



U.S. DEPARTMENT OF
ENERGY

Office of
Science

Basic Energy Sciences Update

BES Advisory Committee Meeting
March 22, 2018

Harriet Kung
Director, Basic Energy Sciences
Office of Science, U.S. Department of Energy

Outline

- DOE & BES News
- FY 2019 President's Budget Request
- FY 2018 Appropriations Status
- BESAC Charge – BES 40th Anniversary



DOE Appointee Status

Deputy Secretary of Energy Nominee Dan Brouillette

- Nomination announced April 3, 2017
- Senate Hearing May 25, 2017
- Senate Confirmation on August 3, 2017
- Sworn in August 7, 2017



Under Secretary for Science Nominee Paul Dabbar

- Nomination announced July 12, 2017
- Senate Hearing July 20, 2017
- Senate Confirmation November 2, 2017
- Sworn in November 7, 2017



Under Secretary for Science Nominee Paul Dabbar

Paul Dabbar is Managing Director in the Global Mergers & Acquisitions Group, and Head of Energy Mergers & Acquisitions at J.P.Morgan, the investment banking division of JPMorgan Chase & Co. He has also led a number of M&A transactions for JPMorgan Chase. He has been financial advisor on over \$300 billion in M&A transactions, including corporate mergers, subsidiary sales and purchases, government privatizations, joint ventures, corporate restructurings, private equity transactions, and unsolicited corporate transactions for companies in the energy sector, including nuclear, as well as in the industrials and financial institutions sectors.

Mr. Dabbar is a member of the Board of the U.S. Department of Energy Environmental Management Advisory Board, and is chairman of his U.S. Naval Academy class fundraising board.

Prior to J.P.Morgan, Mr. Dabbar was a nuclear submarine officer, serving on board the U.S.S. Pintado (SSN-672) out of Mare Island, CA, and Pearl Harbor, HI, where he completed deployments to places including the North Pole and South America. He also worked at the Johns Hopkins Applied Physics Laboratory conducting U.S. Department of Defense research.

Mr. Dabbar has a B.S. with merit in marine engineering from the U.S. Naval Academy (Class of '89) and a M.B.A. from Columbia University. He also completed the U.S. Naval nuclear program's Engineer's School.

<https://energy.gov/em/contributors/paul-m-dabbar>

Office of Basic Energy Sciences

Harriet Kung, Director

BES Budget and Planning

Vacant, Financial Management
Donetta Herbert, Financial Management
Thomas Russell, Senior Technical Advisor

BES Operations

Kerry Hochberger, Program Support Specialist
Robin Hayes, Program Manager
Natalia Melcer, Program Manager
Katie Runkles, Program Analyst / BESAC*
Andy Schwartz, Senior Technical Advisor for EFRCs*

* Basic Energy Sciences Advisory Committee
* Energy Frontier Research Centers

Materials Sciences and Engineering Division

Linda Horton, Director

Teresa Crockett, Program Analyst
Vacant, Secretary

Scientific User Facilities Division

James Murphy, Director

Vacant, Program Support Specialist
Rocio Meneses, Program Assistant

Chemical Sciences, Geosciences, and Biosciences Division

Bruce Garrett, Director

Vacant, Program Assistant

Materials Discovery, Design, and Synthesis

Helen Kerch, Acting
Vacant, P.A.

Condensed Matter and Materials Physics

Jim Horwitz
Vacant, P.A.

Scattering and Instrumentation Sciences

Helen Kerch
Vacant, P.A.

Operations

Construction

Fundamental Interactions

Jeff Krause
Vacant, P.A.

Photochemistry and Biochemistry

Gail McLean
Vacant, P.A.

Chemical Transformations

Raul Miranda
Vacant, P.A.

Materials Chemistry

Craig Henkel
Michael S.

Biomolecular Sciences

Mike Mar

Catalysis Science

Miviane Schwartz
Chris Bradley

Separation Science

Philip Wilk
Chuck Peden
Vacant

Congrats, Mark Spitler & Jim Rhyne!

Program Manager

Solar Photochemistry

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Dr. Spitler joined the U.S. Department of Energy in 2007 as the program manager for the Solar Photochemistry program. Prior to joining DOE, Dr. Spitler was a Senior Scientist at the National Renewable Energy Laboratory (Golden, CA.) From 1997 to 2004 he was President of ChemMotif, Inc., a company formed with former Polaroid colleagues

Program Manager

Neutron and X-ray Scattering Facilities

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Dr. James J. Rhyne joined the Scientific User Facilities Division of DOE's Office of Basic Energy Sciences in February 2013 as a program manager for Neutron and X-ray Scattering Facilities. He had been the Deputy Director for Science of the Lujan Neutron Scattering Center at Los Alamos National Laboratory since 2003

DOE/CF-0144

Department of Energy FY 2019 Congressional Budget Request



Budget in Brief

February 2018

Office of Chief Financial Officer

Message from Secretary Perry

The President's Budget for FY 2019 requests **\$30.6B** for the Department of Energy (DOE) to advance U.S. national security and economic growth through transformative science and technology innovation that promotes affordable and reliable energy through market solutions and meets our nuclear security and environmental cleanup challenges.

The FY 2019 Budget Request provides:

- \$15.1B to modernize and restore the nuclear security enterprise aligned with the Nuclear Posture Review (NPR) and National Security Strategy
- **\$5.4B to conduct cutting-edge, early-stage scientific research and development (R&D) and build state-of-the-art scientific tools and facilities to keep U.S. researchers at the forefront of scientific innovation, including achieving exascale computing in 2021**
- \$2.5B to promote America's energy dominance through technologies that will make our energy supply more affordable, reliable, and efficient
- \$6.6B to continue our commitment for the cleanup of sites resulting from five decades of nuclear weapons development and production and Government-sponsored nuclear energy research



FY 2019 SC Budget Guidance

FY 2017 Enacted: \$5.391B

FY 2018 President's Request: \$4.473B

FY 2019 President's Request: \$5.391B

Priorities:

- Continue operations of the national laboratories
- Continue exascale computing research for delivery in FY 2021
- Expand quantum computing and quantum information science efforts
- Provide sufficient funding to ensure robust cybersecurity program
- Focus on cutting edge, early stage research and development
- Maintain interagency and international partnerships

Office of Science at a Glance

FY 2019 Request: \$5.39B



**Largest Supporter of
Physical Sciences in
the U.S.**



**Funding at >300
Institutions including
all 17 DOE Labs**



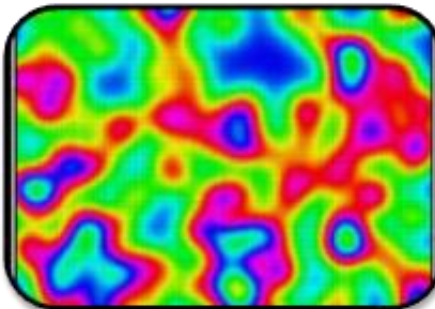
**Over 22,000
Scientists Supported**



**Nearly 32,000 Users
of 26 SC Scientific
Facilities**



**~40% of Research to
Universities**



**Research: 40%,
\$2.15B**



**Facility Operations:
39%, \$2.12B**



**Projects/Other:
21%, \$1.12B**

FY 2019 SC Budget Request

(Dollars in Thousands)

| | FY 2017 | | FY 2018 | | | | FY 2019 | |
|---|------------------|------------------|---------------------|------------------|------------------|----------------------------|---------------------|---|
| | Enacted Approp. | Current Approp. | President's Request | House Mark | Senate Mark | Annualized CR ^b | President's Request | President's Request vs. FY 2017 Enacted |
| ASCR..... | 647,000 | 626,559 | 722,010 | 694,200 | 763,000 | 642,606 | 899,010 | 252,010 38.95% |
| BES..... | 1,871,500 | 1,812,113 | 1,554,500 | 1,871,500 | 1,980,300 | 1,858,791 | 1,850,000 | -21,500 -1.15% |
| BER..... | 612,000 | 588,826 | 348,950 | 582,000 | 633,000 | 607,844 | 500,000 | -112,000 -18.30% |
| FES..... | 380,000 | 368,119 | 309,940 | 395,000 | 232,000 | 377,419 | 340,000 | -40,000 -10.53% |
| HEP..... | 825,000 | 802,849 | 672,700 | 825,000 | 860,000 | 819,397 | 770,000 | -55,000 -6.67% |
| NP..... | 622,000 | 604,473 | 502,700 | 619,200 | 639,200 | 617,776 | 600,000 | -22,000 -3.54% |
| WDTS..... | 19,500 | 19,500 | 14,000 | 19,500 | 19,500 | 19,368 | 19,000 | -500 -2.56% |
| SLI..... | 130,000 | 130,000 | 76,200 | 105,600 | 143,000 | 129,117 | 126,852 | -3,148 -2.42% |
| S&S..... | 103,000 | 103,000 | 103,000 | 103,000 | 103,000 | 102,301 | 106,110 | 3,110 3.02% |
| PD..... | 182,000 | 182,000 | 168,516 | 177,000 | 177,000 | 180,764 | 180,000 | -2,000 -1.10% |
| SBIR/STTR (SC)..... | | 154,561 | | | | | | |
| Subtotal, Science..... | 5,392,000 | 5,392,000 | 4,472,516 | 5,392,000 | 5,550,000 | 5,355,383 | 5,390,972 | -1,028 -0.02% |
| SBIR/STTR (DOE)..... | | 90,813 | | | | | | |
| Rescission of PY Bal ^a | -1,028 | -1,028 | | | | -1,021 | | 1,028 -100.00% |
| Total, Science..... | 5,390,972 | 5,481,785 | 4,472,516 | 5,392,000 | 5,550,000 | 5,354,362 | 5,390,972 | |

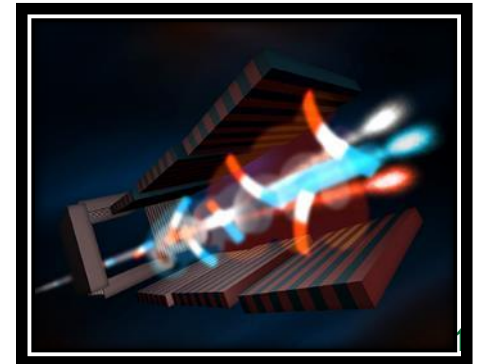
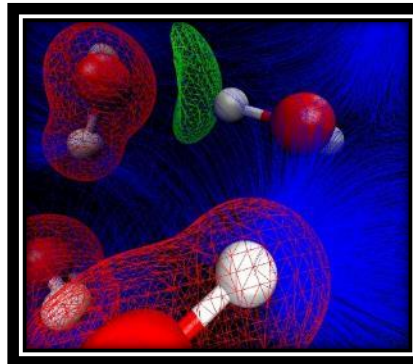
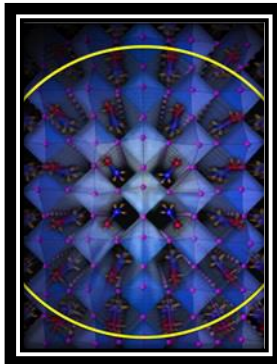
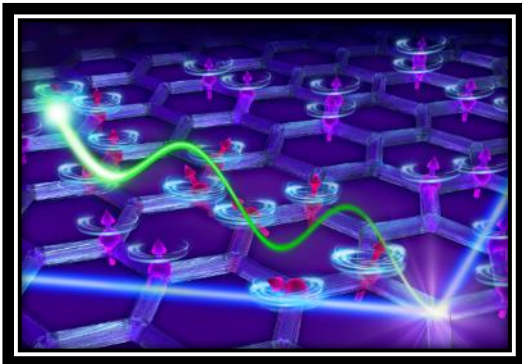
^a Rescission of PY funds in the amount -\$239M for FY 2012 and older; -\$239M for FY 2013; and -\$550M for FY 2014 - FY 2016.

^b FY 2018 Annualized CR column is based on the FY 2017 Enacted minus a 0.6791% reduction totaling \$36.617M

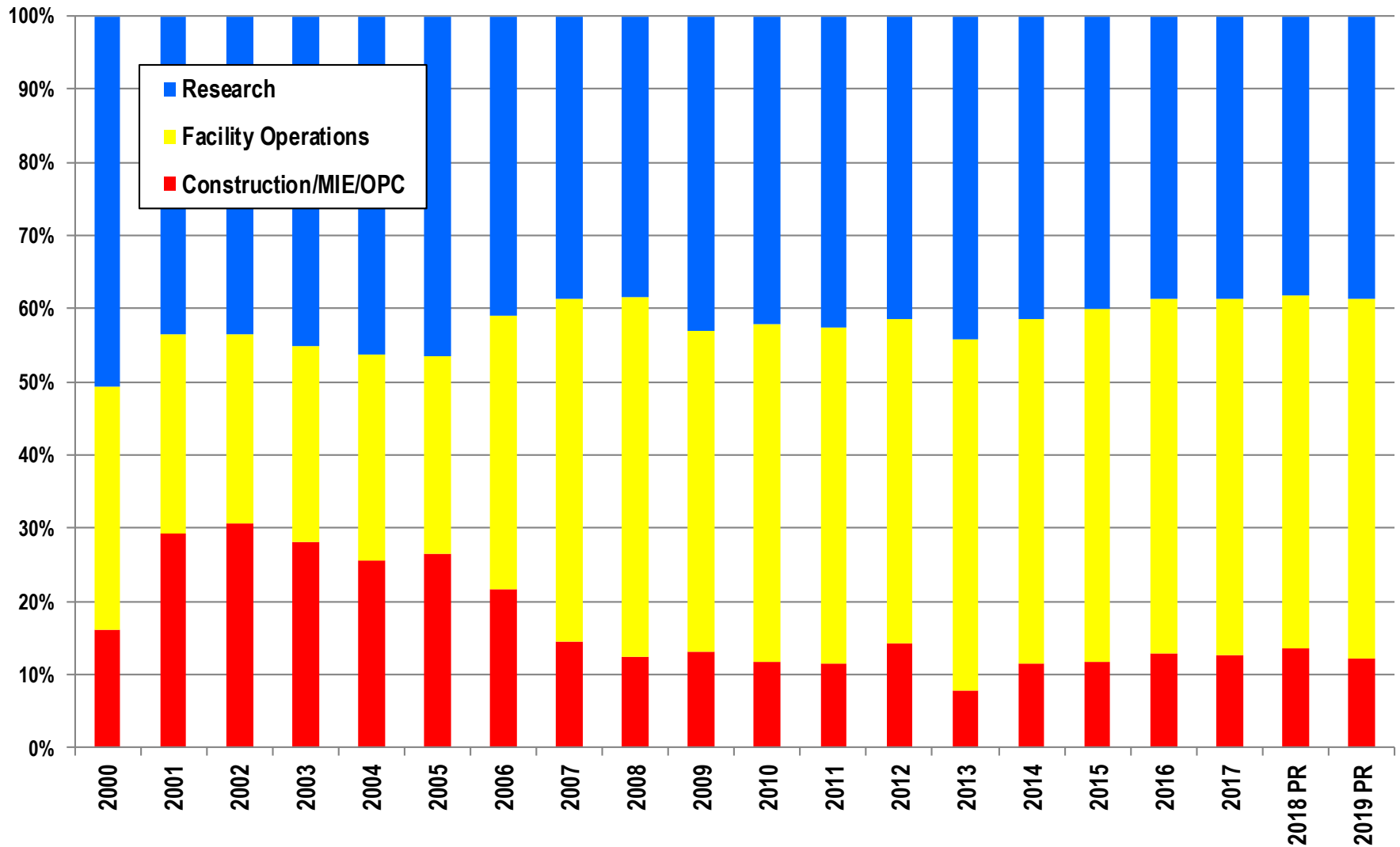
FY 2019 BES Budget Request

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

- The BES FY 2019 Request of **\$1,850.0 million** focuses resources toward the highest priorities in early-stage fundamental research, in operation and maintenance of scientific user facilities, and in facility upgrades.
- **Core research** priorities include quantum information science (QIS), ultrafast science, computational materials and chemical sciences related to the Exascale Computing Initiative, materials and chemical sciences for future nuclear energy, and other priorities identified in recent BES Advisory Committee and “Basic Research Needs” workshop reports.
- Continued funding is requested for **Energy Frontier Research Centers**, two BES-supported **Energy Innovation Hubs**, Batteries and Energy Storage and Fuels from Sunlight, and the DOE Experimental Program to Stimulate Competitive Research.
- All 12 BES **user facilities** operate at 95% optimal levels. No funding is requested for **Long Term Surveillance and Maintenance** or for the disposition of unused equipment for the **Lujan Neutron Scattering Center**.
- To maintain international competitiveness of our facilities, the **Linac Coherent Light Source-II (LCLS-II)** project is fully funded for its last year and the **Advanced Photon Source Upgrade (APS-U)** project continues. The Request also includes funds to initiate the **Advanced Light Source Upgrade (ALS-U)** project at Lawrence Berkeley National Laboratory and the **Linac Coherent Light Source-II High Energy (LCLS-II-HE)** project at SLAC National Accelerator Laboratory.



BES Portfolio Balance: 2000 - 2019



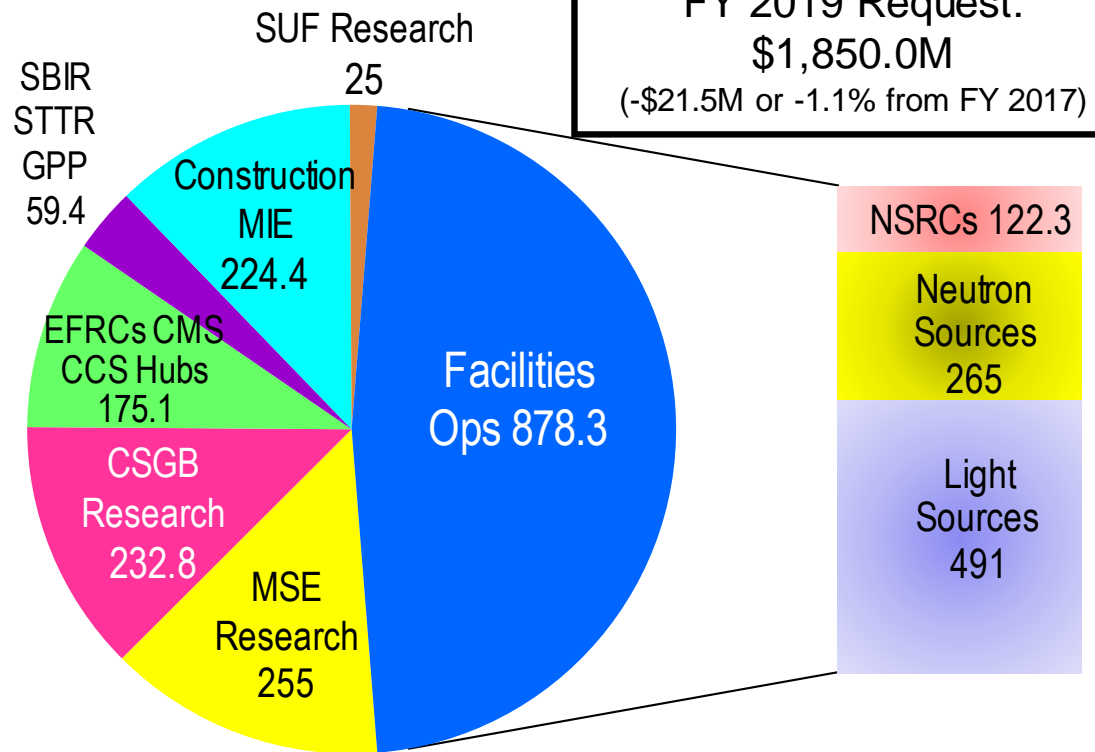
FY 2019 BES Budget Request

Research programs

- Core Research will emphasize quantum materials and chemistry, ultrafast science, and BRN topics (\$513M).
- 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 (\$878.3M)
- No funding is requested for Lujan equipment disposition or Long Term Surveillance and Maintenance



Construction

- Last year of funding for LCLS-II ($\Delta = -\$45M$)
- Advanced Photon Source Upgrade ($\Delta = +17.5M$)
- Two new starts: LCLS-II-HE (\$7M) and ALS-U (\$12M)

BES Research Priorities

- **Quantum Information Science (QIS) – FY18 = \$8M*; FY19 = \$32M***
 - 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.



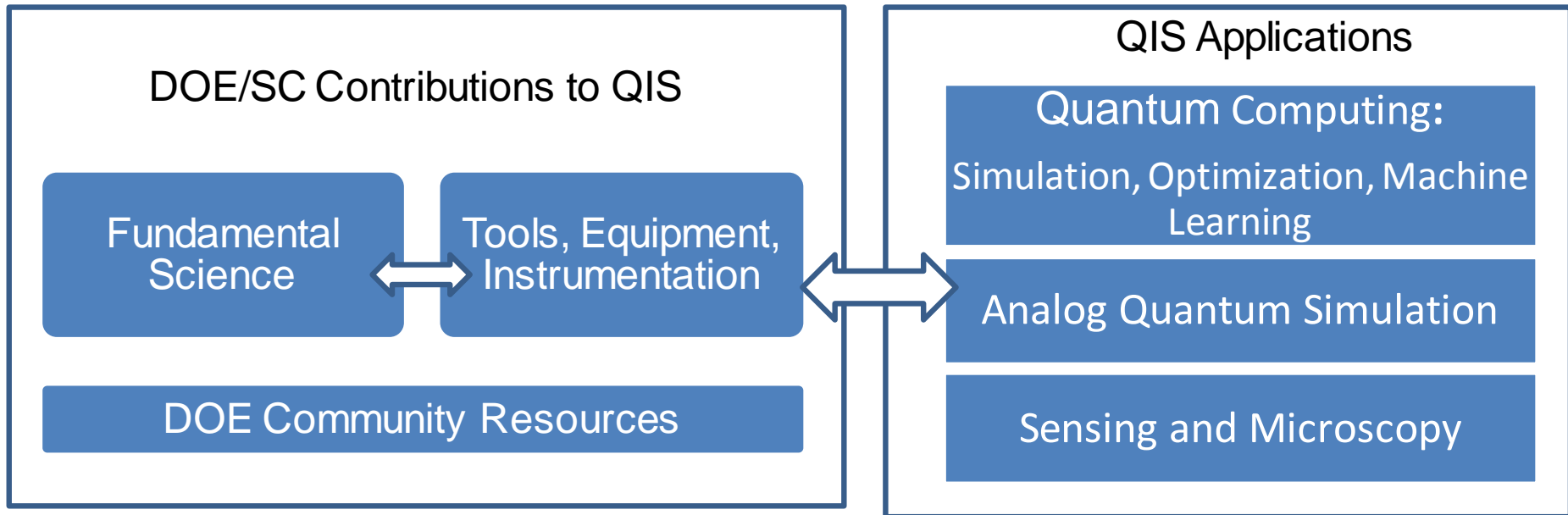
DOE Office of Science Quantum Information Science FY 2019 Investments

The Request also invests \$105M in quantum information science to address the emerging urgency of building U.S. competency and competitiveness in the developing this area of science, including quantum computing and quantum sensor technology. This early stage, fundamental research will concentrate on accelerating progress towards application of quantum computing techniques and quantum sensing to grand challenge science questions.

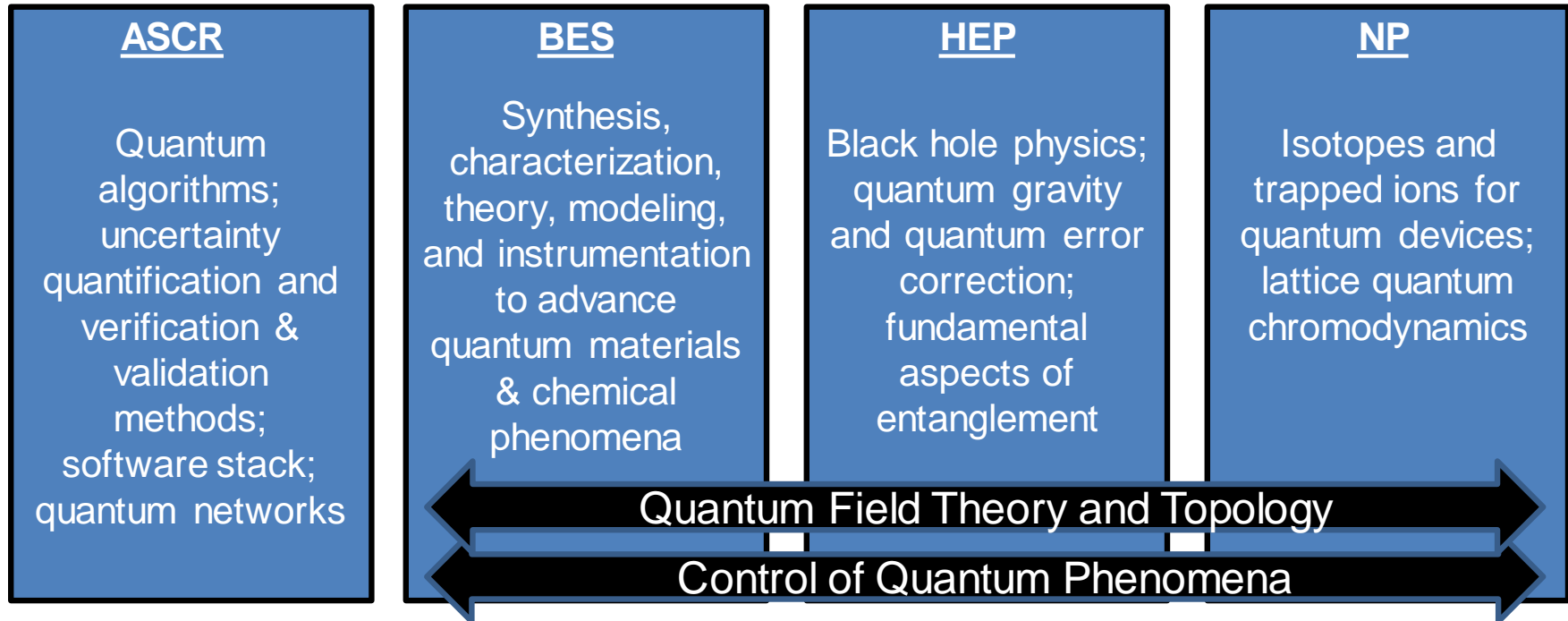
| Quantum Information Science | | | |
|-----------------------------|---------|---------------------|---------------------|
| (\$ in millions) | | | |
| | FY 2017 | FY 2018 | FY 2019 |
| | Enacted | President's Request | President's Request |
| ASCR | 5.801 | 20.801 | 33.507 |
| BES | | 7.708 | 31.561 |
| BER | | 2.000 | 4.500 |
| HEP | | 14.453 | 27.500 |
| NP | | | 8.300 |
| Total | 5.801 | 44.962 | 105.368 |

Office of Science 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, science for next-generation advances, and mission-focused applications



Fundamental Science That Advances QIS



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



Dear Colleague Letter on Accelerating Development of and Research Impacts from Quantum Information Science (QIS) (11/29/17)

In light of significant progress in QIS over the past several years, SC components have held a variety of workshops to define the scientific needs and opportunities. QIS has now been identified as an important cross-cutting topic with potential impact across all SC program offices. To accelerate development of QIS and apply advances in quantum computing, sensing, and other areas to fundamental research questions, quantum information and materials have been emphasized in the DOE SC Fiscal Year 2018 Budget Request. Recent specific FY 2017 program announcements were also issued for National Laboratory-led exploration of hardware approaches to quantum testbeds and development of quantum algorithm teams.

Through this Dear Colleague Letter, DOE SC encourages submission of innovative research ideas in QIS via any appropriate existing mechanism. This letter does not add to the scope of any published announcement and it does not change the review criteria of any published announcement, but it should be taken as a statement of interest in encouraging activity in this field. DOE SC recommends that researchers contact program managers within the most relevant SC program office for details on appropriate programs and specifics on proposal submission; however, it is recognized that many efforts in this area are interdisciplinary and thus may undergo co-review or other joint evaluation by multiple program offices. Activities are particularly encouraged that involve collaboration between academia and DOE National Laboratories, and/or take advantage of the unique resources available in the National Laboratory system.

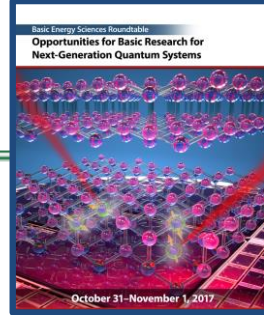
https://science.energy.gov/~media/sc-2/pdf/presentations/2017/DOE-Office_of_Science_Dear_Colleague_Letter_on_QIS.pdf



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 (UChicago/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

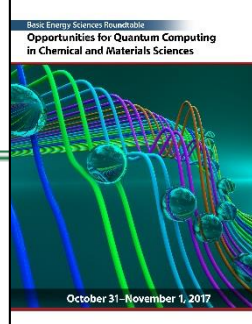
Quantum Information Science: Opportunities for Basic Research for Next Generation Quantum Systems



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 capabilities 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

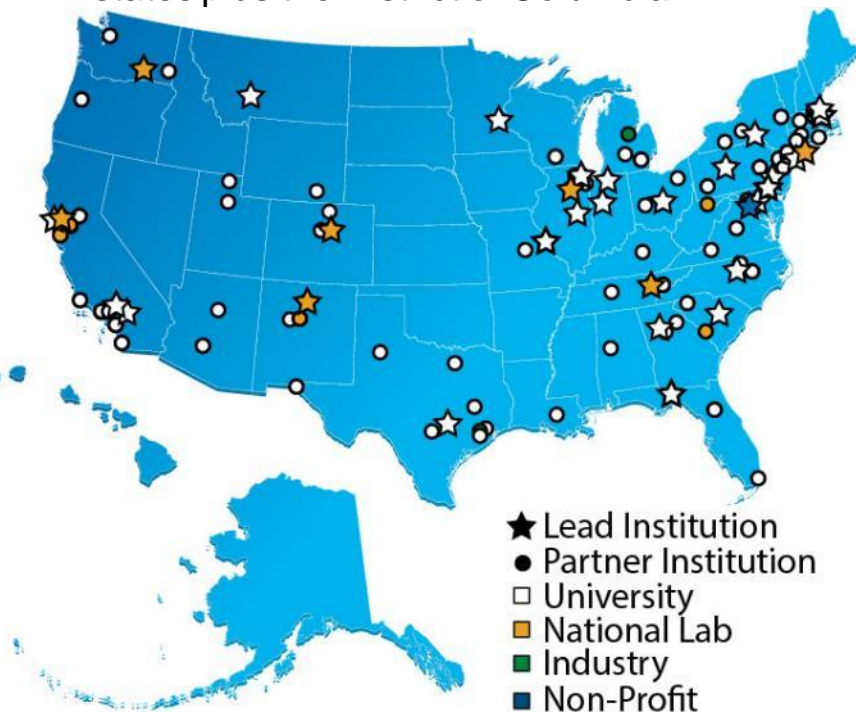


Energy Frontier Research Centers

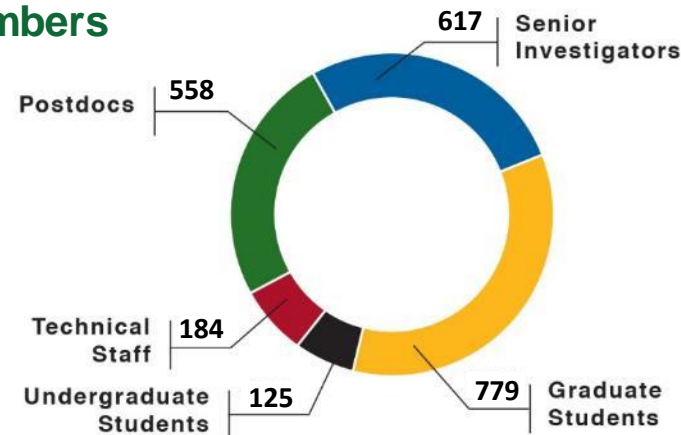
FY 2017 Enacted = \$110M; FY 2019 President's Request = \$110M

Current EFRCs (\$110M in FY 2017)

- 36 awards of \$2-4M per year for 4 years
- Lead institutions by type: **26 universities; 9 DOE national laboratories; 1 nonprofit organization**
- 120 participating institutions, located in 35 states plus the District of Columbia



EFRC Members



FY 2018 Plans

- BES is recompeting the EFRC program in FY 2018, soliciting both renewal proposals from current centers with project periods that end in 2018 as well as proposals for new EFRCs. The recompetition focuses on transformative opportunities and research priorities identified in recent BESAC and Basic Research Needs reports.
- Awards expected to be announced in July 2018.

FY 2019 Request

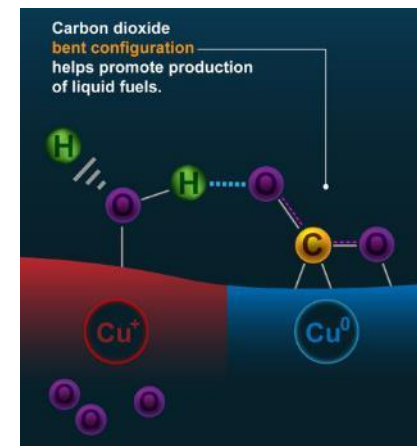
- Provides the fourth year of funding for four EFRCs established in 2016, and the second year of funding for awards resulting from the 2018 recompetition.

Fuels from Sunlight Hub

Joint Center for Artificial Photosynthesis (JCAP)

Research Accomplishments:

- Determined, through combined synchrotron-based X-ray spectroscopy and quantum calculations, the effect of a partial subsurface oxide layer on CO₂ binding by the catalyst copper, revealing an early step in activating CO₂ for subsequent electrocatalytic production of fuels and other products
- Discovered that addition of a specific class of organic molecules to a CO₂ reduction electrolyte can greatly enhance the electrochemical product selectivity toward desired carbon species
- Established a computational model for electrochemical CO₂ reduction on metal surfaces that explains numerous experimental observations and offers insights for identifying new catalysts
- Developed a complete solar-driven CO₂ reduction system that generates ethanol and ethylene with unprecedented efficiency (> 3%)



Ambient pressure X-ray spectroscopy identifies species bound to copper



Schematic illustration of an integrated solar-driven CO₂ reduction prototype

Impact:

- Fundamental understanding of complex catalytic mechanisms and new materials for driving photochemical transformations
- Research prototypes identifying key scientific gaps that should be addressed by basic research and including a stable integrated system that splits water to produce hydrogen with 10% efficiency
- 451 peer-reviewed publications; 78 patent applications, 7 patents granted; alumni include 32 faculty and >35 industry researchers

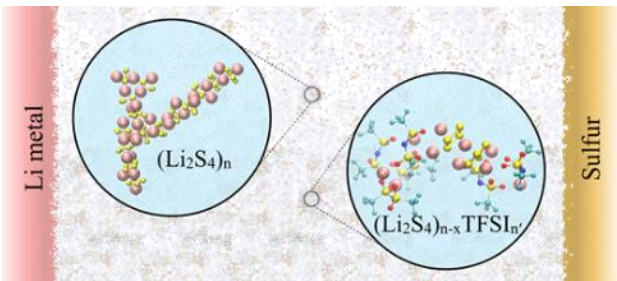
FY 2019 Request

- \$15M is requested to continue support for early-stage fundamental research to establish the foundation for production of hydrocarbon fuels using only sunlight, carbon dioxide, and water as inputs.



Batteries and Energy Storage Hub

Joint Center for Energy Storage Research (JCESR)



Elucidating the solvation structure and dynamics for lithium polysulfides

Research Accomplishments:

JCESR research has significantly advanced new energy storage pathways including:

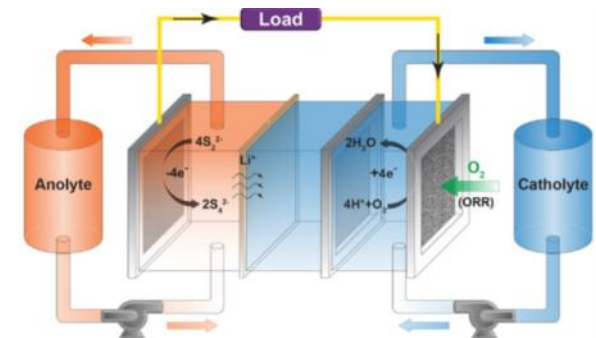
- demonstration of a new class of membranes for flow batteries that can also be used for protection of lithium metal anodes;
- elucidation of the scientific foundations for batteries based on doubly-charged magnesium instead of singly-charged lithium;
- understanding of the chemical and physical processes that must be controlled to greatly improve cycle life in lithium-sulfur batteries; computational screening of over 24,000 potential electrolyte and electrode compounds; and
- creation of new battery concepts and chemistries

Impact:

- Over 350 publications (with >3,500 citations) and ~60 patents
- 3 spin-off companies to commercialize key technologies: solid electrolytes, microporous polymer (PIM) membranes, and air-breathing sulfur battery
- Research on Li-S batteries informed the solicitation/award for EERE's Batt 500 program

FY 2019 Request:

- \$24M is requested to continue support for JCESR with the focus on early-stage research to tackle forefront, basic scientific challenges for next-generation electrochemical energy storage.



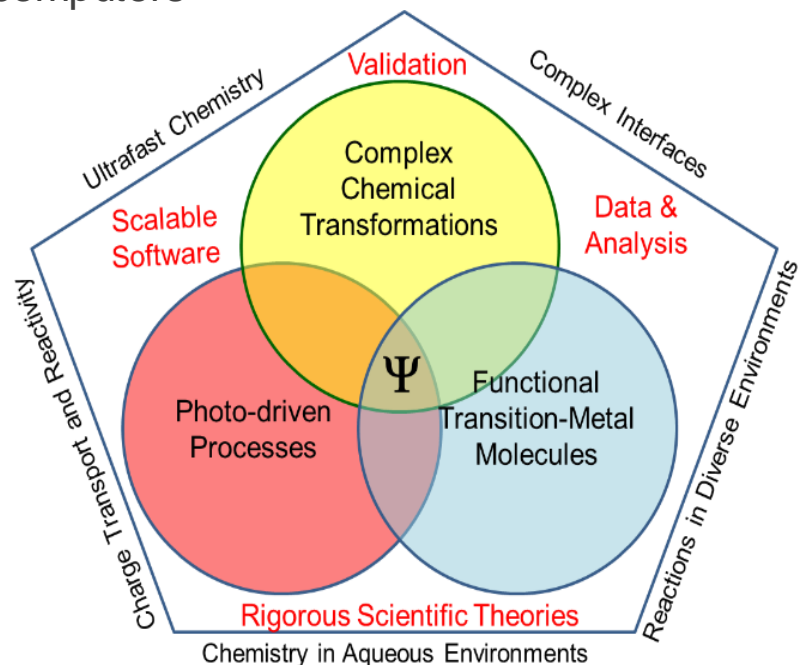
New concept for inexpensive air-breathing sulfur battery for long-term grid energy storage



Computational Chemical Sciences

FY 2019 Request \$13M

- **Ensure sustained U.S. leadership in the development of computational chemistry codes by**
 - Leveraging current leadership in a systematic effort to develop computational chemistry codes that are well adapted to anticipated exascale architecture
 - Delivering open-source community codes to accurately model chemical processes using current petascale and future exascale computers
- **Funding**
 - FY 2017 included \$14M that funded 6 multi-PI awards (2 led by National Labs and 4 led by universities) and 11 single-PI university awards
 - **FY 2018** funding of \$14M (if appropriated) will allow continuation of current projects **and initiation of 3-4 new multi-PI efforts**
 - **FY 2019 funding of \$13M will allow continuation of previously started projects**
 - Ongoing 4-year cycle will allow new solicitations in FY 2021 and FY 2022, pending funding availability



Organization of projects into 3 interacting teams advances computational approaches and tools in important areas of BES chemical sciences

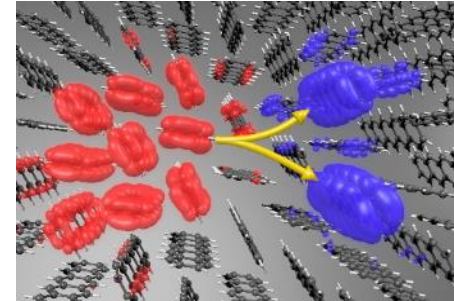


Computational Materials Sciences

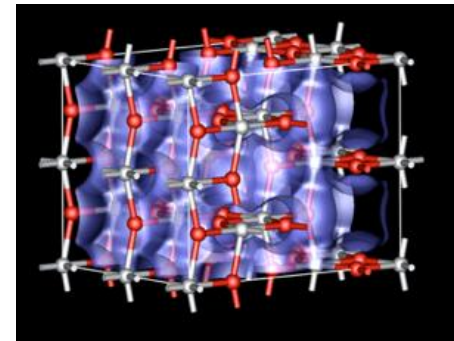
FY 2019 Request \$13M

Computational Materials Sciences -- ensuring U.S. leadership in computing for materials design and discovery

- Research focuses on predictive design of functional materials, taking full advantage of current leadership computers and future exascale capabilities
- Supports integrated theory-computational-experimental teams to perform the basic research required to deliver open-source community codes and the associated experimental and theoretical databases
- Advance tools to predict and validate electronic, magnetic, and strain properties for energy conversion, correlated materials, layered materials, and excited-state phenomena
- **In FY 2019**, a funding opportunity will:
 - **Consider applications for renewal of awards that have successfully completed 4-years of research**
 - **Focus on applications for new awards in the area of predictive design of quantum materials for quantum information science**



Ab-initio theory of decay of an optically excited electron-hole pair (red) into 2 lower energy pairs (blue), while conserving spin



Calculation of the correct electronic charge density of anatase TiO₂ using quantum Monte Carlo and including temperature dependence



BES Scientific User Facilities

- All of the BES user facilities continue operations at approximately 95% of optimum: five x-ray light sources, two neutron scattering sources, and five research centers for nanoscale science.
- LCLS continues operations in support of the BES priority in ultrafast science and also in preparation for completion of the LCLS-II construction project. To allow installation activities for the LCLS-II construction project to proceed, LCLS will be shut down for one year, starting around the second quarter of FY 2019.
- Funding for Long Term Surveillance and Maintenance (LTSM) ends in FY 2018. No funding is requested for LTSM or for the disposition of equipment at the Lujan Neutron Scattering Center.



Light Sources: Global Race to the Top

60+ Facilities Worldwide and Growing

Many other new & upgraded facilities are in the design stage...
 Take Away Message: It's a very competitive landscape!



ALS



APS



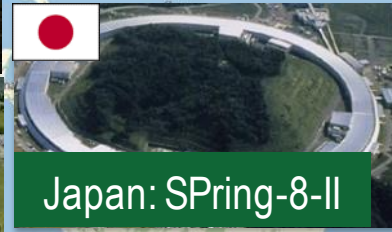
NSLS-II



SSRL



LCLS



Japan: SPring-8-II



Germany: PETRA 3/4



France: ESRF II, 2022



China: BLS



Brazil: SIRIUS, 2019



Sweden: MAX-IV, 2016



SACLA FEL 2011
 8.5 GeV, 30 Hz NC



SWISS FEL 2017
 5.8 GeV, 100 Hz NC



EU XFEL 2017
 17.5 GeV, 3000 x 10 Hz SC

BES Light Sources

Ring Upgrades

New Rings

Upgraded & New FELs

International Developments in Storage Rings and Free Electron Lasers Since 2000

New & Upgraded Storage Rings in USA

NSLS-II (2015)
APS-U
ALS-U

New & Upgraded FELs in USA

LCLS (2010)
LCLS-II
LCLS-II-HE

New & Upgraded Storage Rings

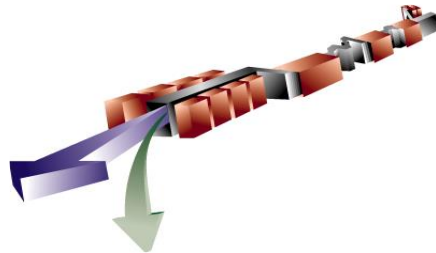
Australia (2007)
Beijing HEPS
Canadian LS (2004)
Diamond (2007)
ESRF-II (2022)
MAX IV (2016)
PETRA III (2009)
Shanghai (2009)
Sirius (2019)
SLS (2000)
Solaris (2016)
Soleil (2006)
Taiwan PS (2015)

New & Upgraded FELs

DESY FLASH (2005)
DESY XFEL (2017)
Pohang FEL (2016)
SACLA FEL (2011)
Swiss FEL (2017)
Shanghai FEL



Storage Ring

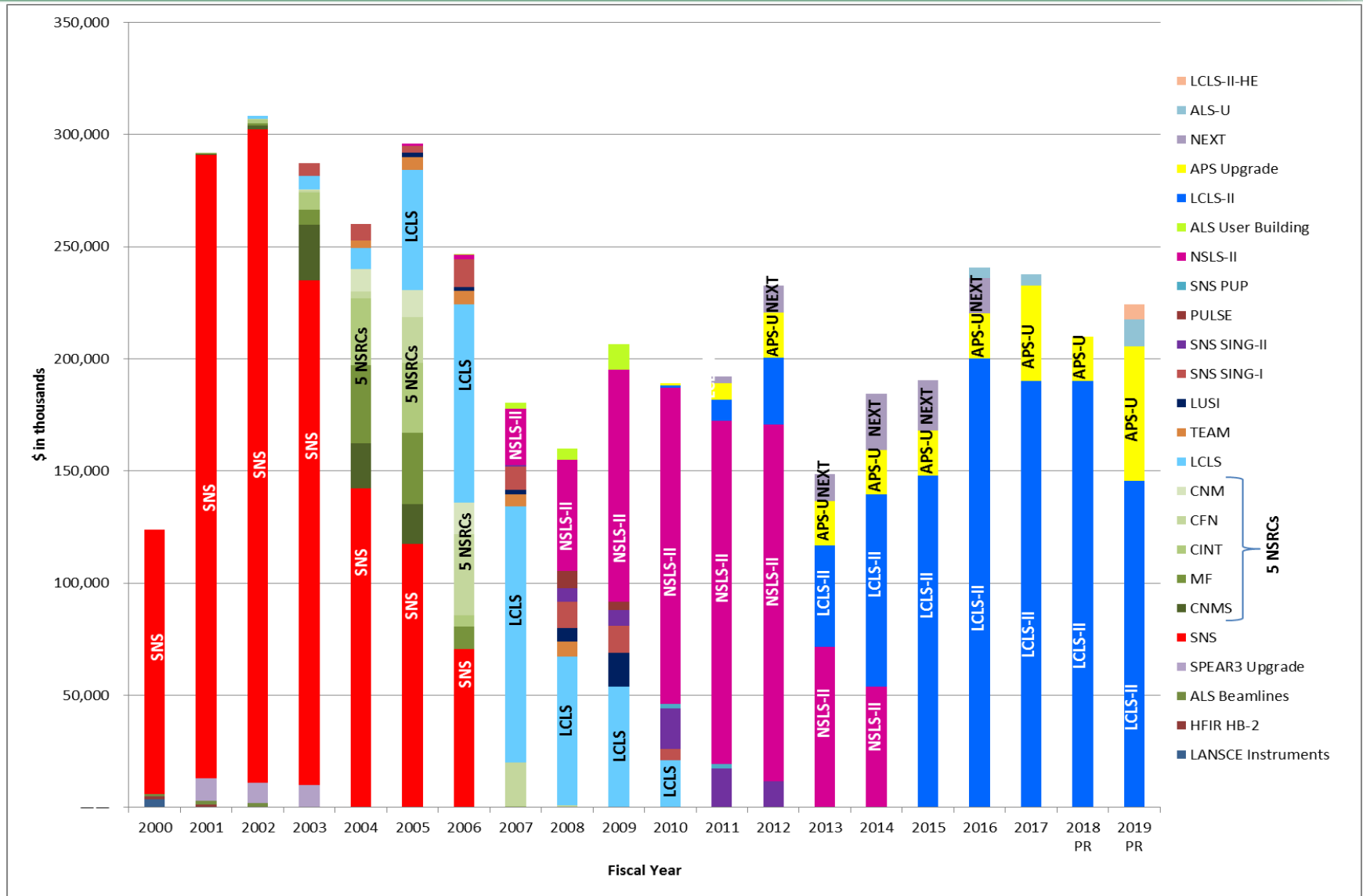


Free Electron Laser

Storage ring & free electron laser sources have complementary properties.



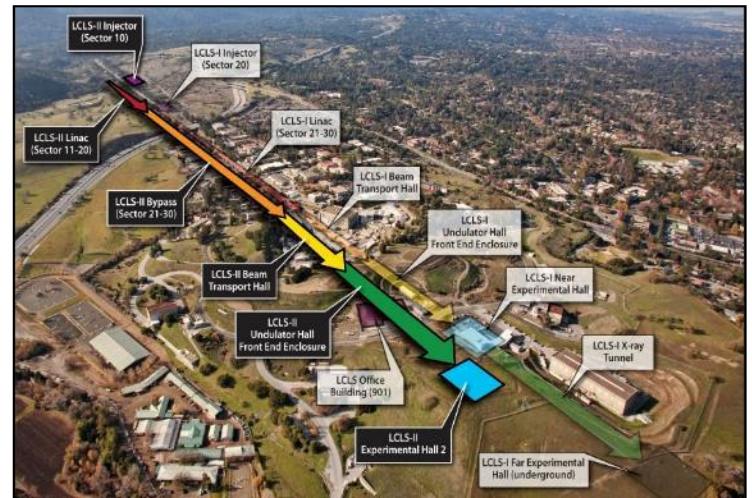
BES Construction/MIE Funding Profile 2000 – 2019



LCLS-II and APS-U Construction Projects

Linac Coherent Light Source-II (LCLS-II)

- FY 2017 = \$190M; FY 2019 = \$145.4M for the final year of funding. FY 2019 activities include R&D, design, prototyping, construction of technical systems, installation, and commissioning.
- When completed, LCLS-II will provide high-repetition-rate, ultra-bright, transform-limited femtosecond x-ray pulses with polarization control and pulse length control.
- The upgrade adds a 4 GeV superconducting linac; an electron injector; a soft x-ray variable gap undulator (200-1,300eV) using the SC linac; and a hard x-ray variable gap undulator capable of operating at 1,000-5,000eV using the SC linac and 1,000-25,000eV using the copper linac with self-seeding capability.



Advanced Photon Source Upgrade (APS-U)

- FY 2017 = \$42.5M; FY 2019 = \$60M for R&D, design, prototyping, testing, fabrication, site preparation, installation, and long lead procurements.
- APS-U will provide an x-ray source with world-leading transverse coherence and extreme brightness.
- The upgrade provides a new storage ring incorporating a multi-bend achromat lattice, new insertion devices, superconducting undulators, and new or upgraded beamlines.



Advanced Light Source Upgrade (ALS-U) at LBNL

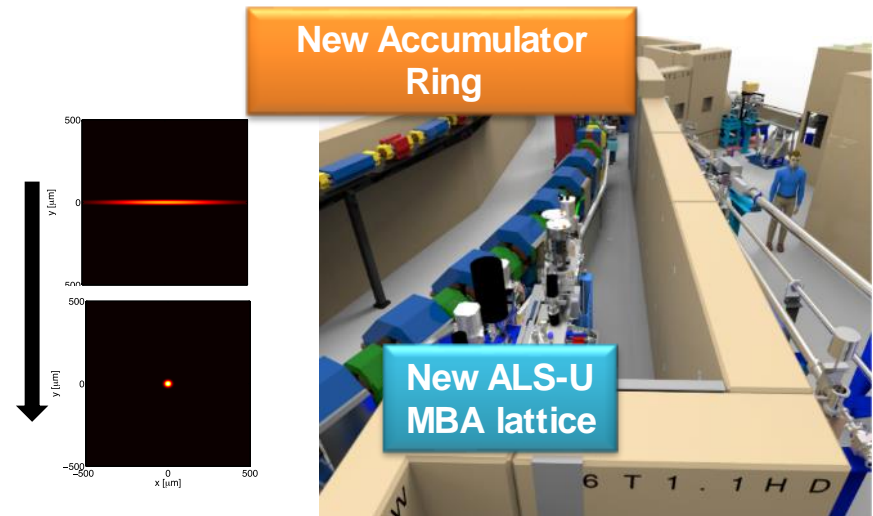
Goal: Generate 1,000 times brighter soft x-rays with higher coherence to resolve nanometer-scale features and enable real-time observation of chemical processes and materials as they function

Project Deliverables:

- Install a multi-bend achromat (MBA) lattice to reduce emittance and produce a “round” x-ray beam
- Develop new advanced instruments that take advantage of the new beam for cutting-edge experiments
- CD-0 approved September 2016, \$260-420M

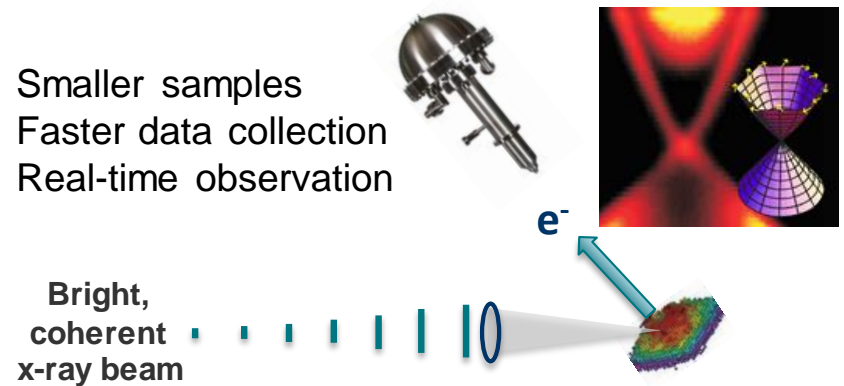
Transformative capabilities with bright, highly coherent soft x-rays

- Increased brightness: fast electronic structural changes in real time during chemical reactions
- Increased coherence: nanoscale imaging techniques to map the 3D electronic, chemical, and magnetic structures
- Tightly focused, bright, coherent soft x-rays: probe electronic structure of single nanoscale domains and gated structures of complex materials



Probe electronic structure of single nanoscale domains

- Smaller samples
- Faster data collection
- Real-time observation



Linac Coherent Light Source II High Energy Upgrade

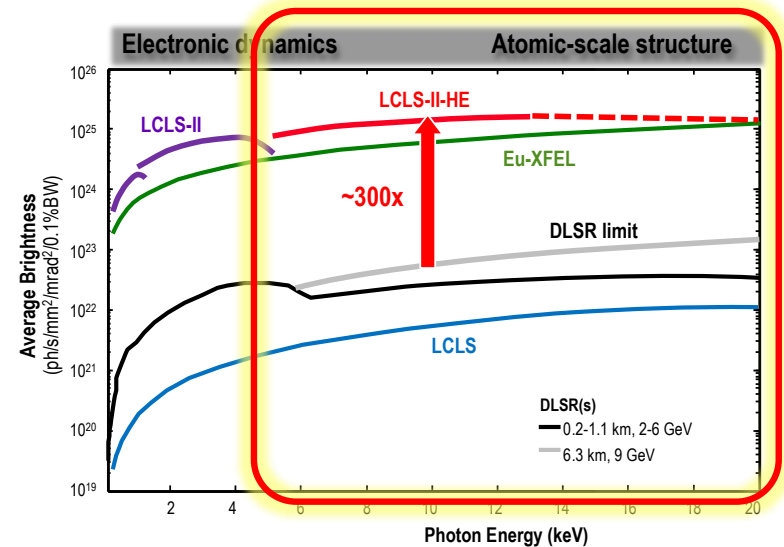
Goal: Increase the repetition rate to 1 MHz at higher energy range (12 keV and beyond)

Project Deliverables:

- Increase the energy of the superconducting linac from 4 to 8 GeV
- Deliver ~1,000-fold higher average brightness hard x-rays at higher energy range (12 keV and beyond)
- CD-0 approved December 2016, \$260-450M

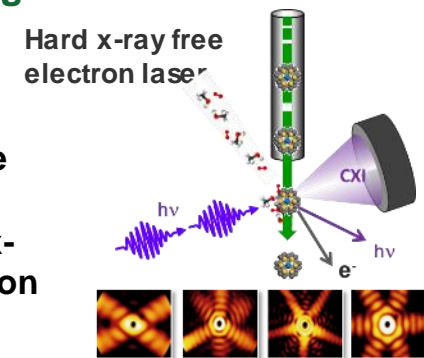
Transformative capabilities with high repetition rate, coherent hard x-rays at higher energy range

- Chemical reactions and material functions studies with excitation energies above 5 keV
- Full coherence: direct structure imaging from coherent x-ray diffraction pattern from non-crystalline nano-particles
- High repetition rate: real time studies of irreversible reaction or atomic or electronic structure changes under external influence



Simultaneously probe electronic and atomic structures during a chemical reaction in real time

- High repetition rate for real time measurements
- Fully coherent x-rays for diffraction imaging



Real time coherent X-ray imaging of heterogeneous nanoparticles

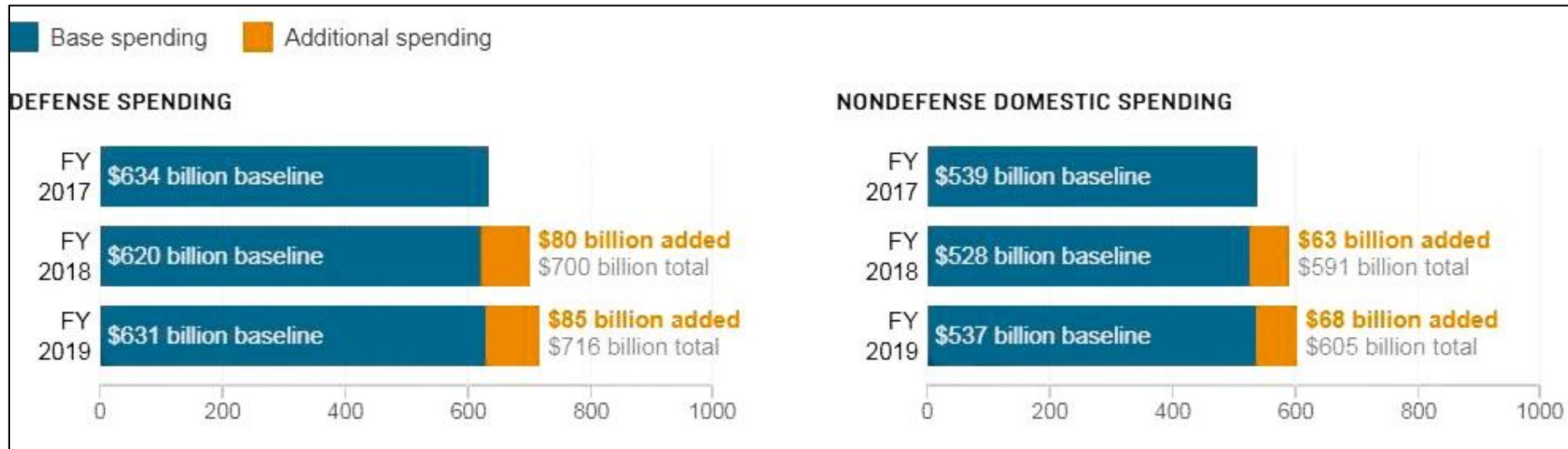
FY 2018 Appropriations Status

Government-Wide Funding Legislation Released

March 21, 2018 The House Appropriations Committee today introduced legislation to provide all discretionary funding for the federal government for the 2018 fiscal year. The bill contains the full legislation and funding for all of the 12 annual Appropriations bills. It totals \$1.3 trillion, including \$78.1 billion in funding for the Global War on Terror (GWOT)/Overseas Contingency Operations (OCO). Total base funding, excluding OCO and emergencies, is \$1.2 trillion.

Congressional Two-Year Budget Deal

- The Budget Control Act of 2011 set annual spending limits for the federal government for FY 2012-2021 as part of an agreement to resolve the debt-ceiling crisis. Any federal spending above those annual limits would be sequestered. Defense and non-defense discretionary spending are tracked separately.
- The Bipartisan Budget Act of 2018, signed by the President on February 9, 2018, raised the annual spending limits for FY 2018-2019 only, as shown below.
- The new non-defense funding cap for FY 2018 is \$117 billion higher than what President Trump requested in his FY 2018 budget request.



FY 2018 Energy and Water Appropriations Bill

DOE Office of Science

Science Research – The bill includes **\$6.26 billion** for science research – an increase of **\$868 million** above the 2017 enacted level. This funding supports basic energy research, the development of high performance computing systems, and research into the next generation of energy sources. These investments lay the groundwork for a more secure energy future, helping to reduce the nation’s dependence on foreign oil and ensuring continued economic growth.

FY 2018 Omnibus Appropriations

To be voted on by midnight Friday, March 23, 2018

| (\$K) | FY 2017 Enacted Approp. | FY 2018 President's Request | FY 2018 Omnibus | FY 2018 Omnibus vs. FY 2017 Enacted | | FY 2018 Omnibus vs. FY 2018 President's Request | |
|----------------------------|-------------------------------|-----------------------------------|--------------------|---|---------------|---|---------------|
| | | | | | | | |
| Research | 1,681,500 | 1,352,400 | 1,744,900 | +63,400 | +3.8% | +392,500 | +29.0% |
| Construction | | | | | | | |
| 13-SC-10 LCLS-II, SLAC | 190,000 | 182,100 | 192,100 | +2,100 | +1.1% | +10,000 | +5.5% |
| 18-SC-10 APS Upgrade, ANL | — | 20,000 | 93,000 | +93,000 | — | +73,000 | +365.0% |
| 18-SC-11 SNS PPU, ORNL | — | — | 36,000 | +36,000 | — | +36,000 | — |
| 18-SC-12 ALS Upgrade, LBNL | — | — | 16,000 | +16,000 | — | +16,000 | — |
| 18-SC-13 LCLS-II-HE, SLAC | — | — | 8,000 | +8,000 | — | +8,000 | — |
| Total, Construction | 190,000 | 202,100 | 345,100 | +155,100 | +81.6% | +143,000 | +70.8% |
| Total | 1,871,500 | 1,554,500 | 2,090,000 | +218,500 | +11.7% | +535,500 | +34.4% |

- EFRCs, CMS, CCS, and both Hubs are all fully funded.
- Light sources increase by 0.2%, neutron facilities increase by 5.6%, and NSRCs increase by 6.7% over FY 2017.
- Construction: LCLS-II fully funded. APS-U ramps up. Three new projects funded: SNS PPU (\$36M), ALS-U (\$30M), LCLS-II-HE (\$10M) including OPC.
- EPSCoR funded at \$20M.
- \$7M for Long Term Surveillance and Maintenance at BNL.

New BESAC Charge from Dr. Binkley (June 16, 2017)



Department of Energy
Office of Science
Washington, DC 20585

Professor Persis Drell
Chair, Basic Energy
Provost
Bldg 10
Stanford University
Stanford, California

Dear Professor Drell,

I very much appreciate the
Advisory Committee's
to express my sincere
inaugural Committee
Innovation Hub, to
BESAC prioritization.

I am writing to ask for
founding of the Basic
highlight a few outstanding
support that have
examples to motivate
research advances
advances often gave
technologies and
from Federal investment
made Federal program
strategy.

The BESAC 2007 annual
opportunities for developing
examining past successes
strategies and approaches
generally, U.S. leadership
such a report will be
it contributes to future
Federal budget outlays
technical details as
each story as it relates to the larger progress of science.

*"I am writing to ask BESAC to produce, during the coming year, a report that commemorates the founding of the Basic Energy Sciences (BES) program four decades ago. The report should highlight **a few outstanding examples of major scientific accomplishments emerging from BES support that have shaped the fields of BES research**, with an eye toward learning from these examples to motivate BES investment strategies for the future. As history has shown, basic research advances have been the bedrock of American innovation and prosperity. **These advances often gave rise to new lines of scientific inquiry and led to inventions of new technologies and industries that transformed our society.** ... By examining past successes, I expect the new BESAC charge report **to illuminate the guiding strategies and approaches that will be key to ensuring future U.S. leadership**, and more generally, **U.S. leadership in the full range of disciplines stewarded by BES.**"*



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2
BES-supported
ances?
an energy,
the greatest
ntify research
strengthen BES in



U.S. DEPARTMENT OF
ENERGY

Office of
Science