumentation and tool development for quantum computers, sensors and metrology



Materials design and synthesis at the atomic level



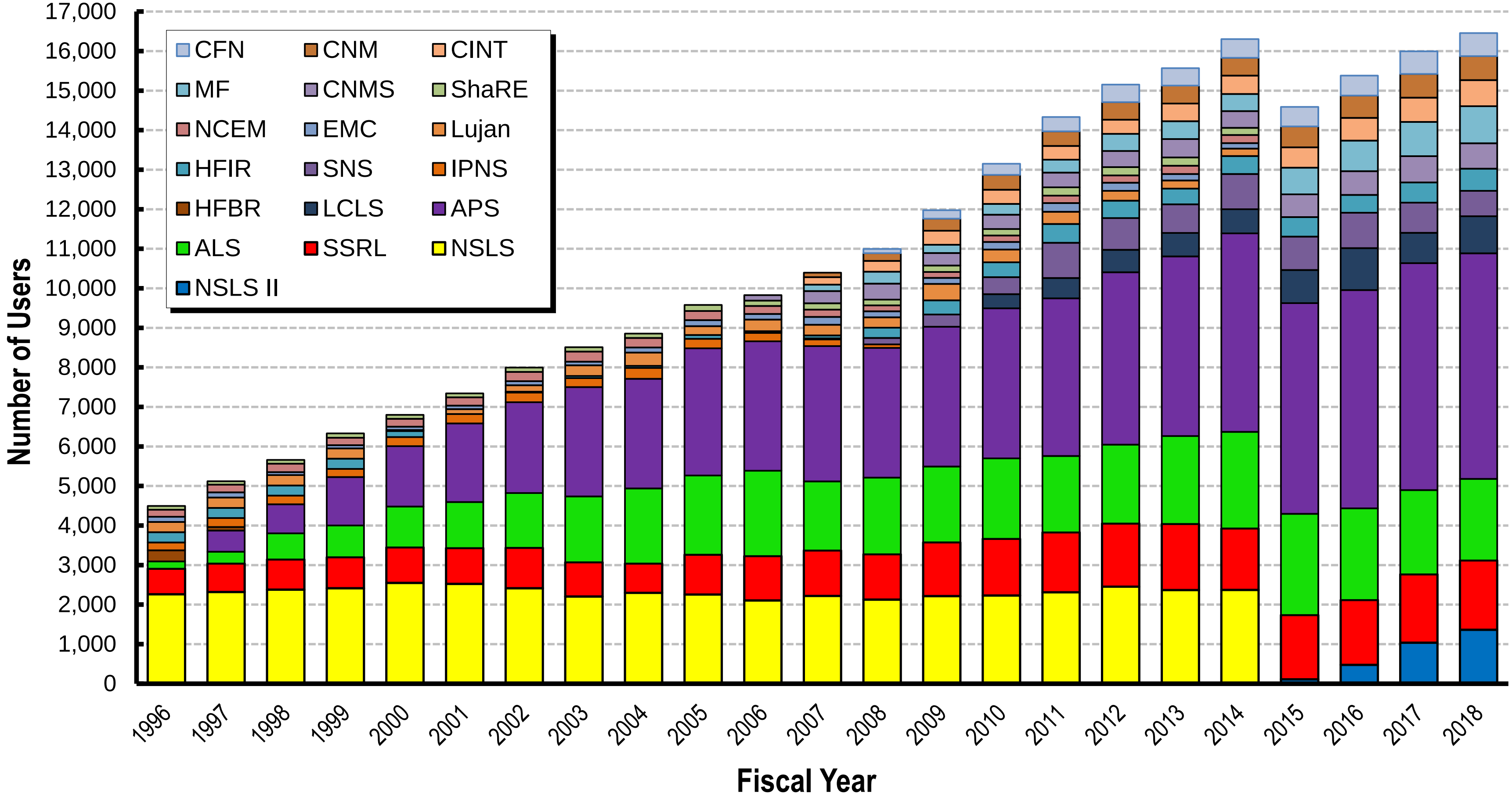
Novel synthesis and 2D materials integration approaches



Revolutionary coherence metrology capabilities

Quantum structure and prototype system testing

BES User Facilities Hosted >16,000 Users in FY 2018



More than 300 companies from various sectors of the manufacturing, chemical, & pharmaceutical industries conducted research at BES scientific user facilities. Over 30 companies were Fortune 500 companies.

Research at APS Contributes to 2018 Chemistry Nobel Prize

Scientific Achievement

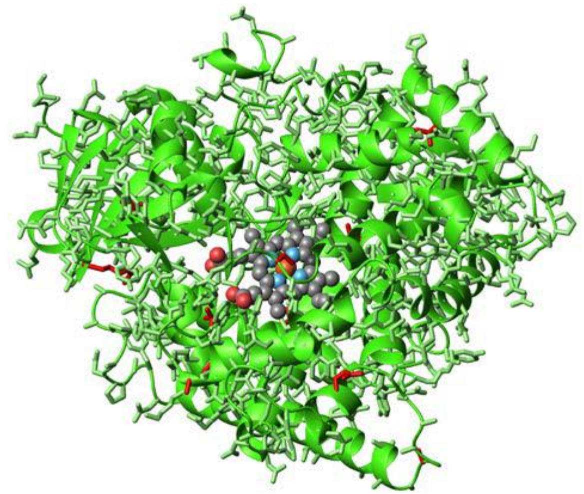
Dr. Frances Arnold (California Institute of Technology) was 1 of 3 2018 Chemistry Nobel awardees for work showing how “directed evolution” can be used to develop proteins or enzymes that have desired enzymatic activity, which can be used to produce chemicals, biofuels, and pharmaceuticals.

Significance and Impact

“The structures were critically important to advancing and understanding the overall evolutionary design successes for which Dr. Arnold has been recognized,” said Matthew Redinbo, William R. Kenan Distinguished Professor of Chemistry, Biochemistry, Microbiology, and Genomics at the University of North Carolina at Chapel Hill, who collaborated on the study.

Research Detail

As part of this research, samples of the enzymes that were created were studied utilizing the General Medical Sciences and Cancer Institutes beamline 23-ID-D at the Advanced Photon Source (APS), a U.S. Department of Energy Office of Science User Facility.



Structure of an evolved biocatalyst for cyclopropanation, determined at the APS.

See: P.S. Coelho et al., Nat. Chem. Biol. **9**, 485 (2013). DOI: 10.1038/nchembio.1278
Contact: frances@cheme.caltech.edu

Scientific Background on the Nobel Prize in Chemistry 2018, “DIRECTED EVOLUTION OF ENZYMES AND BINDING PROTEINS,” 3 OCTOBER 2018, https://www.nobelprize.org/uploads/2018/10/advanced-chemistryprize-2018.pdf

Work performed at Argonne National Laboratory

Successful Demonstration of Fastest Electron Detector Ever Made (Feb 12, 2019)

Accomplishment

Successful installation and testing of the new **4D Camera** that can produce continuous electron images every 11 microseconds. That's about 60X faster than what was possible with previous high speed electron detectors.

Unique Advances Enabled

87,000 frames/second, optimized for high dynamic range through speed and sensitivity

Impact of the New Capability

- Acquisition of pixelated images during high resolution STEM imaging without slowing down the electron probe, leading to real-time phase contrast ptychographic imaging
- Drift mitigation and improvements in signal/noise for beam-sensitive samples (ie- biomolecules)
- Breakthroughs in nanoscale strain mapping and quantification of materials using scanning electron diffraction imaging methods at high resolution

Movie of summed 11 microsecond frames showing accumulation of single electron hits at 91kHz

4D = Dynamic Diffraction Direct Detector

- ***All data will be streamed in real time via a 400 Gbps 1 km optical link to the Cori supercomputer at NERSC for inline processing and analysis.***

Contributors: Jim Ciston, Ian J. Johnson, Brent R. Draney, Peter Ercius, Erin Fong, Azriel Goldschmidt, John M. Joseph, Jason R. Lee, Alexander Mueller, Colin Ophus, Ashwin Selvarajan, David E. Skinner, Thorsten Stezelberger, Craig S. Tindall, Andrew M. Minor, and Peter Denes

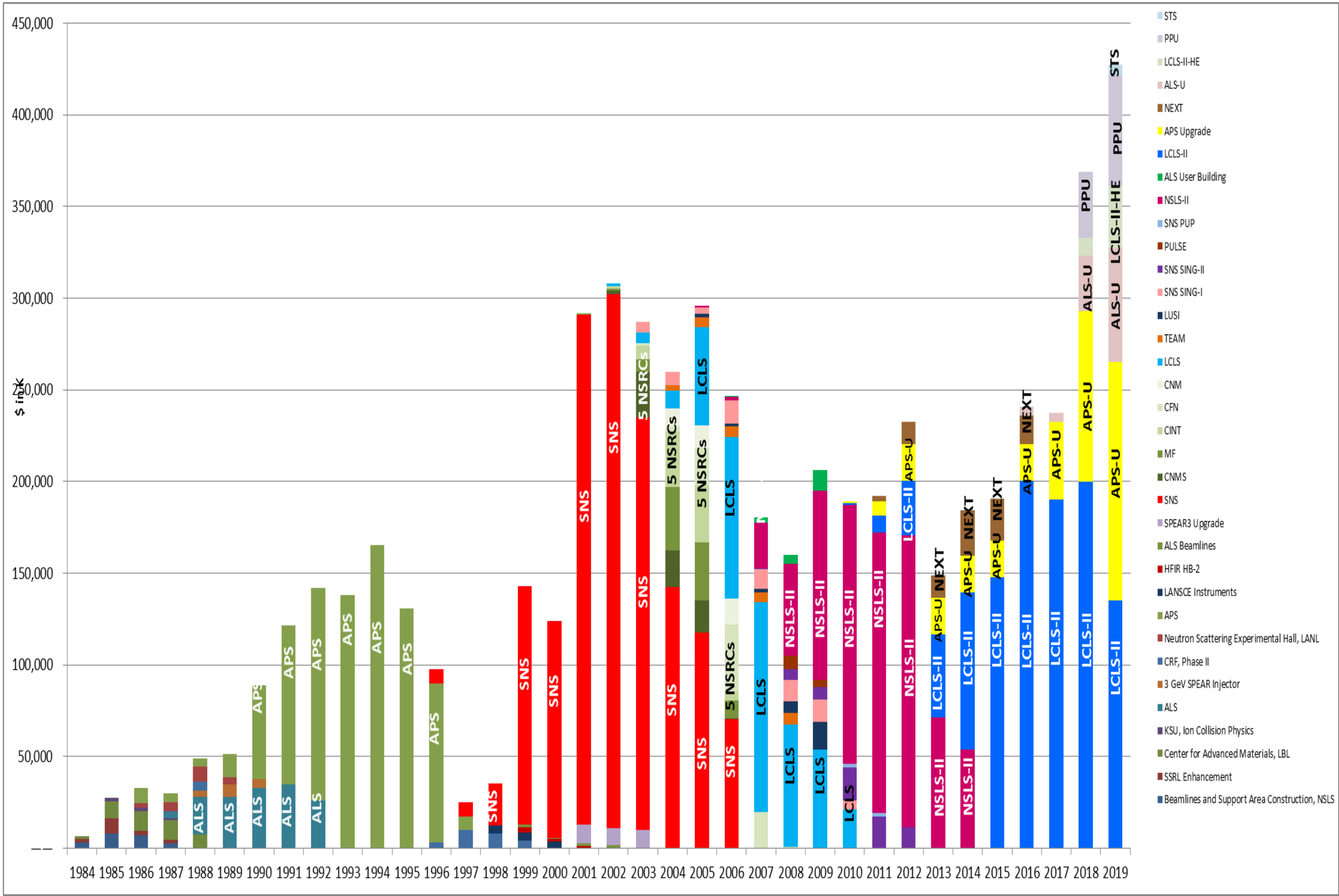
High Flux Isotope Reactor (HFIR) Update

- Reactor shutdown in November 2018, following a slight increase of radioactivity in the Primary Coolant System.
- No release of radiation detected and no staff exposed to any radiation from this event.
- 45 of the 540 fuel plates had deflected.
- DOE, ORNL, and the fuel vendor are investigating the cause
- Most likely due to inadequate fusion between the weld, fuel plate, and support assembly.
- ORNL is developing a restart plan and is aiming to be ready to restart the reactor by the end of Fiscal Year 2019
- By May 1st 2019 an estimated 240 unique and 627 total users will have been impacted, with 252 experiments cancelled

BESAC Report on Facility Upgrades (June 2016)

Project	ANL APS-U	LBNL ALS-U	ORNL SNS PPU	ORNL SNS STS	SLAC LCLS-II	SLAC LCLS-II-HE
Proposed Project	Hard X-ray ~Diffraction Limited 6 GeV MBA Ring	Soft X-ray ~Diffraction Limited 2 GeV MBA Ring	Proton Power Upgrade to 2.5 MW (W Target) 1.3 GeV SC Linac	High Resolution Neutron Science; Second Target Station	High Rep-Rate, Soft X-ray FEL, 4 GeV SC Linac	High Rep-Rate, Medium Energy X-ray FEL, 8 GeV SC Linac
Current Status of Facility	APS is operational since 1996; ring will be replaced	ALS is operational since 1993; ring will be replaced	SNS Linac is operational since 2006 at 0.94 GeV	SNS is operational since 2006	LCLS is operational since 2010; LCLS-II is under construction	LCLS is operational since 2010; LCLS-II is under construction
Worldwide Competition	EU **ESRF** Germany **PETRA3,4** Japan **SPring-6** China **HEPS**	Sweden **MAX-IV** Brazil **SIRIUS** CH **SLS-II**	EU **ESS** Japan **JPARC** China **CSNS** UK **ISIS**	EU **ESS** Japan **JPARC** China **CSNS** UK **ISIS**	EU **XFEL** Japan **SACLA** Korea **PAL XFEL** CH **Swiss FEL**	EU **XFEL** China **SCLF**
Status Q2/19	CD-2 CD-3B	CD-1	CD-1 CD-3A	CD-0	CD-3	CD-1
FY19 Approp	✓	✓	✓	✓	✓	✓

BES Construction/MIE Funding Profile 1984 – 2019



New BESAC Charge from Dr. Binkley (Feb. 5, 2019)

The single Recommendation from the BES40 report asked BES to be bold in choosing new research and facilities to support and experimenting with new funding mechanisms where appropriate. This recommendation is especially timely in view of intensifying globalization in research talent and resources. ... I am writing to ask BESAC to provide input on possible implementation strategies, especially in the context of keeping pace with international competition.

- *Within the BES-supported topical research areas and facility capabilities, in which areas and capabilities is U.S. leadership most threatened, presently or in the foreseeable future?*
- *To preserve and foster U.S. leadership with resource constraints, what are the key efficiencies and balances that should be sought?*
- *For someone deciding whether to pursue a scientific career, or a mature scientist considering whether to stay in the U.S., how can BES programs and facilities be structured and managed to create incentives that will attract and retain talents? What are the key attractions and deterrents of a career in BES-supported science areas? How can the mix of research funding modalities be designed to enhance the attractions and minimize the deterrents?*

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New BESAC Charge from Dr. Binkley (Feb. 25, 2019)

The U.S. Department of Energy (DOE) has maintained long-term stewardship of neutron capabilities for the Nation. The combination of the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR), under the auspices of Basic Energy Sciences (BES) in the Office of Science, has provided the U.S. scientific community with leading neutron capabilities in support of DOE's missions in science, energy, environment, and national security. With the planning process for both the PPU and STS projects under way in 2019, I am writing to seek the input of BESAC on the long-term strategy concerning HFIR, which complements SNS and is among the highest-flux reactor-based sources in the world. With HFIR entering its 6th decade, its long-term future requires careful thought and planning, especially in the context of the U.S. domestic high-performance neutron research facilities.

This charge is also in part informed by the 2018 "Neutrons for the Nation" report, commissioned by the American Physical Society's Panel on Public Affairs, which focuses on the competing goals of reducing nuclear proliferation risk while maintaining intense controlled sources of neutrons for vital scientific and industrial work. The report highlighted the continued need for the U.S. to support its diversity of neutron R&D capabilities, as well as to initiate planning for a new generation of high-performance research reactors.

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New BESAC Charge from Dr. Binkley (Feb. 25, 2019)

I am asking BESAC to form a subcommittee to assess the scientific justification for a U.S. domestic high-performance reactor-based research facility, taking into account current international plans and existing domestic facility infrastructure.

- *What is the merit and significance of the science that could be addressed by a high performance, steady-state reactor, and what is its importance in the overall context of research in materials sciences and related disciplines?*
- *What are the capabilities of other domestic and international facilities, existing and planned, to address the science opportunities afforded by such a domestic research reactor?*
- *What are the benefits to other fields of science and technology and to industry of establishing such a capability in the U.S.? In particular, consider applications such as isotope production, materials irradiation, neutron imaging, dark matter research, and neutron activation for trace element analysis.*
- *What are the strengths and limitations of a steady-state research reactor compared to a pulsed spallation neutron source for science, engineering, and technology?*
- *Are there feasible upgrade paths for HFIR to provide world-leading capabilities in serving the Office of Science missions well into the future?*
- *Can Low Enriched Uranium (LEU) and High Assay LEU (HALEU) fuels (defined as<20% enriched U-235) replace Highly Enriched Uranium fuels in research reactors while preserving the needed characteristics of neutrons produced by steady-state reactors? What R&D would be needed to support LEU and HALEU fuels development?*