Overview

The mission of the Basic Energy Sciences (BES) program is to support fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support Department of Energy (DOE) missions in energy, environment, and national security.

The research disciplines that BES supports—condensed matter and materials physics, chemistry, geosciences, and aspects of biosciences—are those that discover new materials and design new chemical processes that touch virtually every important aspect of energy resources, production, conversion, transmission, storage, efficiency, and waste mitigation. BES research provides a knowledge base to help understand, predict, and ultimately control the natural world and helps build the foundation for achieving a secure and sustainable energy future. BES also supports world-class, open-access scientific user facilities consisting of a complementary set of intense x-ray sources, neutron sources, and research centers for nanoscale science. Capabilities at BES facilities probe materials and chemical systems with ultrahigh spatial, temporal, and energy resolutions to investigate the critical functions of matter—transport, reactivity, fields, excitations, and motion—and answer some of the most challenging grand science questions. BES-supported activities are entering a new era in which materials can be built with atom-by-atom precision, chemical processes at the molecular scale can be controlled with increasing accuracy, and computational models can predict the behavior of materials and chemical processes before they exist.

As history has shown, basic research advances provide the foundation for breakthroughs in new energy technologies. Key to exploiting such discoveries is the ability to create new materials using sophisticated synthesis and processing techniques, to precisely define the atomic arrangements in matter, and to design chemical processes, which will enable control of physical and chemical transformations. The energy systems of the future will revolve around materials and chemical processes that convert energy from one form to another. Such materials will need to be more functional than today's energy materials. The new chemical processes will require ever increasing control to the levels of electrons. Such advances are not found in nature; they must be designed and fabricated to exacting standards using principles revealed by basic science.

Highlights of the FY 2018 Budget Request

The BES FY 2018 Request of $1,554.5 million is a decrease of $294.5 million or 16% from the FY 2016 Enacted level. The Request focuses resources toward the highest priorities in early-stage fundamental research, in operation and maintenance of scientific user facilities, and in facility upgrades. The overall research funding in FY 2018 is reduced by 18% from FY 2016. The magnitude of the decrease requires a significant shift in priorities, with targeted reductions of activities that extend to later-stage fundamental research. No funding is requested for the two BES-supported Energy Innovation Hubs, Batteries and Energy Storage and Fuels from Sunlight, or for the DOE Experimental Program to Stimulate Competitive Research (EPSCoR). In the remaining core research activities, BES emphasizes basic scientific areas with potential to transform the understanding and control of matter and energy. The 2015 Basic Energy Sciences Advisory Committee (BESAC) report, "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science," and the follow-on Basic Research Needs workshop reports outline specific topical areas.[a] The Request continues to support the Energy Frontier Research Center (EFRC) program, which will enable basic energy-relevant research with a scope and complexity beyond that possible in standard single-investigator or small-group awards. Both the core research and the EFRC program will emphasize emerging high priorities in quantum materials and chemistry, catalysis science, synthesis, instrumentation science, and materials and chemical research related to interdependent energy-water issues.

In the Scientific User Facilities subprogram, BES targets resources to maximize capabilities and operational efficiency, with an emphasis on maintaining a balanced suite of complementary tools. Among x-ray light sources, four facilities (Advanced Light Source, Advanced Photon Source, Linac Coherent Light Source, and National Synchrotron Light Source-II) will continue operations and are supported at 6% below the FY 2016 Enacted level. The decrease in funding will reduce operating hours and user support, including shutting down selected beamlines. The Stanford Synchrotron Radiation Lightsource will operate through the first quarter of the fiscal year, then will transition to a warm standby status. Both BES-supported neutron

[a] All reports are available at https://science.energy.gov/bes/community-resources/reports/.

sources, the Spallation Neutron Source and High Flux Isotope Reactor, will be operational in FY 2018 and funded at 10% below the FY 2016 Enacted level with reduced hours and user support. Selected flight paths will be shut down. No funding is requested for the disposition of unused equipment for the Lujan Neutron Scattering Center. Three of the five Nanoscale Science Research Centers will be supported at 6% below the FY 2016 Enacted level, with reduced scientific thrusts and core capabilities. No funding is requested for the Center for Functional Nanomaterials at Brookhaven National Laboratory (BNL) and the Center for Integrated Nanotechnologies at Sandia (SNL) and Los Alamos (LANL) National Laboratories. No funding is requested for Long Term Surveillance and Maintenance at BNL and at SLAC National Accelerator Laboratory (SLAC).

In the Construction subprogram, the Linac Coherent Light Source-II project remains the highest priority construction project in BES and is supported in full per the project plan. The upgrade of the Advanced Photon Source, which was the top-ranked project in the 2015 BESAC facility prioritization report, will be converted from a Major Item of Equipment to a line-item construction project to reflect refinement of project scope and will continue to be supported.

Basic Energy Sciences
Funding ($K)

	FY 2016 Enacted[a]	FY 2017 Annualized CR[b]	FY 2018 Request	FY 2018 vs FY 2016
Materials Sciences and Engineering				
Scattering and Instrumentation Sciences Research	67,350	-	55,830	-11,520
Condensed Matter and Materials Physics Research	113,086	-	113,258	+172
Materials Discovery, Design, and Synthesis Research	70,273	-	64,621	-5,652
Experimental Program to Stimulate Competitive Research (EPSCoR)	14,776	-	0	-14,776
Energy Frontier Research Centers (EFRCs)	55,750	-	50,809	-4,941
Energy Innovation Hubs—Batteries and Energy Storage	24,137	-	0	-24,137
Computational Materials Sciences	12,000	-	10,927	-1,073
SBIR/STTR	12,758	-	11,192	-1,566
Total, Materials Sciences and Engineering	**370,130**	**-**	**306,637**	**-63,493**
Chemical Sciences, Geosciences, and Biosciences				
Fundamental Interactions Research	72,782	-	61,187	-11,595
Chemical Transformations Research	88,918	-	82,004	-6,914
Photochemistry and Biochemistry Research	69,113	-	63,701	-5,412
Energy Frontier Research Centers (EFRCs)	54,250	-	48,065	-6,185
Energy Innovation Hubs—Fuels from Sunlight	15,000	-	0	-15,000
General Plant Projects (GPP)	1,000	-	1,000	0
SBIR/STTR	10,732	-	9,658	-1,074
Total, Chemical Sciences, Geosciences, and Biosciences	**311,795**	**-**	**265,615**	**-46,180**
Scientific User Facilities				
X-Ray Light Sources	482,667	-	428,206	-54,461
High-Flux Neutron Sources	265,082	-	225,620	-39,462
Nanoscale Science Research Centers (NSRCs)	120,575	-	71,135	-49,440
Other Project Costs	0	-	7,900	+7,900
Major Items of Equipment	35,500	-	0	-35,500
Research	31,853	-	19,724	-12,129

[a] The FY 2016 Enacted level includes SBIR and STTR and reflects updates through the end of the fiscal year.
[b] FY 2017 Annualized CR amounts reflect the P.L. 114-254 continuing resolution level annualized to a full year. These amounts are shown only at the congressional control level and above, below that level, a dash (-) is shown.

	FY 2016 Enacted[a]	FY 2017 Annualized CR[b]	FY 2018 Request	FY 2018 vs FY 2016
SBIR/STTR	31,098	-	27,563	-3,535
Total, Scientific User Facilities	**966,775**	**-**	**780,148**	**-186,627**
Subtotal, Basic Energy Sciences	**1,648,700**	**1,645,566**	**1,352,400**	**-296,300**
Construction				
Linac Coherent Light Source-II (LCLS-II), SLAC	200,300	199,919	182,100	-18,200
Advanced Photon Source Upgrade (APS-U), ANL	0	0	20,000	+20,000
Total, Construction	**200,300**	**199,919**	**202,100**	**+1,800**
Total, Basic Energy Sciences	**1,849,000**	**1,845,485**	**1,554,500**	**-294,500**

SBIR/STTR Funding:
- FY 2016 Projected: SBIR $47,468,000 and STTR $7,120,000
- FY 2018 Request: SBIR $42,444,000 and STTR $5,969,000

[a] The FY 2016 Enacted level includes SBIR and STTR and reflects updates through the end of the fiscal year.
[b] FY 2017 Annualized CR amounts reflect the P.L. 114-254 continuing resolution level annualized to a full year. These amounts are shown only at the congressional control level and above, below that level, a dash (-) is shown.

Basic Energy Sciences
Explanation of Major Changes ($K)

	FY 2018 vs FY 2016
Materials Sciences and Engineering: Research will continue to support fundamental scientific opportunities, including those identified as high priorities in the BESAC report on transformative opportunities for discovery science and Basic Research Needs workshops on quantum materials and synthesis science. For the proposed budget reductions, the scope of the subprogram will be reduced to focus on early-stage fundamental research underpinning the Department's mission. The Batteries and Energy Storage Energy Innovation Hub will not be renewed. Funding is terminated for the DOE Experimental Program to Stimulate Competitive Research (EPSCoR). Research on novel materials and theory for quantum information science will be increased.	**-63,493**
Chemical Sciences, Geosciences, and Biosciences: Research will continue in support of fundamental scientific research, including grand challenge science and opportunities identified in the BESAC report on transformative opportunities for discovery science and Basic Research Needs workshops on synthesis science, instrumentation, the energy water nexus, and catalysis. The scope of the subprogram will be reduced while continuing to support those topics that push the frontiers of science and are most strongly aligned with mission drivers. No funding is requested for the Fuels from Sunlight Energy Innovation Hub. Quantum chemistry in support of quantum information science will be increased.	**-46,180**
Scientific User Facilities: Funding is requested to support three Nanoscale Science Research Centers. No funding is requested for the Center for Functional Nanomaterials or the Center for Integrated Nanotechnologies. One light source (Stanford Synchrotron Radiation Lightsource) will operate for one quarter, then transition to warm standby. All remaining scientific user facilities will operate 6–10% below the FY 2016 Enacted level, below optimal operations. Selected light source beamlines and neutron flight paths will be shut down. No funding is requested for the disposition of unused equipment for the Lujan Neutron Scattering Center. No funding is requested for long term surveillance and maintenance. The Advanced Photon Source-Upgrade (APS-U) project is transitioned from a Major Item of Equipment (MIE) to a line item construction project.	**-186,627**
Construction: Funding for the LCLS-II construction project will decrease in FY 2018 per the project plan. The APS-U project is included as a line item construction project in the FY 2018 Request.	**+1,800**
Total, Basic Energy Sciences	**-294,500**

Basic and Applied R&D Coordination

As a program that supports fundamental scientific research relevant to many DOE mission areas, BES strives to build and maintain close connections with other DOE program offices. The Department facilitates coordination between DOE R&D programs through a variety of Departmental activities, including joint participation in research workshops, strategic planning activities, solicitation development, and program review meetings. BES also coordinates with DOE technology offices in the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) program, including topical area planning, solicitations, reviews, and award selections.

BES program managers regularly participate in intra-departmental meetings for information exchange and coordination on solicitations, program reviews, and project selections in the research areas of biofuels derived from biomass; solar energy utilization; building technologies, including solid-state lighting; advanced nuclear energy systems and advanced fuel cycle technologies; vehicle technologies; improving efficiencies in industrial processes; and superconductivity for grid applications. These activities facilitate cooperation and coordination between BES and the DOE technology offices and defense programs. DOE program managers from basic and applied programs have also established formal technical coordination working groups that meet on a regular basis to discuss R&D activities with wide applications. Additionally, DOE technology office personnel participate in reviews of BES research, and BES personnel participate in reviews of research funded by the technology offices.

Co-funding and co-siting of research by BES and DOE technology programs at the same institutions has proven to be a valuable approach to facilitate close integration of basic and applied research. In these cases, teams of researchers benefit by sharing expertise and knowledge of research breakthroughs and program needs. The Department's national laboratory system plays a crucial role in achieving integration of basic and applied research.

Program Accomplishments

Beyond Graphene for Future Electronics. Materials for next-generation electronics will take advantage of quantum effects, as enabled by the controlled reaction of electrons with other parts of the atomic structure. Atomically thin materials may be the foundation for these innovative devices.

- Researchers developed a new process to make ultrafine (5 nm in width) junctions of different semiconductors in specific patterns by combining standard lithography with laser vaporization of sulfur. Applied controllably in planar materials, this process may enable ultrathin microelectronics for smartphones, next-generation solar cells, and solid-state lighting.
- Planar 2-dimensional (2D) layered materials are highly desirable for electronics, but are challenging to form because thermodynamics favors 3D structures in normal growth processes. Atomistic simulations predicted that 2D boron layers could be grown on a reactive metal substrate due to the fact that minor adhesion of boron to the metal will prevent 3D growth. This prediction was confirmed experimentally for deposition of boron on silver, thus demonstrating the first synthesis of a 2D material that does not have its own distinct structure but instead adapts the structure of the metal substrate.
- High surface conductivity was measured on a sandwich structure of graphene and boron nitride layers along the perimeter of the graphene. The high conductivity was attributed to topological phenomena arising from special "edge states" in graphene. These topological edge states were found to coexist with superconductivity (resistance-free electron transport) when two sides of the sandwich layers are in contact with a superconductor. This new discovery brings us closer to applications in future low-power electronics, including fault-tolerant quantum computing.

Efficient Utilization of Carbon-Containing Gases. Methane and carbon dioxide (CO_2), two of the most stable carbon compounds, are greenhouse gases that present challenges as well as opportunities for discovery of new chemical approaches to their conversion into useful fuels or commodity chemicals.

- Scientists identified a new reaction mechanism for converting CO_2 to the more reactive carbon monoxide (CO) as a precursor to chemical fuels. The method involved attaching rhenium-based molecular catalysts to the surface of low-cost graphitic carbons. These novel anchored catalysts have shown activity at least 10 times greater than that of the same catalysts in solution and are more energy efficient than other electrocatalysts. Importantly, this new approach results in the production of only CO, i.e., in 100% selectivity for the desired product, and thus no waste.

- Guided by theoretical results, researchers discovered that nickel-gallium films require less energy to reduce CO_2 to ethylene, ethane, and methanol than copper-based materials, which were previously the best candidate catalysts. Neither nickel nor gallium alone exhibits similar activity; both are needed. Since similar reactions are used in the solar-driven production of hydrocarbons or alcohols from CO_2, this could aid in developing artificial photosynthetic systems that generate renewable transportation fuels.
- Methanogenic microbes are experts at CO_2 reduction. Whether producing or consuming methane, they use the same enzyme for the challenging step of making or breaking the C-H bond. Researchers combined rapid kinetic experiments and computation to provide detailed understanding of the enzymatic mechanism. These results can provide insights for the design of energy-efficient catalysts to convert methane and other one-carbon compounds into liquid fuels and other chemicals.

Electron and Nuclear Dynamics – the Core of Chemical Processes and Properties. Research on electron and atomic displacement is increasing our understanding of both unusual and common mechanisms of energy transformation. Advanced instrumentation and innovative methodology are critical to achieving these insights.

- To generate electricity in organic solar cells, negative and positive charges must be separated over relatively large distances to avoid recombination. Using new terahertz microwave detection methods, researchers found that the charges remained separated in a nanostructure only when the electron is delocalized over an ordered domain. These results suggest that ordered molecular nano-domains play an essential role in efficient organic solar cells.
- Researchers developed a method to produce ultrafast pulses of circularly polarized extreme ultraviolet light in a tabletop setup. With this approach, scientists can easily take tabletop measurements of dynamic processes occurring on ultrafast time scales, such as in novel magnetic materials, and study chiral molecules, such as proteins or DNA, that come in left- and right-handed versions.
- Scientists have confirmed experimentally and with high accuracy the long-held hypothesis that the structure of platinum catalyst nanoparticles, supported on alumina, changes during the catalytic conversion of ethylene to ethane. They designed a miniature reactor to collect nanoscale structural images simultaneously with synchrotron x-ray absorption spectra. This approach provides precise atomic-scale dynamic information to refine models and improve design of supported metal catalysts.

BES user facilities enable U.S. industries to advance technology frontiers and develop new drugs that save lives.

- BES x-ray light sources continue to play a crucial role in helping the pharmaceutical industry advance the fundamental understanding of how diseases function and how to design drugs to treat them. Recently, the U.S. Food and Drug Administration approved Venclexta (venetoclax) to treat chronic lymphocytic leukemia. During the development of this new drug, scientists used structural information obtained at the Advanced Photon Source to understand the function of the BCL-2 protein, which supports cancer growth.
- aBeam Technologies, using a suite of BES light sources and nanocenters, developed a world-leading metrology tool utilizing a fabricated pattern with linewidths down to 1.5 nanometers. aBeam Technologies, together with researchers at the BES user facilities, won an R&D 100 Award for this breakthrough. Metrology tools characterize advanced imaging systems from interferometers to electron microscopes.
- Researchers from Honeywell used the VULCAN instrument at the Spallation Neutron Source to measure residual stresses in a titanium fan jet engine blade that was manufactured by linear friction welding. Residual stress information is crucial to the manufacture of these components due to the detrimental effects the stresses can have on overall mechanical properties.

New optics, insertion device concepts, and accelerator improvements deliver advanced capabilities at BES user facilities.

- Scientists at the National Synchrotron Light Source-II (NSLS-II) developed a hard x-ray scanning microscope employing novel nanofocusing optics that produces a tiny x-ray beam with unprecedented spatial resolution. The microscope provides researchers a unique capability that opens up new scientific frontiers of high-resolution x-ray imaging, taking full advantage of the brightness of NSLS-II. This development won a 2016 Microscopy Today Innovation Award and a 2016 R&D 100 award.

- A new instrument for ultrafast electron diffraction at SLAC National Accelerator Laboratory enables groundbreaking research on complex dynamic systems. Using this superfast high-resolution “electron camera,” with a record shutter speed of 100 quadrillionths of a second, researchers have captured the world’s fastest images of nitrogen molecules rotating in a gas.
- Physicists at the Advanced Photon Source (APS) developed an innovative horizontal-gap vertical-polarization undulator for the Linac Coherent Light Source-II (LCLS-II) project. The new undulator satisfies stringent LCLS-II requirements for control of the magnetic gap, through the use of specially designed springs that exactly match the gap dependence of the magnetic force. Instead of the conventional vertical gap, the horizontal gap generates vertically polarized x-rays to dramatically simplify the design and performance of downstream scientific instruments.

Description

Materials are critical to nearly every aspect of energy generation and end-use. Materials limitations are often the barrier to improved energy efficiencies, longer lifetimes of infrastructure and devices, or the introduction of new energy technologies. The latest BESAC report on transformative opportunities for discovery science, coupled with the Basic Research Needs workshop reports on quantum materials and synthesis science, provide further documentation of the importance of materials sciences in forefront research for next generation scientific and technology advances. The Materials Sciences and Engineering subprogram supports research to provide the fundamental understanding of materials synthesis, behavior, and performance that will enable solutions to wide-ranging energy generation and end-use challenges as well as opening new directions that are not foreseen based on existing knowledge. The research explores the origin of macroscopic material behaviors; their fundamental connections to atomic, molecular, and electronic structures; and their evolution as materials move from nanoscale building blocks to mesoscale systems. At the core of the subprogram is experimental, theory/computational, and instrumentation research that will enable the predictive design and discovery of new materials with novel structures, functions, and properties. Such understanding and control are critical to science-guided design of highly efficient energy conversion processes, multi-functional nanoporous and mesoporous structures for optimum ionic and electronic transport in batteries and fuel cells, materials with longer lifetimes in extreme environments through better materials design and self-healing processes, and new materials with novel, emergent properties that will open new avenues for technological innovation.

To accomplish these goals, the portfolio includes three integrated research activities:

- **Scattering and Instrumentation Sciences**—Advancing science using new tools and techniques to characterize materials structure and dynamics across multiple length and time scales, and to correlate this data with materials performance under real world conditions.

- **Condensed Matter and Materials Physics**—Understanding the foundations of material functionality and behavior including electronic, thermal, optical, and mechanical properties.

- **Materials Discovery, Design, and Synthesis**—Developing the knowledge base and synthesis strategies to design and precisely assemble structures to control properties and enable discovery of new materials with unprecedented functionalities.

The portfolio emphasizes understanding of how to direct and control energy flow in materials systems over multiple time (from femtoseconds to seconds) and length scales (from the nanoscale to mesoscale), and translation of this understanding to prediction of material behavior, transformations, and processes in challenging real-world systems. An example of this research is examination of the transformations that take place in materials with many atomic constituents, complex structures, and a broad range of defects when these materials are exposed to extreme environments, including extremes in temperature, pressure, stress, photon and radiation flux, electromagnetic fields, and chemical exposures – such as those found in fossil energy, nuclear energy, and most industrial settings. To maintain leadership in materials discovery, the research explores new frontiers of unpredicted, emergent materials behavior; utilization of nanoscale control; and materials systems that are metastable or far from equilibrium. The research includes investigation of the interfaces between physical and biological sciences to explore new approaches to novel materials design. Also essential is development of advanced characterization tools, instruments and techniques that can assess a wide range of space and time scales, especially in combination and under dynamic *in operando* conditions to analyze non-equilibrium materials, conditions, and excited-state phenomena.

In addition to single-investigator and small-group research, this subprogram supports Computational Materials Sciences and EFRCs. These research modalities support multi-investigator, multidisciplinary research and focus on forefront scientific challenges that relate to the DOE energy mission. The Computational Materials Sciences activity, initiated in FY 2015, supports integrated, multidisciplinary teams of theorists and experimentalists who focus on development of validated community codes and the associated databases for predictive design of materials. The EFRCs support teams of investigators to perform basic research to accelerate transformative scientific advances for the most challenging topics in materials sciences. The recompetition of the EFRC program scheduled for FY 2018 will focus on the transformative opportunities related to materials sciences identified in the recent BESAC report; the research priorities identified in the Basic Research Needs reports on quantum materials, synthesis science, and instrumentation science; and tackling the scientific challenges required to enable future generations of electrical energy storage and advanced energy generation identified in community-based Basic Research Needs reports.

The Batteries and Energy Storage Hub will receive no additional funding in FY 2018. The goal of this large, tightly integrated team and research was to provide the scientific understanding to enable the next generation of electrochemical energy storage for vehicles and the electrical grid, and its research will be completed at the end of its 5-year award period.

In addition, DOE funding for EPSCoR will be terminated in FY 2018. DOE will continue its long-standing support of energy research and development (R&D) in the regions targeted by the EPSCoR program that include states that are the home of national laboratories for national security and energy research.

Scattering and Instrumentation Sciences Research

Advanced characterization tools with very high precision in space and time are essential to understand, predict, and ultimately control matter and energy at the electronic, atomic, and nanoscale levels. Research in Scattering and Instrumentation Science supports innovative technique and instrumentation development for advanced materials science research with scattering, spectroscopy, and imaging using electrons, scanning probes, neutrons, and x-rays. These tools provide precise and complementary information on the atomic structure, dynamics, and relationship between structure and properties. The use of DOE's world-leading electron, neutron, and x-ray scattering facilities in major advances in materials sciences provides continuing evidence of the importance of this research field. In addition, the BESAC report on transformative opportunities for discovery science, identified imaging as one of the pillars for transformational advances for the future. The use of multimodal platforms to reveal the most critical features of a material was a major finding of the June 2016 workshop "Basic Research Needs Workshop for Innovation and Discovery of Transformative Experimental Tools: Solving Grand Challenges in the Energy Sciences."

The unique interactions of electrons, neutrons and x-rays with matter enable a range of complementary tools with different sensitivities and resolution for the characterization of materials at length- and time-scales spanning many orders of magnitude. A distinct aspect of this activity is the development of innovative instrumentation concepts and techniques for scattering, spectroscopy, and imaging needed to correlate the microscopic and macroscopic properties of energy materials. Characterization of multiscale phenomena to extract heretofore unattainable information on multiple length and time scales is a growing aspect of this research, as is the use of combined scattering and imaging techniques.

Understanding how extreme environments (temperature, pressure, stress, photon and radiation flux, electromagnetic fields, and electrochemical potentials) impact materials at the atomic and nanoscale level and cause changes that eventually result in materials failure is required to design transformational new materials for energy-related applications. Advances in characterization tools, including ultrafast techniques, are needed to measure non-equilibrium and excited-state phenomena at the core of the complex, interrelated physical and chemical processes that underlie materials performance in these conditions. Information from these characterization tools is the foundation for the creation of new materials that have extraordinary tolerance and can function within an extreme environment without property degradation.

Condensed Matter and Materials Physics Research

Understanding and controlling the fundamental properties of materials are critical to improving their functionality on every level and are essential to fulfilling DOE's energy mission. The Condensed Matter and Materials Physics activity supports experimental and theoretical research to advance our understanding of phenomena in condensed matter—solids with structures that vary in size from the nanoscale to the mesoscale. These materials make up the infrastructure for energy technologies, including electronic, magnetic, optical, thermal, and structural materials.

A central focus of this research program is to characterize and understand materials whose properties are derived from the interactions of electrons in their structure, such as unconventional superconductors and magnetic materials. An emerging topic is "quantum materials"—materials whose properties result from strong and coherent interactions of the constituent electrons with each other, the atomic lattice, or light. This activity emphasizes investigation of low-dimensional systems, including nanostructures and two-dimensional layered structures such as graphene, multilayered structures of two-dimensional materials, and studies of the electronic properties of materials at ultra-low temperatures and in high magnetic fields. The research advances the fundamental understanding of the elementary energy conversion steps related to photovoltaics, and the electron spin-phenomena and basic semiconductor physics relevant to next generation electronics and information technologies. Fundamental studies of the quantum mechanical behavior of electrons in materials will lead to an improved understanding of optical, electrical, magnetic, and thermal properties for a wide range of material systems.

This activity also emphasizes research to understand how materials respond to their environments, including the influence of temperature, electromagnetic fields, radiation, and corrosive chemicals. This research includes the defects in materials and their effects on materials' electronic properties, strength, structure, deformation, and failure over a wide range of length and time scales that will enable the design of materials with superior properties and resistance to change under the influence of radiation.

There is a critical need to advance the theories that are being used to describe material properties across a broad range of length and time scales, from the atomic scale to properties at the macroscale where the influence of size, shape, and composition is not adequately understood and the time evolution of these properties from femtoseconds to seconds to much longer times. Theoretical research also includes development of advanced computational and data-oriented techniques and predictive theory and modeling for discovery of materials with targeted properties.

Materials Discovery, Design, and Synthesis Research

The discovery and development of new materials has long been recognized as the engine that drives science frontiers and technology innovations. Predictive design and discovery of new forms of matter with desired properties continues to be a significant challenge for materials sciences. A strong, vibrant research enterprise in the discovery of new materials is critical to world leadership—scientifically, technologically, and economically. One of the goals of this activity is to grow and maintain U.S. leadership in materials discovery by investing in advanced synthesis capabilities and by coupling these with state-of-the-art user facilities and advanced computational capabilities at DOE national laboratories.

The BESAC report on transformative opportunities for discovery science reinforced the importance of the continued growth of synthesis science, recognizing the transformational opportunity to realize targeted functionality in materials by controlling the synthesis and assembly of hierarchical architectures and beyond equilibrium matter. In addition to research on chemical and physical synthesis processes, an important element of this portfolio is research to understand how to use bio-mimetic and bio-inspired approaches to design and synthesize novel materials with some of the unique properties found in nature, e.g., self-repair and adaptability to the changing environment. Major research directions include the controlled synthesis and assembly of nanoscale materials into functional materials with desired properties; porous materials with customized porosities and reactivities; mimicking the energy-efficient, low temperature synthesis approaches of biology to produce materials under mild conditions; bio-inspired materials that assemble autonomously and, in response to external stimuli, dynamically assemble and disassemble to form non-equilibrium structures; and adaptive and resilient materials that also possess self-repairing capabilities. The portfolio also supports fundamental research in solid state chemistry to enable discovery of new functional materials and the development of new crystal growth methods and thin film deposition techniques to create complex materials with targeted structure and properties. An important element of this activity is the development of real-time monitoring tools, *in situ* diagnostic techniques, and instrumentation that can provide information on the progression of structure and properties as a material is formed, in order to understand the underlying physical mechanisms and to gain atomic level control of material synthesis and processing.

Experimental Program to Stimulate Competitive Research (EPSCoR)

Historically, DOE has had an ancillary role in the EPSCoR program, a small program that funded activities across all of DOE to support basic and applied research in states and territories that have historically received lower levels of Federal research funding than others. EPSCoR programs have been supported by multiple federal agencies. Eligibility determination and principal financial investment for EPSCoR are led by the National Science Foundation (NSF) and the National Institutes of Health (NIH). The goal of the various agencies' EPSCoR activities is to support development of infrastructure and research capabilities to advance their ability to successfully compete for research funding through open research solicitations.

No funding is requested for the DOE EPSCoR program for FY 2018. Analysis of DOE funding shows that outside of the EPSCoR program, DOE is providing significant investments in several EPSCoR states, including through national laboratories for both energy and national security. Overall, the states identified as EPSCoR states (based on the NSF eligibility analysis) received approximately 33% of DOE's total funding. Of this funding, the EPSCoR program represents a small fraction, only 0.1%. In addition, the Request focuses BES investments in early stage research and reduces activities like EPSCoR that extend to later-stage or applied research.

<u>Energy Frontier Research Centers (EFRCs)</u>

The EFRC program, initiated in FY 2009, is a unique research modality, bringing together the skills and talents of teams of investigators to perform energy-relevant, basic research with a scope and complexity beyond what is possible in standard single-investigator or small-group awards. These multi-investigator, multi-disciplinary centers foster, encourage, and enable transformative scientific advances for the most challenging topics in materials sciences. The EFRCs supported in this subprogram have historically focused on: the design, discovery, synthesis, characterization, and understanding of novel, solid-state materials that convert energy into electricity; the understanding of materials and processes that are foundational for electrical energy storage, gas separation, and defect evolution in radiation environments; and the exploration of phenomena such as superconductivity and spintronics that can optimize energy flow and transmission. After seven years of research activity, the program has produced an impressive breadth of scientific accomplishments, including over 7,500 peer-reviewed journal publications.

BES's active management of the EFRCs continues to be an important feature of the program. The program uses a variety of methods to regularly assess the progress of the EFRCs, including annual progress reports, monthly phone calls with the EFRC Directors, periodic Directors' meetings, and on-site visits by program managers. BES also conducts in-person reviews by outside experts. Each EFRC undergoes a review of its management structure and approach in the first year of the award and a midterm assessment of scientific progress compared to its scientific goals. To facilitate communication of results to other EFRCs and DOE, meetings of the EFRC researchers are held biennially.

The recompetition of the EFRC program in FY 2018 will focus on use of the team research modality to tackle the transformative opportunities related to materials sciences that have been identified in the recent BESAC report on transformative opportunities for discovery science and the research priorities identified in the Basic Research Needs reports on quantum materials, synthesis science, instrumentation science, and next-generation electrical energy storage.

<u>Energy Innovation Hubs—Batteries and Energy Storage</u>

Over the past four years, the Batteries and Energy Storage Energy Innovation Hub has focused on advancing the understanding of the fundamental electrochemistry and addressing the materials challenges required for advanced electrical energy storage solutions that are critical to the Nation for a reliable electrical grid and improved batteries for vehicles. The Joint Center for Energy Storage Research (JCESR) is led by Argonne National Laboratory (ANL) in collaboration with four other national laboratories, ten universities, and five industrial participants.

JCESR research activities have focused on the development of an atomic-level understanding of reaction pathways and development of universal design rules for electrolyte function for battery systems that go beyond lithium-ion with an emphasis on discovery of new energy storage chemistries. JCESR pioneered the use of technoeconomic modeling to provide a "cost" consideration in setting its fundamental research directions for next generation batteries. JCESR created a library of fundamental scientific knowledge of the phenomena and materials of energy storage at the atomic and molecular level and demonstrated a new paradigm for battery R&D—integrating discovery science, innovative architectures, computational methodologies, and research prototyping in a single highly interactive organization. JCESR research has significantly advanced new energy storage pathways including: demonstration of a new class of membranes for anode protection and flow batteries; elucidation of the characteristics required for multi-valent intercalation electrodes; understanding of the chemical and physical processes that must be controlled to protect the inventories of active materials in lithium-sulfur batteries and greatly improve cycle life; and computational screening of over 16,000 potential electrolyte compounds using the Electrolyte Genome protocols.

The Request focuses resources toward the highest priorities in early-stage fundamental research, with targeted reductions of activities that extend to later-stage fundamental research. JCESR will complete its last year of research in 2018 using funds appropriated in FY 2017; no additional funding is requested.

Computational Materials Sciences

Major strides in materials synthesis, processing, and characterization, combined with concurrent advances in computational science—enabled by enormous improvements in high-performance computing capabilities—have opened an unprecedented opportunity to design new materials with specific function and properties. The goal is to leap beyond simple extensions of current theory and models of materials towards a paradigm shift in which specialized computational codes and software enable the design, discovery, and development of new materials, and in turn, create new advanced, innovative technologies. Given the importance of materials to virtually all technologies, computational materials sciences are critical for United States competitiveness and global leadership in innovation.

This paradigm shift will accelerate the design of revolutionary materials to meet the Nation's energy security and enhance economic competitiveness. Development of fundamentally new design principles could enable stand-alone research codes and integrated software packages to address multiple length and time scales for prediction of the total functionality of materials over a lifetime of use. Examples include dynamics and strongly correlated matter, conversion of solar energy to electricity, design of new catalysts for a wide range of industrial uses, and transport in materials for improved electronics. Success will require extensive R&D with the goal of creating experimentally validated, robust community codes that will enable functional materials innovation.

BES launched 4-year research awards to perform computational materials research in FY 2015 (3 teams) and FY 2016 (2 additional teams), which focused on the creation of computational codes and associated experimental/computational databases for the design of functional materials. This research is performed by fully integrated teams, combining the skills of experts in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication. The research includes development of new *ab initio* theory, mining the data from both experimental and theoretical databases, performing advanced *in situ/in operando* characterization to generate the specific parameters needed to validate computational models, and well-controlled synthesis to confirm the predictions of the codes. It uses the unique world leading tools and instruments at DOE's user facilities, from ultrafast free electron lasers to aberration-corrected electron microscopes and neutron and x-ray scattering and includes instrumentation for atomically controlled synthesis. The computational codes will advance the predictive capability for functional materials, use DOE's leadership class computational capabilities, and be positioned to take advantage of today's petascale and tomorrow's exascale leadership class computers. This research will result in publicly accessible databases of experimental/computational data and open source, robust, validated, user friendly software that captures the essential physics and chemistry of relevant materials systems. The ultimate goal is use of these codes/data by the broader research community and by industry to dramatically accelerate the design of new functional materials.

Computational materials science research activities are managed using the approaches developed by BES for similar large team modalities. Management reviews by a peer review panel are held in the first year of the award, followed by a mid-term peer review to assess scientific progress, with quarterly teleconferences, annual progress reports, and active management by BES throughout the performance period.

Activities and Explanation of Changes

FY 2016 Enacted	FY 2018 Request	Explanation of Changes FY 2018 vs FY 2016
Materials Sciences and Engineering $370,130,000	**$306,637,000**	**-$63,493,000**
Scattering and Instrumentation Sciences Research $67,350,000	**$55,830,000**	**-$11,520,000**
Research emphasized the use of advanced characterization techniques to tackle forefront science on energy-relevant materials science phenomena. Ultrafast science continued to be a priority research area. Investments emphasized hypothesis-driven research with existing ultrafast science capabilities, including lab-based and x-ray free electron laser sources, to establish a more complete understanding of materials properties and behaviors. Neutron scattering sciences stressed innovative time-of-flight scattering and imaging and their effective use in transformational research. New advances in spectroscopy, high-resolution analyses of energy-relevant soft matter, and quantitative *in situ* analysis capabilities under perturbing parameters such as temperature, stress, chemical environment, and magnetic and electric fields were pursued. Research that uses traditional diffraction, imaging, and spectroscopy techniques continued at a reduced level.	Research will continue to support the development and use of the most advanced characterization tools and techniques to address forefront scientific challenges to understand materials and related phenomena, including ultrafast science and quantum materials. Quantitative *in situ* and *in operando* analysis capabilities under perturbing parameters such as temperature, stress, chemical environment, and magnetic and electric fields will be pursued. Investments in x-ray science will emphasize hypothesis driven research with x-ray free electron laser sources, tailored excitations with pumped laser control, and coherent x-ray imaging. Neutron scattering research will emphasize research on thermodynamics of charged polymer systems and emergent quantum phenomena at interfaces and in the bulk. Electron scattering research will focus on innovative and multimodal techniques to assess charge-orbital-spin coupling and quantum phenomena, ultrafast techniques, and high energy resolution imaging and spectroscopy.	Research will continue at the forefront of instrumentation and technique development for materials science research. This activity will emphasize ultrafast techniques in electron scattering, novel and emergent quantum materials phenomena especially with neutron scattering, and assessments of high-speed dynamic phenomena and non-equilibrium systems with x-ray scattering. Imaging and characterization have been identified as key requirements for transformative research by numerous workshop reports. However, the funding decrease requires reduction in program scope. This activity will de-emphasize conventional and heavy fermion superconductivity, lower time resolution dynamic electron scattering, and x-ray scattering for bulk material systems, steady state analysis, and equilibrium systems.
Condensed Matter and Materials Physics Research $113,086,000	**$113,258,000**	**+$172**
The program continued to support fundamental experimental and theoretical research on the properties of materials. It focused on structural, optical, and electrical properties and control of material functionality in response to external stimuli including temperature, pressure, magnetic and electric fields, and radiation. Phenomena in materials	The program will continue to support fundamental experimental and theoretical research on the properties of materials. The experimental and theoretical condensed matter physics research will emphasize quantum materials, focusing on new and emergent behavior including quantum magnetism, spintronics, topological states, and novel 2D materials.	Research will continue at the leading edge of condensed matter and materials physics research to obtain a fundamental understanding of the phenomena that control the properties of materials. This activity will emphasize experimental and theoretic assessments of new and emerging quantum materials and fundamental aspects of physical and

FY 2016 Enacted	FY 2018 Request	Explanation of Changes FY 2018 vs FY 2016
were investigated from atomistic through nanoscale to mesoscale length scales. The research supported continued to address defect structures in materials and how these influence materials properties, especially in energy relevant materials. There was an ongoing emphasis on understanding the relationship between electronic structure and properties in materials that exhibit correlation effects. Research on spin physics, focusing on coupling across heterogeneous boundaries through spin orbit and exchange interactions and studies involving novel magneto-dynamics, were continued. Research involving theory and computational data coupled to experimental characterization of material properties continued to grow. Research on superconducting vortex matter, isolated nanoparticles, quantum Hall behavior, and low dimensional phenomena in carbon nanotubes and graphene continued at a reduced level.	Advancement of theory and computational tools will focus on materials discovery, including data-driven and machine learning techniques; novel approaches, and non-equilibrium systems. Physical behavior research will emphasize innovative science to understand optical, thermal and electronic phenomena. For mechanical behavior and radiation effects, there will be increased focus on understanding defect evolution in radiation environments.	mechanical behavior, including radiation effects. Research in condensed matter physics, physical behavior, and mechanical behavior are major topics for fundamental energy research and have been identified as priorities in community workshops and National Academies studies. Increases for quantum materials and quantum information science will be offset by decreases in long-standing research challenges including heavy fermion superconductivity, Bose-Einstein condensates, compound semiconductor physics, cold atom physics, surface chemistry, shape memory and piezoelectric effects, and plasmonics.
Materials Discovery, Design, and Synthesis Research **$70,273,000**	**$64,621,000**	**-$5,652,000**
Research continued to focus on the predictive design and synthesis of materials across multiple length scales with a particular emphasis on the mesoscale, where functionalities begin to emerge. Within this framework, a fundamental understanding of assembly, both self and directed, and interfacial phenomena, ubiquitous in all materials, were developed. Additionally, synthesis pathways were better understood by use of *in situ* diagnostics and characterization so that they can be controlled more precisely and dynamically. This research helps realize the visionary goals of atom- and energy-efficient syntheses of new forms of matter. Research on recent energy materials on the scene, such as perovskite photovoltaic materials and those with 2D topologies, was strengthened to take advantage of the	Research to develop a scientific understanding for predictive design and synthesis of materials across multiple length scales will continue. Emphasis will be on innovative approaches, including use of *in situ* and *in operando* diagnostics, to understand the mechanisms of chemical, physical, and biomimetic synthesis of materials to enhance discovery of new and improved materials. Continued emphasis will be placed on research that incorporates both experiment and theory with the goal of advancing broad mechanistic insights. Fundamentals of growth kinetics, self-assembly, directed assembly, and the role of interfaces, including organic-in organic systems, will be stressed. In materials chemistry, fundamental research related to polymer chemistry, nanomaterial synthesis, liquids, electrochemistry, and	Pioneering scientific research to advance knowledge of how to make materials and use this understanding to discover new and improved materials will continue, emphasizing innovative research on kinetics and mechanisms for synthesis. Synthesis science and biomimetic research have been the focus of several National Academies studies as well as being identified as research required to enable transformative basic research advances. However, the funding decrease requires reduction in program scope. Topics to be deemphasized include control of synthesis to direct materials properties, molecular materials chemistry, and aspects of biocentric/biohybrid research approaches.

FY 2016 Enacted	FY 2018 Request	Explanation of Changes FY 2018 vs FY 2016
opportunities to realize a more thorough understanding of these materials and their potential for bringing about transformational advances in energy and information technologies. Research on nanomaterials, traditional semiconductors, liquid crystals, and thin film transistor synthesis continued at a reduced level.	control of porosity will continue. For biomolecular materials, research on assembly of materials that incorporates error correction and defect management mechanisms for beyond equilibrium, multicomponent materials will be emphasized.	
Experimental Program to Stimulate Competitive Research (EPSCoR) $14,776,000	**$0**	**-$14,776,000**
Efforts continued to span science in support of the DOE mission, with continued emphasis on science that underpins DOE energy technology programs. Implementation grants, state-laboratory partnerships, and investment in early career research staff from EPSCoR states are sustained. Single investigator research that supports topics related to DOE mission areas, especially through the state-laboratory partnerships component of the program was emphasized.	Funding for EPSCoR is terminated in FY 2018. Research will continue on grants fully funded with EPSCoR funds from prior fiscal years.	No further funding is requested for the DOE EPSCoR program. Analysis of DOE funding shows that DOE provides significant investments in several EPSCoR states, including national laboratories for both energy research and national security. Overall, the EPSCoR states (based on the NSF eligibility analysis) received 33% of DOE funding. Of this funding, the DOE EPSCoR program represents a small fraction, only 0.1%. In addition, the Request focuses investments in early stage research and reduces activities like EPSCoR that extend to later-stage or applied research.
Energy Frontier Research Centers (EFRCs) $55,750,000	**$50,809,000**	**-$4,941,000**
The EFRCs continued to perform fundamental multi-disciplinary research aimed at accelerating scientific innovation. BES conducted a mid-term review of all EFRCs in FY 2016 to assess progress toward meeting scientific research goals. DOE issued a Funding Opportunity Announcement for up to five new EFRC awards in FY 2016.	The recompetition of the EFRC program in FY 2018 will focus on use of the team research modality to tackle the transformative opportunities related to materials sciences and the research priorities identified in the Basic Research Needs reports on quantum materials, synthesis science, instrumentation science, and next-generation electrical energy storage.	The EFRC program will continue to perform fundamental multi-disciplinary research aimed at accelerating scientific innovation. In order to address the priority research directions identified in recent community-based Basic Research Needs workshops and reports, topics to be deemphasized in the FY 2018 competition include phenomena related to traditional solar photovoltaic systems, thermoelectric materials, and solid state lighting.
Energy Innovation Hubs—Batteries and Energy Storage $24,137,000	**$0**	**-$24,137,000**
The Hub, in its fourth year, continued to follow its project plan with an increasing focus on developing lab-scale prototypes to supplement the ongoing fundamental research science underpinning batteries	No funding is requested for FY 2018. JCESR will continue research funded in FY 2017 to complete the five-year award. Its research activities will continue to focus on the development of an atomic-level	The Request focuses resources toward the highest priorities in early-stage fundamental research, with targeted reductions of activities that extend to later-stage fundamental research. The Batteries and Energy

FY 2016 Enacted	FY 2018 Request	Explanation of Changes FY 2018 vs FY 2016
for transportation and the grid, as well as cross-cutting research on materials characterization, theory, and modeling. JCESR completed self-consistent system analyses using techno-economic modeling of three electrochemical couples identified through materials discovery, including output from the electrolyte genome, that have the potential to meet technical performance and cost criteria.	understanding of reaction pathways and development of universal design rules for electrolyte function for battery systems that go beyond lithium-ion with an emphasis on discovery of new energy storage chemistries.	Storage Hub, established in December 2012, will complete its last year of research in 2018; no additional funding is requested.
Computational Materials Sciences $12,000,000	**$10,927,000**	**-$1,073,000**
The computational materials sciences teams that started in FY 2015 performed the first year of research in FY 2016 as outlined in their proposals focused on basic science necessary to develop research-oriented, open-source, experimentally validated software and the associated databases required to predictively design materials with specific functionality; the software utilized current and future leadership class computers. Funding supported additional multi-year awards for research teams focused on functional materials topics not supported by the FY 2015 awards. Early in the award period, each team is peer reviewed to assess management and early research activities.	Research will continue on the computational materials sciences awards focused on basic science necessary to develop research-oriented, open-source, experimentally validated software and the associated databases required to predictively design materials with specific functionality. The software utilizes leadership class computers and incorporates frameworks that are suited for future exascale computer systems. The FY 2016 awards will have their mid-term review by a panel of external peer reviewers in FY 2018. The FY 2015 awards will adjust their research plans based on the mid-term reviews held in FY 2017.	Midterm reviews will be used to assess and focus the research being performed. Lower priority research tasks within each project, based on external peer review and assessment by BES, will be deemphasized to reduce FY 2018 budget requirements.

Description

Transformations of energy among forms, and rearrangements of matter at the atomic, molecular, and nano-scales, are essential in every energy technology. The Chemical Sciences, Geosciences, and Biosciences subprogram supports research to discover fundamental knowledge of chemical reactivity and energy conversion that is the foundation for energy-relevant chemical processes, such as catalysis, synthesis, and light-induced chemical transformation. Research addresses the challenge of understanding how physical and chemical phenomena at the scales of electrons, atoms, and molecules control complex and collective behavior of macro-scale energy conversion systems. At the most fundamental level, understanding of the quantum mechanical behavior of electrons, atoms, and molecules is rapidly evolving into the ability to control and direct such behavior to achieve desired outcomes. This subprogram seeks to extend the new era of control science to include the capability to tailor chemical transformations with atomic and molecular precision. Here, the challenge is to achieve fully predictive understanding of complex chemical, geochemical, and biochemical systems at the same level of detail now known for simple molecular systems.

To address these challenges, the portfolio includes coordinated research activities in three areas:

- **Fundamental Interactions**—Discover the factors controlling chemical reactivity and dynamics in the gas phase, condensed phases and at interfaces, based upon a quantum description of the interactions among photons, electrons, atoms, molecules and nanostructures.

- **Chemical Transformations**—Understand and control the mechanisms of chemical catalysis, synthesis, separation, stabilization and transport in complex chemical systems, from atomic to geologic scales.

- **Photochemistry and Biochemistry**—Elucidate the molecular mechanisms of the capture of light energy and its conversion into electrical and chemical energy through biological and chemical pathways.

This portfolio encompasses several synergistic and cross-cutting fundamental research themes. *Ultrafast Science* develops and applies approaches to probe the dynamics of electrons that control chemical bonding and reactivity; to understand energy flow underlying energy conversions in molecular, condensed phase, and interfacial systems; and to elucidate structural dynamics accompanying bond breaking and bond making in chemical transformations. *Chemistry at Complex Interfaces* addresses the challenge of understanding how the complex environment created at interfaces influences chemical phenomena such as reactivity and transport that are important in photochemical, catalytic, separations, biochemical and geochemical systems. These complex interfaces are structurally and functionally disordered, exhibit complex dynamic behavior, and have disparate properties in each phase. *Charge Transport and Reactivity* explores how the dynamics of charges contribute to energy flow and conversion and how the charge transport and reactivity are coupled. *Catalytic Mechanisms* elucidates the factors controlling chemical transformations through an understanding of the sequence of reaction steps and the catalytic functionalities that control their rates in synthetic or natural catalysts, providing foundational knowledge for the discovery of novel catalytic pathways with unprecedented activity and selectivity. *Chemistry in Aqueous Environments* addresses the unique properties of water, particularly how they manifest in extreme environments such as confinement and complex solutions, and the role aqueous systems play in energy and chemical conversions. The advancement of characterization tools and instrumentation with high spatial and temporal resolution and ability to study real-world systems under operating conditions, as well as computational and theoretical tools that provide predictive capabilities for studies of progressively complex systems, are essential for advancing fundamental science.

In addition to single-investigator and small-group research, the subprogram supports EFRCs, which are multi-investigator, multidisciplinary research efforts focused on forefront scientific challenges that relate to the DOE energy mission. The EFRCs support teams of investigators to perform basic research to accelerate transformative scientific advances for the most challenging topics in chemical sciences, geosciences, and biosciences. The recompetition of the EFRC program scheduled for FY 2018 will focus on transformative opportunities related to chemical sciences, geosciences, and biosciences identified in recent BESAC reports as well as the research topics identified in community-based Basic Research Needs reports on synthesis science, instrumentation science, catalysis science, and the role of water in energy production and use.

The Request focuses resources toward the highest priorities in early-stage fundamental research, with targeted reductions of activities that extend to later-stage fundamental research. No funding is requested for the Fuels from Sunlight Energy Innovation Hub in FY 2018. This Hub was renewed in FY 2015 with research conducted by the large, tightly integrated team focused on providing fundamental scientific understanding to enable the next generation of technologies for direct conversion of sunlight to chemical fuels.

Fundamental Interactions Research

This activity emphasizes structural and dynamical studies of atoms, molecules, and nanostructures, and the description of their interactions in full quantum detail. The goal is to achieve a complete understanding of reactive chemistry in the gas phase, condensed phase, and at interfaces. Using techniques and tools developed for *Ultrafast Sciences*, novel sources of photons, electrons, and ions are used to probe and control atomic, molecular, and nanoscale matter. Ultrafast optical and x-ray sources are developed and used to study and direct molecular dynamics and chemical reactions to increase basic understanding of *Charge Transport and Reactivity* and *Catalytic Mechanisms,* and to understand how the dynamics of molecular environments influence reactivity and transport that is important in the *Chemistry at Complex Interfaces* and *Chemistry in Aqueous Environments.* Research encompasses structural and dynamical studies of chemical systems in the gas and liquid phases. New algorithms for computational chemistry are developed for an accurate and efficient description of chemical processes to better understand *Chemical Mechanisms*, *Charge Transport and Reactivity, Chemistry at Complex Interfaces,* and *Ultrafast Sciences*. These theoretical and computational approaches are applied in close coordination with experiment. The knowledge and techniques produced by Fundamental Interactions research form a science base that underpins numerous aspects of the DOE mission.

The principal research thrusts in this activity are atomic, molecular, and optical sciences (AMOS) and three areas of chemical physics: gas phase chemical physics, condensed phase and interfacial molecular science, and computational and theoretical chemistry. AMOS research emphasizes the fundamental interactions of atoms, molecules, and nanostructures with photons, particularly intense, ultrafast x-ray pulses, to characterize and control their behavior and provide the foundation for understanding the making and breaking of chemical bonds. The goal is to develop accurate quantum mechanical descriptions of ultrafast dynamical processes such as chemical bond breaking and forming, interactions in strong fields, and electron correlation. Novel attosecond sources are used to image the dynamics of electrons and charge transport. Chemical physics research builds from the AMO foundation by examining the reactive chemistry of molecules whose chemistry is profoundly affected by the environment, especially at complex interfaces. The transition from molecular-scale chemistry to collective phenomena is explored at a molecular level in condensed phase systems, such as the effects of solvation or interfaces on chemical structure and reactivity. The goal is to understand reactivity and dynamical processes in liquid systems and at complex interfaces using model systems. Understanding of such collective behavior is critical in a wide range of energy and environmental applications, from solar energy conversion to radiolytic effects in condensed phases and interfacial systems, to catalysis. Gas-phase chemical physics emphasizes experimental and theoretical studies of the ultrafast dynamics and rates of chemical reactions, as well as the chemical and physical properties of key intermediates relevant to catalysis. Computational and theoretical research supports the development and integration of new and existing theoretical and computational approaches for accurate and efficient descriptions of ultrafast processes relevant to catalysis and charge transport. Of special interest is foundational research on computational design of molecular- to meso-scale materials, and on next-generation simulation of complex dynamical processes. Research in this area is crucial to utilize planned exascale computing facilities and to optimize use of existing petascale computers, leveraging U.S. leadership in the development of computational chemistry codes.

Chemical Transformations Research

Fundamentally, Chemical Transformations Research emphasizes advancing the knowledge of chemical reactivity, matter transport, and chemical separation and stabilization processes that will ultimately impact fuel science, separations science, heavy element chemistry and geosciences. The research uses tools from *Ultrafast Sciences* to identify transient species during reactions and refine theories of reactivity; advances understanding of *Charge Transport and Reactivity* important in electrocatalytic and geochemical redox processes; explores *Chemistry at Complex Interfaces* in catalytic, geochemical and separations systems; and develops understanding of *Chemistry in Aqueous Environments* that play important roles in separations, particularly for heavy elements. This research breadth demands a broad coverage of scientific disciplines and analytical tools. Hence, Chemical Transformations comprise four core areas: Catalysis Science, Separations Science, Heavy Element Chemistry and Geosciences.

Catalytic Mechanisms represent a major fraction of the research in this activity, particularly focused on achieving predictability and control of catalytic conversions, which are dominated by correlated structural and electronic dynamics under reaction conditions. This chemistry encompasses interfacial dynamics of catalytic particles, transient or reactive interfacial species, multifunctional membranes, nanostructured electrodes, and multiphase electrolytes. This activity supports development and application of theoretical and computational approaches to achieve a deeper understanding of reaction and separation pathways and processes; design new catalysts, membranes or separation media; and predict transport and reaction processes in the Earth's subsurface. This activity contains the largest federally funded program in non-biological Catalysis Science.

This activity supports fundamental separation science to resolve complex organic or inorganic mixtures, extract actinides from complex solutions, or recover targeted species from streams. Controlling the interaction of electric fields and matter allows for improved separations and controlled reactions. Controlling charge transport and reactivity is essential to efficiently control electroseparations as well as redox processes in fuel cells, electrocatalysts, reactive membranes or mineral interfaces.

Fundamental studies of the structure and reactivity of actinide-containing molecules provide foundational knowledge for future nuclear energy approaches. Radionuclides and heavy elements under extreme radiation environments exhibit unique dynamic and kinetic behavior. The challenges are further compounded by the evolution of these chemical mixtures over time. The chemistry of aqueous systems plays an important role in understanding the science of separations for these mixtures as well as their evolution.

Geosciences research provides the fundamental scientific basis underlying the subsurface chemistry and physics of natural substances under extreme conditions of pressure in solid or confined environments (e.g., porous media). Understanding chemistry of aqueous solutions at mineral interfaces and in confined environments is a common theme for this research activity, which advances knowledge of subsurface fracture, fluid flow and complex chemistry occurring over multiple scales of time and space.

Photochemistry and Biochemistry Research

This activity supports research on the molecular mechanisms that capture light energy and convert it into electrical and chemical energy in both natural and man-made systems. An important component of this activity is its leadership role in the support of basic research in both solar photochemistry and natural photosynthesis. A breadth of approaches and unique tools, such as those in *Ultrafast Sciences*, are developed and used to investigate the structural and chemical dynamics of energy absorption, transfer, conversion and storage across multiple spatial and temporal scales to better understand *Charge Transport and Reactivity*. Such efforts target the basic understanding of mechanisms and dynamics of chemical processes such as water oxidation, charge transfer, and redox interconversion of small molecules (e.g. carbon dioxide/methane, nitrogen/ammonia, and protons/hydrogen). Crosscutting research underpins a fundamental understanding of the synthesis, dynamics, and function of natural and artificial membranes and nano- to mesoscale-structures and develops new knowledge of the *Chemistry at Complex Interfaces* as well as *Chemistry in Aqueous Environments*. Structural, functional and mechanistic properties of enzymes, enzyme systems, and energy-relevant biological reactions are studied to identify principles important for catalyst function, selectivity, and stability. This synergistic research in *Catalytic Mechanisms* is illustrated by studies of the mechanism of the complex water splitting reaction catalyzed by the metallocluster of the oxygen evolving complex in natural photosynthesis. The fundamental chemical and physical concepts resulting from studies of both natural systems (e.g. photosynthetic and affiliated downstream biological processes) and man-made chemical systems provide crucial foundational knowledge on processes of energy capture, conversion, and storage.

Studies of natural photosynthesis provide an understanding of the dynamic mechanisms of solar energy capture and conversion in biological systems, from the atomic scale through the mesoscale. Research efforts encompass light harvesting, electron and proton transport, and the assembly, repair, and regulation of photosynthetic complexes. Physical science tools are used extensively to elucidate the molecular and chemical mechanisms of biological energy transduction, including complex multielectron redox reactions and processes beyond primary photosynthesis such as carbon dioxide reduction and subsequent deposition of the reduced carbon into energy-dense carbohydrates and lipids. Complementary research on solar energy conversion in chemical and artificial systems incorporates organic and inorganic photochemistry, electrochemistry, light-driven energy and electron transfer processes, and molecular assemblies for electricity generation and artificial photosynthetic fuel production.

Energy Frontier Research Centers (EFRCs)
The EFRC program, initiated in FY 2009, is a unique research modality, bringing together the skills and talents of teams of investigators to perform energy-relevant, basic research with a scope and complexity beyond what is possible in standard single-investigator or small-group awards. These multi-investigator, multi-disciplinary centers foster, encourage, and accelerate basic research to enable transformative scientific advances for the most challenging topics in chemical sciences, geosciences, and biosciences. The EFRCs supported in this subprogram have historically focused on the following topics: the design, discovery, characterization, and control of the chemical, biochemical, and geological moieties and processes for the advanced conversion of solar energy into chemical fuels and for improved electrochemical storage of energy; the understanding of catalytic chemistry and biochemistry that are foundational for fuels, chemicals, and separations; and advanced interrogation and characterization of the earth's subsurface. After seven years of research activity, the program has produced an impressive breadth of accomplishments, including over 7,500 peer-reviewed journal publications.

BES's active management of the EFRCs continues to be an important feature of the program. A variety of methods are used to regularly assess the progress of the EFRCs, including annual progress reports, monthly phone calls with the EFRC Directors, periodic Directors' meetings, and on-site visits by program managers. BES also conducts in-person reviews by outside experts. Each EFRC undergoes a review of its management structure and approach in the first year of the award and a midterm assessment of scientific progress compared to its scientific goals. To facilitate communication of results to other EFRCs and DOE, meetings of the EFRC researchers are held biennially.

The recompetition of the EFRC program in FY 2018 will focus on use of the team research modality to tackle the transformative opportunities related to chemical sciences, geosciences, and biosciences that have been identified in the recent BESAC report on transformative opportunities for discovery science and the research topics identified in Basic Research Needs reports on synthesis science, instrumentation science, and energy-water issues (e.g., the efficient use of water in energy production and energy-intensive industrial processes and the efficient use of energy in water production).

Energy Innovation Hubs—Fuels from Sunlight
Established in September 2010 and renewed in 2015, the Fuels from Sunlight Hub, called the Joint Center for Artificial Photosynthesis (JCAP), is a multi-disciplinary, multi-investigator, multi-institutional effort to create the scientific foundation for transformative advances in the development of artificial photosynthetic systems for the conversion of sunlight, water, and carbon dioxide into a range of commercially useful fuels. JCAP is led by the California Institute of Technology (Caltech) in primary partnership with Lawrence Berkeley National Laboratory (LBNL). Other partners include the SLAC National Accelerator Laboratory and University of California institutions.

During the initial award, JCAP achieved the scientific and technical advances needed to reach its five-year goal to design and construct a photocatalytic prototype that could generate fuel from sunlight, developing a stable integrated prototype that split water to produce hydrogen at greater than 10% efficiency. Based on the outcome of external peer review, JCAP was renewed by BES for a final five-year award term starting on September 30, 2015, at an annual funding level of $15M. In the second award, JCAP is focusing on the fundamental science of carbon dioxide reduction to establish the foundation for production of hydrocarbon fuels using only sunlight, carbon dioxide, and water as inputs. Research objectives for the JCAP renewal project include discovery and understanding of highly selective catalytic mechanisms for carbon dioxide reduction and oxygen evolution; accelerated discovery of electrocatalytic and photoelectrocatalytic materials and light-absorber photoelectrodes for selective and efficient carbon dioxide reduction; and, using JCAP prototypes, demonstration of highly efficient and selective artificial photosynthetic carbon dioxide reduction and oxygen evolution components.

JCAP has demonstrated progress in several key areas of the renewal project. Guided by theoretical results, scientists discovered that nickel-gallium films require less energy to reduce carbon dioxide to ethylene, ethane, and methanol than copper-based materials, which were previously considered to be the best candidate catalysts. The research team combined JCAP's unique computational and experimental high-throughput capabilities to discover new earth-abundant metal vanadates that meet demanding requirements for water-splitting photoanodes. These results nearly doubled the number of materials that could considered for this key component of solar fuel generators and are helping researchers understand how material properties can be tuned for a specific function. Theoretical and experimental photocatalysis efforts also produced nanocrystals that exhibited the first demonstration of plasmon-enhanced photocurrent in carbon dioxide reduction and are being used to understand the interplay between plasmon and single particle excitation, providing insight into the possible use of plasmons in photo-induced chemical reactions.

No funding is requested for JCAP in FY 2018. The Request focuses resources toward the highest priorities in early-stage fundamental research, with targeted reductions of activities that extend to later-stage fundamental research.

General Plant Projects (GPP)
GPP funding is provided for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems at the Ames Laboratory. Funding of this type is essential for maintaining the productivity and usefulness of Department-owned facilities and for meeting requirements for safe and reliable facilities operation. The total estimated cost of each GPP project will not exceed $10,000,000.

Activities and Explanation of Changes

FY 2016 Enacted	FY 2018 Request	Explanation of Changes FY 2018 vs FY 2016
Chemical Sciences, Geosciences, and Biosciences $311,795,000	**$265,615,000**	**-$46,180,000**
Fundamental Interactions Research $72,782,000	**$61,187,000**	**-$11,595,000**
Research continued to develop and apply forefront ultrafast x-ray and optical probes of matter, utilizing the LCLS, BES synchrotron light sources, and table-top laser-based ultrafast light sources, to probe and control atomic, molecular, nanoscale and mesoscale matter. The program continued to develop advanced theoretical methods to guide and interpret ultrafast measurements and to design new experiments. It also continued to emphasize time-resolved electron and x-ray probes of matter at unprecedented short time scales and in systems of increasing complexity. Computational efforts stressed the development of improved methods to calculate electronically excited states in molecules and extended mesoscale systems. Work continued on advanced combustion research to accelerate the predictive simulation of highly efficient and clean internal combustion engines. Increased emphasis was on investigating properties of combustion in high-pressure or multiphase systems. The program deemphasized research at the interface of nanoscience with molecular physics.	This program will continue to develop and apply forefront ultrafast x-ray and optical probes of matter, utilizing the LCLS, BES synchrotron light sources, and table-top laser-based ultrafast light sources, to probe and control atomic, molecular, nanoscale and mesoscale matter. Attosecond light sources will be used to image the dynamics of electrons and charge transport in increasingly complex systems. The program continues to develop advanced theoretical methods to guide and interpret ultrafast measurements and catalysts such as metal-organic frameworks. Computational efforts stress the development of improved methods to calculate electronically excited states in molecules and extended mesoscale systems that can be scaled to operate on exascale computers. Research will extend efforts to understand and control chemical processes and dynamics in aqueous systems and at complex interfaces at a molecular level. Gas phase research will examine the structure and dynamics of reactive intermediates important to catalysis.	Research will continue leading efforts to discover the factors controlling chemical reactivity and dynamics in the gas phase, condensed phases and at interfaces, based upon fundamental knowledge of the interactions among photons, electrons, atoms, molecules and nanostructures. This activity will emphasize quantum chemistry, imaging studies of molecular dynamics using ultrafast BES light sources, research to understand increasingly complex interfacial systems, and advanced computational and theoretical tools for exascale computing. This activity is a major supporter of ultrafast chemical sciences and chemical physics, underpinning energy conversion and transformation phenomena. However, the funding decrease requires reduction in program scope. The activity will de-emphasize aspects of nanoscience and combustion research in favor of higher priorities.
Chemical Transformations Research $88,918,000	**$82,004,000**	**-$6,914,000**
Synthesis, guided by theory and computation, continued to explore novel catalytic materials at the nano- and mesoscale for the efficient conversion of traditional and new feedstocks into higher-value fuels and other chemicals. The program emphasized catalytic conversion of biomass to fuels and other energy related chemical products as well as the search for catalysts for new ammonia production routes that	This activity will continue to support predictive fundamental research on the design and synthesis of novel catalysts to efficiently convert chemical feedstocks, particularly small hydrocarbons (e.g., with 1-4 carbon atoms) and bio-derived molecules, to high-value fuels and chemicals. New routes to the efficient synthesis of hydrogen, ammonia, methanol, syngas, and others, will continue to be pursued. Fundamental	Research will continue to lead the development of fundamental knowledge of mechanisms of chemical catalysis, synthesis, separation, stabilization and transport required to control chemical processes in complex systems. This activity will emphasize advancing catalytic mechanisms that operate efficiently at lower temperatures and pressures, enhance efforts in electro-catalytic synthesis, and

FY 2016 Enacted	FY 2018 Request	Explanation of Changes FY 2018 vs FY 2016
avoid the generation of greenhouse gases. To support these new emphases, the program deemphasized the development of mass spectrometric techniques. Likewise, coupled predictive theory and synthesis of designer mesoporous membranes and filter materials sought more efficient separation of carbon dioxide from power plant effluents or of oxygen from air relevant to oxycombustion approaches. Subsurface geochemistry and geophysics sought to provide data and mechanistic interpretation for models of reactive flow and transport important for carbon sequestration and extraction of tight gas and oil. Actinide research continued to emphasize new insights in actinides chemical bonding enabling new chemistry for separation and related nuclear fuels and waste form processes especially using ionic liquids. Fundamental research activities in geochemistry and geophysics of the subsurface continued in parallel with efforts in other offices as coordinated by the Subsurface Science, Technology and Engineering R&D (Subsurface) crosscut.	separations science research will continue on efficient processes for separating chemical mixtures. Operando characterization of chemical conversions and separations will continue to be supported, as will predictive theory for separation processes molecular recognition, transport and resolution. Geochemistry and geophysics will continue to develop mechanisms of reaction and transport processes of substances introduced to the subsurface environments. Heavy Element research will continue to pursue new chemistry of actinide reactivity, bonding, synthesis, and separation.	initiate studies of integrated catalytic-separation approaches. This activity is the major supporter of catalysis and heavy element chemistry that have been the focus of community workshops and National Academies studies. However, the funding decrease requires reduction in program scope. The activity will de-emphasize research on chiral catalysis and catalytic synthesis of nanomaterials, geophysics of microfluidics in natural porous system, and chemical analysis not aligned with separations science.
Photochemistry and Biochemistry Research		
$69,113,000	**$63,701,000**	**-$5,412,000**
Research continued to emphasize a fundamental understanding of light energy capture and conversion in non-biological and biological (photosynthetic) systems. These studies established a foundation for direct conversion of solar energy to electricity, fuels, and high value chemicals. The program continued to support efforts in computation and modeling as such approaches can facilitate design and fabrication of semiconductor/polymer interfaces, dye-sensitized solar cells, inorganic-organic molecular complexes, and bio-inspired/biohybrid light harvesting complexes. The program continued to emphasize research to understand the fundamental mechanisms of water-splitting, redox, cell wall biosynthesis, and	The program will continue to support fundamental research on light energy capture and conversion into chemical and electrical energy through non-biological (chemical) and biological (photosynthetic) pathways. Studies of light absorption, energy transfer, and charge transport and separation will continue to be emphasized. Research to uncover the fundamental mechanisms of photocatalysis and biocatalysis will continue to be a focus of the program and will make use of innovative ultrafast methodologies as well as computation and modeling. Enhanced efforts will target a fundamental understanding of reactivity across complex interfaces and in aqueous environments. Research will address a greater	Cutting-edge research will continue to develop fundamental knowledge and innovative approaches to understand physical and chemical processes of light energy capture and conversion in non-biological and biological systems. Research on charge transport, energy transfer, and catalytic mechanisms will be enhanced by increased efforts that address the chemistry of complex interfaces and water-driven processes. This activity is important for understanding chemical processes and dynamics during energy conversion and is viewed by community workshops as key for transformative science. However, the funding decrease requires reduction in program scope. Efforts in plant cell wall biosynthesis and structure, light

FY 2016 Enacted	FY 2018 Request	Explanation of Changes FY 2018 vs FY 2016
other energy-relevant biological (enzymatic) reactions, from the nano- to the mesoscale. These studies provided new insights for developing novel bio-inspired catalysts based on earth-abundant materials and for controlling and optimizing chemical reactions important for energy capture, conversion, and storage. The program deemphasized research on fundamental mechanisms of carbon capture.	understanding of how water drives formation of mesoscale structures for energy capture and conversion in natural systems and the chemistry and structure of water within the field of highly ionizing radiation.	signaling in plant development, and combinatorial studies of catalytic semiconductors will be de-emphasized in favor of higher priorities.
Energy Frontier Research Centers (EFRCs) **$54,250,000**	**$48,065,000**	**-$6,185,000**
The EFRCs continued to perform fundamental multi-disciplinary research aimed at accelerating scientific innovation. BES conducted a mid-term review of all EFRCs in FY 2016 to assess progress toward meeting scientific research goals. DOE issued a Funding Opportunity Announcement for up to five new EFRC awards in FY 2016.	The recompetition of the EFRC program in FY 2018 will focus on use of the team research modality to tackle the transformative opportunities related to chemical sciences, geosciences and biosciences and the research priorities identified in the Basic Research Needs reports on synthesis science, instrumentation science, and energy-water issues.	The EFRC program will continue to perform fundamental multi-disciplinary research aimed at accelerating scientific innovation. In order to address the priority research directions identified in recent community-based Basic Research Needs workshops and reports, topics to be deemphasized in the FY 2018 competition include phenomena related to radioactive waste management, CO_2 sequestration, aspects of cellulosic degradation, and more mature areas of solar photovoltaics.
Energy Innovation Hubs—Fuels From Sunlight **$15,000,000**	**$0**	**-$15,000,000**
The Fuels from Sunlight Hub was renewed for a final award term of up to 5 years starting in September 2015. Research in the renewal focuses on the fundamental science needed to enable efficient, sustainable and scalable photochemical reduction of carbon dioxide for production of liquid transportation fuels. The renewal allows JCAP to further advance research efforts addressing critical needs in solar fuels development and to capitalize on its achievements and infrastructure development from the initial funding period. BES conducted scientific and merit review in FY 2016 to assess progress toward meeting project milestones and goals.	No funding is requested for FY 2018. JCAP will continue research funded in FY 2017. These activities will focus on the renewal project goal to conduct fundamental research for a mechanistic understanding of the photochemical reduction of carbon dioxide for fuel production.	The Request focuses resources toward the highest priorities in early-stage fundamental research, with targeted reductions of activities that extend to later-stage fundamental research. The Fuels from Sunlight Hub was established in December 2010 and renewed in FY 2015. No funding is requested in FY 2018.

FY 2016 Enacted	FY 2018 Request	Explanation of Changes FY 2018 vs FY 2016
General Plant Projects $1,000,000	**$1,000,000**	**$0**
Funding supports minor facility improvements at Ames Laboratory.	Funding supports minor facility improvements at Ames Laboratory.	Funding is flat with the FY 2016 Enacted level.

Basic Energy Sciences
Scientific User Facilities

Description

The Scientific User Facilities subprogram supports the operation of a geographically diverse suite of major research facilities that provide thousands of researchers from universities, industry, and government laboratories unique tools to advance a wide range of sciences. These user facilities are operated on an open access, competitive merit review basis, enabling scientists from every state and many disciplines from academia, national laboratories, and industry to utilize the facilities' unique capabilities and sophisticated instrumentation.

Studying matter at the level of atoms and molecules requires instruments that can probe structures that are one thousand times smaller than those detectable by the most advanced light microscopes. Thus, to characterize structures with atomic detail, we must use probes such as x-rays, electrons, and neutrons with wavelengths at least as small as the structures being investigated. The BES user facilities portfolio consists of a complementary set of intense x-ray sources, neutron scattering centers, and research centers for nanoscale science. These facilities allow researchers to probe materials in space, time, and energy with the appropriate resolutions that can interrogate the inner workings of matter to answer some of the most challenging grand science questions. By taking advantage of the intrinsic charge, mass, and magnetic characteristics of x-rays, neutrons, and electrons, these tools offer unique capabilities to help understand the fundamental aspects of the natural world.

Advances in tools and instruments often drive scientific discovery. The continual development and upgrade of the instrumental capabilities include new x-ray and neutron experimental stations, improved core facilities, and new stand-alone instruments. The subprogram also supports research in accelerator and detector development to explore technology options for the next generations of x-ray and neutron sources.

In FY 2016, the BES scientific facilities were used by more than 15,000 scientists and engineers in many fields of science and technology. These facilities provide unique capabilities to the scientific community and industry and are a critical component of maintaining U.S. leadership in the physical sciences. Collectively, these user facilities and enabling tools contribute to important research results that span the continuum from basic to applied research and embrace the full range of scientific and technological endeavors, including chemistry, physics, geology, materials science, environmental science, biology, and biomedical science. These capabilities enable scientific insights that can lead to the discovery and design of advanced materials and novel chemical processes with broad societal impacts, from energy applications to information technologies and biopharmaceutical discoveries. The advances enabled by these facilities extend from energy-efficient catalysts to spin-based electronics and new drugs for cancer therapy. For approved, peer-reviewed projects, operating time is available at no cost to researchers who intend to publish their results in the open literature.

X-Ray Light Sources

X-rays are an essential tool for studying the structure of matter and have long been used to peer into material through which visible light cannot penetrate. Today's light source facilities produce x-rays that are billions of times brighter than medical x-rays. Scientists use these highly focused, intense beams of x-rays to reveal the identity and arrangement of atoms in a wide range of materials. The tiny wavelength of x-rays allows us to see things that visible light cannot resolve, such as the arrangement of atoms in metals, semiconductors, biological molecules, and other materials. The fundamental tenet of materials research is that structure determines function. The practical corollary that converts materials research from an intellectual exercise into a foundation of our modern technology-driven economy is that structure can be manipulated to construct materials with particular desired behaviors. To this end, x-rays have become a primary tool for probing the atomic and electronic structure of materials internally and on their surfaces.

From its first systematic use as an experimental tool in the 1960s, large scale light source facilities have vastly enhanced the utility of pre-existing and contemporary techniques, such as x-ray diffraction, x-ray spectroscopy, and imaging and have given rise to scores of new ways to do experiments that would not otherwise be feasible with conventional x-ray machines. Moreover, the wavelength can be selected over a broad range (from the infrared to hard x-rays) to match the needs of particular experiments. Together with additional features, such as controllable polarization, coherence, and ultrafast pulsed time structure, these characteristics make x-ray light sources an important tool for a wide range of materials research. The wavelengths of the emitted photons span a range of dimensions from the atom to biological cells, thereby providing incisive probes for advanced research in a wide range of areas, including materials science, physical and chemical sciences, metrology, geosciences, environmental sciences, biosciences, medical sciences, and pharmaceutical sciences. BES operates a suite of five light sources, including a free electron laser, the Linac Coherent Light Source (LCLS) at SLAC and four storage ring based light sources—the Advanced Light Source (ALS) at LBNL, Advanced Photon Source (APS) at ANL, Stanford Synchrotron Radiation Lightsource (SSRL) at SLAC, and the newly constructed National Synchrotron Light Source-II (NSLS-II) at BNL. BES also provides funds to support facility operations, enable cutting-edge research and technical support, and to administer the user program at these facilities, which are made available to all researchers with access determined via peer review of user proposals.

High Flux Neutron Sources

One of the goals of modern materials science is to understand the factors that determine the properties of matter on the atomic scale and to use this knowledge to optimize those properties or to develop new materials and functionality. This process regularly involves the discovery of fascinating new physics, which itself may lead to previously unexpected applications. Among the different probes used to investigate atomic-scale structure and dynamics, thermal neutrons have unique advantages:

- they have a wavelength similar to the spacing between atoms, allowing atomic resolution studies of structure, and have an energy similar to the elementary excitations of atoms and magnetic spins in materials, thus allowing an investigation of material dynamics;
- they have no charge, allowing deep penetration into a bulk material;
- they are scattered to a similar extent by both light and heavy atoms but differently by different isotopes of the same element, so that different chemical sites can be distinguished via isotope substitution experiments, for example in organic and biological materials;
- they have a magnetic moment, and thus can probe magnetism in condensed matter systems; and
- their scattering cross-section is precisely measurable on an absolute scale, facilitating straightforward comparison with theory and computer modeling.

The High Flux Isotope Reactor (HFIR) at ORNL generates neutrons via fission in a research reactor. HFIR operates at 85 megawatts and provides state-of-the-art facilities for neutron scattering, materials irradiation, and neutron activation analysis. It is the world's leading production source of elements heavier than plutonium for medical, industrial, and research applications. There are 12 instruments in the user program at HFIR and the adjacent cold neutron beam guide hall, which include world-class inelastic scattering spectrometers, small angle scattering, powder and single crystal diffractometers, neutron imaging, and an engineering diffraction machine.

Another approach for generating neutron beams is to use an accelerator to generate protons that strike a heavy-metal target. As a result of the impact, neutrons are produced in a process known as spallation. The Spallation Neutron Source (SNS) at ORNL is the world's brightest pulsed neutron facility and presently includes 19 instruments. These instruments include very high resolution inelastic and quasi-elastic scattering capabilities, powder and single crystal diffraction, polarized and unpolarized beam reflectometry, spin echo and small angle scattering spectrometers. A full suite of high and low temperature, high magnetic field, and high pressure sample environment equipment is available on each instrument. All the SNS instruments are in high demand by researchers world-wide in a range of disciplines from biology to materials sciences and condensed matter physics.

Nanoscale Science Research Centers (NSRCs)

Nanoscience is the study of materials and their behaviors at the nanometer scale—probing and assembling single atoms, clusters of atoms, and molecular structures. The scientific quest is to design new nanoscale materials and structures not found in nature, and observe and understand how they function and interact with their environment. Developments at the nanoscale and mesoscale have the potential to make major contributions to delivering remarkable scientific discoveries that transform our understanding of energy and matter and advance national, economic, and energy security.

The NSRCs focus on interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. They are a different class of facility than the x-ray and neutron sources, as NSRCs are not based on a large accelerator or reactor but are comprised of a suite of smaller unique tools and expert scientific staff. The five NSRCs are the Center for Nanoscale Materials at ANL, Center for Functional Nanomaterials at BNL, Molecular Foundry at LBNL, Center for Nanophase Materials Sciences at ORNL, and Center for Integrated Nanotechnologies at SNL and LANL. Each center has particular expertise and capabilities, such as nanomaterials synthesis and assembly; theory, modeling and simulation; imaging and spectroscopy including electron microscopy; and nanostructure fabrication and integration. Selected thematic areas include catalysis, electronic materials, nanoscale photonics, and soft and biological materials. The centers are housed in custom-designed laboratory buildings near one or more other major BES facilities for x-ray, neutron, electron scattering, or computation which complement and leverage the capabilities of the NSRCs. These laboratories contain clean rooms, nanofabrication resources, one-of-a-kind signature instruments, and other instruments not generally available except at major user facilities. The NSRC electron microscopy capabilities provide superior atomic-scale spatial resolution and the ability to simultaneously obtain structural, chemical, and other types of information from sub-nanometer regions at short time scales. Operating funds enable cutting-edge research and technical support and to administer the user program at these facilities, which are made available to academic, government, and industry researchers with access determined through external peer review of user proposals.

<u>Other Project Costs</u>
The total project cost (TPC) of DOE's construction projects comprises two major components—the total estimated cost (TEC) and other project costs (OPC). The TEC includes project costs incurred after Critical Decision-1, such as costs associated with all engineering design and inspection; the acquisition of land and land rights; direct and indirect construction/fabrication; and the initial equipment necessary to place the facility or installation in operation; and facility construction costs and other costs specifically related to those construction efforts. OPC represents all other costs related to the projects that are not included in the TEC. Generally, other project costs are incurred during the project's initiation and definition phase for planning, conceptual design, research, and development, and during the execution phase for R&D, startup, and commissioning. OPC is always funded via operating funds.

<u>Major Items of Equipment</u>
BES supports major item of equipment (MIE) projects to ensure the continual development and upgrade of major scientific instrument capabilities, including fabricating new x-ray and neutron experimental stations, improving core facilities, and providing new stand-alone instruments. In general, each MIE with a total project cost greater than $5,000,000 and all line item construction projects follow the DOE Project Management Order 413.3B, which requires formal reviews to obtain critical decisions that advance the developmental stages of a project. Additional reviews may be required depending on the complexity and needs of the projects in question.

<u>Research</u>
This activity supports targeted basic research in accelerator physics, x-ray and neutron detectors, and developments of advanced x-ray optics. Accelerator research is the cornerstone for the development of new technologies that will improve performance of accelerator-based light sources and neutron scattering facilities. Research areas include ultrashort pulse free electron lasers (FELs), new seeding techniques and other optical manipulation to reduce the cost and complexity and improve performance of next generation FELs, and development of intense laser-based THz sources to study non-equilibrium behavior in complex materials. Detector research is a crucial component to enable the optimal utilization of user facilities, together with the development of innovative optics instrumentation to advance photon-based sciences, and data management techniques. The emphasis of the detector activity is on research leading to new and more efficient photon and neutron detectors. X-ray optics research involves development of systems for time-resolved x-ray science that preserve the spatial, temporal, and spectral properties of x-rays. Research includes studies on creating, manipulating, transporting, and performing diagnostics of ultrahigh brightness beams and developing ultrafast electron diffraction systems that complement the capabilities of x-ray FELs. This activity also includes research in sophisticated data management tools to address the vastly accelerated pace and volume of data generated by faster, higher resolution detectors and brighter light sources. This activity also supports training in the field of particle beams and their associated accelerator technologies.

This activity also includes long term surveillance and maintenance (LTSM) responsibilities and legacy cleanup work at BNL and SLAC. No funding is requested for LTSM in FY 2018.

Activities and Explanation of Changes

FY 2016 Enacted	FY 2018 Request	Explanation of Changes FY 2018 vs FY 2016
Scientific User Facilities $966,775,000	**$780,148,000**	**-$186,627,000**
Synchrotron Radiation Light Sources $482,667,000	**$428,206,000**	**-$54,461,000**
Funding supported near optimal operations of the five BES light sources, including the first full year of operations for the newly constructed NSLS-II. $5M is for R&D in support of the Advanced Light Source Upgrade.	The FY 2018 Request prioritizes funding for four BES light sources (APS, ALS, NSLS-II, and LCLS). These facilities will reduce operating hours and user support, including shutting down selected beamlines. Maintenance, upgrades, and procurement activities will be deferred. SSRL will operate through the first quarter of the fiscal year, then the facility will transition to a warm standby status.	The funding decrease will support below optimal operations for four BES light sources. SSRL will operate for limited hours and then transition to a warm standby status. SSRL has the lowest user demand of the BES light sources in steady-state operations. No funding is requested for the Advanced Light Source Upgrade.
High-Flux Neutron Sources $265,082,000	**$225,620,000**	**-$39,462,000**
Funding supported the operation of HFIR and SNS at near optimal levels. Limited funding is included for the Lujan Neutron Scattering Center for the removal of hazardous materials and planning of the disposition of unused equipment. $10M is provided to accelerate the progress towards critical decision-1 for the Second Target Station at SNS.	The FY 2018 Request provides funding for HFIR and SNS. These facilities will reduce operating hours and user support, including shutting down selected flight paths. Maintenance, upgrades, and procurement activities will be deferred. No funding is requested to the Lujan Neutron Scattering Center for the disposition of unused equipment.	The funding decrease will support below optimal operations for HFIR and SNS. No funding is requested for the Lujan Neutron Scattering Center or for the Second Target Station at SNS.
Nanoscale Science Research Centers $120,575,000	**$71,135,000**	**-$49,440,000**
Funding supported operations at the NSRCs at near optimal levels. Program emphasis continued to cultivate and expand the user base from universities, national laboratories, and industry. Planning efforts continued to advance the cutting-edge nanostructure characterization capabilities, with an emphasis on coupling multi-probes of photon, neutron, and electron, and planning for future electron scattering needs that could address scientific roadblocks toward observing ultrafast chemical and physical phenomena at ultra-small size scales in different sample environments.	The Request provides funding for three BES Nanoscale Science Research Centers (CNM, CNMS, and TMF). These centers will reduce the number of scientific thrusts and core capabilities, and eliminate user support in selected areas. Maintenance and procurement activities will be deferred. No funding is requested for operations at CINT and CFN.	The funding decrease will support below optimal operations for three NSRCs. No funding is requested for operations at CINT and CFN.

FY 2016 Enacted	FY 2018 Request	Explanation of Changes FY 2018 vs FY 2016
Other Project Costs $0	**$7,900,000**	**+$7,900,000**
No funds are requested for Other Project Costs.	Funds are requested for Other Project Costs for the LCLS-II project at SLAC National Accelerator Laboratory per the project plan.	Other Project Costs increases according to the LCLS-II project plan.
Major Items of Equipment $35,500,000	**$0**	**-$35,500,000**
The Advanced Photon Source-Upgrade (APS-U) project continued with planning and facility design, magnet prototyping, and R&D related to implementation of the multi-bend achromat lattice during FY 2016.	APS-U is transitioned from a Major Item of Equipment (MIE) to line item construction project. No MIE funds are requested for APS-U.	APS-U is included as a construction project in the FY 2018 Request.
The NSLS-II Experimental Tools (NEXT) project continued with the design, procurements, construction/fabrication, installation, testing and commissioning of equipment during FY 2016.	No funds are requested for NEXT in FY 2018.	FY 2016 was the last year of funding for NEXT per the project plan.
Research $31,853,000	**$19,724,000**	**-$12,129,000**
The research funding for the scientific user facilities continued to support selected, high-priority research activities. This funding supported activities to ensure that the scientific user facilities continue to demonstrate performance excellence, with focused efforts to address next generation facilities research needs. Emphasis is placed on detectors and optics instrumentation to allow full utilization of neutron and photon beams. Funding continued the long term surveillance and maintenance responsibilities at BNL and SLAC is included.	The FY 2018 Request will support limited high-priority research activities for detectors and optics instrumentation. No funding is requested for long term surveillance and maintenance at BNL and SLAC.	The funding decrease will support limited accelerator and detector research activities. No funding is requested for long term surveillance and maintenance.

Basic Energy Sciences
Construction

Description

Reactor-based neutron sources, accelerator-based x-ray light sources, and accelerator-based pulsed neutron sources are essential user facilities that enable critical DOE mission-driven science. These user facilities provide the academic, laboratory, and industrial research communities with the tools to fabricate, characterize, and develop new materials and chemical processes to advance basic and applied research, advancing chemistry, physics, earth science, materials science, environmental science, biology, and biomedical science. Regular investments in construction of new user facilities and upgrades to existing user facilities are essential to maintaining U.S. leadership in these research areas.

The Linac Coherent Light Source-II (LCLS-II) project will provide a second source of electrons at LCLS by constructing a 4 GeV, high repetition rate, superconducting linear accelerator in addition to adding two new variable gap undulators to generate an unprecedented high-repetition-rate free-electron laser. This new x-ray source will solidify the LCLS complex as the world leader in ultrafast x-ray science for decades to come.

Critical Decision-3B (CD-3B), Approve Long Lead Procurements, was approved for the LCLS-II project on May 28, 2015, authorizing long lead and advanced procurements for key components of the cryoplant and the superconducting linac which were on the critical path for the project. The project received approval for CD-2, Approve Performance Baseline, and CD-3, Approve Start of Construction, on March 21, 2016, establishing a Total Project Cost (TPC) of $1,045,000,000 and a CD-4, Project Completion date of June 30, 2022.

The Advanced Photon Source Upgrade (APS-U) project will provide scientists with an x-ray source possessing world-leading transverse coherence and extreme brightness. The magnetic lattice of the APS storage ring will be upgraded to a multi-bend achromat configuration to provide 100-1000 times increased brightness and coherent flux. APS-U will ensure that the APS remains a world leader in hard x-ray science.

Critical Decision-3B, Approve Long-Lead Procurements, was approved for APS-U on October 6, 2016, authorizing long lead and advanced procurements for accelerator components and associated systems. The project has a preliminary Total Project Cost (TPC) range of $700,000,000-$1,000,000,000 and TPC point estimate of $770,000,000. The proposed CD-4, Approve Project Completion, is FY 2026.

All BES construction projects are conceived and planned with the scientific community and, during construction, adhere to the highest standards of safety and are executed on schedule and within cost through best practices in project management. In accordance with DOE Order 413.3B, each project is closely monitored and must perform within 10% of the cost and schedule performance baselines, established at Critical Decision 2, Approve Performance Baseline, which are reproduced in the construction project data sheet.

Activities and Explanation of Changes

FY 2016 Enacted	FY 2018 Request	Explanation of Changes FY 2018 vs FY 2016
Construction $200,300,000	**$202,100,000**	**+$1,800,000**
Linac Coherent Light Source-II (LCLS-II) $200,300,000	**$182,100,000**	**-$18,200,000**
The project continued with facility design, initiated critical long-lead procurements of technical materials and cryogenic systems, continued R&D and prototyping activities, and fabricated technical equipment.	FY 2018 funding will support the completion of the major cryomodule and undulator productions lines and the start of critical installation activities requiring the shutdown of the LCLS facility. Commissioning activities for some technical systems will begin in FY 2018. In addition, the design, long lead and advance procurements, R&D, prototyping, site preparation activities, fabrication, installation and testing activities continue until they have been completed.	Funding for the LCLS-II construction project will decrease in FY 2018 per the project plan.
Advanced Photon Source-Upgrade (APS-U) $0	**$20,000,000**	**+$20,000,000**
APS-U was included as a Major Item of Equipment project in FY 2016.	In FY 2018, APS-U will continue with R&D, engineering design, equipment prototyping, fabrication, and long lead and advance procurements. In November 2016, the APS-U project completed the prioritization of project beamlines needed to conduct cutting edge science with the upgraded source. Two of these best-in-class beamlines require conventional civil construction to extend the beamlines beyond the existing APS Experimental Hall to achieve the desired nano-focused beam spot size. As a result, the FY 2018 Request proposes to convert the APS-U project into a line item construction project.	The project is converted to a line-item construction project in the FY 2018 Request; the increase is offset by a corresponding decrease in research, where the project was funded as an MIE. APS-U funding continues at the FY 2016 level, consistent with the approved project plan.

Basic Energy Sciences
Performance Measures

In accordance with the GPRA Modernization Act of 2010, the Department sets targets for, and tracks progress toward, achieving performance goals for each program.

	FY 2016	FY 2017	FY 2018
Performance Goal (Measure)	**BES Construction/MIE Cost & Schedule - Cost-weighted mean percentage variance from established cost and schedule baselines for major construction, upgrade, or equipment procurement projects**		
Target	< 10 %	< 10 %	< 10 %
Result	Met	TBD	TBD
Endpoint Target	Adhering to the cost and schedule baselines for a complex, large scale, science project is critical to meeting the scientific requirements for the project and for being good stewards of the taxpayers' investment in the project.		
Performance Goal (Measure)	**BES Energy Storage - Deliver two high-performance research energy storage prototypes for transportation and the grid that project at the battery pack level to be five times the energy density at 1/5 the cost of the 2011 commercial baseline.**		
Target	Complete self-consistent system analyses using techno-economic modeling of three electrochemical couples, identified through materials discovery including output from the electrolyte genome, that have the potential to meet technical performance and cost criteria.	Develop and demonstrate energy storage research prototypes that are scalable for transportation and grid applications using concepts beyond lithium ion (multivalent ions, chemical transformation, and non-aqueous redox flow), as identified through materials discovery and techno-economic modeling.	N/A
Result	Met	TBD	N/A
Endpoint Target	Three specific outcomes: 1) A library of the fundamental science of the materials and phenomena of energy storage at atomic and molecular levels; 2) two prototypes, one for transportation and one for the electricity grid, that, when scaled up to manufacturing, have the potential to meet the Joint Center for Energy Storage Research's (JCESR) 5-5-5 goals; 3) A new paradigm for battery R&D that integrates discovery science, battery design, research prototyping and manufacturing collaboration in a single highly interactive organization.		
Performance Goal (Measure)	**BES Facility Operations - Average achieved operation time of BES user facilities as a percentage of total scheduled annual operation time**		
Target	≥ 90 %	≥ 90 %	≥ 90 %
Result	Met	TBD	TBD
Endpoint Target	Many of the research projects that are undertaken at the Office of Science's scientific user facilities take a great deal of time, money, and effort to prepare and regularly have a very short window of opportunity to run. If the facility is not operating as expected the experiment could be ruined or critically setback. In addition, taxpayers have invested millions or even hundreds of millions of dollars in these facilities. The greater the period of reliable operations, the greater the return on the taxpayers' investment.		
Performance Goal (Measure)	**BES Research - Conduct discovery-focused research to increase our understanding of matter, materials and their properties**		

	FY 2016	FY 2017	FY 2018
Target	N/A	N/A	Expand computational materials and chemical discovery through increased data production and additional online computational resources: add elastic and electronic properties data for 5000 compounds and 5,000 reaction energies for catalytic reactions to publicly available databases; add new or expanded functionality to on-line, high performance computer software/codes for prediction of materials properties.
Result	N/A	N/A	TBD
Endpoint Target	Understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels		

Basic Energy Science
Capital Summary ($K)

	Total	Prior Years	FY 2016 Enacted	FY 2017 Annualized CR*[a]	FY 2018 Request	FY 2018 vs FY 2016
Capital Operating Expenses Summary						
Capital Equipment	n/a	n/a	86,475	-	21,500	-64,975
General Plant Projects (GPP)	n/a	n/a	11,000	-	1,000	-10,000
Accelerator Improvement Projects (AIP)	n/a	n/a	8,540	-	3,500	-5,040
Total, Capital Operating Expenses	**n/a**	**n/a**	**106,015**	**-**	**26,000**	**-80,015**
Capital Equipment						
Major Items of Equipment						
Advanced Photon Source Upgrade (APS-U), ANL (TPC TBD)	—	80,000	20,000	-	0	-20,000
Linac Coherent Light Source-II (LCLS-II), SLAC[b,c]	—	85,600	0	-	0	0
NSLS-II Experimental Tools (NEXT), BNL (TPC $90,000)	90,000	52,000	15,500	-	0	-15,500
Total, Major Items of Equipment	n/a	n/a	35,500	-	0	-35,500
Total, Non-MIE Capital Equipment	n/a	n/a	50,975	-	21,500	-29,475
Total, Capital equipment	**n/a**	**n/a**	**86,475**	**-**	**21,500**	**-64,975**
General Plant Projects (GPP)						
Other general plant projects under $5 million TEC	n/a	n/a	11,000	-	1,000	-10,000
Accelerator Improvement Projects (AIP)						
Accelerator improvement projects under $5 million TEC	n/a	n/a	8,540	-	3,500	-5,040

[a] FY 2017 Annualized CR amounts reflect the P.L. 114-254 continuing resolution level annualized to a full year. These amounts are shown only at the congressional control level and above, below that level, a dash (-) is shown.

[b] LCLS-II is requested as a line item construction project beginning in FY 2014.

[c] LCLS-II received $85,600,000 in FY 2010–FY 2013 as an MIE.

Construction Projects Summary ($K)

	Total	Prior Years	FY 2016 Enacted	FY 2017 Enacted	FY 2018 Request	FY 2018 vs FY 2016
13-SC-10, Linac Coherent Light Source-II (LCLS-II), SLAC						
TEC	993,100	142,700	200,300	190,000	182,100	-18,200
OPC	51,900	28,600	0	-	7,900	+7,900
TPC	**1,045,000**	**171,300**[a]	**200,300**	**190,000**	**190,000**	**-10,300**
18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL						
TEC	—	0	0	0	20,000	+20,000
OPC	—	0	0	0	0	0
TPC	**770,000**	**0**	**0**	**0**	**20,000**	**+20,000**
Total, Construction						
TEC	n/a	n/a	200,300	190,000	202,100	+1,800
OPC	n/a	n/a	0	0	7,900	+7,900
TPC	**n/a**	**n/a**	**200,300**	**190,000**	**210,000**	**+9,700**

Funding Summary ($K)

	FY 2016 Enacted	FY 2017 Annualized CR[b]	FY 2018 Request	FY 2018 vs FY 2016
Research	689,288	-	570,126	-119,162
Scientific User Facilities Operations	868,324	-	732,861	-135,463
Major Items of Equipment	35,500	-	0	-35,500
Construction Projects (includes OPC)	200,300	-	202,100	+1,800
Other[c]	55,588	-	49,413	-6,175
Total, Basic Energy Sciences	**1,849,000**	**1,845,485**	**1,554,500**	**-294,500**

[a] LCLS-II received $85,600,000 in FY 2010-FY 2013 as an MIE.

[b] FY 2017 Annualized CR amounts reflect the P.L. 114-254 continuing resolution level annualized to a full year. These amounts are shown only at the congressional control level and above, below that level, a dash (-) is shown.

[c] Includes SBIR/STTR funding and non-Facility related GPP.

Scientific User Facility Operations ($K)

The treatment of user facilities is distinguished between two types: TYPE A facilities that offer users resources dependent on a single, large-scale machine; TYPE B facilities that offer users a suite of resources that is not dependent on a single, large-scale machine.

Definitions:
Achieved Operating Hours – The amount of time (in hours) the facility was available for users.
Planned Operating Hours –

- For Past Fiscal Year (PY), the amount of time (in hours) the facility was planned to be available for users.
- For Current Fiscal Year (CY), the amount of time (in hours) the facility is planned to be available for users.
- For the Budget Fiscal Year (BY), based on the proposed budget request the amount of time (in hours) the facility is anticipated to be available for users.

Optimal Hours – The amount of time (in hours) a facility would be available to satisfy the needs of the user community if unconstrained by funding levels.

Percent of Optimal Hours – An indication of utilization effectiveness in the context of available funding; it is not a direct indication of scientific or facility productivity.

- For BY and CY, Planned Operating Hours divided by Optimal Hours expressed as a percentage.
- For PY, Achieved Operating Hours divided by Optimal Hours.

Unscheduled Downtime Hours - The amount of time (in hours) the facility was unavailable to users due to unscheduled events. NOTE: For type "A" facilities, zero Unscheduled Downtime Hours indicates Achieved Operating Hours equals Planned Operating Hours.

	FY 2016 Enacted	FY 2017 Annualized CR*	FY 2018 Request	FY 2018 vs FY 2016
TYPE A FACILITIES				
Advanced Light Source	**$68,240**	-	**$59,010**	**-$9,230**
Number of Users	2,317	-	2,000	-317
Achieved operating hours	5,017	-	N/A	N/A
Planned operating hours	4,550	-	4,500	-50
Optimal hours	5,300	-	5,300	0
Percent optimal hours	94.7%	-	84.9%	N/A
Unscheduled downtime hours	<10%	-	<10%	N/A

* FY 2017 Annualized CR amounts reflect the P.L. 114-254 continuing resolution level annualized to a full year. These amounts are shown only at the congressional control level and above, below that level, a dash (-) is shown.

	FY 2016 Enacted	FY 2017 Annualized CR*	FY 2018 Request	FY 2018 vs FY 2016
Advanced Photon Source	**$130,670**	**-**	**$122,075**	**-$8,595**
Number of Users	5,521	-	4,800	-721
Achieved operating hours	4,934	-	N/A	N/A
Planned operating hours	5,000	-	4,300	-700
Optimal hours	5,000	-	5,000	0
Percent optimal hours	98.7%	-	86.0%	N/A
Unscheduled downtime hours	<10%	-	<10%	N/A
National Synchrotron Light Source-II, BNL	**$110,000**	**-**	**$102,952**	**-$7,048**
Number of Users	477	-	800	+323
Achieved operating hours	3,446	-	N/A	N/A
Planned operating hours	3,740	-	4,300	+560
Optimal hours	3,300	-	5,000[a]	+1,700
Percent optimal hours	104.4%	-	86.0%	N/A
Unscheduled downtime hours	N/A	-	<10%	N/A
Stanford Synchrotron Radiation Lightsource	**$41,088**	**-**	**$20,000**	**-$21,088**
Number of Users	1,641	-	400	-1,241
Achieved operating hours	4,892	-	N/A	N/A
Planned operating hours	5,000	-	1,300	-3,700
Optimal hours	5,400	-	5,400	0
Percent optimal hours	90.6%	-	24.1%	N/A
Unscheduled downtime hours	<10%	-	<10%	N/A

[a] Optimal hours increased as the facility is in a ramp up phase.

	FY 2016 Enacted	FY 2017 Annualized CR*	FY 2018 Request	FY 2018 vs FY 2016
Linac Coherent Light Source	**$132,669**	-	**$124,169**	**-$8,500**
Number of Users	1,062	-	850	-212
Achieved operating hours	5,277	-	N/A	N/A
Planned operating hours	5,500	-	4,300	-1,200
Optimal hours	5,500	-	5,000	-500
Percent optimal hours	95.9%	-	86.0%	N/A
Unscheduled downtime hours	<10%	-	<10%	N/A
High Flux Isotope Reactor	**$63,419**	-	**$56,773**	**-$6,646**
Number of Users	450	-	370	-80
Achieved operating hours	4,076	-	N/A	N/A
Planned operating hours	3,700	-	3,100	-600
Optimal hours	3,700	-	3,700	0
Percent optimal hours	110.2%	-	83.8%	N/A
Unscheduled downtime hours	<10%	-	<10%	N/A
Lujan Neutron Scattering Center	**$3,000**	-	**$0**	**-$3,000**
Achieved operating hours	N/A	-	N/A	N/A
Planned operating hours	0	-	0	0
Optimal hours	0	-	0	0
Percent optimal hours	N/A	-	N/A	N/A
Unscheduled downtime hours	N/A	-	N/A	N/A
Spallation Neutron Source	**$198,663**	-	**$168,847**	**-$29,816**
Number of Users	893	-	650	-243
Achieved operating hours	4,972	-	N/A	N/A
Planned operating hours	4,700	-	3,700	-1,000
Optimal hours	4,700	-	4,500[a]	-200
Percent optimal hours	105.8%	-	82.2%	N/A
Unscheduled downtime hours	<10%	-	<10%	N/A

[a] Optimal hours decreased for scheduled maintenance.

	FY 2016 Enacted	FY 2017 Annualized CR*	FY 2018 Request	FY 2018 vs FY 2016
TYPE B FACILITIES				
Center for Nanoscale Materials	**$24,877**	-	**$22,913**	**-$1,964**
Number of users	566	-	400	-166
Center for Functional Nanomaterials	**$21,344**	-	**$0**	**-$21,344**
Number of users	505	-	0	-505
Molecular Foundry	**$28,017**	-	**$25,823**	**-$2,194**
Number of users	774	-	500	-274
Center for Nanophase Materials Sciences	**$24,232**	-	**$22,399**	**-$1,833**
Number of users	601	-	400	-201
Center for Integrated Nanotechnologies	**$22,105**	-	**$0**	**-$22,105**
Number of users	574	-	0	-574
Total, All Facilities	**$868,324**	-	**$724,961**	**-$143,363**
Number of Users	15,381	-	11,170	-4,211
Achieved operating hours	32,614	-	N/A	N/A
Planned operating hours	32,190	-	25,500	-6,690
Optimal hours	32,900	-	33,900	+1,000
Percent of optimal hours	101.1%	-	82.8%	N/A
Unscheduled downtime hours	<10%	-	<10%	N/A

Scientific Employment

	FY 2016 Enacted	FY 2017 Annualized CR[a]	FY 2018 Estimate	FY 2018 vs FY 2016
Number of permanent Ph.D.'s (FTEs)	4,330	-	3,730	-600
Number of postdoctoral associates (FTEs)	1,120	-	1,020	-100
Number of graduate students (FTEs)	1,660	-	1,580	-80
Other[b]	2,900	-	2,360	-540

[a]FY 2017 Annualized CR amounts reflect the P.L. 114-254 continuing resolution level annualized to a full year. These amounts are shown only at the congressional control level and above, below that level, a dash (-) is shown.

[b]Includes technicians, support staff, and similar positions.

13-SC-10, Linac Coherent Light Source-II
SLAC National Accelerator Laboratory, Menlo Park, California
Project is for Design and Construction

1. Significant Changes and Summary

Significant Changes

This Construction Project Data Sheet (CPDS) is an update of the FY 2017 CPDS and does not include a new start for the budget year.

The FY 2018 Request for the Linac Coherent Light Source-II (LCLS-II) is $182,100,000. In March 2016, the project received approval of CD-2, Approve Performance Baseline and CD-3, Approve Start of Construction. The total project cost (TPC) is $1,045,000,000 and CD-4 is June 2022.

Summary

The most recent DOE 413.3B approved Critical Decisions (CD) are CD-2/3, (Approve Performance Baseline and Approve Start of Construction) that were approved on March 21, 2016.

A Federal Project Director has been assigned to this project and has approved this CPDS.

The LCLS-II project will construct a new high repetition rate electron injector and replace the first kilometer of the existing linac with a 4 GeV superconducting linac to create the electron beam required for x-ray production in the 0.2–5 keV range with a repetition rate near 1 MHz. The new electron beam will be transported to the existing undulator hall and will be capable of feeding either of the two new variable gap undulators. At the completion of the LCLS-II project, the facility will operate two independent electron linacs and two independent x-ray sources, supporting up to six experiment stations. A liquid helium refrigeration plant is required to cool the linac to superconducting temperatures and a building will be constructed to house the refrigeration plant equipment. Modifications to the existing experimental halls, beam transport and switchyard areas, and to the experimental equipment will be made as necessary to maximize the use of the new x-ray source.

FY 2016 funding continued activities for design, long lead and advance procurements (LLP/APs), R&D, prototyping, site preparation activities (which includes the removal of original linac equipment), fabrication, installation, and construction activities after CD-2/CD-3 approval. FY 2017 funding is critical for the procurement of materials and equipment needed to maintain the project schedule and expand the construction efforts. Design, LLP/APs, R&D, prototyping, site preparation activities, fabrication, and installation also continue in FY 2017. FY 2018 funding will support the completion of the major cryomodule and undulator production lines and the start of critical installation activities requiring the shutdown of the LCLS facility. Commissioning activities for some technical systems will begin in FY 2018. In addition, the design, LLP/APs, R&D, prototyping, site preparation activities, fabrication, installation, and testing activities from FY 2017 will carry forward into FY 2018 and beyond until they have been completed.

2. Critical Milestone History

(fiscal quarter or date)

	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2013	4/22/2010		10/14/2011	1Q FY 2013	4Q FY 2016	3Q FY 2013	N/A	4Q FY 2019
FY 2014	4/22/2010		10/14/2011	4Q FY 2013	4Q FY 2016	4Q FY 2013	N/A	4Q FY 2019
FY 2015	4/22/2010		10/14/2011	4Q FY 2015	4Q FY 2017	4Q FY 2016	N/A	4Q FY 2021
FY 2016	4/22/2010	1/21/2014	8/22/2014	2Q FY 2016	4Q FY 2017	2Q FY 2016	N/A	4Q FY 2021
FY 2017	4/22/2010	1/21/2014	8/22/2014	2Q FY 2016	4Q FY 2017	2Q FY 2016	N/A	3Q FY 2022
FY 2018	4/22/2010	1/21/2014	8/22/2014	3/21/2016	4Q FY 2017	3/21/2016	N/A	6/30/2022

CD-0 – Approve Mission Need for a construction project with a conceptual scope and cost range
Conceptual Design Complete – Actual date the conceptual design was completed (if applicable)
CD-1 – Approve Alternative Selection and Cost Range
CD-2 – Approve Performance Baseline
Final Design Complete – Estimated/Actual date the project design will be/was complete (d)
CD-3 – Approve Start of Construction
D&D Complete – Completion of D&D work
CD-4 – Approve Start of Operations or Project Closeout

	Performance Baseline Validation	CD-3A[a]	CD-3B
FY 2013	1Q FY 2013	3/14/2012	
FY 2014	4Q FY 2013	3/14/2012	
FY 2015	4Q FY 2015	3/14/2012	
FY 2016	2Q FY 2016	3/14/2012	3Q FY 2015
FY 2017	2Q FY 2016	3/14/2012	5/28/2015
FY 2018	3/21/2016	3/14/2012	5/28/2015

CD-3A – Approve Long-Lead Procurements, Original Scope
CD-3B – Approve Long-Lead Procurements, Revised Scope

3. Project Cost History

(dollars in thousands)

	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, D&D	OPC, Total	TPC
FY 2013	18,000	367,000	385,000	20,000	N/A	20,000	405,000
FY 2014	18,000	367,000	385,000	20,000	N/A	20,000	405,000
FY 2015	47,000	799,400	846,400	48,600	N/A	48,600	895,000
FY 2016	47,000	869,400	916,400	48,600	N/A	48,600	965,000
FY 2017	47,000	946,100	993,100	51,900	N/A	51,900	1,045,000
FY 2018[b]	47,000	946,100	993,100	51,900	N/A	51,900	1,045,000

4. Project Scope and Justification

Scope

The SLAC National Accelerator Laboratory's (SLAC) advances in the creation, compression, transport, and monitoring of bright electron beams have spawned a new generation of x-ray radiation sources based on linear accelerators rather than on storage rings. The Linac Coherent Light Source (LCLS) produces a high-brightness x-ray beam with properties vastly exceeding those of current x-ray sources in three key areas: peak brightness, coherence, and ultrashort pulses. The peak brightness of the LCLS is 10 billion times greater than current synchrotrons, providing up to 10^{12} x-ray photons in a pulse with duration in the range of 3–500 femtoseconds. These characteristics of the LCLS have opened new realms of research in the chemical, material, and biological sciences. LCLS-II will build on the success of LCLS by expanding the spectral range of hard x-rays produced at the facility by adding a new high repetition rate, spectrally tunable x-ray source. The repetition rate for x-ray production in the 0.2–5 keV range will be increased by at least a factor of 1,000 to yield unprecedented high average brightness x-rays that will be unique worldwide.

[a] CD-3A was approved as part of the original project scope prior to the July 2013 BESAC recommendation. All original project scope long lead procurement work was suspended.
[b] Includes MIE funding of $7,000,000 for the design phase and $60,000,000 for the construction phase, which results in $67,000,000 of TEC funding, as well as $18,600,000 of OPC funding, for a total of $85,600,000 of MIE funding in the TPC.

LCLS is based on the existing SLAC linear accelerator (linac), which is not a superconducting linac. The linac was originally designed to accelerate electrons and positrons to 50 GeV for colliding beam experiments and for nuclear and high energy physics experiments on fixed targets. It was later adapted for use as a free electron laser (FEL, the LCLS facility) and for advanced accelerator research. At present, the last third of the 3 kilometer linac is being used to operate the LCLS facility, and the first 2 kilometers are used for advanced accelerator research.

The revised scope of the LCLS-II project is based on the July 2013 Basic Energy Sciences Advisory Committee (BESAC) report and will construct a new high repetition rate electron injector and replace the first kilometer of the linac with a 4 GeV superconducting linac to create the electron beam required for x-ray production in the 0.2–5 keV range with a repetition rate near 1 MHz. The new electron beam will be transported to the existing undulator hall and will be capable of feeding either of the two new variable gap undulators. The revised project will require cryogenic cooling to operate the linac at superconducting temperatures. The increased cryogenic capacity will require increasing the cryogenic equipment building size to approximately 20,000 square foot.

The third kilometer of the linac will continue to produce 14 GeV electron bunches for hard x-ray production at a 120 Hz repetition rate. The electron bunches will be sent to both of the new undulators to produce two simultaneous x-ray beams. The x-ray beams will span a tunable photon energy range of 1 to 25 keV, beyond the range of the existing LCLS facility, and they will incorporate "self-seeding sections" to greatly enhance the longitudinal coherence of the x-ray beams. The middle kilometer of the existing linac will not be used as part of LCLS-II but will continue to be used for advanced accelerator research. It would be available for future expansion of the LCLS-II capabilities.

At the completion of the LCLS-II project, the facility will operate two independent electron linacs and two independent x-ray sources, supporting up to six experiment stations. Both the capability and capacity of the facility will be significantly enhanced. The combined characteristics (spectral content, peak power, average brightness, pulse duration, and coherence) of the new x-ray sources will surpass the present capabilities of the LCLS beam in spectral tuning range and brightness. The high repetition rate will accommodate more experiments. Furthermore, the two new undulators will be independently controlled to enable more experiments to be conducted simultaneously.

Experience with LCLS has, for the first time, provided data on performance of the x-ray instrumentation and optics required for scientific experiments with the LCLS. The LCLS-II project will take advantage of this knowledge base to design LCLS-II x-ray transport, optics, and diagnostics matched to the characteristics of these sources. The LCLS-II project scope is able to leverage the existing suite of LCLS instrumentation for characterization of the x-ray sources with moderate upgrades primarily to address the higher repetition rate operation.

The existing LCLS Beam Transport and Undulator Hall will be modified as necessary to house the new undulators, electron beam dumps, and x-ray optics. The existing experimental stations will be updated as necessary for the exploitation of the new x-ray sources. In contrast to the initial version of the project, construction of a new undulator tunnel and a new instrument suite will not be required.

The LCLS-II project developed strategic partnerships with other SC laboratories for the design, fabrication, installation, and commissioning of the new superconducting linear accelerator, the high repetition rate electron injector and the new variable gap undulators.

Prior to implementing the revised LCLS-II project, the original LCLS-II scope included construction of the Sector 10 Annex with a total cost of $8.2M. The construction costs are included in the preliminary Total Project Cost of $1,045M.

Justification

The LCLS-II project's purpose is to expand the x-ray spectral operating range and the user capacity of the existing LCLS facility. The expanded spectral range will enable researchers to tackle new research frontiers. The capacity increase is critically needed as the demand for LCLS capabilities far exceeds the available time allocation to users. In FY 2015, only about 20% of the experiment proposals received beam time. The addition of a second x-ray source will allow two or more experiments to be run simultaneously. The revised LCLS-II presented here is informed by the 2013 BESAC recommendations to provide "high repetition rate, ultra-bright, transform limited, femtosecond x-ray pulses over a broad photon energy (about 0.2–5 keV) with full spatial and temporal coherence" and the "linac should feed multiple independently tunable undulators each of which could have multiple endstations." Collectively, the project will enable groundbreaking research in a wide range of scientific disciplines in chemical, material and biological sciences.

Based on the factors described above, the most effective and timely approach for DOE to meet the Mission Need and realize the full potential of the LCLS is upgrading the existing x-ray free electron laser at SLAC with a new superconducting accelerator and x-ray sources.

The project is being conducted in accordance with the project management requirements in DOE O 413.3B, Program and Project Management for the Acquisition of Capital Assets.

Key Performance Parameters (KPPs)

The Threshold KPPs, represent the minimum acceptable performance that the project must achieve. Achievement of the Threshold KPPs will be a prerequisite for approval of CD-4, Project Completion. The Objective KPPs represent the desired project performance. If project performance is sustained and funds are available, the project will strive to attain the Objective KPPs.

Preliminary LCLS-II Key Performance Parameters

Performance Measure	Threshold	Objective
Variable gap undulators	2 (soft and hard x-ray)	2 (soft and hard x-ray)
Superconducting linac-based FEL system		
Superconducting linac electron beam energy	3.5 GeV	≥ 4 GeV
Superconducting linac repetition rate	93 kHz	929 kHz
Superconducting linac charge per bunch	0.02 nC	0.1 nC
Photon beam energy range	250–3,800 eV	200–5,000 eV
High repetition rate capable end stations	≥ 1	≥ 2
FEL photon quantity (10^{-3} BW[a])	5×10^8 (10x spontaneous @ 2,500 eV)	> 10^{11} @ 3,800 eV
Normal conducting linac-based system		
Normal conducting linac electron beam energy	13.6 GeV	15 GeV
Normal conducting linac repetition rate	120 Hz	120 Hz
Normal conducting linac charge per bunch	0.1 nC	0.25 nC
Photon beam energy range	1,000–15,000 eV	1,000–25,000 eV
Low repetition rate capable end stations	≥ 2	≥ 3
FEL photon quantity (10^{-3} BW[a])	10^{10} (lasing @ 15,000 eV)	> 10^{12} @ 15,000 eV

[a] Fractional bandwidth. The specified KPPs are the number of photons with an energy within 0.1% of the specified central value.

5. **Preliminary Financial Schedule**

	(dollars in thousands)		
	Appropriations	Obligations	Costs[a]
Total Estimated Cost (TEC)			
Design phase			
MIE funding			
FY 2012	2,000	2,000	2,000
FY 2013[b]	5,000	5,000	5,000
Total, MIE funding	7,000	7,000	7,000
Line item construction funding			
FY 2014	4,000	4,000	2,040
FY 2015	21,000	21,000	9,089
FY 2016	15,000	15,000	20,500
FY 2017	0	0	8,371
Total, Line item construction funding	40,000	40,000	40,000
Total, Design phase	47,000	47,000	47,000
Construction phase			
MIE funding			
FY 2012	42,500[c]	20,000	13,862
FY 2013[c]	17,500	40,000	33,423
FY 2014	0	0	12,256
FY 2015	0	0	455
FY 2016	0	0	0
FY 2017	0	0	4
Total, MIE funding	60,000	60,000	60,000
Line item construction funding			
FY 2014	71,700	71,700	16,673
FY 2015	117,700	117,700	65,442
FY 2016	185,300	185,300	125,476
FY 2017	190,000	190,000	312,079
FY 2018	182,100	182,100	221,374
FY 2019	139,300	139,300	139,600
FY 2020	0	0	5,456
Total, Line item construction funding	886,100	886,100	886,100
Total, Construction phase	946,100	946,100	946,100

[a] Costs through FY 2016 reflect actual costs; costs for FY 2017 and the outyears are estimates. The split between design costs and construction costs were updated for FY 2014 and FY 2015.

[b] FY 2013 funding was requested as a line item, but due to a Continuing Resolution, FY 2013 funds were executed as an MIE.

[c] FY 2012 funding shown includes $22,500,000 of prior year balances from FY 2012 that was reallocated to the LCLS-II project during FY 2013.

[b] Costs through FY 2016 reflect actual costs; costs for FY 2017 and the outyears are estimates. The split between design costs and construction costs were updated for FY 2014 and FY 2015.

[c] FY 2013 funding was requested as a line item, but due to a Continuing Resolution, FY 2013 funds were executed as an MIE.

[d] Amounts shown include MIE funding of $67,000,000 in the TEC, $18,600,000 in the OPC, and $85,600,000 in the TPC.

	(dollars in thousands)		
	Appropriations	Obligations	Costs[a]
TEC			
MIE funding			
FY 2012	44,500[a]	22,000	15,862
FY 2013 [c]	22,500	45,000	38,423
FY 2014	0	0	12,256
FY 2015	0	0	455
FY 2016	0	0	0
FY 2017	0	0	4
Total, MIE funding	67,000	67,000	67,000
Line item construction funding			
FY 2014	75,700	75,700	18,713
FY 2015	138,700	138,700	74,531
FY 2016	200,300	200,300	145,976
FY 2017	190,000	190,000	320,450
FY 2018	182,100	182,100	221,374
FY 2019	139,300	139,300	139,600
FY 2020	0	0	5,456
Total, Line item construction funding	926,100	926,100	926,100
Total, TEC[d]	993,100	993,100	993,100
Other Project Cost (OPC)			
OPC except D&D			
MIE funding			
FY 2010	1,126	1,126	938
FY 2011	9,474	9,474	8,033
FY 2012	8,000	8,000	8,893
FY 2013[a]	0	0	116
FY 2014	0	0	439
FY 2015	0	0	10
FY 2016	0	0	0
FY 2017	0	0	171
Total, MIE funding	18,600	18,600	18,600
Line item construction funding			
FY 2014	10,000	10,000	8,142
FY 2015	9,300	9,300	2,650
FY 2016	0	0	34
FY 2017	0	0	2,000
FY 2018	7,900	7,900	10,000
FY 2019	6,100	6,100	9,966
FY 2020	0	0	508
Total, Line item construction funding	33,300	33,300	33,300
Total, OPC	51,900	51,900	51,900

[a] FY 2013 funding was requested as a line item, but due to a Continuing Resolution, FY 2013 funds were executed as an MIE.

	(dollars in thousands)		
	Appropriations	Obligations	Costs[a]
Total Project Cost (TPC)			
MIE funding			
FY 2010	1,126	1,126	938
FY 2011	9,474	9,474	8,033
FY 2012	52,500[c]	30,000	24,755
FY 2013[a]	22,500	45,000	38,539
FY 2014	0	0	12,695
FY 2015	0	0	465
FY 2016	0	0	0
FY 2017	0	0	175
Total, MIE funding	85,600	85,600	85,600
Line item construction funding			
FY 2014	85,700	85,700	26,855
FY 2015	148,000	148,000	77,181
FY 2016	200,300	200,300	146,010
FY 2017	190,000	190,000	322,450
FY 2018	190,000	190,000	231,374
FY 2019	145,400	145,400	149,566
FY 2020	0	0	5,964
Total, Line item construction funding	959,400	959,400	959,400
Total, TPC[d]	1,045,000	1,045,000	1,045,000

6. Details of Project Cost Estimate

	(dollars in thousands)		
	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design			
Design	42,400	40,750	42,125
Contingency	4,600	6,250	4,875
Total, Design	47,000	47,000	47,000
Construction			
Site Preparation	24,700	24,700	24,700
Equipment	692,742	672,900	678,205
Other Construction	58,500	58,500	58,500
Contingency	170,158	190,000	184,695
Total, Construction	946,100	946,100	946,100
Total, TEC[b]	993,100	993,100	993,100
Contingency, TEC	174,758	196,250	189,570

Other Project Cost (OPC)
OPC except D&D

---

[b] Costs through FY 2016 reflect actual costs; costs for FY 2017 and the outyears are estimates. The split between design costs and construction costs were updated for FY 2014 and FY 2015.
[c] FY 2012 funding shown includes $22,500,000 of prior year balances from FY 2012 that was reallocated to the LCLS-II project during FY 2013.
[d] Costs through FY 2016 reflect actual costs; costs for FY 2017 and the outyears are estimates.
[b] Amounts shown include MIE funding of $67,000,000 in the TEC, $18,600,000 in the OPC, and $85,600,000 in the TPC.

	(dollars in thousands)		
	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Conceptual Planning	1,980	1,980	1,980
Conceptual Design	23,408	23,408	23,408
Research and Development	1,972	1,972	1,972
Start-Up	15,790	15,790	15,790
Contingency	8,750	8,750	8,750
Total, OPC	51,900	51,900	51,900
Contingency, OPC	8,750	8,750	8,750
Total, TPC[b]	1,045,000	1,045,000	1,045,000
Total, Contingency	183,508	205,000	198,320

7. Schedule of Appropriations Requests

(dollars in thousands)

Request		Prior Years	FY 2015	FY 2016	FY 2017	FY 2018	FY 2019	FY 2020	Outyears	Total
FY 2012 (MIE)	TEC	22,000	TBD	TBD	TBD	TBD	TBD	TBD	TBD	TBD
	OPC	18,600	TBD	TBD	TBD	TBD	TBD	TBD	TBD	TBD
	TPC	40,600	TBD	TBD	TBD	TBD	TBD	TBD	TBD	TBD
FY 2013[a] (MIE)	TEC	165,800	94,000	105,300	19,900	0	0	0	0	385,000
	OPC	19,300	0	700	0	0	0	0	0	20,000
	TPC	185,100	94,000	106,000	19,900	0	0	0	0	405,000
FY 2014	TEC	162,000	122,500	100,500	0	0	0	0	0	385,000
	OPC	19,300	0	700	0	0	0	0	0	20,000
	TPC	181,300	122,500	101,200	0	0	0	0	0	405,000
FY 2015	TEC	142,700	138,700	204,000	185,100	156,000	19,900	0	0	846,400
	OPC	28,600	9,300	0	0	5,900	4,800	0	0	48,600
	TPC	171,300	148,000	204,000	185,100	161,900	24,700	0	0	895,000
FY 2016	TEC	142,700	138,700	200,300	189,100	176,000	69,600	0	0	916,400
	OPC	28,600	9,300	0	0	5,900	4,800	0	0	48,600
	TPC	171,300	148,000	200,300	189,100	181,900	74,400	0	0	965,000
FY 2017	TEC	142,700	138,700	200,300	190,000	192,100	129,300	0	0	993,100
	OPC	28,600	9,300	0	0	7,900	6,100	0	0	51,900
	TPC	171,300	148,000	200,300	190,000	200,000	135,400	0	0	1,045,000
FY 2018	TEC	142,700	138,700	200,300	190,000	182,100	139,300	0	0	993,100
	OPC	28,600	9,300	0	0	7,900	6,100	0	0	51,900
	TPC	171,300	148,000	200,300	190,000	190,000	145,400	0	0	1,045,000

8. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy (fiscal quarter or date)	4Q FY 2021
Expected Useful Life (number of years)	25
Expected Future Start of D&D of this capital asset (fiscal quarter)	4Q FY 2046

(Related Funding Requirements)

[a] FY 2013 funding was requested as a line item, but due to a Continuing Resolution, FY 2013 funds were executed as an MIE.

	Annual Costs		Life Cycle Costs	
	Current Total Estimate	Previous Total Estimate	Current Total Estimate	Previous Total Estimate
Operations and Maintenance	$38.6M	$38.6M	$1,317.0M	$1,317.0M

The numbers presented are the incremental lifecycle operations and maintenance costs above the existing LCLS. The estimate will be updated as the project is executed.

9. D&D Information

The new area being constructed in this project is not replacing existing facilities.

	Square Feet
New area being constructed by this project at SLAC	~20,000
Area of D&D in this project at SLAC	0
Area at SLAC to be transferred, sold, and/or D&D outside the project including area previously "banked"	~20,000
Area of D&D in this project at other sites..	0
Area at other sites to be transferred, sold, and/or D&D outside the project including area previously "banked"	0
Total area eliminated	~20,000

Prior to implementing the revised LCLS-II project, the original LCLS-II scope included construction of the Sector 10 Annex. This facility is 2,275 ft^2 and was offset by demolition of a 1,630 ft^2 building with the balance offset using banked space. The information above reflects only the new construction associated with the revised project.

10. Acquisition Approach

DOE has determined that the LCLS-II project will be acquired by the SLAC National Accelerator Laboratory under the existing DOE management and operations (M&O) contract.

A Conceptual Design Report for the LCLS-II project has been completed and will be revised based on the new technical parameters. Key design activities, requirements, and high-risk subsystem components will be identified to reduce cost and schedule risk to the project and expedite the startup. The necessary project management systems are fully up-to-date, operating, and are maintained as a SLAC-wide resource.

SLAC is partnering with other SC laboratories for design and procurement of key technical subsystem components. Technical system designs will require research and development activities. Preliminary cost estimates for these systems are based on actual costs from LCLS and other similar facilities, to the extent practicable. Recent cost data has been exploited fully in planning and budgeting for the project. Design of the technical systems will be completed by SLAC or partner laboratory staff. Technical equipment will either be fabricated in-house or subcontracted to vendors with the necessary capabilities.

All subcontracts will be competitively bid and awarded based on best value to the government. Project performance metrics for SLAC are included in the M&O contractor's annual performance evaluation and measurement plan.

Lessons learned from the LCLS Project and other similar facilities will be exploited fully in planning and executing LCLS-II.

18-SC-10, Advanced Photon Source-Upgrade
Argonne National Laboratory, Argonne, Illinois
Project Data Sheet is for PED/Construction

1. Significant Changes and Summary

Significant Changes

This is the first project data sheet submitted for the Advanced Photon Source-Upgrade (APS-U) as a line item construction project. APS-U was first proposed as a Major Item of Equipment (MIE) project in the FY 2012 President's Budget Request. In November 2016, the APS-U project completed the prioritization of project beamlines needed to conduct cutting edge science with the upgraded source. Two of these best-in-class beamlines require conventional civil construction to extend the beamlines beyond the existing APS Experimental Hall to achieve the desired nano-focused beam spot size. As a result, the FY 2018 Request proposes to convert the APS-U MIE project into a line item construction project.

Summary

The most recent DOE O 413.3B approved Critical Decision, CD-3B (Approve Long-Lead Procurements), was approved on October 6, 2016. The project has a preliminary Total Project Cost (TPC) range of $700,000,000-$1,000,000,000 and TPC point estimate of $770,000,000. The proposed CD-4, Approve Project Completion, is FY 2026.

A Federal Project Director has been assigned to this project and is certified to level IV.

The APS-U project will deliver a next-generation high-energy x-ray storage ring optimized for providing hard x-rays (>20 keV) to experiments. The APS-U project includes advanced beamlines, optics and detectors, and will result in narrow nano-focused x-ray beams ideal for imaging. This project includes the design and construction of the APS-U accelerator incorporating a multi-bend achromat (MBA) magnet lattice, insertion devices, front ends, beamlines/experimental stations, and any required modifications to the linac, booster, and radio frequency (RF) systems. APS-U will exceed the current APS performance by 2 to 3 orders of magnitude in brightness and coherent flux. The upgrade will provide brighter and more intense beams at all beamline locations and improved performance capabilities.

In FY 2016, APS-U continued activities associated with research and development (R&D), engineering design, equipment prototyping, and equipment fabrication in preparation for long lead procurements. In FY 2017, APS-U continues with R&D, engineering design, pre-production prototyping, fabrication, and long lead and advance procurements (LLP/APs) of critical systems. In FY 2018, APS-U continues with R&D, engineering design, equipment prototyping, fabrication, and LLP/APs.

2. Critical Milestone History

(fiscal quarter or date)

	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2018[a]	4/22/2010	9/18/2015	2/04/2016	1Q FY 2019	2Q FY 2020	4Q FY 2019	N/A	1Q FY 2026

CD-0 – Approve Mission Need for a construction project with a conceptual scope and cost range
Conceptual Design Complete – Actual date the conceptual design was completed (if applicable)
CD-1 – Approve Design Scope and Project Cost and Schedule Ranges
CD-2 – Approve Project Performance Baseline
Final Design Complete – Estimated/Actual date the project design will be/was complete(d)
CD-3 – Approve Start of Construction

[a] This project is pre-CD-2; the estimated cost and schedule are preliminary. Construction will not be executed without appropriate CD approvals.

D&D Complete – Completion of D&D work
CD-4 – Approve Project Completion

	Performance Baseline Validation	CD-3A	CD-3B
FY 2018	1Q FY 2019	8/30/2012	10/6/2016

CD-3A – Approve Long-Lead Procurements for the Resonant Inelastic X-ray Scattering (RIXS) beamline.
CD-3B – Approve Long-Lead Procurements for accelerator components and associated systems.

3. Project Cost History

(dollars in thousands)

	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, D&D	OPC, Total	TPC
FY 2018[a]	141,015	577,985	719,000	51,000	N/A	51,000	770,000

4. Project Scope and Justification

<u>Scope</u>
There is a growing need to study materials under real conditions in real time through the use of groundbreaking scientific techniques. These techniques must provide the capability to observe, understand, and ultimately control the functions of materials down to the nanoscale and beyond with atomic resolution. To sustain U.S. leadership in this technology frontier, DOE's Office of Basic Energy Sciences (BES) will upgrade an existing hard x-ray synchrotron radiation facility to provide world-leading coherence and brightness at levels that are orders of magnitude higher than currently available. High-energy penetrating x-rays are critical for probing materials under real working environments, such as in a battery or fuel cell under load conditions.

By building on the existing APS facility at Argonne National Laboratory (ANL), for significantly less than the replacement cost of APS, the APS-U will provide a world-leading hard x-ray synchrotron radiation facility, which will be a unique asset in the U.S. portfolio of scientific user facilities. The APS-U is a critical and cost effective next step in the photon science strategy that will keep the U.S. at the forefront of scientific research, combining with other facilities to give the U.S. a complementary set of storage ring and free-electron laser x-ray light sources.

The APS-U project will upgrade the existing APS to provide scientists with an x-ray source possessing world-leading transverse coherence and extreme brightness. The APS-U project supports activities to develop, design, build, install, and test the equipment necessary to upgrade the APS, an existing third-generation synchrotron light source facility.

The APS-U project includes a new storage ring incorporating a multi-bend achromat (MBA) lattice utilizing the existing tunnel, new insertion devices optimized for brightness and flux, superconducting undulators for selected beamlines, new or upgraded front-ends, and any required modifications to the linac, booster, and radio frequency (RF) systems. The MBA lattice will provide 100-1000 times increased brightness and coherent flux. The project will construct new beamlines and incorporate substantial refurbishment of existing beamlines, along with new optics and detectors that will enable the beamlines to take advantage of the improved accelerator performance. Two best-in-class beamlines require conventional civil construction to extend the beamlines beyond the existing APS Experimental Hall to achieve the desired nano-focused beam spot size.

---

[a] This project is pre-CD-2; the estimated cost and schedule are preliminary. Construction will not be executed without appropriate CD approvals.

With the ever increasing demand for higher penetration power for probing real world materials and applications, the high energy hard x-rays (20 keV and above) produced at APS provide unique capabilities in the suite of U.S. x-ray light sources that are a pre-requisite for tackling the grand science and energy challenges of the 21st Century. The APS-U will ensure that the APS remains a world leader in hard x-ray science.

Justification

BES's mission is to "support fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security." APS-U is in direct support of the DOE Strategic Plan, 2014-2018, Strategic Objective 3 which includes a strategy to "provide the nation's researchers with world-class scientific user facilities that enable mission-focused research and advance scientific discovery."

Worldwide investments in accelerator-based x-ray light source user facilities threaten U.S. leadership in light source technology within the next 6-10 years. The European Synchrotron Radiation Facility (ESRF) in France, PETRA-III in Germany, and SPring-8 in Japan are well into campaigns of major upgrades of beamlines and are also incorporating technological advancements in accelerator science to enhance performance. In 2015, China announced its intention to construct a next generation 6 GeV hard x-ray synchrotron light source.

The APS-U will upgrade the APS by replacing the existing 20 year old storage ring with a multi-bend achromat (MBA)-based machine, and will provide a beam with a natural emittance that is orders of magnitude lower than what is currently available with third-generation light sources. With this investment and the current APS infrastructure, the APS-U will position the APS as the leading storage ring-based hard x-ray source in the U.S. for decades to come.

The high-energy penetrating x-rays will provide a unique scientific capability directly relevant to problems in energy, the environment, new and improved materials, and biological studies. The upgraded APS will complement the capabilities of x-ray free electron lasers (e.g., the Linac Coherent Light Source and Linac Coherent Light Source-II), which occupy different spectral, flux, and temporal range of technical specifications.

The project is being conducted in accordance with the project management requirements in DOE O 413.3B, Program and Project Management for the Acquisition of Capital Assets.

Key Performance Parameters (KPPs)

The threshold KPPs, which will define the official performance baseline at CD-2, Approve Project Performance Baseline, represent the minimum acceptable performance that the project must achieve. Achievement of the threshold KPPs will be a prerequisite for CD-4, Approve Project Completion. The objective KPPs represent the desired project performance. If project performance is sustained and funds are available, the project will strive to attain the objective KPPs. The KPPs presented here are preliminary, pre-baseline values. The final key parameters will be established as part of CD-2, Approve Project Performance Baseline.

Preliminary APS-U Key Performance Parameters

Performance Measure	Threshold	Objective
Storage Ring Energy	> 5.7 GeV, with systems installed for 6 GeV operation	6 GeV
Beam Current	> 25 mA in top-up with systems installed for 200 mA operation	200 mA in top-up
Horizontal Emittance	< 150 pm-rad	75 pm-rad
Brightness @ 20 keV[1]	> 2×10^{20}	2.5×10^{21}
Brightness @ 65 keV[2]	> 2×10^{19}	6×10^{20}
New MBA Beamlines	5	6

Performance Measure	Threshold	Objective

[1]Units = photons/sec/0.1% BW/mm^2/$mrad^2$; determined from a 2.75 cm period, 2.4 m long permanent magnet undulator

[2]Units = photons/sec/0.1% BW/mm^2/$mrad^2$; determined from a 1.6 cm period, 1.5 m long superconducting undulator

5. Preliminary Financial Schedule

	(dollars in thousands)		
	Appropriations	Obligations	Costs
Total Estimated Cost (TEC)			
Design phase			
MIE funding			
FY 2012	19,200	19,200	8,679
FY 2013	15,000	15,000	17,825
FY 2014	17,015	17,015	13,122
FY 2015	20,000	20,000	19,678
FY 2016	20,000	20,000	22,529
FY 2017	30,000	30,000	27,000
FY 2018	0	0	11,000
FY 2019	0	0	1,382
Total, MIE funding	121,215	121,215	121,215
Line item construction funding			
FY 2018	9,300	9,300	8,500
FY 2019	23,000	23,000	22,500
FY 2020	3,500	3,500	3,000
FY 2021	0	0	1,400
FY 2022	0	0	400
Total, Line item construction funding	35,800	35,800	35,800
Total, Design phase	157,015	157,015	157,015
Construction phase			
MIE funding			
FY 2012	800	800	416
FY 2013	5,000	5,000	3,391
FY 2014	2,985	2,985	4,301
FY 2015	0	0	677
FY 2016	0	0	0
FY 2017	12,500	12,500	11,800
FY 2018	0	0	700
Total, MIE funding	14,785	14,785	14,785
Line item construction funding			
FY 2018	10,700	10,700	9,500
FY 2019	68,691	68,691	65,000
FY 2020	161,500	161,500	153,000
FY 2021	160,000	160,000	151,000
FY 2022	82,500	82,500	80,000
FY 2023	79,809	79,809	74,000
FY 2024	0	0	24,000
FY 2025	0	0	6,700
Total, Line item construction funding	563,200	563,200	563,200
Total, Construction phase	577,985	577,985	577,985

	(dollars in thousands)		
	Appropriations	Obligations	Costs
TEC			
MIE funding			
FY 2012	20,000	20,000	9,095
FY 2013	20,000	20,000	21,216
FY 2014	20,000	20,000	17,423
FY 2015	20,000	20,000	20,355
FY 2016	20,000	20,000	22,529
FY 2017	20,000	20,000	23,300
FY 2018	0	0	4,700
FY 2019	0	0	1,382
Total, MIE funding	120,000	120,000	120,000
Line item construction funding			
FY 2018	20,000	20,000	18,000
FY 2019	91,691	91,691	87,500
FY 2020	165,000	165,000	156,000
FY 2021	160,000	160,000	152,400
FY 2022	82,500	82,500	80,400
FY 2023	79,809	79,809	74,000
FY 2024	0	0	24,000
FY 2025	0	0	6,700
Total, Line item construction funding	599,000	599,000	599,000
Total, TEC	719,000	719,000	719,000
Other Project Cost (OPC)			
OPC except D&D			
MIE funding			
FY 2010	1,000	1,000	587
FY 2011	7,500	7,500	3,696
FY 2012	0	0	4,217
Total MIE funding	8,500	8,500	8,500
Line item construction funding			
FY 2021	5,000	5,000	4,500
FY 2022	27,500	27,500	26,500
FY 2023	10,000	10,000	9,400
FY 2024	0	0	1,700
FY 2025	0	0	400
Total, Line item construction funding	42,500	42,500	42,500
Total, OPC	51,000	51,000	51,000

	(dollars in thousands)		
	Appropriations	Obligations	Costs
Total Project Cost (TPC)			
MIE funding			
FY 2010	1,000	1,000	587
FY 2011	7,500	7,500	3,696
FY 2012	20,000	20,000	13,312
FY 2013	20,000	20,000	21,216
FY 2014	20,000	20,000	17,423
FY 2015	20,000	20,000	20,355
FY 2016	20,000	20,000	22,529
FY 2017	20,000	20,000	23,300
FY 2018	0	0	4,700
FY 2019	0	0	1,382
Total, MIE funding	128,500	128,500	128,500
Line item construction funding			
FY 2018	20,000	20,000	18,000
FY 2019	91,691	91,691	87,500
FY 2020	165,000	165,000	156,000
FY 2021	165,000	165,000	156,900
FY 2022	110,000	110,000	106,900
FY 2023	89,809	89,809	83,400
FY 2024	0	0	25,700
FY 2025	0	0	7,100
Total, Line item construction funding	641,500	641,500	641,500
Total, TPC	770,000	770,000	770,000

6. Details of Project Cost Estimate

	(dollars in thousands)		
	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design			
Design	135,375	N/A	N/A
Contingency	5,640	N/A	N/A
Total, Design	141,015	N/A	N/A
Construction			
Equipment	411,625	N/A	N/A
Other Construction	12,700	N/A	N/A
Contingency	153,660	N/A	N/A
Total, Construction	577,985	N/A	N/A
Total, TEC	719,000	N/A	N/A
Contingency, TEC	159,300	N/A	N/A
Other Project Cost (OPC)			
OPC except D&D			
Conceptual Planning	1,000	N/A	N/A
Conceptual Design	7,500	N/A	N/A
Start-Up	31,800	N/A	N/A
Contingency	10,700	N/A	N/A
Total, OPC	51,000	N/A	N/A

	(dollars in thousands)		
	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Contingency, OPC	10,700	N/A	N/A
Total, TPC	770,000	N/A	N/A
Total, Contingency	170,000	N/A	N/A

7. Schedule of Appropriations Requests

(dollars in thousands)

Request		Prior Years	FY 2016	FY 2017	FY 2018	FY 2019	FY 2020	FY 2021	Outyears	Total
FY 2018[a]	TEC	80,000	20,000	20,000	20,000	91,691	165,000	160,000	162,309	719,000
	OPC	8,500	0	0	0	0	0	5,000	37,500	51,000
	TPC	88,500	20,000	20,000	20,000	91,691	165,000	165,000	199,809	770,000

8. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy (fiscal quarter or date)	1Q FY 2026
Expected Useful Life (number of years)	25
Expected Future Start of D&D of this capital asset (fiscal quarter)	1Q FY 2051

(Related Funding Requirements)

	Annual Costs		Life Cycle Costs	
	Current Total Estimate	Previous Total Estimate	Current Total Estimate	Previous Total Estimate
Operations and Maintenance	$0M	N/A	$0M	N/A

The numbers presented are the incremental lifecycle operations and maintenance costs above the existing APS. The operations and maintenance costs are not anticipated to increase. The estimate will be updated and additional details will be provided after CD-2, Approve Project Performance Baseline.

9. D&D Information

	Square Feet
New area being constructed by this project at ANL	7,000-10,000
Area of D&D in this project at ANL	0
Area at ANL to be transferred, sold, and/or D&D outside the project including area previously "banked"	7,000-10,000
Area of D&D in this project at other sites...	0
Area at other sites to be transferred, sold, and/or D&D outside the project including area previously "banked"	0
Total area eliminated	0

[a] This project has not yet received CD-2 approval; funding and cost estimates are preliminary.

Approximately 7,000-10,000 square feet of new construction is needed for the 2 beamlines extending beyond the current APS experimental facility.

10. Acquisition Approach

The APS-U project will be acquired by ANL under the existing DOE management and operations (M&O) contract between DOE and UChicago Argonne, LLC, which operates ANL. The acquisition of equipment and systems for large research facilities is within the scope of the DOE contract for the management and operations of ANL and consistent with the general expectation of the responsibilities of DOE M&O contractors.

ANL will have prime responsibility for oversight of all contracts required to execute this project, which will include managing the design and construction of the APS-U accelerator incorporating a multi-bend achromat (MBA) magnet lattice, insertion devices, front ends, beamlines/experimental stations, and any required modifications to the linac, booster, and radio frequency (RF) systems. ANL has established an APS-U project organization with project management, procurement management, and ES&H management with staff qualified to specify, select and oversee procurement and installation of the accelerator and beamline components and other technical equipment. These items will be procured from a variety of sources, depending on the item. Procurements will be competitively bid on a 'best value' basis following all applicable ANL procurement requirements. The APS-U project will most likely be accomplished using the design-bid-fabricate method. This proven approach provides the project with direct control over the accelerator components and beamline design, equipment specification and selection, and all contractors.