Basic Energy Sciences

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 2019 Budget Request

The BES FY 2019 Request of $1,850.0 million focuses resources toward the highest priorities in early-stage fundamental research, in operation and maintenance of scientific user facilities, and in facility upgrades. Core research priorities in the FY 2019 Request include quantum information science (QIS), ultrafast science, and computational materials and chemical sciences related to the Exascale Computing Initiative, as well as research in support of future nuclear energy systems. 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 Centers (EFRCs), 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 EFRCs will emphasize emerging high priorities in quantum materials and chemistry, catalysis science, synthesis, instrumentation science, materials and chemical research related to interdependent energy-water issues, future nuclear energy systems, and next-generation electrical energy storage. The Request also supports the two BES-supported Energy Innovation Hubs, and the DOE Established Program to Stimulate Competitive Research (EPSCoR).

In the Scientific User Facilities subprogram, BES maintains a balanced suite of complementary tools. The Linac Coherent Light Source (LCLS) continues operations in support of the BES priority in ultrafast science and also in preparation for completion of the LCLS-II construction project. To allow installation activities for the LCLS-II construction project to proceed, LCLS will be shut down for one year, starting around the second quarter of FY 2019. The Advanced Light Source, Advanced Photon Source, National Synchrotron Light Source-II, and the Stanford Synchrotron Radiation Lightsource will continue operations and are supported at 95% of optimum. Both BES-supported neutron sources, the Spallation Neutron Source and the High Flux Isotope Reactor, will be operational in FY 2019 and funded at approximately 95% of optimum. All five

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

Nanoscale Science Research Centers will be supported, with part of the funding designated for tool development for QIS. The BES commitment for long term surveillance and maintenance ends in FY 2018. No funding is requested for these activities in FY 2019.

In the Construction subprogram, the LCLS-II project remains the highest priority construction project in BES and is fully supported for the last year of funding for the project. The Request provides continued support for the Advanced Photon Source Upgrade (APS-U) project, and funds to initiate the Advanced Light Source Upgrade (ALS-U) project at Lawrence Berkeley National Laboratory and the Linac Coherent Light Source-II High Energy (LCLS-II-HE) project at SLAC National Accelerator Laboratory.

Basic Energy Sciences
Funding ($K)

	FY 2017 Enacted	FY 2018 Annualized CR[a]	FY 2019 Request	FY 2019 Request vs FY 2017 Enacted
Materials Sciences and Engineering				
Scattering and Instrumentation Sciences Research	76,598	—	60,925	-15,673
Condensed Matter and Materials Physics Research	101,645	—	123,790	+22,145
Materials Discovery, Design, and Synthesis Research	61,931	—	62,551	+620
Established Program to Stimulate Competitive Research (EPSCoR)	14,452	—	7,708	-6,744
Energy Frontier Research Centers (EFRCs)	55,800	—	55,800	0
Energy Innovation Hubs—Batteries and Energy Storage	24,088	—	24,088	0
Computational Materials Sciences	12,000	—	13,000	+1,000
SBIR/STTR	13,127	—	13,178	+51
Total, Materials Sciences and Engineering	**359,641**	**—**	**361,040**	**+1,399**
Chemical Sciences, Geosciences, and Biosciences				
Fundamental Interactions Research	62,606	—	69,581	+6,975
Chemical Transformations Research	81,687	—	88,869	+7,182
Photochemistry and Biochemistry Research	89,168	—	74,386	-14,782
Energy Frontier Research Centers (EFRCs)	54,200	—	54,200	0
Energy Innovation Hubs—Fuels from Sunlight	15,000	—	15,000	0
Computational Chemical Sciences (CCS)	13,489	—	13,000	-489
General Plant Projects (GPP)	1,000	—	1,000	0
SBIR/STTR	11,977	—	11,934	-43
Total, Chemical Sciences, Geosciences, and Biosciences	**329,127**	**—**	**327,970**	**-1,157**
Scientific User Facilities				
X-Ray Light Sources	489,059	—	491,059	+2,000
High-Flux Neutron Sources	266,000	—	265,000	-1,000
Nanoscale Science Research Centers (NSRCs)	122,272	—	122,272	0
Other Project Costs	5,000	—	10,100	+5,100
Major Items of Equipment	42,500	—	0	-42,500
Research	34,618	—	25,000	-9,618
SBIR/STTR	33,283	—	33,259	-24
Total, Scientific User Facilities	**992,732**	**—**	**946,690**	**-46,042**
Subtotal, Basic Energy Sciences	**1,681,500**	**1,670,081**	**1,635,700**	**-45,800**

[a] A full-year 2018 appropriation for this account was not enacted at the time the budget was prepared; therefore, the budget assumes this account is operating under the Continuing Appropriations Act, 2018 (Division D of P.L. 115-56, as amended). The amounts included for 2018 reflect the annualized level provided by the continuing resolution. (These amounts are shown only at the Congressional control level and above; below that level, a dash (—) is shown).

	FY 2017 Enacted	FY 2018 Annualized CR[a]	FY 2019 Request	FY 2019 Request vs FY 2017 Enacted
Construction				
13-SC-10, Linac Coherent Light Source-II (LCLS-II), SLAC	190,000	188,710	139,300	-50,700
18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL	0	—	60,000	+60,000
19-SC-10, Advanced Light Source Upgrade (ALS-U), LBNL	0	—	10,000	+10,000
19-SC-11, Linac Coherent Light Source-II-HE (LCLS-II-HE), SLAC	0	—	5,000	+5,000
Total, Construction	**190,000**	**188,710**	**214,300**	**+24,300**
Total, Basic Energy Sciences	**1,871,500**	**1,858,791**	**1,850,000**	**-21,500**

SBIR/STTR Funding:

- FY 2017 Enacted: SBIR $51,189,000; and STTR $7,198,000
- FY 2019 Request: SBIR $51,175,000; and STTR $7,196,000

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Explanation of Major Changes ($K)

	FY 2019 Request vs FY 2017 Enacted
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, with a special emphasis on quantum materials. Research priorities include ultrafast science to understand the initial stages of materials phenomena and dynamics, materials science theory for computational applications that take full advantage of exascale computing, and materials under extreme environments for future nuclear energy. The Request emphasizes research on novel materials and theory for QIS. Funding is requested for continued support of the Batteries and Energy Storage Energy Innovation Hub and the DOE Established Program to Stimulate Competitive Research (EPSCoR).	**+1,399**
Chemical Sciences, Geosciences, and Biosciences: Research will continue to support fundamental science, 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, energy-water issues, catalysis science, and future nuclear energy. Ultrafast science research will continue to be emphasized to probe the dynamics of electrons that control chemical bonding and reactivity; to investigate energy flow underlying energy conversions; and to elucidate structural dynamics accompanying bond breaking and bond making in chemical transformations. Research on QIS remains a priority to understand the quantum nature of atomic and molecular systems important for developing quantum information systems and to exploit recent advances in quantum computing to address scientific challenges that are beyond the capabilities of classical computers. Funding is requested for continued support of the Fuels from Sunlight Energy Innovation Hub.	**-1,157**
Scientific User Facilities: The Linac Coherent Light Source (LCLS) continues operations in support of ultrafast science and also in preparation for completion of the LCLS-II construction project. To allow installation activities for the LCLS-II construction project to proceed, LCLS will be shut down for one year, starting around the second quarter of FY 2019. All remaining scientific user facilities will operate at approximately 95% of optimum. Funding for the Nanoscale Science Research Centers will include support for QIS-related tools development. No funding is requested for the disposition of unused equipment for the Lujan Neutron Scattering Center. The BES commitment for long term surveillance and maintenance ends in FY 2018. No funding is requested for these activities in FY 2019.	**-46,042**
Construction: LCLS-II is fully supported for the last year of funding for the project. Support for the APS-U project continues. The Request includes funds to initiate the Advanced Light Source Upgrade (ALS-U) project at LBNL and the Linac Coherent Light Source-II High Energy (LCLS-II-HE) project at SLAC.	**+24,300**
Total, Basic Energy Sciences	**-21,500**

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 recommendations.

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
Ultrafast Chemistry. Controlling chemical transformations requires knowledge of the fundamental processes that direct energy flow and bond rearrangement in chemical reactions. New capabilities to probe ultrafast phenomena, such as light-activated processes occurring on timescales of attoseconds to nanoseconds, allow unprecedented insight into chemical transformations underlying energy technologies.

- Femtosecond-duration soft x-ray pulses from a free-electron laser revealed the ultrafast relaxation of thymine, a DNA building block, following absorption of ultraviolet light. The new understanding of this protective ultrafast mechanism, which dissipates the absorbed energy before harmful chemical reactions can affect the thymine molecules, settles a long-standing scientific quest. The new experimental technique promises to lead to insights on the ultrafast response of other organic molecules to light, including processes relevant to photosynthesis as well as human vision.
- By transient absorption of femtosecond soft x-ray pulses from a laboratory-scale table-top source in combination with theoretical simulations, scientists made an x-ray spectroscopic "movie" of the electrons in cyclohexadiene as it opens from a ring to a linear shape in hundreds of femtoseconds after exposure to ultraviolet light. This approach uncovers details of the ultrafast exchange of energy in coupled electronic and nuclear dynamics leading to ring opening in cyclohexadiene, and is applicable to a wide range of light-activated chemical reactions that are ubiquitous in photobiology and in optoelectronic technologies.
- During photosynthesis, the Photosystem II (PSII) protein complex uses light energy to extract electrons from water, splitting water into oxygen and hydrogen. Scientists combined femtosecond pulses from a free electron laser and a new sample delivery method to obtain the first high-resolution, 3D view of PSII in action at room temperature. These images provide new insights into the chemistry of natural photosynthetic water splitting and could aid development of artificial photosynthesis approaches for renewable energy production.

Probing the Ultrasmall World through Unprecedented Precise Measurements. Much of modern science and technology relies on highly complex materials where defects and disorder disrupt ordered, periodic crystallinity to create internal boundaries between small regions called grains. Researchers are gaining insight into the behavior of a wide variety of such materials through a range of new high-precision measurement techniques that elucidate the defect or grain structure. This information can then be correlated to functional material properties, with the potential for controlled design of improved energy materials.

- In an iron-platinum nanoparticle, the 3D coordinates of 6,569 iron and 16,627 platinum atoms were determined with 22 picometer precision by a new imaging technique, atomic electron tomography. Further, the chemical order/disorder were correlated with material properties at the single-atom level. Similar “single-atom” correlations of properties for a wide range of nanostructured materials could transform our understanding of structure-property relationships at the most fundamental level.
- A new x-ray technique, Bragg coherent diffraction imaging, characterized the dynamics of crystal defects in individual, nanoscale grains of gold during annealing. The technique provided 3D detailed structure with extraordinary resolution (10 nm spatial and sub-angstrom displacement field resolution). The approaches could shed light on the response of many polycrystalline materials under external stimuli, such as stress, temperature, or exposure to chemicals common to materials used for energy applications.
- Two-dimensional (2D) materials, such as graphene, have electronic and chemical properties that are sensitive to atomic defects. In “MXene” phases, a 2D transition metal carbide, high-resolution electron microscopy revealed that the concentration of an important defect in the structure – missing atoms called vacancies – could be controlled during chemical processing. Coupled theoretical results demonstrated that vacancies influence the surface morphology and chemistry of the 2D material. Such advances could lead to new catalytic substrates and electrodes for energy storage.

Chemistry at Complex Interfaces. Complex environments created at interfaces (characterized by structural and functional disorder and dynamic behavior) influence chemical phenomena such as reactivity and transport that are important in photochemical, catalytic, separation, biochemical, and geochemical systems. Manipulating non-covalent interactions holds the promise of gaining control over chemical processes at these complex interfaces.

- At mineral-water interfaces, a quantitative description of ion exchange with the surrounding fluids can aid in the design of chemical processes such as solid nucleation, growth, and water purification. This exchange depends in part on the rates of adsorption and desorption to and from the surface. With time-resolved x-ray reflectivity measurements at a mica-water interface, scientists demonstrated that rubidium cations adsorb at a greater rate than they desorb, because of direct adsorption from solution to the surface and an additional resistance to full hydration from the surface back into solution.
- The by-products of electrochemical reduction of carbon dioxide are typically mostly hydrogen and carbon monoxide, with a minor fraction of desirable multi-carbon compounds. Scientists discovered several chemical additives that can greatly increase the yield of multi-carbons; for instance, adding specific nitrogen-containing aromatics increased ethylene and ethanol output to more than 75% of the total. This research provides new insights into how additives impact the composition of the interfaces, influencing selectivity, and can inform our understanding of the role of non-covalent interactions on these processes.
- The activity and selectivity of heterogeneous catalysis depends on the stability of reaction intermediates at the catalyst interfaces. For oxidative coupling of alcohols catalyzed by gold, scientists combined experiment with theory to demonstrate the critical further dependence of stability of intermediates on non-covalent interactions. For alkoxide intermediates, they found that the influence of non-covalent interactions on stability of intermediates depended on the internal molecular structure of the intermediates, affecting the selectivity of catalysis differently for the different intermediates.

The Science of Spin. The spin of an electron plays a prominent role in materials properties and functionality. Common examples are magnetism, computer memory, and electronics. For the future, isolated spins in materials are candidates for the development of quantum information and quantum sensing technologies. In addition, the collective behavior of spins is producing new, emergent behavior that could lead to the development of next-generation energy-relevant technologies.

- Next-generation quantum-based electronics requires long-range, efficient control of spin states of the electrons and associated atomic structures. This may be possible with hybrid architectures combining different properties, such as nanodiamond particles on top of a ferromagnetic thin film. Research found that microwaves could generate spin waves in the film that excited single electron spins in the particles at distances approaching millimeter-scale, a two-orders-of-magnitude increase. This is a notable step toward ultra-efficient control of solid-state qubits for quantum information processing and nanoscale sensing.

- Under certain conditions, atoms in a material can be oriented such that the electron spins find so many stable orientations that a randomly oriented spin structure or "spin ice" is formed. However, it is difficult to achieve tailored long-range ordering of these configurations. This was solved by using a magnetic force microscope to control the magnetic charge orientations and produce localized regions of aligned spin. This nanoscale control could create novel phenomena associated with the spin orientation and may enable write-read-erase multi-functionality for information storage on a nanometer length scale.
- In spintronics, extreme-low-power transmission of electrical information uses the spin of the electron, rather than moving electrons as in conventional electronics. However, spin currents are harder to detect and to amplify. Researchers demonstrated the ability to manipulate and amplify the spin current in a material, similar to amplifying a conventional electrical current with a transistor, using layered structures of an antiferromagnetic and an insulating material. The layered structure showed a factor of ten increase in the spin polarized current, laying the path to use in computing and high-efficiency electronics.

BES user facilities contribute to world leading science and help U.S. industries advance the technology frontiers.

- The advanced imaging capabilities at BES synchrotron facilities have assisted the aviation industry to gain insights into the components of their engines. The 3D micro-structure information about these engine materials under operating environments provides understanding of the features and the interaction between micro-structures, and of damage evolution of the materials. This will allow the industry to develop safer and more fuel-efficient engines.
- The VISION inelastic scattering instrument at the Spallation Neutron Source (SNS) has been employed by a commercial research laboratory (Toyota Research Institute) to study the fundamental internal chemical reactions taking place in a new type of electrolyte material called "molten redox" that may lead to improved performance of future batteries.
- Researchers at the Center for Nanoscale Materials invented a new nano-enabled foam called the Oleo Sponge that not only easily adsorbs oil from water, but is also reusable and can pull dispersed oil from an entire water column, not just the surface. Successful tests in New Jersey's Ohmsett—The National Oil Spill Response Research and Renewable Energy Test Facility—giant seawater tank indicate that this new technology could have significant impact in oil and other contaminant remediation.

New advanced capabilities and instrumentations at BES user facilities enable ground breaking science.

- The NSLS-II Experimental Tools (NEXT) project has delivered five world-class scientific instruments at NSLS-II. These new instruments provide the researchers the most advanced scientific research capabilities to resolve fundamental scientific problems, to examine materials under various environmental conditions, and to conduct in situ and operando studies of reactions. This will facilitate the discovery of new materials and the development of new devices that address national challenges.
- Experiments using SLAC's Ultrafast Electron Diffraction system demonstrated that light whirls atoms around in perovskites, possibly facilitating the transport of electric charge through the composite, and potentially explaining the high efficiency of these next-generation solar cell materials. Perovskites are cheap, easy to produce and very efficient at converting light into electricity.
- Using the Oak Ridge Leadership Computing Facility, SNS scientists and the ORNL Applied Math Group have developed the capability for real-time theoretical modeling of inelastic neutron scattering results. This development has enabled researchers to instantly compare experimental data to relevant theory and to determine if the theoretical and experimental results are demonstrating equivalent physical phenomena. This comparison allows researchers to adjust parameters in the theory in real-time based on the scattering data results and likewise to determine aspects of the experimental data that need more statistical detail.
- The Molecular Foundry scientists developed a new electron microscopy imaging technique that greatly improves images of light elements while using fewer electrons. The MIDI-STEM method may solve the challenge of seeing structures with a mixture of heavy and light elements in close proximity, thereby allowing scientists to use high-resolution electron microscopy on a broader set of hard and soft material combinations. The high resolution, speed, and non-invasiveness could transform the way key biomolecular interactions are studied for sensors, biology, and biomedicine.

Basic Energy Sciences
Materials Sciences and Engineering

Description

Materials are critical to nearly every aspect of energy generation and end-use. Materials limitations are often a significant 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, provide further documentation of the importance of materials sciences in forefront research for next generation scientific and technological 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. A growing area for insight on materials behavior is the understanding of dynamic processes, especially those in the ultrafast regime that only recently has been accessible for materials research. 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, including ultrafast science, 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, and quantum materials whose properties arise from the effects of quantum mechanics.

- **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, including rare earth and other critical materials.

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 *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, EFRCs, and the Batteries and Energy Storage Hub. 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 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 that will take advantage of advanced exascale computing platforms. The EFRCs support teams of investigators to perform basic research to accelerate transformative scientific advances for the most challenging topics in materials sciences. Early stage research in the Batteries and Energy Storage Hub focuses on developing the scientific understanding required to advance next generation energy storage for the grid, transportation, and other national priorities.

The Materials Sciences and Engineering subprogram also includes DOE EPSCoR. Previously referred to as the "Experimental Program to Stimulate Competitive Research," this program has been renamed the "Established Program to Stimulate Competitive Research" as directed in the American Innovation and Competitiveness Act, Public Law 114–329, §103(e)(2)(A). The DOE EPSCoR program strengthens investments in early stage energy research for states and US territories that do not historically have large academic research programs.

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, including development of science to understand ultrafast dynamics. 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, emphasizing 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. These tools and techniques are also critical in advancing understanding and discovery of novel quantum materials, including materials for next generation systems to advance QIS.

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 and related entities in their structure, such as unconventional superconductors and magnetic materials. There is a growing emphasis on "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 quantum 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 growing emphasis on extending knowledge of radiation effects to enable predictive capabilities for the multiple extreme environments envisioned for future nuclear reactors.

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.

Quantum materials research as it relates to QIS is a priority with important connections to national security and energy, including the development of the understanding to enable future generations of sensors, computers, and related technologies. Research priorities are being established through community engagement in roundtable discussions, interactions with other SC program offices, and at the interagency level, to define a unique BES role in this critical field. The research will couple materials expertise in quantum materials, theory for materials discovery, and prototypes of next generation devices.

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. This program will be enhanced to expand the application of materials discovery and synthesis research to understand the unique properties of rare earth and other critical materials, with the goal of reducing their use through development of substitutes, reducing the quantities required for specific properties, and developing novel synthesis techniques.

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 research to understand 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, including the extraordinary challenges for synthesis of quantum materials.

Established Program to Stimulate Competitive Research (EPSCoR)
The DOE EPSCoR program funds early stage research that supports the agency's energy mission in states and territories with historically lower levels of Federal research funding. Eligibility determination for the DOE EPSCoR program follows the National Science Foundation (NSF) eligibility analysis.

The DOE EPSCoR program emphasizes research that will improve the capability of designated states and territories to conduct sustainable and nationally competitive energy-related research; jumpstart research capabilities in designated states and territories through training scientists and engineers in energy-related areas; and build beneficial relationships between scientists and engineers in the designated jurisdictions with world-class laboratories managed by the DOE, leverage DOE national user facilities, and take advantage of opportunities for intellectual collaboration across the DOE system. Through broadened participation, DOE EPSCoR seeks to augment the network of energy-related research performers across the nation.

Energy Frontier Research Centers (EFRCs)
The EFRC program 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 related to quantum materials that can optimize energy flow and transmission. After eight years of research activity, the program has produced an impressive breadth of scientific accomplishments, including over 9,600 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, BES holds meetings of the EFRC researchers biennially.

Energy Innovation Hubs—Batteries and Energy Storage
The Joint Center for Energy Storage Research (JCESR) focuses 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, improved batteries for vehicles, and other national priorities. JCESR is a multi-institutional research team led by Argonne National Laboratory (ANL) in collaboration with four other national laboratories, ten universities, and five industrial participants. In the initial 5-year award (2013-2018), JCESR research activities focused on the development of an atomic-level understanding of reaction pathways and elucidation of design rules for electrolyte and electrode 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 prioritizing its fundamental research directions for next generation batteries. JCESR created a library of fundamental scientific knowledge 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 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 renewal of JCESR will continue the focus on early stage research to tackle forefront, basic scientific challenges for next-generation electrochemical energy storage. The research will be consistent with the priorities established in the recent BES workshop report *Basic Research Needs for Next Generation Electrical Energy Storage,* including discovery science for exploration of new battery chemistries and materials with novel functionality. It is anticipated that advances will elucidate cross-cutting scientific principles for electrochemical stability; ionic and electronic transport at interfaces/interphases, in bulk materials or membranes; solvation structures and dynamics in electrolytes; nucleation and growth of materials, new phases, or defects; coupling of electrochemical and mechanical processes; and kinetic factors that govern reversible and irreversible reactions. Close coupling of theory, simulation, and experimentation is expected to accelerate scientific progress; to unravel the complex, coupled phenomena of electrochemical energy storage; to bridge gaps in knowledge across length and temporal scales; and to enhance the predictive capability of electrochemical models.

<u>Computational Materials Sciences</u>
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 functions 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 American 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 electrical and thermal 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.

Awards in this program focus 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 regular teleconferences, annual progress reports, and active management by BES throughout the performance period.

Activities and Explanation of Changes

FY 2017 Enacted	FY 2019 Request	Explanation of Changes FY 2019 Request vs FY 2017 Enacted
Materials Sciences and Engineering $359,641,000	**$361,040,000**	**+$1,399,000**
Scattering and Instrumentation Sciences Research $76,598,000	**$60,925,000**	**-$15,673,000**
Research supported advanced characterization tools and techniques to address forefront scientific challenges to understand materials and related phenomena. Quantitative *in situ* and *in operando* analysis capabilities under perturbing parameters such as temperature, stress, chemical environment, and magnetic and electric fields were investigated. Investments in x-ray science emphasized hypothesis driven research with x-ray free electron laser sources, tailored excitations with pumped laser control, and coherent x-ray imaging. Neutron scattering research emphasized research on thermodynamics of charged polymer systems and emergent quantum phenomena at interfaces and in the bulk. Electron scattering research focused 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 emphasize the development and use of forefront characterization tools to address challenges in materials science including understanding of quantum phenomena, with an increasing emphasis on ultrafast techniques. In addition to high spatial resolution, the research will emphasize dynamics – understanding how material structures and phenomena evolve with time and in environments that reflect the challenges for energy generation and use. 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 in emergent quantum phenomena, especially research involving interfaces. Electron scattering research will focus on innovative techniques to assess quantum phenomena, especially with ultrafast techniques.	Research will emphasize development of novel ultrafast techniques, especially using x-ray free electron lasers, and their use to assess materials dynamics including processes related to quantum phenomena. Research that uses long-standing x-ray, neutron scattering, and electron microscopy techniques and research focused on traditional superconductivity and organic electronics will be deemphasized.

FY 2017 Enacted	FY 2019 Request	Explanation of Changes FY 2019 Request vs FY 2017 Enacted
Condensed Matter and Materials Physics Research **$101,645,000**	**$123,790,000**	**+$22,145,000**
The program continued to support fundamental experimental and theoretical research on the properties of materials. The experimental and theoretical condensed matter physics research emphasized quantum materials, focusing on new and emergent behavior including quantum magnetism, spintronics, topological states, and novel 2D materials. Advancement of theory and computational tools focused on materials discovery, including data-driven and machine learning techniques; novel approaches; and non-equilibrium systems. Physical behavior research emphasized innovative science to understand optical, thermal, and electronic phenomena. For mechanical behavior and radiation effects, there was an increased focus on understanding defect evolution in radiation environments.	Research on fundamental experimental and theoretical research on the properties of materials, emphasizing quantum phenomena, will be continued. Experimental and theoretical condensed matter physics research will emphasize quantum materials, focusing on new and emergent behavior for QIS, including spintronics, topological states and novel 2D materials. Physical behavior research will emphasize innovative science to understand optical and electronic phenomena. Mechanical behavior and radiation effects research will continue to focus on the mechanisms of materials failure due to mechanical strain, corrosion, and radiation environments, including the coupled extremes envisioned for future nuclear reactors.	Research will emphasize forefront research in the topical areas covered by this subprogram. Research will increase focus on quantum materials research, including research relevant for QIS for both experimental and theoretical approaches. Also emphasized is radiation effects research that will illuminate the scientific understanding of materials intended for future nuclear reactors. Topics to be deemphasized include research on traditional superconductivity; theory related to soft matter, glassy systems, granular materials, ionic liquids, surface chemistry, and mechanics; and high-strain-rate deformation behavior.
Materials Discovery, Design, and Synthesis Research **$61,931,000**	**$62,551,000**	**+$620,000**
Research to develop a scientific understanding for predictive design and synthesis of materials across multiple length scales continued. Emphasis was 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 was 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-inorganic systems, were stressed. In materials chemistry, fundamental research related to polymer chemistry, nanomaterial	Research will continue to focus on understanding the fundamentals of predictive design and synthesis of materials using chemical, physical and bio-inspired techniques. Understanding the dynamics and evolution of materials structure and chemistry during the early stages of materials synthesis will be emphasized, as will 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 and defect management will be stressed for complex materials including quantum materials, organic systems, nanomaterials, electrochemical materials, polymers, and high fidelity mesoscale systems.	Research will emphasize forefront science to understand synthesis related to novel functionalities and elucidating the roles of interfaces, especially for quantum and critical materials. Topics to be de-emphasized include research related to optimization of synthetic methods, research focused on specific properties of materials for applications, and research with a primary goal of device fabrication and testing.

FY 2017 Enacted	FY 2019 Request	Explanation of Changes FY 2019 Request vs FY 2017 Enacted
synthesis, liquids, electrochemistry, and control of porosity continued. For biomolecular materials, research on assembly of materials that incorporate error correction and defect management mechanisms for beyond equilibrium, multicomponent materials was emphasized.		
Established Program to Stimulate Competitive Research (EPSCoR) $14,452,000	**$7,708,000**	**-$6,744,000**
Research supported science crosscutting 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 was sustained. Single investigator research through the state-laboratory partnerships component of the program was emphasized.	Efforts will continue to span science in support of the DOE mission, with emphasis on early stage science that underpins DOE energy technology programs. Research will emphasize broadening EPSCoR jurisdiction-laboratory partnerships and investment in early career research faculty from EPSCoR designated jurisdictions.	Research support is reduced compared to the FY 2017 Enacted level, taking into consideration overall funding for core research to institutions in EPSCoR states and emphasis on support for early stage, basic research.
Energy Frontier Research Centers (EFRCs) $55,800,000	**$55,800,000**	**$0**
FY 2017 funds provided the fourth year of funding for awards made in FY 2014, as well as the second year of funding for new awards made in FY 2016.	FY 2019 funds will continue to support four-year EFRC awards that were made in FY 2016 and FY 2018.	As a result of the recompetition of the EFRC program in FY 2018, emphasis is placed on tackling 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, next-generation electrical energy storage, and future nuclear energy. In order to address these priorities, the following topical areas are deemphasized: phenomena related to more mature areas of solar photovoltaics, thermoelectrics, and solid-state lighting.

FY 2017 Enacted	FY 2019 Request	Explanation of Changes FY 2019 Request vs FY 2017 Enacted
Energy Innovation Hubs—Batteries and Energy Storage $24,088,000	**$24,088,000**	**$0**
FY 2017 funding supported the research for JCESR to complete the five-year award (research continued through mid-FY 2018). Its research activities 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.	Research will continue to focus on early stage research to tackle forefront, basic scientific challenges for next-generation electrochemical energy storage. The research will emphasize discovery science, elucidation of cross-cutting scientific principles for electrical energy storage, and integration of theory, experiment, and computational approaches to accelerate progress.	Funding will support renewal of the JCESR award at the same funding level.
Computational Materials Sciences $12,000,000	**$13,000,000**	**+$1,000,000**
Research continued 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. For these four-year awards, management reviews are held in the first year of the award, and full peer reviews are held after two years. Renewal, based on full peer review, is an option to ensure maximum impact.	Research will continue on the computational materials sciences awards, with ongoing focus 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. Software will be developed that utilizes leadership class computers, and made available to the broad research community. In addition, the codes will incorporate frameworks that are suited for future exascale computer systems. Awards that complete their fourth year of research will be considered for renewal in a solicitation that also considers new applications.	The additional funds will support awards related to theory for predictive design of quantum materials for next generation QIS.
SBIR/STTR $13,127,000	**$13,178,000**	**+$51,000**
In FY 2017, SBIR/STTR funding was set at 3.65% of non-capital funding.	In FY 2019, SBIR/STTR funding is set at 3.65% of non-capital funding.	

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, and molecules.

- **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 five synergistic, fundamental research themes that are at the intersections of multiple research focus areas. An important component of ultrafast science, *Ultrafast Chemistry,* 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, separation, 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 charge transport and reactivity are coupled. *Reaction Pathways in Diverse Environments* discovers the influence of nonequilibrium, heterogeneous, nanoscale, and extreme environments on complex reaction mechanisms in chemical conversions. Research in this area increases understanding of the factors controlling chemical processes and provides mechanistic insights into the efficiency, control, and selectivity of reaction pathways. *Chemistry in Aqueous Environments* addresses the unique properties of water, particularly how they manifest in extreme environments such as confinement (e.g., nanoscale pores) and multi-component, multi-phase solutions (e.g., concentrated electrolytes), 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 more complex systems, are essential for advancing fundamental science in these areas.

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 FY 2019 Request focuses resources toward the highest priorities in early-stage fundamental research, with targeted reductions of activities that extend to later-stage fundamental research. High priority areas include ultrafast science, particularly through the cross-cutting research theme in *Ultrafast Chemistry* and complemented by research supported in other research themes, QIS to understand the quantum nature of atomic and molecular systems and research to exploit recent advances in quantum computing to address scientific challenges that are beyond the capabilities of classical computers, and chemical processes in extreme environments, in particular the extremes of radiation, temperature, stress, and chemical reactivity, to provide fundamental knowledge needed to understand as well as advance nuclear energy systems.

<u>Fundamental Interactions Research</u>

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 atoms and molecules. 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 *Reaction Pathways in Diverse Environments,* and to understand how the dynamics of molecular environments influence reactivity and transport that is important in *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 *Reaction Pathways in Diverse Environments*, *Charge Transport and Reactivity, Chemistry at Complex Interfaces,* and *Ultrafast Chemistry*. 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 and molecules with electrons and 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 and to understand quantum effects, such as coherence in molecular systems, that are the foundation for creating novel QIS systems. 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. Additional emphasis will be placed on codes that contribute to a fundamental understanding of how molecules might function as components of quantum computers.

<u>Chemical Transformations Research</u>

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, separation science, heavy element chemistry and geosciences. The research uses tools from *Ultrafast Chemistry* 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 separation systems; and develops understanding of *Chemistry in Aqueous Environments* that play important roles in geochemical transformations and chemical separations, including heavy elements. This research breadth demands a broad coverage of scientific disciplines and analytical tools. Hence, Chemical Transformations comprise four core areas: Catalysis Science, Separation Science, Heavy Element Chemistry and Geosciences.

Reaction Pathways in Diverse Environments 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. The fundamental knowledge gained from this research activity provides the foundation for replacing critical elements such as noble metals in catalytic processes.

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. The fundamental knowledge gained from this research activity provides the foundations for extracting and purifying critical elements from waste as well as new resources.

Foundational knowledge for future nuclear energy approaches is provided through fundamental studies of the structure and reactivity of actinide-containing molecules in extreme environments such as those in nuclear reactors and nuclear waste containment. 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.

<u>Photochemistry and Biochemistry Research</u>
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 Chemistry*, are developed and used to investigate the structural and chemical dynamics of energy absorption, transfer, conversion and storage across multiple spatial and temporal scales as well as 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*. To develop knowledge of *Reaction Pathways in Diverse Environments*, structural, functional and mechanistic properties of enzymes, enzyme systems, and energy-relevant biological reactions are studied, identifying principles important for catalyst function, selectivity, and stability. These cross-cutting synergistic efforts are illustrated by studies of the mechanism of the 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, photosynthetic electron and proton transport, photosynthetic uptake and reduction of carbon dioxide, and mechanisms of self-assembly, self-regulation, and self-repair exhibited by the proteins, membranes and cellular compartments that perform natural photosynthesis. Physical science tools, such as those used for *Ultrafast Chemistry*, are used extensively to probe structural, functional, and mechanistic properties of enzymes, enzyme systems, and energy-relevant biological reactions and pathways related to energy capture, conversion, and storage, including complex multielectron redox reactions, electron transfer and bifurcation, and processes beyond primary photosynthesis such as nitrogen reduction and deposition of the reduced carbon into energy-dense carbohydrates and lipids. Complementary research on solar energy conversion in chemical and artificial systems focuses on the elementary steps of light absorption, charge separation, and charge transport within a number of chemical systems. Supported research incorporates organic and inorganic photochemistry, catalysis and photocatalysis, light-driven electron and energy transfer in the condensed phase and across interfaces, photoelectrochemistry, and artificial assemblies for charge separation and transport and provides fundamental insights for electricity generation from sunlight and artificial photosynthetic fuel production.

This activity also supports radiation science, investigating fundamental physical and chemical effects produced by the absorption of energy from ionizing radiation. These fundamental studies provide understanding of the chemical reactions that occur in radiation fields of nuclear reactors, including in their fuel and coolants. A common theme is the exploration of radiolytic processes that occur across solid-liquid and solid-gas interfaces, where surface chemistry can be activated and changed by radiolysis.

Energy Frontier Research Centers (EFRCs)

The EFRC program 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 eight years of research activity, the program has produced an impressive breadth of accomplishments, including over 9,600 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, BES holds meetings of the EFRC researchers biennially.

Energy Innovation Hubs—Fuels from Sunlight

Established in September 2010, 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 was renewed by BES for a final five-year award term starting on September 30, 2015, at an annual funding level of $15M. 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.

In the second award, JCAP focused 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. 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.

The FY 2019 Request continues to focus resources toward the highest priorities in early-stage fundamental research on carbon dioxide reduction, with targeted decreases in activities that extend to later-stage fundamental research.

<u>Computational Chemical Sciences</u>

Software solutions and infrastructure provide the enabling tools for an effective scientific strategy to address the nation's energy challenges. BES-supported activities are entering a new era in which chemical reactions can be controlled and matter can be built with atom-by-atom precision. At the foundation of this new era are computational models that can accurately predict the behavior of molecules and materials based on theoretical calculations prior to their experimental synthesis. Open-source and commercial codes have established American dominance in computational chemistry. However, that dominance is being challenged with the transition to predominantly massively-parallel high performance computing (HPC) platforms, because most existing computational chemistry codes are unable to use efficiently more than one percent of the processors available on existing leadership-class supercomputers. While recent breakthroughs in computational chemistry provide a strong foundation for future success, a multidisciplinary team effort is critically needed to modify or replace existing computational chemistry codes with codes that are well-adapted to current petascale and anticipated exascale architectures.

BES launched research awards in FY 2017 to perform computational chemistry research that focus on the creation of computational codes and associated experimental/computational databases for the design of chemical processes and assemblies. These research efforts combine the skills of experts in theoretical chemistry, modeling, computation, and applied mathematics. The research includes development of new *ab initio* theory, mining data from both experimental and theoretical databases, and experimental validation of the codes. The computational codes will advance the predictive capability for chemical processes and assemblies, using DOE's scientific user facilities (including both advanced experimental as well as leadership class computational capabilities). 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 chemical systems. The ultimate goal is use of these codes/data by the broader research community and by industry to dramatically accelerate chemical research in the United States.

Computational chemical 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 monthly teleconferences, annual progress reports, and active management by BES throughout the performance period.

<u>General Plant Projects (GPP)</u>

GPP funding provides for minor new construction, for other capital alterations and additions, and for improvements to land, buildings, and utility systems to maintain the productivity and usefulness of Department-owned facilities and to meet requirements for safe and reliable facilities operation.

Activities and Explanation of Changes

FY 2017 Enacted	FY 2019 Request	Explanation of Changes FY 2019 Request vs FY 2017 Enacted
Chemical Sciences, Geosciences, and Biosciences $329,127,000	**$327,970,000**	**-$1,157,000**
Fundamental Interactions Research $62,606,000	**$69,581,000**	**+$6,975,000**
This activity is a major supporter of ultrafast chemical sciences and chemical physics, underpinning energy conversion and chemical transformation phenomena. This activity supported structural and dynamical studies of atoms and molecules, and the description of their interactions in full quantum detail, with the aim of providing a complete understanding of reactive chemistry in the gas phase, condensed phase, and at interfaces. Novel sources of photons, electrons, and ions were used to probe and control atomic, molecular, and nanoscale matter. Ultrafast optical and x-ray techniques were developed and used to study and direct molecular, dynamics, and chemical reactions.	This activity will continue to develop and apply forefront ultrafast x-ray and optical probes of matter to study and control energy flow and bond rearrangements. Gas phase research will continue to develop and apply approaches to examine the structure and dynamics of reactive intermediates and how they impact reaction pathways in heterogeneous environments. Research will extend efforts to understand and control chemical processes and dynamics, at the molecular level, in increasingly complex aqueous and interfacial systems. Research will expand the use of ultrafast techniques to study gas-phase, condensed phase and interfacial chemical phenomena. The activity will develop advanced theoretical methods for electronic structure calculations that can be scaled to operate on exascale computers. Research will support the development of new computational tools to calculate electronically excited states in molecules and extended mesoscale systems, to guide and interpret ultrafast measurements, and to develop new catalysts. The activity will emphasize efforts to drive advances in the application of quantum computing for molecular calculations.	The Request emphasizes imaging studies of molecular dynamics using as well as developing ultrafast capabilities at BES light sources, research to understand increasingly complex interfacial systems, advances in computational and theoretical chemistry for molecular systems of increasing complexity, advanced computational tools, and exascale computing. This activity 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, and molecules. This activity will increase research in support of the application of quantum computing to calculations of molecular structure and dynamics. The activity will de-emphasize aspects of nanoscience and combustion research.

FY 2017 Enacted	FY 2019 Request	Explanation of Changes FY 2019 Request vs FY 2017 Enacted
Chemical Transformations Research $81,687,000	**$88,869,000**	**+$7,182,000**
This activity is a major supporter of catalysis and heavy element chemistry that have been the focus of community workshops and National Academy studies. This activity supported fundamental research for the characterization, control, and optimization of chemistry in many forms. Catalysis science supported the design of new catalytic methods for the clean and efficient production of fuels and chemicals through thermally and non-thermally induced reaction pathways. It involved catalysts of various types: inorganic and organic complexes, nanostructured and macromolecular phases, and solids and interfaces in complex environments. Heavy element chemistry explored the unique molecular bonding of the actinide and transactinide elements using experiment and theory to elucidate electronic and molecular structure as well as reaction thermodynamics. Research on chemical separations focused on understanding pathways and developing principles for how to control atomic and molecular interactions with separation media, including solvents, inorganic and organic/hybrid membranes, confined environments, complex mixtures and interfaces. Geosciences research covered molecular to mesoscale processes underlying interfacial geochemistry, flow and transport, and geomechanics.	This activity will continue to support predictive fundamental research on the design and synthesis of novel catalysts to efficiently convert chemical feedstocks to high-value fuels and chemicals. New routes to the efficient synthesis of high-energy chemicals such as hydrogen, ammonia, methanol, and others, will continue to be pursued. Fundamental separation science research will continue on innovative approaches for separating chemical mixtures. Molecular recognition at complex interfaces, predictive theory for transport and separation in confined environments, and multiscale methods for bonding and dynamics will continue to be supported, increasingly with exascale capabilities. Geochemical and geophysical mechanisms of reaction and transport processes in the subsurface environments, such as nucleation, growth and mineralization, solvation in aqueous environments at extreme conditions, and dynamics at mineral-water interfaces will continue to be supported. Heavy element research will continue to expand the knowledge of the chemistry of actinide reactivity, bonding, synthesis, and separation, and also support training in nuclear chemistry. Theoretical methods will continue to be advanced to accurately describe the chemistry of f-element compounds.	This Request emphasizes efforts in ultrafast spectroscopy for detailed studies of pathways, electronic structure calculations for systems of increasing molecular and solid complexity, and multiscale modeling and simulations for complex bonding or reaction and transport processes. Research will continue to lead the development of fundamental knowledge of mechanisms of chemical catalysis, synthesis, separations, stabilization and transport required to control chemical processes in complex systems. This activity will emphasize fundamental studies of the chemical processes that occur in nuclear environments, aimed towards an understanding of the structure, dynamics, and energetics of molten salt coolants and fuels as well as of the chemical and physical properties of interfaces and heavy elements. Also emphasized are the catalytic and separation mechanisms that operate within diverse environments created by complex atomic architectures, solvents, electric or mechanical fields, at various temperatures and pressures. It will provide new knowledge on reaction systems that integrate multiple steps, including chemical conversion, energy conversion and chemical separation steps that are resilient and adaptable to multiple sources of energy and feedstocks. The activity will de-emphasize research on chemical analysis, synthesis of nanomaterials, physics of fluids in rock systems, and biocatalytic reactions that are better aligned under other activities.

FY 2017 Enacted	FY 2019 Request	Explanation of Changes FY 2019 Request vs FY 2017 Enacted
Photochemistry and Biochemistry Research **$89,168,000**	**$74,386,000**	**-$14,782,000**
This activity is a major supporter of solar photochemistry and natural photosynthesis research, and central to understanding chemical processes and dynamics during energy capture and conversion. Research supported the molecular mechanisms involved in the capture of light energy and its conversion into chemical and electrical energy through biological and chemical pathways. Study of natural photosynthetic systems provided insights for artificial and bio-hybrid systems that exhibit the biological traits of self-assembly, regulation, and self-repair. Complementary research encompassed organic and inorganic photochemistry, photo-electrochemistry, electron and energy transfer, photo- and bio-catalysis, and molecular assemblies for artificial photosynthesis.	The activity 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 in both natural and artificial systems. Research of the fundamental mechanisms of photocatalysis and biocatalysis will continue to make use of innovative ultrafast methodologies as well as computation and modeling. Efforts to understand processes and reactions on ultrafast timescales for energy conversion in natural and artificial systems will continue to be supported and will target a fundamental understanding of ultrafast chemistry and of reactivity across complex interfaces, in aqueous environments, and under dynamic conditions. Research will also continue to examine how water drives formation of mesoscale structures for energy capture and conversion in natural systems and the chemistry and structure of water and other molecules within the field of highly ionizing radiation.	The Request emphasizes the use and development of ultrafast techniques and theory and computation to understand excited-state dynamics and charge and energy transfer in photochemical and biochemical processes. Cutting-edge research will continue to develop fundamental knowledge and innovative approaches to understand physical, chemical, and biochemical processes of light energy capture and conversion in non-biological and biological systems. Research in fundamental radiation chemistry will be emphasized to provide a foundation for prediction and control of radiation-chemical transformations in complex and extreme environmental systems. Fundamental research on charge transport, energy transfer, and catalytic mechanisms will provide new knowledge of processes important for energy capture, conversion, and storage as will efforts in the chemistry of ultrafast processes, complex interfaces, and water-driven processes. The activity will de-emphasize efforts in plant cell wall biosynthesis and structure, light signaling in plant development, and polyelectrolytes in solar photoconversion.
Energy Frontier Research Centers (EFRCs) **$54,200,000**	**$54,200,000**	**$0**
FY 2017 funds provided the fourth year of funding for awards made in FY 2014, as well as the second year of funding for new awards made in FY 2016.	The Request will continue to support four-year EFRC awards that were made in FY 2016 and FY 2018.	As a result of the recompetition of the EFRC program in FY 2018, the FY 2019 Request will emphasize tackling the transformative opportunities related to chemical sciences, geosciences, and biosciences and the research priorities identified in the Basic Research Needs reports on catalysis science, synthesis science, instrumentation science, energy-water issues, and future nuclear energy. In order to address these priorities, the following topical areas are

FY 2017 Enacted	FY 2019 Request	Explanation of Changes FY 2019 Request vs FY 2017 Enacted
		deemphasized: phenomena related to more mature areas of solar photovoltaics; carbon dioxide sequestration; and biologically-mediated breakdown and conversion of lignocellulosic biomass.
Energy Innovation Hubs—Fuels from Sunlight $15,000,000	**$15,000,000**	**$0**
The Fuels from Sunlight Hub continued to perform research on the fundamental science of carbon dioxide reduction needed to enable efficient, sustainable solar-driven production of liquid transportation fuels. JCAP underwent a scientific and merit review in FY 2017 to assess progress toward meeting project milestones and goals.	FY 2019 funds will continue to support JCAP's fundamental research on the science of carbon dioxide reduction.	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.
Computational Chemical Sciences $13,489,000	**$13,000,000**	**-$489,000**
Computational Chemical Sciences (CCS) projects were initiated to develop open-source modular software tools that can be reused and tailored for fundamental research needs of the chemistry community. This investment builds on current quantum chemistry software, seeking to create new codes that fully leverage massively-parallel high performance computing platforms and target implementation on future exascale computer systems. Funded research areas included: hierarchical and scalable software for spectra, transformation and separation; transition-metal molecules for chemical control and quantum systems; and photocatalytic and field-driven chemistry and transport.	FY 2019 funds will continue to support CCS awards that were made in FY 2017 and any new awards in complementary research areas made in FY 2018.	The Request will support awards that enable the use of leadership class computing and exascale computer systems for research areas complementary to the FY 2017 awards, including to understand quantum mechanical behavior of molecular systems for next generation QIS.
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.	No changes.
SBIR/STTR $11,977,000	**$11,934,000**	**-$43,000**
In FY 2017, SBIR/STTR funding was set at 3.65% of non-capital funding.	In FY 2019, SBIR/STTR funding is set at 3.65% of non-capital funding.	

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 2017, the BES scientific facilities were used by nearly 16,000 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.

<u>X-Ray Light Sources</u>

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, the Advanced Photon Source (APS) at ANL, the 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, to 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.

<u>High Flux Neutron Sources</u>

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, and 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.

<u>Nanoscale Science Research Centers (NSRCs)</u>

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 BES currently supports are the Center for Nanoscale Materials at ANL, the Center for Functional Nanomaterials at BNL, the Molecular Foundry at LBNL, the Center for Nanophase Materials Sciences at ORNL, and the 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.

The emerging field of quantum information science (QIS) exploits intricate quantum mechanical phenomena such as entanglement to create fundamentally new ways of obtaining and processing information. Harnessing these counterintuitive properties of matter promises to yield revolutionary new approaches to computing, sensing, communication, and metrology, as well as far-reaching advances in our understanding of the world around us. A part of the FY 2019 BES funding for the NSRCs will be used to develop QIS related research infrastructure for materials synthesis, fabrication, metrology, modeling and simulation. The goal is to develop a flexible and enabling infrastructure so that U.S. institutions and industry can rapidly develop and commercialize the new discoveries and innovations.

<u>Other Project Costs</u>
The total project cost (TPC) of DOE's construction projects is comprised of 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; 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, such as costs that are incurred during the project's initiation and definition phase for planning, conceptual design, research, and development, and those incurred 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. The BES commitment for LTSM ends in FY 2018. No funding is requested in FY 2019.

Activities and Explanation of Changes

FY 2017 Enacted	FY 2019 Request	Explanation of Changes FY 2019 Request vs FY 2017 Enacted
Scientific User Facilities $992,732,000	**$946,690,000**	**-$46,042,000**
X-Ray Light Sources $489,059,000	**$491,059,000**	**+$2,000,000**
Funding supported near optimal operations of the five BES light sources. The light sources supported over 11,000 users in FY 2017. In addition, $5M was appropriated for R&D in support of the Advanced Light Source Upgrade.	LCLS operations will continue in preparation for completion of the LCLS-II project and in support of the BES priority in ultrafast science. To allow installation activities for the LCLS-II construction project to proceed, LCLS will be shut down for one year, starting around 2Q FY 2019. During the shutdown, LCLS will continue to maintain critical systems, advance linac remediation activities, and develop new instruments and capabilities for experiments. APS, ALS, NSLS-II and SSRL operations will continue at 95% of optimum.	The increase supports LCLS operations in preparation for completion of the LCLS-II project and in support of the BES priority in ultrafast science.
High-Flux Neutron Sources $266,000,000	**$265,000,000**	**-$1,000,000**
Funding supported the operation of HFIR and SNS at near optimal levels. The neutron facilities supported over 1,200 users in FY 2017. Limited funding was provided to the Lujan Neutron Scattering Center for the disposition of unused equipment.	SNS and HFIR operations will continue at 95% of optimum. No funding is requested for the Lujan Neutron Scattering Center for the disposition of unused equipment.	No funding is requested for the disposition of unused equipment at the Lujan Neutron Scattering Center.
Nanoscale Science Research Centers $122,272,000	**$122,272,000**	**$0**
Funding supported operations at the five BES NSRCs at near optimal levels. The NSRCs continued to expand the user base from universities, national laboratories, and industry. In FY 2017, the NSRCs supported over 3,300 users.	All five NSRCs will be supported, with part of the funding designated for tool development for QIS.	No change.

FY 2017 Enacted	FY 2019 Request	Explanation of Changes FY 2019 Request vs FY 2017 Enacted
Other Project Costs $5,000,000	**$10,100,000**	**+$5,100,000**
OPC funds were appropriated by Congress for the Advanced Light Source Upgrade (ALS-U) project.	Funds are requested for Other Project Costs for the LCLS-II project at SLAC National Accelerator Laboratory, ALS-U at Argonne National Laboratory, and LCLS-II-HE at SLAC per the project plans.	Other Project Costs increase according to the project plans.
Major Items of Equipment $42,500,000	**$0**	**-$42,500,000**
The Advanced Photon Source Upgrade (APS-U) project continued with R&D, engineering design, prototyping, fabrication, and long lead and advance procurements of critical systems.	APS-U was proposed to be transitioned from a Major Item of Equipment (MIE) to a separate line item construction project in the FY 2018 Request. No MIE funds are requested in this program in FY 2019.	APS-U is included as a separate line-item construction project in the FY 2019 Request.
Research $34,618,000	**$25,000,000**	**-$9,618,000**
Research funding for the scientific user facilities continued to support selected, high-priority research activities for detectors and optics. Funding continued for long term surveillance and maintenance activities at BNL and SLAC.	The Request will support limited high-priority research activities for detectors and optics instrumentation. The BES commitment for long term surveillance and maintenance at BNL and SLAC ends in FY 2018. No funding is requested for these activities in FY 2019.	No funding is requested for long term surveillance and maintenance.
SBIR/STTR $33,283,000	**$33,259,000**	**-$24,000**
In FY 2017, SBIR/STTR funding was set at 3.65% of non-capital funding.	In FY 2019, SBIR/STTR funding is set at 3.65% of non-capital funding.	

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. 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 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.

The **Advanced Light Source Upgrade (ALS-U)** project will upgrade the existing Advanced Light Source facility by replacing the existing electron storage ring with a new electron storage ring based on a multi-bend achromat lattice design which will provide a soft x-ray source that is brighter, up to 1000 times greater brightness, and with a significantly higher coherent flux fraction. ALS-U will leverage two decades of investments in scientific tools at the ALS by making use of the existing beamlines and infrastructure. ALS-U will ensure that the ALS facility remains a world leader in soft x-ray science. Critical Decision-0 (CD-0), Approve Mission Need, was approved for ALS-U on September 27, 2016. The preliminary TPC range, based on early concepts under consideration, is $260,000,000 - $420,000,000.

The **Linac Coherent Light Source-II-HE (LCLS-II-HE)** project will increase the energy of the superconducting linac currently under construction as part of the LCLS-II project from 4 GeV to 8 GeV and thereby expand the high rep rate operation (1 million pulses per second) of this unique FEL into the hard x-ray regime (5-12 keV). LCLS-II-HE will add new and upgraded instrumentation to augment existing capabilities and upgrade the facility infrastructure as needed. The LCLS-II-HE project will upgrade and expand the capabilities of the LCLS-II to maintain U.S. leadership in ultrafast x-ray science. Critical Decision-0 (CD-0), Approve Mission Need, was approved for LCLS-II-HE on December 15, 2016. The preliminary TPC range, based on early concepts under consideration, is $260,000,000 - $450,000,000.

All BES construction projects are conceived and planned with the scientific community, 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 2017 Enacted	FY 2019 Request	Explanation of Changes FY 2019 Request vs FY 2017 Enacted
Construction $190,000,000	**$214,300,000**	**+$24,300,000**
Linac Coherent Light Source-II (LCLS-II) $190,000,000	**$139,300,000**	**-$50,700,000**
FY 2017 funding supported critical procurement of materials and equipment needed to maintain the project schedule and expand the construction efforts. Design, long lead and advance procurements, R&D, prototyping, site preparation activities, fabrication, and installation also continued in FY 2017.	FY 2019 funding will be used for installation of major accelerator and x-ray systems and facilities including the linear accelerator and its cryogenic refrigeration facilities, electron beam transport, undulator x-ray sources, x-ray optics and experimental systems and supporting infrastructure.	Funding for the LCLS-II construction project decreases per the project plan. FY 2019 will be the last year of funding for the project.
Advanced Photon Source Upgrade (APS-U) $0	**$60,000,000**	**+$60,000,000**
APS-U was included as a Major Item of Equipment project in FY 2017.	The FY 2018 Request proposed to transition APS-U from a MIE to a line item construction project. FY 2019 funding will be used for targeted R&D, engineering design, equipment prototyping, testing, fabrication, site preparation, installation, and long lead and advance procurements.	The Request continues funding for the APS-U construction project.
Advanced Light Source Upgrade (ALS-U) $0	**$10,000,000**	**+$10,000,000**
N/A	FY 2019 funding will be used for R&D, engineering design, equipment prototyping, testing and other activities required to advance the ALS-U project.	This is the first request for the ALS-U project.
Linac Coherent Light Source-II High Energy (LCLS-II-HE) $0	**$5,000,000**	**+$5,000,000**
N/A	FY 2019 funding will be used for R&D, engineering design, equipment prototyping, testing and other activities required to advance the LCLS-II-HE project.	This is the first request for the LCLS-II-HE project.

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 2017	FY 2018	FY 2019
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	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	N/A
Result	Met	N/A	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

	FY 2017	FY 2018	FY 2019
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**		
Target	N/A	Expand computational materials and chemical discovery through increased data production and additional online computational resources: add electronic properties data for 7,000 compounds, elastic properties data for 3,000 compounds and reaction energies for 5,000 catalytic reactions to publicly available databases; add new or expanded functionality to on-line, high performance computer software/codes for prediction of materials properties.	Expand computational materials and chemical discovery through increased data production and open source software: add 2000 adsorption energies for chemicals in nanoporous materials to publically available databases; add new or expanded functionality to 10 online, high performance computer software/codes for prediction of materials and chemical properties.
Result	N/A	TBD	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 2017 Enacted	FY 2018 Annualized CR[a]	FY 2019 Request	FY 2019 Request vs FY 2017 Enacted
Capital Operating Expenses Summary						
Capital Equipment	n/a	n/a	60,188	—	24,500	-35,688
General Plant Projects (GPP)	n/a	n/a	4,005	—	1,000	-3,005
Accelerator Improvement Projects (AIP)	n/a	n/a	7,000	—	11,000	+4,000
Total, Capital Operating Expenses	**n/a**	**n/a**	**71,193**	—	**36,500**	**-34,693**
Capital Equipment						
Major Items of Equipment						
Advanced Photon Source Upgrade (APS-U), ANL (TPC TBD)[b]	151,000	108,500	42,500	—	0	-42,500
Linac Coherent Light Source-II (LCLS-II), SLAC[c,d]	85,600	85,600	0	—	0	0
NSLS-II Experimental Tools (NEXT), BNL (TPC $90,000)	90,000	90,000	0	—	0	0
Total, Major Items of Equipment	n/a	n/a	42,500	—	0	-42,500
Total, Non-MIE Capital Equipment	n/a	n/a	17,688	—	24,500	+6,812
Total, Capital equipment	**n/a**	**n/a**	**60,188**	—	**24,500**	**-35,688**
General Plant Projects (GPP)						
Other general plant projects under $5 million TEC	n/a	n/a	4,005	—	1,000	-3,005
Accelerator Improvement Projects (AIP)						
Accelerator improvement projects under $5 million TEC	n/a	n/a	7,000	—	11,000	+4,000

[a] A full-year 2018 appropriation for this account was not enacted at the time the budget was prepared; therefore, the budget assumes this account is operating under the Continuing Appropriations Act, 2018 (Division D of P.L. 115-56, as amended). The amounts included for 2018 reflect the annualized level provided by the continuing resolution. (These amounts are shown only at the Congressional control level and above; below that level, a dash (—) is shown).

[b] APS-U is requested as a line item construction project beginning in FY 2018.

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

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

Construction Projects Summary ($K)

	Total	Prior Years	FY 2017 Enacted	FY 2018 Annualized CR[a]	FY 2019 Request	FY 2019 Request vs FY 2017 Enacted
13-SC-10, Linac Coherent Light Source-II (LCLS-II), SLAC						
TEC	993,100	343,000	190,000	188,710	139,300	-50,700
OPC	51,900	28,600	0	7,900	6,100	+6,100
TPC	**1,045,000**	**371,600[b]**	**190,000**	**196,610**	**145,400**	**-44,600**
18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL						
TEC	770,000	0	0	—	60,000	+60,000
OPC	0	0	0	—	0	0
TPC	**770,000**	**0[c]**	0	—	**60,000**	**+60,000**
19-SC-10, Advanced Light Source Upgrade (ALS-U), LBNL						
TEC	282,000	0	0	—	10,000	+10,000
OPC	38,000	5,000	5,000	—	2,000	-3,000
TPC	**320,000**	**5,000**	**5,000**	—	**12,000**	**+7,000**
19-SC-11, Linac Coherent Light Source-II-HE (LCLS-II-HE), SLAC						
TEC	300,000	0	0	—	5,000	+5,000
OPC	20,000	0	0	—	2,000	+2,000
TPC	**320,000**	0	0	—	**7,000**	**+7,000**
Total, Construction						
TEC	n/a	n/a	190,000	188,710	214,300	+24,300
OPC	n/a	n/a	5,000	7,900	10,100	+5,100
TPC	**n/a**	**n/a**	**195,000**	**196,610**	**224,400**	**+29,400**

[a] A full-year 2018 appropriation for this account was not enacted at the time the budget was prepared; therefore, the budget assumes this account is operating under the Continuing Appropriations Act, 2018 (Division D of P.L. 115-56, as amended). The amounts included for 2018 reflect the annualized level provided by the continuing resolution. (These amounts are shown only at the Congressional control level and above; below that level, a dash (—) is shown).

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

[c] APS-U received $151,000,000 in FY 2010-FY 2017 as an MIE.

Funding Summary ($K)

	FY 2017 Enacted	FY 2018 Annualized CR[a]	FY 2019 Request	FY 2019 Request vs FY 2017 Enacted
Research	755,669	—	746,269	-9,400
Scientific User Facilities Operations	877,331	—	878,331	+1,000
Projects				
Major Items of Equipment	42,500	—	0	-42,500
Construction Projects (includes OPC)	195,000	—	224,400	+29,400
Total Projects	237,500	—	224,400	-13,100
Other[b]	1,000	—	1,000	0
Total, Basic Energy Sciences	**1,871,500**	**1,858,791**	**1,850,000**	**-21,500**

[a] A full-year 2018 appropriation for this account was not enacted at the time the budget was prepared; therefore, the budget assumes this account is operating under the Continuing Appropriations Act, 2018 (Division D of P.L. 115-56, as amended). The amounts included for 2018 reflect the annualized level provided by the continuing resolution. (These amounts are shown only at the Congressional control level and above; below that level, a dash (—) is shown).

[b] Includes 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 2017 Enacted	FY 2018 Annualized CR[a]	FY 2019 Request	FY 2019 Request vs FY 2017 Enacted
TYPE A FACILITIES				
Advanced Light Source	**$64,950**	—	**$64,950**	**$0**
Number of Users	2,129	—	2,000	-129
Achieved operating hours	4,587	—	N/A	N/A
Planned operating hours	4,900	—	4,850	-50
Optimal hours	5,300	—	5,300	0
Percent optimal hours	86.5%	—	91.5%	N/A
Unscheduled downtime hours	<10%	—	<10%	N/A

[a] A full-year 2018 appropriation for this account was not enacted at the time the budget was prepared; therefore, the budget assumes this account is operating under the Continuing Appropriations Act, 2018 (Division D of P.L. 115-56, as amended). The amounts included for 2018 reflect the annualized level provided by the continuing resolution. (These amounts are shown only at the Congressional control level and above; below that level, a dash (—) is shown).

	FY 2017 Enacted	FY 2018 Annualized CR[a]	FY 2019 Request	FY 2019 Request vs FY 2017 Enacted
Advanced Photon Source	**$133,995**	—	**$133,995**	**$0**
Number of Users	5,742	—	5,400	-342
Achieved operating hours	4,936	—	N/A	N/A
Planned operating hours	5,000	—	4,900	-100
Optimal hours	5,000	—	5,000	0
Percent optimal hours	98.7%	—	98.0%	N/A
Unscheduled downtime hours	<10%	—	<10%	N/A
National Synchrotron Light Source-II, BNL	**$111,834**	—	**$111,834**	**$0**
Number of Users	1,037	—	1,100	+63
Achieved operating hours	4,402	—	N/A	N/A
Planned operating hours	4,500	—	4,750	+250
Optimal hours	4,700	—	5,000	+300
Percent optimal hours	93.7%	—	95.0%	N/A
Unscheduled downtime hours	<10%	—	<10%	N/A
Stanford Synchrotron Radiation Lightsource	**$41,986**	—	**$41,986**	**$0**
Number of Users	1,729	—	1,500	-229
Achieved operating hours	5,169	—	N/A	N/A
Planned operating hours	5,100	—	5,000	-100
Optimal hours	5,400	—	5,400	0
Percent optimal hours	95.7%	—	92.6%	N/A
Unscheduled downtime hours	<10%	—	<10%	N/A

[a] A full-year 2018 appropriation for this account was not enacted at the time the budget was prepared; therefore, the budget assumes this account is operating under the Continuing Appropriations Act, 2018 (Division D of P.L. 115-56, as amended). The amounts included for 2018 reflect the annualized level provided by the continuing resolution. (These amounts are shown only at the Congressional control level and above; below that level, a dash (—) is shown).

	FY 2017 Enacted	FY 2018 Annualized CR[a]	FY 2019 Request	FY 2019 Request vs FY 2017 Enacted
Linac Coherent Light Source	**$136,294**	—	**$138,294**	**+$2,000**
Number of Users	766	—	250	-516
Achieved operating hours	3,212	—	N/A	N/A
Planned operating hours	3,000	—	1,350	-1,650
Optimal hours	3,100	—	1,400[b]	-1,700
Percent optimal hours	103.6%	—	96.4%	N/A
Unscheduled downtime hours	<10%	—	<10%	N/A
High Flux Isotope Reactor	**$65,000**	—	**$65,000**	**$0**
Number of Users	511	—	460	-51
Achieved operating hours	4,165	—	N/A	N/A
Planned operating hours	3,900	—	3,750	-150
Optimal hours	4,000	—	4,000	0
Percent optimal hours	104.1%	—	93.8%	N/A
Unscheduled downtime hours	<10%	—	<10%	N/A
Lujan Neutron Scattering Center	**$1,000**	—	**$0**	**-$1,000**
Achieved operating hours	N/A	—	N/A	N/A
Planned operating hours	0	—	0	N/A
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	**$200,000**	—	**$200,000**	**$0**
Number of Users	764	—	780	+16
Achieved operating hours	4,807	—	N/A	N/A
Planned operating hours	4,800	—	4,750	-50
Optimal hours	5,000	—	5,000	0
Percent optimal hours	96.1%	—	95.0%	N/A
Unscheduled downtime hours	<10%	—	<10%	N/A

[a] A full-year 2018 appropriation for this account was not enacted at the time the budget was prepared; therefore, the budget assumes this account is operating under the Continuing Appropriations Act, 2018 (Division D of P.L. 115-56, as amended). The amounts included for 2018 reflect the annualized level provided by the continuing resolution. (These amounts are shown only at the Congressional control level and above; below that level, a dash (—) is shown).

[b] LCLS Optimal hours reduced in preparation for LCLS-II.

	FY 2017 Enacted	FY 2018 Annualized CR[a]	FY 2019 Request	FY 2019 Request vs FY 2017 Enacted
TYPE B FACILITIES				
Center for Nanoscale Materials	**$25,205**	—	**$25,205**	**$0**
Number of users	598	—	500	-98
Center for Functional Nanomaterials	**$21,418**	—	**$21,418**	**$0**
Number of users	571	—	500	-71
Molecular Foundry	**$28,406**	—	**$28,406**	**$0**
Number of users	866	—	600	-266
Center for Nanophase Materials Sciences	**$24,638**	—	**$24,638**	**$0**
Number of users	666	—	500	-166
Center for Integrated Nanotechnologies	**$22,605**	—	**$22,605**	**$0**
Number of users	614	—	500	-114
Total, All Facilities	**$877,331**	—	**$878,331**	**+$1,000**
Number of Users	15,993	—	14,090	-1,903
Achieved operating hours	31,278	—	N/A	N/A
Planned operating hours	31,200	—	29,350	-1,850
Optimal hours	32,500	—	31,100	-1,400
Percent of optimal hours	97.4%	—	95.3%	N/A
Unscheduled downtime hours	<10%	—	<10%	N/A

[a] A full-year 2018 appropriation for this account was not enacted at the time the budget was prepared; therefore, the budget assumes this account is operating under the Continuing Appropriations Act, 2018 (Division D of P.L. 115-56, as amended). The amounts included for 2018 reflect the annualized level provided by the continuing resolution. (These amounts are shown only at the Congressional control level and above; below that level, a dash (—) is shown).

Scientific Employment

	FY 2017 Enacted	FY 2018 Annualized CR[a]	FY 2019 Request	FY 2019 Request vs FY 2017 Enacted
Number of permanent Ph.D.'s (FTEs)	4,460	—	4,410	-50
Number of postdoctoral associates (FTEs)	1,180	—	1,200	20
Number of graduate students (FTEs)	1,810	—	1,870	60
Other[b]	2,900	—	2,810	-90

[a] A full-year 2018 appropriation for this account was not enacted at the time the budget was prepared; therefore, the budget assumes this account is operating under the Continuing Appropriations Act, 2018 (Division D of P.L. 115-56, as amended). The amounts included for 2018 reflect the annualized level provided by the continuing resolution. (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 2018 CPDS and does not include a new start for the budget year. There are no significant changes to the project.

Summary

The FY 2019 Request for the Linac Coherent Light Source-II (LCLS-II) is $145,400,000, including $139,300,000 in Total Estimated Cost (TEC) funds and $6,100,000 in Other Project Costs (OPC) funds, consistent with the approved baseline funding profile. FY 2019 will be the last year of construction funding for the project. The most recent DOE Order 413.3B approved Critical Decisions (CD) are CD-2/3, (Approve Performance Baseline and Approve Start of Construction), which were approved on March 21, 2016.

A Federal Project Director, certified to level IV, 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 2017 funding supported critical procurement of materials and equipment needed to maintain the project schedule and expand the construction efforts. Design, long lead and advance procurements (LLP/APs), R&D, prototyping, site preparation activities, fabrication, and installation also continued 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 will carry forward into FY 2019 and beyond until they have been completed. FY 2019 funding will be used to complete installation of all major accelerator and x-ray systems and facilities including the linear accelerator and its cryogenic refrigeration facilities, electron beam transport, undulator x-ray sources, x-ray optics, and experimental systems and supporting infrastructure.

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
FY 2019	4/22/2010	1/21/2014	8/22/2014	3/21/2016	4Q FY 2018	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
FY 2019	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	47,000	946,100	993,100	51,900	N/A	51,900	1,045,000
FY 2019[b]	47,000	946,100	993,100	51,900	N/A	51,900	1,045,000

4. Project Scope and Justification

Scope

SLAC's 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

[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.

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.

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 three kilometer linac is being used to operate the LCLS facility, and the first two 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 feet.

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 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 Order 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])	$5x10^8$ (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	6,040
FY 2018	0	0	2,331
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[b]	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	226,933
FY 2018	182,100	182,100	270,000
FY 2019	139,300	139,300	180,000
FY 2020	0	0	1,576
Total, Line item construction funding	886,100	886,100	886,100
Total, Construction phase	946,100	946,100	946,100
TEC			
MIE funding			
FY 2012	44,500[c]	22,000	15,862
FY 2013[b]	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

[a] Costs through FY 2017 reflect actual costs; costs for FY 2018 and the outyears are estimates.
[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 LCLC-II project during FY 2013.

	(dollars in thousands)		
	Appropriations	Obligations	Costs[a]
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	232,973
FY 2018	182,100	182,100	272,331
FY 2019	139,300	139,300	180,000
FY 2020	0	0	1,576
Total, Line item construction funding	926,100	926,100	926,100
Total, TEC[b]	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[c]	0	0	116
FY 2014	0	0	439
FY 2015	0	0	10
FY 2016	0	0	0
FY 2017	0	0	0
FY 2018	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	758
FY 2018	7,900	7,900	12,000
FY 2019	6,100	6,100	9,000
FY 2020	0	0	716
Total, Line item construction funding	33,300	33,300	33,300
Total, OPC	51,900	51,900	51,900
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	30,000	24,755
FY 2013[c]	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	4
FY 2018	0	0	171
Total, MIE funding	85,600	85,600	85,600

[a] Costs through FY 2017 reflect actual costs; costs for FY 2018 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.
[c] 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]
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	233,731
FY 2018	190,000	190,000	284,331
FY 2019	145,400	145,400	189,000
FY 2020	0	0	2,292
Total, Line item construction funding	959,400	959,400	959,400
Total, TPC[b]	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	43,200	42,400	42,125
Contingency	3,800	4,600	4,875
Total, Design	47,000	47,000	47,000
Construction			
Site Preparation	24,700	24,700	24,700
Equipment	776,112	692,742	678,205
Other Construction	58,500	58,500	58,500
Contingency	86,788	170,158	184,695
Total, Construction	946,100	946,100	946,100
Total, TEC[b]	993,100	993,100	993,100
Contingency, TEC	90,588	174,758	189,570
Other Project Cost (OPC)			
OPC except D&D			
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	99,338	183,508	198,320

[a] Costs through FY 2017 reflect actual costs; costs for FY 2018 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.

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	TEC	22,000	TBD	TBD	TBD	TBD	TBD	TBD	TBD	TBD
(MIE)	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]	TEC	165,800	94,000	105,300	19,900	0	0	0	0	385,000
(MIE)	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	199,919	182,100	129,381	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	199,919	190,000	135,481	0	0	1,045,000
FY 2019	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)

	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.

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

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 determined that the LCLS-II project was to be acquired by the SLAC National Accelerator Laboratory under the existing DOE M&O contract.

A Conceptual Design Report for the LCLS-II project was completed and was revised based on the new technical parameters. Key design activities, requirements, and high-risk subsystem components were 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 is for Design and Construction

1. Significant Changes and Summary

Significant Changes

This Construction Project Data Sheet (CPDS) is an update of the FY 2018 CPDS and does not include a new start for the budget year. The FY 2018 CPDS included removal and installation of storage ring components in preparation for commissioning as part of Other Project Costs (OPC) in FY 2021-2023. These activities are properly classified as construction costs and included in Total Estimated Cost (TEC). The FY 2019 CPDS has been updated for this change. The preliminary estimate for Total Project Cost (TPC) of $770,000,000 is unchanged.

Summary

The FY 2019 Request for the Advanced Photon Source-Upgrade (APS-U) project is $60,000,000. The most recent DOE Order 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, certified to level IV, has been assigned to this project and has approved this CPDS.

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 2017, APS-U continued with R&D, engineering design, pre-production prototyping, fabrication, and initiated long lead and advanced procurements (LLP/APs) of critical systems. In FY 2018 funding will support targeted R&D, engineering design, equipment prototyping, testing, fabrication, site preparation, installation, and additional LLP/APs. Planned activities for FY 2019 include targeted R&D, engineering design, equipment prototyping, testing, fabrication, site preparation, installation, 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	04/22/2010	09/18/2015	02/04/2016	1Q FY 2019	2Q FY 2020	4Q FY 2019	N/A	1Q FY 2026
FY 2019[a]	04/22/2010	09/18/2015	02/04/2016	2Q FY 2019	4Q FY 2021	1Q FY 2020	N/A	2Q 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)

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

CD-3 – Approve Start of Construction
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
FY 2019	2Q 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	157,015	561,985	719,000	51,000	N/A	51,000	770,000
FY 2019[a]	167,000	590,100	757,100	12,900	N/A	12,900	770,000

4. Project Scope and Justification

Scope

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, the U.S. Department of Energy's (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 capability on the existing APS facility, for significantly less than the replacement cost of the 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 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 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

The BES 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 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 Order 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. The KPPs presented here are preliminary and may change as the project continues towards CD-2. 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

[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	16,441
FY 2018	0	0	14,000
FY 2019	0	0	8,941
Total, MIE funding	121,215	121,215	121,215
Line item construction funding			
FY 2018	9,300	9,300	8,500
FY 2019	27,985	27,985	26,000
FY 2020	8,500	8,500	8,000
FY 2021	0	0	2,885
FY 2022	0	0	400
Total, Line item construction funding	45,785	45,785	45,785
Total, Design phase	167,000	167,000	167,000
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	7,046
FY 2018	0	0	5,454
Total, MIE funding	21,285	21,285	21,285
Line item construction funding			
FY 2018	10,700	10,700	9,500
FY 2019	32,015	32,015	31,515
FY 2020	141,500	141,500	130,600
FY 2021	159,780	159,780	150,000
FY 2022	133,100	133,100	125,500
FY 2023	91,720	91,720	82,000
FY 2024	0	0	26,000
FY 2025	0	0	13,700
Total, Line item construction funding	568,815	568,815	568,815
Total, Construction phase	590,100	590,100	590,100

	(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	42,500	42,500	23,487
FY 2018	0	0	19,454
FY 2019	0	0	8,941
Total, MIE funding	142,500	142,500	142,500
Line item construction funding			
FY 2018	20,000	20,000	18,000
FY 2019	60,000	60,000	57,515
FY 2020	150,000	150,000	138,600
FY 2021	159,780	159,780	152,885
FY 2022	133,100	133,100	125,900
FY 2023	91,720	91,720	82,000
FY 2024	0	0	26,000
FY 2025	0	0	13,700
Total, Line item construction funding	614,600	614,600	614,600
Total, TEC	757,100	757,100	757,100
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 2022	2,200	2,200	2,000
FY 2023	2,200	2,200	2,000
FY 2024	0	0	400
Total, Line item construction funding	4,400	4,400	4,400
Total, OPC	12,900	12,900	12,900

	(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	42,500	42,500	23,487
FY 2018	0	0	19,454
FY 2019	0	0	8,941
Total, MIE funding	151,000	151,000	151,000
Line item construction funding			
FY 2018	20,000	20,000	18,000
FY 2019	60,000	60,000	57,515
FY 2020	150,000	150,000	138,600
FY 2021	159,780	159,780	152,885
FY 2022	135,300	135,300	127,900
FY 2023	93,920	93,920	84,000
FY 2024	0	0	26,400
FY 2025	0	0	13,700
Total, Line item construction funding	619,000	619,000	619,000
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	157,150	151,375	N/A
Contingency	9,850	5,640	N/A
Total, Design	167,000	157,015	N/A
Construction			
Equipment	426,420	395,625	N/A
Other Construction	14,680	12,700	N/A
Contingency	149,000	153,660	N/A
Total, Construction	590,100	561,985	N/A
Total, TEC	757,100	719,000	N/A
Contingency, TEC	158,850	159,300	N/A

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Other Project Cost (OPC)			
OPC except D&D			
Conceptual Planning	1,000	1,000	N/A
Conceptual Design	7,500	7,500	N/A
Start-Up	3,250	31,800	N/A
Contingency	1,150	10,700	N/A
Total, OPC	12,900	51,000	N/A
Contingency, OPC	1,150	10,700	N/A
Total, TPC	770,000	770,000	N/A
Total, Contingency	160,000	170,000	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	TEC	80,000	20,000	42,500	20,000	81,772	152,419	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	42,500	20,000	81,772	152,419	165,000	199,809	770,000
FY 2019[a]	TEC	80,000	20,000	42,500	20,000	60,000	150,000	159,780	224,820	757,100
	OPC	8,500	0	0	0	0	0	0	4,400	12,900
	TPC	88,500	20,000	42,500	20,000	60,000	150,000	159,780	229,220	770,000

8. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy (fiscal quarter or date)	2Q FY 2026
Expected Useful Life (number of years)	25
Expected Future Start of D&D of this capital asset (fiscal quarter)	2Q 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	$12M	N/A	$300M	N/A

The numbers presented are the incremental lifecycle operations and maintenance costs above the existing APS. The estimate will be updated and additional details will be provided after CD-2, Approve Project Performance Baseline.

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

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

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 the Argonne National Laboratory (ANL) under the existing DOE 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 MBA magnet lattice, insertion devices, front ends, beamlines/experimental stations, and any required modifications to the linac, booster, and 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.

19-SC-10, Advanced Light Source Upgrade
Lawrence Berkeley National Laboratory, Berkeley, California
Project is for Design and Construction

1. Significant Changes and Summary

Significant Changes
This Construction Project Data Sheet (CPDS) is new and includes a new start for the budget year.

Summary
The FY 2019 Request for the Advanced Light Source Upgrade (ALS-U) project is $12,000,000, including $10,000,000 in Total Estimated Cost (TEC) funds and $2,000,000 in Other Project Costs (OPC) funds. The most recent DOE Order 413.3B approved Critical Decisions (CD) is CD-0 (Approve Mission Need), approved September 27, 2016. The preliminary total project cost (TPC) range, based on early concepts under consideration, is $260,000,000 - $420,000,000.

A Federal Project Director, certified to level III, has been assigned to this project and has approved this CPDS.

The ALS-U project will upgrade the existing ALS facility by replacing the existing electron storage ring with a new electron storage ring based on a multi-bend achromat lattice design to provide a soft x-ray source that is orders of magnitudes brighter—a 10-1000 times increase in brightness over the current ALS—and to provide a significantly higher fraction of coherent light in the soft x-ray region (~50-2,000 eV) than is currently available at ALS. With an aggressive accelerator design, ALS-U will provide the highest coherent flux of any existing or planned storage ring facility worldwide, up to a photon energy of about 3.5 keV. This range covers the entire soft x-ray regime. To make use of the new source, the project may also include construction activities to build new beamlines or reconfigure existing beamlines. The ALS-U project is the most cost effective way to meet the soft x-ray capability gap stated in the mission need statement at this stage of project development.

FY 2019 funding will be used for planning, engineering design, R&D and prototyping activities.

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 2019[a]	9/27/2016	4Q FY 2019	4Q FY 2019	4Q FY 2020	4Q FY 2022	4Q FY 2021	N/A	4Q 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 Alternative Selection and Cost Range
CD-2 – Approve Performance Baseline
Final Design Complete – Estimated/Actual date the project design will be/was completed
CD-3 – Approve Start of Construction
D&D Complete – Completion of D&D work
CD-4 – Approve Start of Operations or Project Closeout

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

	Performance Baseline Validation	CD-3A
FY 2019[a]	4Q FY 2020	4Q FY 2020

CD-3A – Approve Long-Lead Procurements: As the project planning and design matures, long lead procurement may be requested in FY 2020 to mitigate cost and schedule risk to the project.

3. Project Cost History

(dollars in thousands)

	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, D&D	OPC, Total	TPC
FY 2019[a]	39,000	243,000	282,000	38,000	N/A	38,000	320,000

4. Project Scope and Justification

Scope

The ALS-U project will upgrade the existing ALS facility by replacing the existing electron storage ring with a new electron storage ring based on a multi-bend achromat (MBA) lattice design to provide a soft x-ray source that is orders of magnitudes brighter—a 10-1000 times increase in brightness over the current ALS—and to provide a significantly higher fraction of coherent light in the soft x-ray region (~50-2,000 eV) than is currently available at ALS. The project will replace the existing triple-bend achromat storage ring with a new, high-performance storage ring based on a nine-bend achromat design. In addition, the project will add a low-emittance, full-energy accumulator ring to the existing tunnel to enable on-axis, swap-out injection using fast kicker magnets. The new source will require upgrading x-ray optics on existing beamlines with some beamlines being realigned or relocated. The project adds three new undulator beamlines that are optimized for the novel science made possible by the beam's new high coherent flux. If possible, the project intends to reuse the existing building, utilities, electron gun, linac, and booster synchrotron equipment currently at ALS. Related scope may be added as necessary to optimize the final design and provide the maximum performance achievable to support the science needs and goals contained in the Mission Need Statement. With an aggressive accelerator design, ALS-U will provide the highest coherent flux of any existing or planned storage ring facility worldwide, up to a photon energy of about 3.5 keV. This range covers the entire soft x-ray regime.

Justification

At this time, our ability to observe and understand materials and material phenomena in real-time and as they emerge and evolve is limited. Soft x-rays (~50 to 2,000 eV) are ideally suited for revealing the chemical, electronic, and magnetic properties of materials, as well as the chemical reactions that underpin these properties. This knowledge is crucial for the design and control of new advanced materials that address the challenges of new energy technologies.

Existing storage ring light sources lack a key attribute that would revolutionize x-ray science: stable, nearly continuous soft x-rays with high brightness and high coherent flux—that is, smooth, well organized soft x-ray wave fronts. Such a stable, high brightness, high coherent flux source would enable 3D imaging with nanometer resolution and the measurement of spontaneous nanoscale motion with nanosecond resolution—all with electronic structure sensitivity.

Currently the Office of Basic Energy Sciences (BES) operates advanced ring-based light sources that produce soft x-rays. The National Synchrotron Light Source-II (NSLS-II), commissioned in 2015, is the brightest soft x-ray source in the U.S. The ALS, completed in 1993, is competitive with NSLS-II for x-rays below 200 eV but not above that. NSLS-II is somewhat lower in brightness than the new Swedish light source, MAX-IV, which is currently under commissioning and represents the first use of a MBA lattice design in a light source facility. Neither NSLS-II nor ALS make use of the newer MBA lattice design.

[a] The project is pre-CD-2 and is not baselined. The cost and schedule shown are preliminary and may change as the project matures towards CD-2. Construction will not be executed without appropriate CD approvals.

Switzerland's SLS-2 (an MBA-based design in the planning stage) will be a brighter soft x-ray light source than both NSLS-II and MAX-IV when it is built and brought into operation. These international light sources, and those that follow, will present a significant challenge to U.S. light source community to provide competitive x-ray sources to domestic users. Neither NSLS-II nor ALS soft x-ray light sources possess sufficient brightness or coherent flux to provide the capability to meet the mission need in their current configurations.

BES is currently supporting two major light source upgrade projects, the Advanced Photon Source-Upgrade (APS-U) and the Linac Coherent Light Source-II (LCLS-II). These two projects will upgrade existing x-ray facilities in the U.S. and will provide significant increases in brightness and coherent flux. These upgrades will not address the specific research needs that demand stable, nearly continuous soft x-rays with high brightness and high coherence.

APS-U (in planning and design) will deploy the MBA lattice design optimized for its higher 6 GeV electron energy and to produce higher energy (hard) x-rays in the range of 10-100 keV. Because the ring will be optimized for high energy, the soft x-ray light it produces will not be sufficiently bright to meet the research needs described above.

LCLS-II (under construction) is a high repetition rate (up to 1 MHz) free electron laser (FEL) designed to produce high brightness, coherent x-rays, but in extremely short bursts rather than as a nearly continuous beam. Storage rings offer higher stability than FELs. In addition, there is a need for a facility that can support a larger number of concurrent experiments than LCLS-II can in its current configuration. This is critical for serving the large and expanding soft x-ray research community. LCLS-II will not meet this mission need.

The ALS is a 1.9 GeV storage ring operating at 500 mA of beam current. It is optimized to produce intense beams of soft x-rays, which offer spectroscopic contrast, nanometer-scale resolution, and broad temporal sensitivity. The ALS facility includes an accelerator complex and photon delivery system that are capable of providing the foundations for an upgrade that will achieve world-leading soft x-ray coherent flux. The existing ALS provides a ready-made foundation, including conventional facilities, a $500M scientific infrastructure investment and a vibrant user community of over 2,500 users per year already attuned to the potential scientific opportunities an upgrade offers. The facility also includes extensive (up to 40) simultaneously operating beamlines and instrumentation, an experimental hall, computing resources, ancillary laboratories, offices, and related infrastructure that will be heavily utilized in an upgrade scenario. Furthermore, the upgrade leverages the ALS staff, who are experts in the scientific and technical aspects of the proposed upgrade.
In summary, the capabilities at our existing x-ray light source facilities are insufficient to develop the next generation of tools that combine high resolution spatial imaging together with precise energy resolving spectroscopic techniques in the soft x-ray range. To enable these cutting edge experimental techniques, it is necessary to possess an ultra-bright source of soft x-ray light that generates the high coherent x-ray flux required to resolve nanometer-scale features and interactions, and to allow the real-time observation and understanding of materials and phenomena as they emerge and evolve. Developing such a light source will ensure the U.S. has the tools to maintain its leadership in soft x-ray science and will significantly accelerate the advancement of the fundamental sciences that underlie a broad range of emerging and future energy applications.

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

<u>Key Performance Parameters (KPPs)</u>
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. The KPPs presented here are preliminary and may change as the project continues towards CD-2. The final key parameters will be established as part of CD-2, Approve Project Performance Baseline.

Preliminary Key Performance Parameters

Performance Measure	Threshold	Objective
Storage Ring Energy	≥ 1.9 GeV	2.0 GeV
Beam Current	> 25 mA	500 mA
Horizontal Emittance	< 150 pm-rad	<75 pm-rad
Brightness @ 1 keV[1]	> 2×10^{19}	2×10^{21}
New MBA Beamlines	2	3

5. Preliminary Financial Schedule

	(dollars in thousands)		
	Appropriations	Obligations	Costs
Total Estimated Cost (TEC)			
Design			
FY 2019	6,000	6,000	2,000
FY 2020	15,000	15,000	13,000
FY 2021	12,000	12,000	12,000
FY 2022	6,000	6,000	9,000
FY 2023	0	0	3,000
Total, Design	39,000	39,000	39,000
Construction			
FY 2019	4,000	4,000	4,000
FY 2020	11,540	11,540	11,000
FY 2021	20,640	20,640	20,000
FY 2022	45,560	45,560	45,000
FY 2023	63,530	63,530	65,000
FY 2024	63,350	63,350	60,000
FY 2025	34,380	34,380	30,000
FY 2026	0	0	8,000
Total, Construction	243,000	243,000	243,000
TEC			
FY 2019	10,000	10,000	6,000
FY 2020	26,540	26,540	24,000
FY 2021	32,640	32,640	32,000
FY 2022	51,560	51,560	54,000
FY 2023	63,530	63,530	68,000
FY 2024	63,350	63,350	60,000
FY 2025	34,380	34,380	30,000
FY 2026	0	0	8,000
Total, TEC	282,000	282,000	282,000

	(dollars in thousands)		
	Appropriations	Obligations	Costs
Other Project Cost (OPC)			
OPC except D&D			
FY 2016	5,000	5,000	1,500
FY 2017	5,000	5,000	5,500
FY 2018	0	0	3,000
FY 2019	2,000	2,000	2,000
FY 2020	5,000	5,000	5,000
FY 2021	0	0	0
FY 2022	0	0	0
FY 2023	5,000	5,000	3,000
FY 2024	6,000	6,000	6,000
FY 2025	10,000	10,000	8,000
FY 2026	0	0	4,000
Total, OPC	38,000	38,000	38,000
Total Project Cost (TPC)			
FY 2016	5,000	5,000	1,500
FY 2017	5,000	5,000	5,500
FY 2018	0	0	3,000
FY 2019	12,000	12,000	8,000
FY 2020	31,540	31,540	29,000
FY 2021	32,640	32,640	32,000
FY 2022	51,560	51,560	54,000
FY 2023	68,530	68,530	71,000
FY 2024	69,350	69,350	66,000
FY 2025	44,380	44,380	38,000
FY 2026	0	0	12,000
Total, TPC[a]	320,000	320,000	320,000

6. Details of Preliminary Project Cost Estimate

	(dollars in thousands)		
	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design			
Design	30,000	N/A	N/A
Contingency	9,000	N/A	N/A
Total, Design	39,000	N/A	N/A
Construction		N/A	N/A
Site Preparation	5,000	N/A	N/A
Equipment	170,000	N/A	N/A
Other Construction	0	N/A	N/A
Contingency	68,000	N/A	N/A
Total, Construction	243,000	N/A	N/A
Total, TEC	282,000	N/A	N/A
Contingency, TEC	77,000	N/A	N/A

[a] The project is pre-CD-2 and is not baselined. The cost and schedule shown are preliminary and may change as the project matures towards CD-2. Construction will not be executed without appropriate CD approvals.

	(dollars in thousands)		
	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Other Project Cost (OPC)		N/A	N/A
OPC except D&D		N/A	N/A
Conceptual Planning	2,000	N/A	N/A
Conceptual Design	12,000	N/A	N/A
Research and Development	10,000	N/A	N/A
Start-Up	6,000	N/A	N/A
Contingency	8,000	N/A	N/A
Total, OPC	38,000	N/A	N/A
Contingency, OPC	8,000	N/A	N/A
Total, TPC[a]	320,000	N/A	N/A
Total, Contingency	85,000	N/A	N/A

7. Schedule of Appropriations Requests

(dollars in thousands)

Request		Prior Years	FY 2019	FY 2020	FY 2021	FY 2022	FY 2023	FY 2024	Outyears	Total
FY 2019	TEC	0	10,000	26,540	32,640	51,560	63,530	63,350	34,380	282,000
	OPC	10,000	2,000	5,000	0	0	5,000	6,000	10,000	38,000
	TPC	10,000	12,000	31,540	32,640	51,560	68,530	69,350	44,380	320,000

8. Related Operations and Maintenance Funding Requirements

Operations and maintenance funding requirements will be provided when the project receives CD-2 approval.

9. D&D Information

At this stage of project planning and development, it is anticipated that there will be no new area being constructed in the construction project.

10. Preliminary Acquisition Approach

DOE has determined that the ALS-U project will be acquired by the Lawrence Berkeley National Laboratory under the existing DOE M&O contract.

A Conceptual Design Report for the ALS-U project will be prepared. 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 will be fully up-to-date, operating, and are maintained as a LBNL-wide resource.

LBNL may partner with other 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 ALS actual costs and other similar facilities, to the extent practicable. Recent cost data from similar projects will be exploited fully in planning and budgeting for the project. Design of the technical systems will be completed by LBNL 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.

Lessons learned from other Office of Science projects and other similar facilities will be exploited fully in planning and executing ALS-U.

[a] The project is pre-CD-2 and is not baselined. The cost and schedule shown are preliminary and may change as the project matures towards CD-2. Construction will not be executed without appropriate CD approvals.

19-SC-11, Linac Coherent Light Source-II High Energy
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 new and includes a new start for the FY 2019 budget year.

Summary

The FY 2019 Request for the Linac Coherent Light Source-II High Energy (LCLS-II-HE) project is $7,000,000, including $5,000,000 in Total Estimated Cost (TEC) funds and $2,000,000 in Other Project Costs (OPC) funds. The most recent DOE Order 413.3B approved Critical Decisions (CD) is CD-0 (Approve Mission Need), approved on December 15, 2016. The preliminary total project cost (TPC) range, based on early concepts under consideration, is $260,000,000 - $450,000,000.

A Federal Project Director, certified to level IV, has been assigned to this project and has approved this CPDS.

The Linac Coherent Light Source-II High Energy (LCLS-II-HE) project will increase the energy of the superconducting linac currently under construction as part of the LCLS-II project from 4 GeV to 8 GeV. To make use of the new source, the project may also include construction activities to build new beamlines or reconfigure existing beamlines. The project will upgrade the facility infrastructure as needed. The LCLS-II-HE project is the most cost effective way to meet the hard x-ray capability gap described in the mission need statement.

FY 2019 funding will be used for planning, engineering, design, R&D, prototyping activities, and long lead procurements.

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 2019[a]	12/15/2016	3Q FY 2019	3Q FY 2019	1Q FY 2021	1Q FY 2023	2Q FY 2022	N/A	2Q 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 Alternative Selection and Cost Range
CD-2 – Approve Performance Baseline
Final Design Complete – Estimated/Actual date the project design will be/was completed
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
FY 2019[a]	1Q FY 2021	4Q FY 2019

CD-3A – Approve Long-Lead Procurements: As the project planning and design matures, long lead procurement may be requested in FY 2019 to mitigate cost and schedule risk to the project.

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

3. Project Cost History

(dollars in thousands)

	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, D&D	OPC, Total	TPC
FY 2019[a]	34,000	266,000	300,000	20,000	N/A	20,000	320,000

4. Project Scope and Justification

Scope

There is a limited ability to observe and understand the structural dynamics of complex matter at the atomic scale with hard x-rays, at ultrafast time scales, and in operational environments. Overcoming this capability gap is crucial for the design, control and understanding of new advanced materials necessary to develop new energy technologies. To achieve this objective, the Department needs a hard x-ray source capable of producing high energy ultrafast bursts, with full spatial and temporal coherence, at high repetition rates. Possession of a hard x-ray source with a photon energy range from 5 keV to 12 keV and beyond would enable spectroscopic analysis of additional key elements in the periodic table, deeper penetration into materials, and enhanced resolution. This capability cannot be provided by any existing or planned light source.

The Linac Coherent Light Source-II (LCLS-II) project at SLAC National Accelerator Laboratory (SLAC), which is currently under construction and will begin operations in 2020-2021, only partially addresses this capability gap. LCLS-II will be the premier x-ray free electron laser (XFEL) facility in the world at energies ranging from 200 eV up to approximately 5 keV. The cryomodule technology that underpins LCLS-II is a major advance from prior designs that will allow continuous operation up to 1 MHz.

When completed, LCLS-II will be powered by SLAC's 4 GeV superconducting electron linear accelerator (linac). Over the past years, the cryomodule design for LCLS-II has performed beyond expectations, providing the technical basis to double the electron beam energy. It is therefore conceivable to add additional acceleration capacity at SLAC to double the electron beam energy from 4 GeV to 8 GeV. Calculations indicate that an 8 GeV linac will deliver a hard x-ray photon beam with peak energy of 12.8 keV, which will meet the mission need.

The LCLS-II High Energy (LCLS-II-HE) project will upgrade the LCLS-II to maintain U.S. leadership in XFEL science. The upgrade will provide world leading experimental capabilities for the U.S. research community by extending the x-ray energy of LCLS-II from 5 keV to 12 keV and beyond. The flexibility and detailed pulse structure associated with the proposed LCLS-II-HE facility will not be matched by other facilities under development worldwide.

The LCLS-II-HE project will increase the superconducting linac energy from 4 GeV to 8 GeV by installing additional cryomodules in the first kilometer of the existing linac tunnel. The electron beam will be transported to the existing undulator hall to extend the x-ray energy to 12 keV and beyond. The project will also modify or upgrade existing infrastructure and x-ray transport, optics and diagnostics system, and provide new or upgraded instrumentation to augment existing and planned capabilities.

Justification

The leadership position of LCLS-II will be challenged by the European XFEL at DESY in Hamburg, Germany, which began operations in 2017. The European XFEL has a higher electron energy, which allows production of shorter (i.e., harder) x-ray wavelength pulses compared to LCLS-II. More recent plans emerging from DESY have revealed how the European XFEL could be extended from a pulsed operation mode to continuous operation, which would create a profound capability gap compared to LCLS-II. The continuous operation improves the stability of the electron beam and provides uniformly spaced

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

pulses of x-rays or, if desired, the ability to customize the sequence of x-ray pulses provided to experiments to optimize the measurements being made.

In the face of this challenge to U.S. scientific leadership, extending the energy reach of x-rays beyond the upper limit of LCLS-II (5 keV) is a high priority. 12 keV x-rays correspond to an x-ray wavelength of approximately 1 Ångstrom, which is particularly important for high resolution structural determination experiments since this is the characteristic distance between bound atoms in matter. Expanding the photon energy range beyond 5 keV will allow U.S. researchers to probe earth-abundant elements that will be needed for large-scale deployment of photo-catalysts for electricity and fuel production; it allows the study of strong spin-orbit coupling that underpins many aspects of quantum materials; and it reaches the biologically important selenium k-edge, used for protein crystallography.

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 facility is by upgrading the LCLS-II, currently under construction at SLAC, by increasing the energy of the superconducting accelerator and upgrading the existing infrastructure and instrumentation.

The project is being conducted in accordance with the project management requirements in DOE Order 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. The KPPs presented here are preliminary and may change as the project continues towards CD-2. The final key parameters will be established as part of CD-2, Approve Project Performance Baseline.

Preliminary Key Performance Parameters

Performance Parameters	Threshold	Objective
Superconducting linac electron beam energy	≥ 7 GeV	≥ 8 GeV
Electron bunch repetition rate	93 kHz	929 kHz
Superconducting linac charge per bunch	0.02 nC	0.1 nC
Photon beam energy range	200 to ≥ 8,000 eV	200 to ≥ 12,000 eV
High repetition rate capable, hard X-ray end stations	≥ 3	≥ 5
FEL photon quantity (10^{-3} BW)	$5x10^{8}$ (10x spontaneous @8 keV)	> 10^{11} @ 12 keV

5. Preliminary Financial Schedule

	(dollars in thousands)		
	Appropriations	Obligations	Costs
Total Estimated Cost (TEC)			
Design			
FY 2019	2,000	2,000	2,000
FY 2020	8,000	8,000	8,000
FY 2021	10,000	10,000	10,000
FY 2022	10,000	10,000	10,000
FY 2023	4,000	4,000	4,000
Total, Design	34,000	34,000	34,000

	(dollars in thousands)		
	Appropriations	Obligations	Costs
Construction			
FY 2019	3,000	3,000	3,000
FY 2020	12,060	12,060	12,000
FY 2021	15,000	15,000	15,000
FY 2022	40,000	40,000	40,000
FY 2023	57,375	57,375	55,000
FY 2024	78,000	78,000	78,000
FY 2025	60,565	60,565	55,000
FY 2026	0	0	8,000
Total, Construction	266,000	266,000	266,000
TEC			
FY 2019	5,000	5,000	5,000
FY 2020	20,060	20,060	20,000
FY 2021	25,000	25,000	25,000
FY 2022	50,000	50,000	50,000
FY 2023	61,375	61,375	59,000
FY 2024	78,000	78,000	78,000
FY 2025	60,565	60,565	55,000
FY 2026	0	0	8,000
Total, TEC	300,000	300,000	300,000
Other Project Cost (OPC)			
OPC except D&D			
FY 2019	2,000	2,000	2,000
FY 2020	4,000	4,000	3,000
FY 2021	0	0	1,000
FY 2022	0	0	0
FY 2023	0	0	0
FY 2024	4,000	4,000	4,000
FY 2025	10,000	10,000	9,000
FY 2026	0	0	1,000
Total, OPC	20,000	20,000	20,000
Total Project Cost (TPC)			
FY 2019	7,000	7,000	7,000
FY 2020	24,060	24,060	23,000
FY 2021	25,000	25,000	26,000
FY 2022	50,000	50,000	50,000
FY 2023	61,375	61,375	59,000
FY 2024	82,000	82,000	82,000
FY 2025	70,565	70,565	64,000
FY 2026	0	0	9,000
Total, TPC[a]	320,000	320,000	320,000

[a] The project is pre-CD-2 and is not baselined. The cost and schedule shown are preliminary and may change as the project matures towards CD-2. Construction will not be executed without appropriate CD approvals.

6. Details of Preliminary Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design			
Design	30,500	N/A	N/A
Contingency	3,500	N/A	N/A
Total, Design	34,000	N/A	N/A
Construction			
Site Preparation	3,000	N/A	N/A
Equipment	182,000	N/A	N/A
Other Construction	9,000	N/A	N/A
Contingency	72,000	N/A	N/A
Total, Construction	266,000	N/A	N/A
Total, TEC	300,000	N/A	N/A
Contingency, TEC	75,500	N/A	N/A
Other Project Cost (OPC)			
OPC except D&D			
Conceptual Planning	1,500	N/A	N/A
Conceptual Design	4,000	N/A	N/A
Research and Development	4,000	N/A	N/A
Start-Up	8,000	N/A	N/A
Contingency	2,500	N/A	N/A
Total, OPC	20,000	N/A	N/A
Contingency, OPC	2,500	N/A	N/A
Total, TPC[a]	320,000	N/A	N/A
Total, Contingency	78,000	N/A	N/A

7. Schedule of Appropriations Requests

(dollars in thousands)

Request		Prior Years	FY 2019	FY 2020	FY 2021	FY 2022	FY 2023	FY 2024	Outyears	Total
FY 2019	TEC	0	5,000	20,060	25,000	50,000	61,375	78,000	60,565	300,000
	OPC	0	2,000	4,000	0	0	0	4,000	10,000	20,000
	TPC	0	7,000	24,060	25,000	50,000	61,375	82,000	70,565	320,000

8. Related Operations and Maintenance Funding Requirements

Operations and maintenance funding requirements will be provided when the project receives CD-2 approval.

9. D&D Information

At this stage of project planning and development, it is anticipated that there will be no new area being constructed in the construction project.

[a] The project is pre-CD-2 and is not baselined. The cost and schedule shown are preliminary and may change as the project matures towards CD-2. Construction will not be executed without appropriate CD approvals.

10. Preliminary Acquisition Approach

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

A Conceptual Design Report for the LCLS-II-HE project will be prepared. 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 will be fully up-to-date, operating, and are maintained as a SLAC-wide resource.

SLAC may partner with other 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-II 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.

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