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. BES accomplishes its mission through excellence in scientific discovery in the energy sciences, and through stewardship of world-class scientific user facilities that enable cutting-edge research and development.

The research disciplines that BES supports—condensed matter and materials physics, chemistry, geosciences, and aspects of biosciences—touch virtually every important aspect of energy resources, production, conversion, transmission, storage, efficiency, and waste mitigation, providing a knowledge base for achieving a secure and sustainable energy future. The 2018 Basic Energy Sciences Advisory Committee (BESAC) report, "A Remarkable Return on Investment in Fundamental Research",[a] provides key examples of major technological, commercial, and national security impacts directly traceable to BES-supported basic research. This mission-relevance of BES research results from a long-standing established strategic planning process, which encompasses BESAC reports, topical in-depth community workshops and reports, and rigorous program reviews.

BES scientific user facilities consist 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 science questions. The above-noted BESAC report recounts the central role of these shared resources as a key to U.S. scientific and industrial leadership. BES has a long history of delivering major construction projects on time and on budget, and of providing reliable availability and support to users for operating facilities. This record follows from rigorous community-based processes for conceptualization, planning, and execution of projects, and from performance assessment of operating facilities.

Key to exploiting scientific discoveries for future energy systems 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 and conversions of energy from one form to another. Such materials will need to be more functional than today's energy materials. These new chemical processes will require ever-increasing control to the levels of electrons. These advances are not found in nature; they must be designed and fabricated to exacting standards using principles revealed by basic science. Today, 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. Collectively, these new tools and capabilities convey a significant strategic advantage for the Nation to advance the scientific frontiers while laying the foundation for future innovations and economic prosperity.

DOE envisions a future in which the cross-cutting field of quantum information science (QIS) increasingly drives these scientific frontiers and innovations toward realizing the full potential of quantum-based applications, from computing, to communication, to sensing. This will require precise control at the atomic and molecular levels for the understanding, design, prediction, synthesis, fabrication, and integration of quantum systems. In support of the National Quantum Initiative[b], SC QIS Centers, coupled with a robust core research portfolio stewarded by the individual Office of Science (SC) programs including BES, will create the ecosystem across universities, national labs, and industry that is needed to foster these developments.

The Office of Science has been an important facilitator and sponsor of research at the cutting edge of microelectronics. Its programs have made major contributions to the scientific understanding and advanced instrumentation that enabled Moore's law scaling, and have driven transformative advances in microelectronics in response to the challenging demands of DOE's high performance computing and science facilities. Sustained and rapid progress in microelectronics science and

[a] All reports are available at https://science.energy.gov/bes/community-resources/reports/.
[b] Section 402 of the National Quantum Initiative Act, PL 115-368

technology is essential if DOE is to continue pushing the boundaries of science and, more significantly, continue to lead the global information technology revolution.

Highlights of the FY 2020 Request

The BES FY 2020 Request of $1,858,285,000 focuses resources toward the highest priorities in early-stage fundamental research, in operation and maintenance of scientific user facilities, and in facility upgrades.

Key elements in the FY 2020 Request include:

Research

Core research priorities in the FY 2020 Request include QIS, next-generation microelectronics, and data analytics and machine learning for data-driven science. BES will partner with SC's Offices of Advanced Scientific Computing Research (ASCR) and High Energy Physics (HEP) to establish at least one multi-disciplinary QIS center to promote basic research and early stage development to accelerate the advancement of QIS through vertical integration between systems and theory and hardware and software. The Request increases funding for the Energy Frontier Research Centers (EFRCs) with a planned solicitation in FY 2020 to expand the EFRC portfolio in topical areas of the highest priority to the Department, including QIS, microelectronics, and other program priorities. This EFRC solicitation will also recompete funding for science relevant to the Department's environmental management mission. The Request continues support for computational materials and chemical sciences to deliver shared software infrastructure to the research communities as part of the Exascale Computing Initiative. The BES-supported Batteries and Energy Storage Energy Innovation Hub continues. The Fuels from Sunlight Energy Innovation Hub will complete its second five-year term with FY 2019 funding. FY 2020 funding is requested to continue support of early-stage fundamental research on solar fuels generation that builds on the Hub's unique capabilities and accomplishments to date. BES will issue an open competition in FY 2020 for new multi-investigator, cross-disciplinary solar fuels research to address emerging new directions as well as long-standing challenges in this transformational area of energy science.

Facility Operations

In the Scientific User Facilities subprogram, BES maintains a balanced suite of complementary tools. Linac Coherent Light Source (LCLS) operations will resume in the second quarter of FY 2020 on completion of installation of LCLS-II accelerator components. The Advanced Light Source (ALS), Advanced Photon Source (APS), National Synchrotron Light Source-II (NSLS-II), and the Stanford Synchrotron Radiation Lightsource (SSRL) will continue operations and are supported at approximately 87% of optimum. Both BES-supported neutron sources, the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR), will be operational in FY 2020 and funded at approximately 87% of optimum. All five Nanoscale Science Research Centers (NSRCs) will be supported with funding designated for nanoscience as well as QIS research and related tools development.

Projects

In the Construction subprogram, the LCLS-II project received its last year of funding in FY 2019, per the project plan. The FY 2020 Request provides continued support for the Advanced Photon Source Upgrade (APS-U) project, the Advanced Light Source Upgrade (ALS-U) project, the Linac Coherent Light Source-II High Energy (LCLS-II-HE) project, the Proton Power Upgrade (PPU) project, and the Second Target Station (STS) project at SNS. The FY 2020 Request includes two new Major Item of Equipment projects: the NSLS-II Experimental Tools-II (NEXT-II) project to continue the phased build-out of beamlines at NSLS-II, and the NSRC Recapitalization project.

The Basic Energy Sciences program supports the following FY 2020 Administration Priorities:

FY 2020 Administration Priorities

	(dollars in thousands)			
	Exascale Computing Initiative (ECI)	**Artificial Intelligence (AI)**	**Quantum Information Science (QIS)**	**Microelectronics**
Basic Energy Sciences	26,000	10,000	52,503	25,000

Basic Energy Sciences
Funding

(dollars in thousands)

	FY 2018 Enacted	FY 2019 Enacted	FY 2020 Request	FY 2020 Request vs FY 2019 Enacted
Materials Sciences and Engineering				
Scattering and Instrumentation Sciences Research	73,569	71,235	65,205	-6,030
Condensed Matter and Materials Physics Research	127,984	132,463	140,625	+8,162
Materials Discovery, Design, and Synthesis Research	67,588	65,443	59,989	-5,454
Established Program to Stimulate Competitive Research (EPSCoR)	19,270	19,270	7,323	-11,947
Energy Frontier Research Centers (EFRCs)	55,800	55,800	65,000	+9,200
Energy Innovation Hubs—Batteries and Energy Storage	24,088	24,088	24,088	—
Computational Materials Sciences	13,000	13,000	13,000	—
SBIR/STTR	14,445	14,445	14,215	-230
Total, Materials Sciences and Engineering	**395,744**	**395,744**	**389,445**	**-6,299**
Chemical Sciences, Geosciences, and Biosciences				
Fundamental Interactions Research	86,053	89,067	84,111	-4,956
Chemical Transformations Research	99,886	97,836	83,635	-14,201
Photochemistry and Biochemistry Research	76,688	75,724	64,163	-11,561
Energy Frontier Research Centers (EFRCs)	54,200	54,200	65,000	+10,800
Energy Innovation Hubs—Fuels from Sunlight	15,000	15,000	20,000	+5,000
Computational Chemical Sciences (CCS)	13,000	13,000	13,000	—
General Plant Projects (GPP)	1,000	1,000	1,000	—
SBIR/STTR	13,063	13,063	12,498	-565
Total, Chemical Sciences, Geosciences, and Biosciences	**358,890**	**358,890**	**343,407**	**-15,483**

	FY 2018 Enacted	FY 2019 Enacted	FY 2020 Request	FY 2020 Request vs FY 2019 Enacted
	(dollars in thousands)			
Scientific User Facilities				
X-Ray Light Sources	488,903	505,000	484,514	-20,486
High-Flux Neutron Sources	279,768	282,000	254,665	-27,335
Nanoscale Science Research Centers (NSRCs)	129,926	135,000	127,229	-7,771
Other Project Costs	23,900	19,100	6,000	-13,100
Major Items of Equipment	—	—	2,000	+2,000
Research	34,080	29,457	36,118	+6,661
SBIR/STTR	33,689	32,509	31,907	-602
Total, Scientific User Facilities	**990,266**	**1,003,066**	**942,433**	**-60,633**
Subtotal, Basic Energy Sciences	**1,744,900**	**1,757,700**	**1,675,285**	**-82,415**
Construction				
19-SC-14 Second Target Station (STS), ORNL	—	1,000	1,000	—
18-SC-10 Advanced Photon Source Upgrade (APS-U), ANL	93,000	130,000	150,000	+20,000
18-SC-11 Spallation Neutron Source Proton Power Upgrade (PPU), ORNL	36,000	60,000	5,000	-55,000
18-SC-12 Advanced Light Source Upgrade (ALS-U), LBNL (19-SC-10 in FY 2019 President's Request)	16,000	60,000	13,000	-47,000
18-SC-13 Linac Coherent Light Source-II-High Energy (LCLS-II-HE), SLAC (19-SC-11 in FY 2019 President's Request)	8,000	28,000	14,000	-14,000
13-SC-10 Linac Coherent Light Source-II (LCLS-II), SLAC	192,100	129,300	—	-129,300
Total, Construction	**345,100**	**408,300**	**183,000**	**-225,300**
Total, Basic Energy Sciences	**2,090,000**	**2,166,000**	**1,858,285**	**-307,715**

SBIR/STTR Funding:

- FY 2018 Enacted: SBIR $53,652,000 and STTR $7,545,000
- FY 2019 Enacted: SBIR $52,617,000 and STTR $7,400,000
- FY 2020 Request: SBIR $51,393,000 and STTR $7,227,000

Basic Energy Sciences
Explanation of Major Changes

	(dollars in thousands) FY 2020 Request vs FY 2019 Enacted
Materials Sciences and Engineering Research will continue to support fundamental scientific opportunities, including those identified as high priorities in recent BESAC and Basic Research Needs workshop reports. Research priorities include increased support for novel materials and theory for QIS and next-generation microelectronics, continued emphasis on materials science theory for computational applications that take full advantage of exascale computing, and new directions in the use of data analytics and machine learning for data-driven materials science. The Request increases funding for the EFRCs with a planned solicitation in FY 2020 to expand the EFRC portfolio in topical areas of the highest priority to the Department and to recompete funding for science relevant to the Department's environmental management mission. The Request also includes funding for continued support of the Batteries and Energy Storage Energy Innovation Hub.	**-6,299**
Chemical Sciences, Geosciences, and Biosciences Research will continue to support fundamental science, including grand challenge science and opportunities identified in recent BESAC and Basic Research Needs workshop reports. Priority research areas include QIS research to understand the quantum nature of atomic and molecular systems and to exploit advances in quantum computing for solutions to currently intractable problems; next-generation microelectronics; chemical science theory for computational applications that take full advantage of exascale computing; chemical conversion of increasingly complex chemical systems such as polymers; and the use of data analytics and machine learning for data-driven science. The Request increases funding for the EFRCs with a planned solicitation in FY 2020 to expand the EFRC portfolio in topical areas of the highest priority to the Department and to recompete funding for science relevant to the Department's environmental management mission. The Fuels from Sunlight Energy Innovation Hub will complete its second five-year term with FY 2019 funding. An open competition in FY 2020 will solicit early-stage fundamental research on solar fuels generation that builds on the Hub's unique capabilities and accomplishments to date.	**-15,483**
Scientific User Facilities Linac Coherent Light Source (LCLS) operations will resume in the second quarter of FY 2020 on completion of installation activities for the LCLS-II construction project. All remaining scientific user facilities will operate at a reduced level, approximately 87% of optimum. Funding for the Nanoscale Science Research Centers will include support for nanoscience and QIS research and related tools development. Research priorities include applications of artificial intelligence methods and machine learning techniques to accelerator optimization, control, prognostics, and data analysis. The Request includes funds to initiate two major items of equipment: the NEXT-II beamline project for NSLS-II and the NSRC recapitalization project.	**-60,633**
Construction The Request continues support for the Advanced Photon Source-Upgrade (APS-U) project, the Advanced Light Source Upgrade (ALS-U) project, the Linac Coherent Light Source-II High Energy (LCLS-II-HE) project, the Proton Power Upgrade (PPU) project at the Spallation Neutron Source (SNS), and the Second Target Station (STS) project at SNS.	**-225,300**
Total, Basic Energy Sciences	**-307,715**

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. BES coordinates with 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, including solar fuels; 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
Control of Chemical Reaction Pathways. Catalytic conversion of feedstocks to fuels; extraction of energy from fuels such as in combustion; and capture, conversion, and storage of energy in biological organisms involve complex, multistep chemical reaction mechanisms. The specific reaction pathways determine what is produced and vary widely depending on the reaction environment. New computational tools and experimental approaches allow understanding of how diverse reaction environments provide control of chemical reaction pathways.

- Plants and algae adjust photosynthetic rates to prevent damage under environmental stresses like cold and limited nutrients. Researchers discovered that, when exposed to environmental stress, an algal enzyme was activated and reduced the amount of a major lipid in the membranes that house the photosynthetic machinery. This structural change altered the arrangement of photosynthetic proteins in the membranes and contributed to regulating the amount of sunlight captured and used for photosynthesis to mitigate damage.
- A mechanistic understanding of the electrochemical reduction of CO_2 is needed to enable efficient production of solar fuels and other chemicals. Using sophisticated X-ray spectroscopy and high-resolution microscopy, researchers analyzed the oxidation state and surface structure of metal catalysts under reaction conditions. Building on these molecular-level details, multiscale computational techniques were developed to understand the complex influence of electrolyte composition on catalyst surface chemistry.
- The dry reforming of propane, derived from shale gas, with CO_2 may follow two pathways leading to valuable products, one that produces propylene and another yielding CO and H_2 (syngas). Both pathways are catalyzed by nickel alloys. Researchers predicted the mechanisms and successfully showed, via experiments, the atomic-level detail of the structures, compositions, and oxidation states of the iron-nickel alloy that exclusively produces propylene and the platinum-nickel alloy that produces syngas.

Energy Storage. Advances in energy storage are essential for a wide range of energy technologies, notably improvements to the stability of the electrical grid and increased lifetimes and safety for future batteries. Understanding the fundamentals of electrochemistry and the interactions of the materials used in batteries are key enablers for next generation technologies.

- Batteries could dramatically increase their capacity, the amount of energy they can deliver, if they could use two electrons, rather than just the one electron in current devices. For the first time, researchers reversibly inserted and extracted two lithium ions from a multi-electron lithium ion battery cathode (ε-$VOPO_4$), with full recovery upon recharging. The key was low temperature synthesis of nanoparticles, which preserved their crystallinity, and a conductive graphene coating.

- Lithium metal electrodes hold great promise for next-generation battery systems due to its superior energy density, but dendrites can form during charging and short circuit the battery, leading to premature failure. Researchers added very high molecular weight polymers that suppressed localized instabilities near the electrode surfaces, which reduced the formation of dendrites and also extended the range of operating voltages. This advance opens a new approach for utilizing high-energy metal anodes such as lithium and aluminum without forming dendrites.
- Lithium-sulfur (Li-S) batteries are one of the most promising alternatives to today's lithium ion batteries; however, the sluggish and partially irreversible formation of new phases when the batteries discharge during use has been identified as a critical hurdle for attaining high energy capacity and long cycle life. A new discharge pathway has been discovered that forms stable and inherently self-healing phases (Li_2S_2) in micropores, opening the door to the design of higher capacity, more reversible Li-S batteries.

Computational Materials and Chemical Sciences. BES supports basic research to develop open-source, experimentally validated software and the associated databases required to predictively design materials and chemical processes and assemblies with specific functionality. Software is targeted for today's leadership class computing facilities but is broadly applicable on smaller machines. Software is also being developed for exascale computing facilities as these become available.

- The Materials Project provides a unique collection of computed properties of materials for more than 80,000 compounds plus downloadable software for data analysis. The site has more than 38,000 registered users. Online properties include electrochemical and electronic structure, mechanical properties, phase stability and corrosion resistance. Data has been used to explore performance of novel battery designs, among other energy applications.
- A new mechanism has been discovered for generation of current in organic photovoltaic materials that could lead to greatly improved performance and lower cost solar cell technology. Software developed for these studies has performed well on pre-exascale computers with up to 500,000 processor cores.
- Understanding charge transfer processes in complex molecular systems is challenging because they depend on multiple factors including local environment and molecular structure. Computational chemical scientists employed a multiscale approach to a photosynthetic reaction center mimic to show how the solvent environment modifies the propensity of a molecule to bend, causing the quantum analog of an electrical short circuit. These insights will enhance knowledge of Nature's light-harvesting systems that, in turn, will enable predictions of novel artificial solar energy systems.

Science for Environmental Management. The cleanup and long term storage of large quantities of highly complex nuclear waste remains one of DOE's greatest challenges. Studies of the fundamental chemical and physical properties of radioactive and other elements present in the waste, as well as the creation of novel storage materials, will enable more efficient, cost-effective, and safer solutions.

- Dissolution and precipitation of gibbsite (an aluminum-based compound) is important in radioactive waste treatment and industrial aluminum production. Real-time experiments revealed that the aluminum does not transition between a 4-coordinate species in solution to a 6-coordinate species as a solid, but involves an intermediate 5-coordinate species that depends on the composition of the solution. Such studies support the development of new methods for processing high level radioactive wastes at Hanford and Savannah River, and provide potentially less energy-intensive routes for aluminum production.
- Cerium is often used as an analog for plutonium in experiments that explore the selective binding of actinides for recycling used nuclear fuels. Experiments showed that both plutonium and cerium complexes exhibit the same coordination and structure, but the plutonium complex was more stable and only the plutonium complex exhibited quasi-reversible redox behavior. This work exposes the limits of using cerium as a surrogate for plutonium in future research.
- Separating cesium and chlorine from liquid waste streams is important, the former for its radioactivity and the latter for its incompatibility with borosilicate glasses, the leading nuclear waste form. Researchers showed that spark plasma sintering can be used to form dense pellets of a perovskite material with 23% mass cesium and 38% mass chlorine without decomposition. The leading alternate waste form only incorporates about 11% chlorine. This work could enable a simpler and more efficient treatment of nuclear waste streams that contain chlorine.

BES user facilities contribute to world leading science. Researchers from U.S. industries and academia use the unique capabilities at the BES scientific user facilities to advance science and technology frontiers.

- Intense x-rays delivered from the newly developed helical superconducting undulator at the Advanced Photon Source can image the fuel spray process from an injector with unprecedented resolution without x-ray optics. The auto industry can use this information to gain detailed insights into the relationship between the fuel distribution and mechanical movement of the fuel injector inside a combustion engine. This knowledge will help the industry to develop cleaner and more fuel-efficient engines.
- Center for Integrated Nanotechnologies researchers successfully integrated donor atoms and quantum dots to create quantum bits, or qubits, for quantum computers. For almost two decades, scientists have created theoretical proposals of such a hybrid qubit architecture. Researchers have now made an important step toward the practical realization of silicon qubits. Silicon matters because the qubit manufacturing process could fit within today's manufacturing and computing technologies.
- The VULCAN instrument at the Spallation Neutron Source can measure atomic level details of defects in large engineered components at extreme conditions. Its ability to spatially resolve residual stress enabled researchers from the United States Steel Corporation to perform experiments on how lightweight advanced high-strength steels formed by hydroforming behave at realistic operating conditions. These unique experimental capabilities enable U.S. industries to design and engineer automotive and other components that are lighter, stronger, and more durable.

New capabilities for users at BES facilities. Researchers developed new capabilities and instrumentation at the BES scientific user facilities to enable cutting-edge user experiments.

- A new beamline instrument at the Linac Coherent Light Source was used to split x-ray pulses, creating femtosecond to nanosecond time delays between the pulses. Using this new capability, scientists measured the nanosecond equilibrium dynamics of nanoparticles, allowing the examination of heterogeneous dynamics associated with cooling a liquid. Such dynamics are important in complex synthesis and fabrication of energy-relevant materials.
- The Full Field X-ray Imaging beamline, one of the newest beamlines at NSLS-II, can complete a 3D nanotomography measurement with unprecedented time and spatial resolution. This advanced scientific research tool provides the researchers the ability to examine nanostructures in details and to study the reaction of forming new nanomaterials in real time.
- Center for Nanophase Materials Sciences researchers developed a technique that creates tiny, precise metallic shapes. They rastered a beam from a helium-ion microscope through a liquid precursor to induce chemical reactions. The reactions locally deposit high purity platinum in ribbons only 15 nanometers in diameter. The new high-precision, additive direct ion beam writing capability opens nanofabrication opportunities to improve electronics, drug delivery, chemical separations, and other applications.

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 BESAC report on transformative opportunities for discovery science, coupled with the Basic Research Needs workshop reports on energy technologies and roundtable reports on quantum information and ultrafast science, 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. Growing research activities in quantum materials highlight the importance and challenges for materials science in understanding and guiding the development of systems that realize unique properties for QIS and can contribute to SC QIS Centers. Materials science for next generation microelectronics will provide the needed advances for future computing, sensors, and detectors that are critical for national priorities in energy and for leadership in advanced research over a wide range of fields. Research priorities in this field will be guided by a Basic Research Needs workshop and reports. Another increasingly important aspect of materials research is the growing use of data analytics and machine learning for data-driven science to enhance the utility of both theoretical and experimental data for predictive design and discovery of materials.

In addition to single-investigator and small-group research, this subprogram supports Computational Materials Sciences, EFRCs, and the Batteries and Energy Storage Hub, and in FY 2020 will become a partner in support of at least one SC QIS Center. 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. In support of the National Quantum Initiative, SC QIS Centers will push the current state-of-the-art science and technology toward realizing the full potential of quantum-based applications, from computing to communication to sensing.

The Materials Sciences and Engineering subprogram also includes the DOE Established Program to Stimulate Competitive Research (EPSCoR). The DOE EPSCoR program strengthens investments in early stage energy research for states and U.S. territories that do not historically have large federally-supported 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 techniques and instrumentation development for advanced materials science research with scattering, spectroscopy, and imaging using electrons, neutrons, and x-rays, including development of science to understand ultrafast dynamics. These techniques provide precise and complementary information on the relationship among structure, dynamics, and properties. The major advances in materials sciences from DOE's world-leading electron, neutron, and x-ray scattering facilities provide 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 future transformational advances. 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."[a] 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 and support the work of SC QIS Centers.

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 and techniques for scattering, spectroscopy, and imaging needed to correlate the microscopic and macroscopic properties of energy materials. The use of multiscale and multimodal techniques to extract heretofore unattainable information on multiple length and time scales is a growing aspect of this research. For example, to design transformational new materials for energy-related applications, operando experiments contribute to understanding the atomic and nanoscale changes that lead to materials failure in non-equilibrium and extreme environments (temperature, pressure, stress, radiation, magnetic fields, and electrochemical potentials). Information from these characterization tools is the foundation for the creation of new materials that have extraordinary tolerance and can function within an extreme environment without property degradation.

Condensed Matter and Materials Physics Research

Understanding and controlling the fundamental properties of materials are critical to improving their functionality on every level and are essential to fulfilling DOE's energy mission. The Condensed Matter and Materials Physics activity supports

[a] https://science.energy.gov/bes/community-resources/reports/

experimental and theoretical research to advance the 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. New techniques for data analytics and machine learning for data-driven science are seeing increasing applications in materials science research to extract value from large databases of theoretical calculations and experimental measurements.

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. These advances will be key components of the activities of SC QIS Centers. Related to quantum materials is materials research for next-generation microelectronics, critical for competitiveness for future computers, sensors, and related technologies.

This activity includes the SC QIS Centers which will promote basic research and early stage development to accelerate the advancement of QIS through vertical integration between systems and theory and hardware and software. As identified by BES strategic planning reports including the Basic Research Needs Workshop on Quantum Materials and the Roundtable on Opportunities for Basic Research for Next-Generation Quantum Systems, key materials-related technical areas will include fundamental theory of materials and molecular systems for quantum applications; research leading to materials and molecular systems that meet quantum communication, computation, and sensor requirements; fundamental research on device physics for next generation QIS systems, including interface science and modeling of materials performance; and synthesis and fabrication research for quantum materials and processes, including integration in novel device architectures. In FY 2020, BES will partner with ASCR and HEP to establish at least one multi-disciplinary multi-institutional QIS center, which will be selected through a merit reviewed process conducted early in FY 2020. The scope of the SC QIS center will be on a set of QIS applications or cross-cutting topics that collectively cover the development space that may impact ASCR, BES and HEP and include work on sensors, quantum emulators/simulators and enabling technologies that will pave the path to exploit quantum computing in the longer term.

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 low energy synthesis approaches of biology to produce materials; 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 and self-regulating 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.

Annual EPSCoR funding opportunities alternate between a focus on research performed in collaboration with the DOE national laboratories and a focus on implementation awards that facilitate larger team awards for the development of research infrastructure. The program supports a small cadre of early career scientists from EPSCoR jurisdictions on an annual basis and provides complementary support for research grants to eligible institutions.

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. They allow experts from a variety of disciplines to collaborate on shared challenges, combining their strengths to uncover new and innovative solutions to the most difficult problems in materials sciences. The EFRCs also support numerous graduate students and postdoctoral researchers, educating and training a scientific workforce for the 21st century economy. The EFRCs supported in this subprogram focus on the following topics: 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; future nuclear energy; and quantum materials that can optimize the transmission, utilization, and control of energy and information. After nine years of research activity, the program has produced an impressive breadth of scientific accomplishments, including over 10,500 peer-reviewed journal publications.

BES's active management of the EFRCs continues to be an important feature of the program. The program uses a variety of methods to regularly assess the progress of the EFRCs, including annual progress reports, monthly phone calls with the EFRC Directors, periodic Directors' meetings, and on-site visits by program managers. BES also conducts in-person reviews by outside experts. Each EFRC undergoes a review of its management structure and approach in the first year of the award and a midterm assessment of scientific progress compared to its scientific goals. To facilitate communication of results to other EFRCs and DOE, 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 early stage research to tackle forefront, basic scientific challenges for next-generation electrochemical energy storage. JCESR is a multi-institutional research team led by Argonne National Laboratory (ANL) in collaboration with four other national laboratories, eleven universities, the Army Research Laboratory, and industry. In the initial five-year award (2013-2018), 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 in lithium-sulfur batteries to greatly improve cycle life; and computational screening of over 16,000 potential electrolyte compounds using the Electrolyte Genome protocols.

For the current award (2018-2023, pending annual progress reviews and appropriations), JCESR used its past research to identify a number of critical scientific gaps to serve as a foundation for the proposed research. The research directions are consistent with the priorities established in the recent BES workshop report *Basic Research Needs for Next Generation Electrical Energy Storage,*[a] 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. In the current research, prototypes will be used to demonstrate the impact of materials advances for specific battery architectures and designs.

Based on established best practices for managing large awards, BES will continue to require quarterly reports, frequent teleconferences, and annual progress reports and peer reviews to communicate progress, provide input on the technical directions, and ensure high quality research.

Computational Materials Sciences

Major strides in materials synthesis, processing, and characterization, combined with concurrent advances in computational science—enabled by enormous improvements in high-performance computing capabilities—have opened an unprecedented opportunity to design new materials with specific 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,

[a] https://science.energy.gov/bes/community-resources/reports/

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, appropriate data analytics tools for materials research, 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 2019 Enacted	FY 2020 Request	Explanation of Changes FY 2020 Request vs FY 2019 Enacted
Materials Sciences and Engineering $395,744,000	**$389,445,000**	**-$6,299,000**
Scattering and Instrumentation Sciences Research $71,235,000	$65,205,000	-$6,030,000
The FY 2019 Enacted budget emphasizes the development and use of forefront characterization tools to address challenges in materials science including understanding of quantum phenomena, with a continued emphasis on ultrafast techniques. In addition to high spatial resolution, the research emphasizes 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 emphasizes hypothesis-driven research with x-ray free electron laser sources, tailored excitations with pumped laser control, and coherent x-ray imaging. Neutron scattering research emphasizes research in emergent quantum phenomena, especially research involving interfaces. Electron scattering research focuses on innovative techniques to assess quantum phenomena, especially with ultrafast techniques.	The Request will continue to emphasize the development and use of forefront characterization tools to address challenges in materials science including understanding of quantum phenomena. The research will explore dynamics across many orders of magnitude in length and time scales to understand the evolution of emergent phenomena and in materials and their properties. Research includes complex quantum behavior and performance in the environments experienced by materials used in energy generation and use. Investments in x-ray science will emphasize hypothesis-driven research using x-ray free electron laser (XFEL) sources, exploiting tailored excitations, and imaging with coherent x-rays. Neutron scattering research will focus on emergent quantum phenomena and soft materials, especially at interfaces. Electron scattering research will focus on innovative techniques to assess quantum phenomena.	Emphasis will be on characterization of quantum phenomena using new developments in XFELs, neutron instrumentation, and scanning probes; and combining techniques to produce novel multi-modal approaches to understanding structure and excitations at the quantum level of matter. This activity will de-emphasize conventional and heavy fermion superconductivity, lower time resolution dynamic electron scattering, and x-ray scattering for bulk material systems, steady state analysis, and equilibrium systems. Conventional materials systems and research focused on well-established tools and techniques will be phased out.
Condensed Matter and Materials Physics Research $132,463,000	$140,625,000	+$8,162,000
The FY 2019 Enacted budget continues to focus on fundamental experimental and theoretical research on the properties of materials, emphasizing quantum phenomena, continues. Experimental and theoretical condensed matter physics research emphasizes quantum materials, focusing on new and emergent behavior for QIS, including spintronics, topological	The Request will continue to focus on forefront experimental and theoretical condensed matter research, emphasizing quantum phenomena including new and emergent behavior for QIS such as spintronics, topological states and novel 2D materials. Physical behavior research will emphasize innovative science to understand coherent light-matter interactions. Related activities will advance	Research on quantum materials will continue to increase, including a focus on innovation for new materials systems and use of quantum computing platforms for materials science research. Additionally, the increased funding will support research to provide the scientific foundations for future microelectronics. Also highlighted is

FY 2019 Enacted	FY 2020 Request	Explanation of Changes FY 2020 Request vs FY 2019 Enacted
states and novel 2D materials. Physical behavior research emphasizes innovative science to understand optical and electronic phenomena. Mechanical behavior and radiation effects research continues 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.	the underlying physical science understanding for next generation electronics. 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. BES will partner with ASCR and HEP to establish at least one multi-disciplinary multi-institutional QIS center, which will be selected through a merit reviewed process conducted early in FY 2020. The scope of the SC QIS center will be on a set of QIS applications or cross-cutting topics that collectively cover the development space that may impact ASCR, BES and HEP and include work on sensors, quantum emulators/ simulators and enabling technologies that will pave the path to exploit quantum computing in the longer term.	development and use of advanced computational tools for materials sciences, including data mining. Radiation effects research to address the challenges for next generation nuclear reactors will be emphasized. Topics to be deemphasized include conventional superconductivity, fractional quantum Hall physics, and theory of granular materials. Topics to be phased out include mechanics and theory of soft matter and ionic liquids.
Materials Discovery, Design, and Synthesis Research $65,443,000	$59,989,000	-$5,454,000
The FY 2019 Enacted budget continues 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 is emphasized, as is 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 is stressed for complex materials including quantum materials, organic systems, nanomaterials, electrochemical materials, polymers, and high fidelity mesoscale systems.	The Request will continue to focus on understanding the fundamentals of predictive design and synthesis of materials across multiple length scales using chemical, physical and bio-inspired techniques. Development of insights on the dynamics of materials structure and chemistry during the early stages of materials synthesis will be stressed, as will research that incorporates both experiment and theory. For complex materials and materials systems, research will focus on the fundamentals of growth kinetics, self-assembly, directed and dissipative assembly, and the role of interfaces and defect management. Discovery of new functional materials and new synthesis and computational techniques to create complex materials with targeted structure and properties will be emphasized.	Emphasis will be on forefront research for the synthesis of complex materials for novel functionalities, especially for quantum materials and systems in which interfaces are critical. Topics to be de-emphasized include control of synthesis to direct materials properties, molecular materials chemistry, and aspects of biocentric/biohybrid research approaches. Topics to be phased out include traditional synthesis research for conventional materials systems and optimization of synthetic processes.

FY 2019 Enacted	FY 2020 Request	Explanation of Changes FY 2020 Request vs FY 2019 Enacted
Established Program to Stimulate Competitive Research (EPSCoR) $19,270,000	$7,323,000	-$11,947,000
The FY 2019 Enacted budget continues to span science in support of the DOE mission, with emphasis on early stage science that underpins DOE energy technology programs. Research emphasizes EPSCoR jurisdiction implementation awards and investment in early career research faculty from EPSCoR designated jurisdictions.	The Request will continue to span science in support of the DOE mission, with emphasis on early stage science that underpins DOE energy technology programs. Following the prior year focus on implementation award investments, the focus for this year will be on broadening EPSCoR jurisdiction-laboratory partnerships, leveraging the DOE national laboratory energy research expertise and user facilities. Investment will continue in early career research faculty from EPSCoR designated jurisdictions and in co-investment with other programs for awards to eligible institutions.	FY 2020 funding will focus on research that involves collaboration among researchers in EPSCoR jurisdictions with the DOE national laboratories.
Energy Frontier Research Centers (EFRCs) $55,800,000	$65,000,000	+$9,200,000
The FY 2019 Enacted budget continues to support EFRC awards that were made in FY 2016 and FY 2018.	The Request will continue to support four-year EFRC awards that were made in FY 2018. In addition, FY 2020 funds will support a recompetition of the four-year EFRC awards made in FY 2016, which focused on science relevant to DOE's environmental management mission. Finally, the request will support a solicitation for new EFRCs that are responsive to recent BES strategic planning workshop reports, including use-inspired science relevant to advanced microelectronics and QIS.	Additional funds in FY 2020 will be used to expand the EFRC portfolio in topical areas of the highest priority to DOE, including microelectronics and QIS.
Energy Innovation Hubs—Batteries and Energy Storage $24,088,000	$24,088,000	$—
The FY 2019 Enacted budget continues to focus on early stage research to tackle forefront, basic scientific challenges for next-generation electrochemical energy storage. The research emphasizes discovery science, elucidation of cross-cutting scientific principles for electrical energy storage, and integration of theory,	The Request will continue to focus on early stage research for next generation electrical energy storage for the grid and vehicles. Research will emphasize understanding the fundamentals of electrochemistry (transport, solvation, evolution of chemistries and materials during charge/ discharge) and discovery science, including close coupling of theory, simulation, and experimentation, to elucidate	The funding continues at the same level. Annual peer reviews will be used to fine tune research directions based on annual progress, input from the JCESR team, and peer review.

FY 2019 Enacted	FY 2020 Request	Explanation of Changes FY 2020 Request vs FY 2019 Enacted
experiment, and computational approaches to accelerate progress.	the impact of coupled phenomena and for predictive design of new materials for batteries.	
Computational Materials Sciences $13,000,000	$13,000,000	$—
The FY 2019 Enacted budget continues research on the Computational Materials Sciences (CMS) 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 is developed that utilizes leadership class computers, and made available to the broad research community. In addition, the codes incorporate frameworks that are suited for future exascale computer systems. Awards that complete their fourth year of research are considered for renewal in a solicitation that also considers new applications.	The Request will continue research on current CMS awards that focus on development of research-oriented, open-source, experimentally validated software and the associated databases required to predictively design materials with specific functionality. Software will utilize leadership class computers, and be made available to the broad research community. The codes will also incorporate frameworks 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 FY 2020 solicitation will incorporate materials science research priorities from the most recent BES workshop and roundtable reports on basic research needs related to specific energy technologies, QIS, and next generation electronics, as well as consideration of data analytics and machine learning for data-driven science.
SBIR/STTR $14,445,000	$14,215,000	-$230,000
In FY 2019, SBIR/STTR funding is set at 3.65% of non-capital funding.	In FY 2020, SBIR/STTR funding will be set at 3.65% of non-capital funding.	Funding changes are the direct result of decreases in non-capital funding.

Basic Energy Sciences
Chemical Sciences, Geosciences, and Biosciences

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 multi-investigator, cross-disciplinary teams—through EFRCs, the Energy Innovation Hub for solar fuels, and Computational Chemical Sciences—to focus on forefront scientific challenges that relate to the DOE energy mission. In FY 2020, the subprogram will become a partner in support of at least one SC QIS Center.

The FY 2020 Request continues to focus resources toward the highest priorities in early-stage fundamental research. High priority areas include ultrafast science to probe the dynamics of electrons, atoms, and molecules that underlie photochemical processes, chemical transformations, and energy flow; QIS research 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; photo and electrochemical processes associated with the capture of solar energy and conversion to fuels; chemical conversion of increasingly complex chemical systems such as polymers; the use of data analytics and machine learning for data-driven science; 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.

Fundamental Interactions Research

This activity emphasizes structural and dynamical studies of atoms, molecules, and nanostructures, and the description of their interactions in full quantum detail. The goal is to achieve a complete understanding of reactive chemistry in the gas phase, condensed phase, and at interfaces. Using techniques and tools developed for *Ultrafast Sciences*, novel sources of photons, electrons, and ions are used to probe and control 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. The goal, which will be fundamental to the work of SC QIS Centers, 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 and x-ray free electron laser sources such as the Linac Coherent Light Source (LCLS) are used to image the dynamics of electrons and charge transport. Chemical physics research builds from the AMOS 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, including solar energy conversion, radiolytic effects, and catalysis. In addition, unraveling complex mechanisms of chemical reactions at interfaces can inform the design and synthesis of new materials relevant to microelectronics and QIS. 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 and combustion. 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, which 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; in the context of SC QIS Centers, this research also lays groundwork for applications of future quantum computers to computational quantum chemistry. Additional emphasis will be placed on codes that contribute to a fundamental understanding of how molecules might function as components of quantum computers.

This activity includes the SC QIS Centers which will promote basic research and early stage development to accelerate the advancement of QIS through vertical integration between systems and theory and hardware and software. As identified by BES strategic planning reports including the Roundtable on Opportunities for Quantum Computing in Chemical and

Materials Sciences and the Roundtable on Opportunities for Basic Research for Next-Generation Quantum Systems, key technical areas will include fundamental theory of materials and molecular systems for quantum applications; research leading to materials and molecular systems that meet quantum communication, computation, and sensor requirements; fundamental research on device physics for next generation QIS systems, including interface science; and synthesis and fabrication research for quantum materials and processes, including integration in novel device architectures. In FY 2020, BES will partner with ASCR and HEP to establish at least one multi-disciplinary multi-institutional QIS center, which will be selected through a merit reviewed process conducted early in FY 2020. The scope of the SC QIS center will be on a set of QIS applications or cross-cutting topics that collectively cover the development space that may impact ASCR, BES and HEP and include work on sensors, quantum emulators/simulators and enabling technologies that will pave the path to exploit quantum computing in the longer term.

Chemical Transformations Research

Fundamentally, Chemical Transformations Research advances 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, experimental tools, and theoretical, computational and data analytics approaches. 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, computational and data analytics methods 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 single 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, for enabling the beneficial chemical conversion of complex materials, such as synthetic polymers, and for guiding synthesis mechanisms of novel molecular systems for microelectronics.

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.

Photochemistry and Biochemistry Research

This activity supports research on the molecular mechanisms that capture light energy and convert it into electrical and chemical energy in both natural and man-made systems. An important component of this activity is its leadership role in the support of basic research in both solar photochemistry and natural photosynthesis. 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.

Supported research on the structural and chemical dynamics of energy absorption, transfer, conversion and storage across multiple spatial and temporal scales provides fundamental knowledge of *Charge Transport and Reactivity*. Efforts target the basic understanding of mechanisms and dynamics of chemical and biochemical processes including water oxidation, charge transfer, and redox interconversion of small molecules (e.g. carbon dioxide/methane, nitrogen/ammonia, and protons/hydrogen). A breadth of approaches and tools, such as those in *Ultrafast Chemistry*, are used to investigate quantum phenomena in natural and artificial systems; studies of the potential role and manipulation of photodriven quantum coherence in natural photosynthesis and artificial molecular systems could not only enhance fundamental understanding of energy transfer but also inspire new methods for quantum information processing, potentially in the portfolio of SC QIS Centers. Crosscutting research underpins a fundamental understanding of the synthesis, dynamics, and function of natural and artificial membranes and nano- to meso-scale structures, increasing knowledge of *Chemistry at Complex Interfaces* as well as *Chemistry in Aqueous Environments*. To understand *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 exemplified by studies of the water oxidation reaction and the nitrogen reduction reaction that are catalyzed by complex and unique metalloclusters of the oxygen evolving complex in natural photosynthesis and the nitrogenase enzyme in microbial systems respectively.

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, quantum coherent energy transfer, 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. The resulting mechanistic understanding of natural photosynthesis provides inspiration in the development of bio-hybrid, biomimetic, and artificial photosynthetic systems for solar fuels production and informs strategies to enhance photosynthetic efficiency in natural systems. Physical science tools 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 in natural systems, including complex multielectron redox reactions, electron transfer and bifurcation, and processes beyond primary photosynthesis such as nitrogen reduction and deposition of reduced carbon into energy-dense carbohydrates and lipids. This knowledge of energy conversion and storage in natural systems will identify principles for the design of highly selective and efficient catalysts, for instance, for ammonia synthesis or chemical conversion of polymers; the control of electron flow to achieve desired metabolic products; and the design of next-generation energy conversion/storage technologies.

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, photodriven generation of quantum coherence in artificial molecular systems, and artificial assemblies for charge separation and transport. These studies provide essential foundational knowledge for the use of solar energy for fuel production and electricity generation.

This activity also supports radiation science, investigating fundamental physical and chemical effects produced by the absorption of energy from ionizing radiation. 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. These studies increase fundamental knowledge of the chemical reactions that occur in radiation fields of nuclear reactors, including in their fuel and coolants, and can provide insights for effective nuclear waste remediation, fuel-cycle separation and design of nuclear reactors.

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. They allow experts from a variety of disciplines to collaborate on shared challenges, combining their strengths to uncover new and innovative solutions to the most difficult problems in chemical sciences, geosciences, and biosciences. The EFRCs also support numerous graduate students and postdoctoral researchers, educating and training a scientific workforce for the 21st century economy. The EFRCs supported in this subprogram focus 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; interdependent energy-water issues; future nuclear energy; 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 10,500 peer-reviewed journal publications.

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

JCAP's fundamental research enabled development of experimental artificial photosynthesis systems using earth-abundant catalysts for efficient solar-to-hydrogen conversion, now up to 19%. Central to these systems is JCAP's research leading to the development of transparent electrically conductive coatings for semiconductors that protect against corrosion in the aqueous electrolytes used for solar-fuels generation. JCAP research is also solving the critical and highly complex puzzle of directing the selectivity of carbon dioxide reduction into specific products. Studies revealed that molecular-level modifications to the reaction electrolyte of an electrocatalyst pre-activated carbon dioxide to promote formation of valuable two- and three-carbon products. JCAP used high throughput experimentation and theory to identify unique light absorbers with desired energetics; the combination of light absorbers and selective electrocatalysis is a crucial tool in defining mechanisms of light-driven carbon dioxide reduction.

With the completion of the second five-year term of JCAP, FY 2020 funding is requested for continued support of early-stage fundamental research on solar fuels generation that builds on JCAP's unique capabilities and accomplishments to date. An open competition will be held to solicit new awards of multi-investigator, cross-disciplinary solar fuels research to address emerging new directions as well as long-standing challenges in this transformational area of energy science.

Computational Chemical Sciences
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 chemical sciences research that focuses on the creation of computational codes and associated experimental/computational databases for the design of chemical processes and assemblies. Additional awards were initiated in FY 2018. 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 DOE-owned facilities and to meet requirements for safe and reliable facilities operation.

Basic Energy Sciences
Chemical Sciences, Geosciences, and Biosciences

Activities and Explanation of Changes

FY 2019 Enacted		FY 2020 Request	Explanation of Changes FY 2020 Request vs FY 2019 Enacted
Chemical Sciences, Geosciences, and Biosciences	**$358,890,000**	**$343,407,000**	**-$15,483,000**
Fundamental Interactions Research	$89,067,000	$84,111,000	-$4,956,000
The FY 2019 Enacted budget continues 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 continues to develop and apply approaches to examine the structure and dynamics of reactive intermediates and how they impact reaction pathways in heterogeneous environments. Research efforts are extended to understand and control chemical processes and dynamics, at the molecular level, in increasingly complex aqueous and interfacial systems. Research expands the use of ultrafast techniques to study gas-phase, condensed phase and interfacial chemical phenomena. The activity develops advanced theoretical methods for electronic structure calculations that can be scaled to operate on exascale computers. Research supports 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 emphasizes efforts to drive advances in the application of quantum computing for molecular calculations.		The Request will continue to develop forefront ultrafast approaches, with emphasis on the use of x-ray free electron lasers, to study and control energy flow and bond rearrangements in gas-phase, condensed phase and interfacial chemical phenomena. Gas-phase research will continue studies of how reactive intermediates in heterogeneous environments impact reaction pathways and expand to examine quantum phenomena such as coherence and entanglement in tailored molecules. Research will extend efforts to understand and control chemical processes and quantum phenomena, at the molecular level, in increasingly complex aqueous and interfacial systems. Understanding interfacial chemical reactions and their control will inform the design and synthesis of new materials relevant to microelectronics. The activity will continue to develop advanced theoretical and computational approaches, including data science approaches such as machine learning that can be scaled to operate on exascale computers and apply the approaches to calculations on progressively complex systems to guide and interpret ultrafast measurements and to develop understanding needed to advance catalysis and solar energy research. The activity will continue to emphasize efforts to drive advances in the	Research will emphasize forefront efforts to image molecular dynamics using, as well as developing, ultrafast capabilities at BES light sources, to understand increasingly complex interfacial systems, and to advance exascale-ready computational tools and data science approaches for molecular systems of increasing complexity. Continuing emphasis will remain on 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. Research will emphasize experimental and computational studies of tailored molecular systems in the gas-phase, solutions, and interfacial systems to understand quantum phenomena underlying quantum systems for QIS. Emphasis continues on understanding the molecular mechanisms of charge transport. New efforts will develop an understanding of interfacial processes that inform the design and synthesis of systems with advanced (opto)electronic and spin properties relevant to microelectronics. The application of quantum computing to calculations of molecular structure and dynamics will continue to be emphasized. This activity will continue to de-emphasize aspects of nanoscience and combustion research.

FY 2019 Enacted	FY 2020 Request	Explanation of Changes FY 2020 Request vs FY 2019 Enacted
	application of quantum computing for molecular calculations. BES will partner with ASCR and HEP to establish at least one multi-disciplinary multi-institutional QIS center, which will be selected through a merit reviewed process conducted early in FY 2020. The scope of the SC QIS center will be on a set of QIS applications or cross-cutting topics that collectively cover the development space that may impact ASCR, BES and HEP and include work on sensors, quantum emulators/ simulators and enabling technologies that will pave the path to exploit quantum computing in the longer term.	
Chemical Transformations Research $97,836,000	$83,635,000	-$14,201,000
The FY 2019 Enacted budget continues 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, continues to be pursued. Fundamental separation science research continues 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 continues 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 continues to be supported. Heavy element research continues to expand the knowledge of the chemistry of actinide reactivity, bonding, synthesis, and	The Request will continue to support predictive fundamental research on the design and synthesis of novel catalysts to efficiently convert chemical feedstocks, including synthetic polymers, to high-value fuels and chemicals. Fundamental studies will also target the understanding and control of the synthesis and reconstruction of molecular structures with advanced (opto)electronic and spin properties. Fundamental separation science research will continue on innovative approaches for separating chemical mixtures. This activity will emphasize the use of computational approaches, including data science tools and multi-scale methods, to investigate molecular recognition at complex interfaces, predict transport and separation in confined environments, and bonding and dynamics. 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	Research will emphasize efforts in ultrafast spectroscopy for detailed studies of reaction pathways, electronic structure calculations for systems of increasing molecular and solid complexity, and multiscale modeling, simulations, and data science approaches for complex reaction and transport processes. Research will continue to lead the mechanistic understanding of chemical catalysis, synthesis, separations, stabilization and transport required to control chemical processes in diverse environments created by complex atomic architectures, solvents, electric or mechanical field. It will provide new knowledge of reaction processes that integrate multiple steps, such as chemical conversion and chemical separation steps of multiple sources of energy and feedstocks, including polymeric materials. This activity will emphasize fundamental studies of the structure, dynamics, and energetics of coolants and fuels in extreme nuclear environments, and the chemical and physical properties of interfaces and heavy elements in these environments. Efforts will

FY 2019 Enacted	FY 2020 Request	Explanation of Changes FY 2020 Request vs FY 2019 Enacted
separation, and also support training in nuclear chemistry. Theoretical methods continue to be advanced to accurately describe the chemistry of f-element compounds.	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.	explore molecular mechanisms central to the synthesis of novel molecular systems for microelectronics. This activity will continue to de-emphasize research on chemical analysis, synthesis of nanomaterials, physics of fluids in rock systems, and biocatalytic reactions.
Photochemistry and Biochemistry Research $75,724,000	$64,163,000	-$11,561,000
The FY 2019 Enacted budget continues to support fundamental research on photon 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 continues to be emphasized in both natural and artificial systems. Research of the fundamental mechanisms of photocatalysis and biocatalysis 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 continue to be supported and target a fundamental understanding of ultrafast chemistry and of reactivity across complex interfaces, in aqueous environments, and under dynamic conditions. Research also continues 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 will continue to support fundamental research and innovative approaches to understand physical, chemical, and biochemical processes of light energy capture and conversion in chemical and biological systems. Studies of light absorption, energy transfer, charge transport and separation, and photocatalysis will continue to be emphasized in both natural and artificial systems to advance foundational knowledge of solar energy capture and conversion with an emphasis on solar fuels generation. Understanding of molecular mechanisms of photon capture and electron transfer will advance solar fuels research as well as provide insights into quantum phenomena in energy transfer. Research on biocatalysis will continue to focus on a mechanistic understanding of enzyme structure and function with a particular emphasis on multi-electron redox reactions, electron bifurcation, and co-factor tuning. Efforts to understand processes and reactions on ultrafast timescales for energy conversion in natural and artificial systems will continue as will studies of reactivity across complex interfaces, in aqueous environments, and under dynamic conditions.	Research will emphasize cutting-edge science of charge transport, energy transfer, photo- and bio-catalytic mechanisms, and excited-state dynamics of processes important for energy capture and conversion in chemical and biological systems. Studies will increase focus on quantum phenomena in photochemical and biochemical processes, such as quantum coherence in energy transfer. Studies of biocatalysis and biological energy conversion will emphasize multi-electron reactions and control of electron flow to identify fundamental principles for catalyst and pathway design, for example, for targeted chemical production or for chemical conversion of complex materials such as polymers. Research in fundamental radiation chemistry will continue to be emphasized to provide a foundation for prediction and control of radiation-chemical transformations in complex systems. Emphasis on light capture and charge transfer will include fundamental phenomena important for quantum information science. This activity will continue to de-emphasize efforts in plant cell wall biosynthesis and structure, light signaling in plant development, organismal level studies, and molecular solar thermal energy storage.

FY 2019 Enacted	FY 2020 Request	Explanation of Changes FY 2020 Request vs FY 2019 Enacted
Energy Frontier Research Centers (EFRCs) $54,200,000	$65,000,000	+$10,800,000
The FY 2019 Enacted budget continues to support EFRC awards that were made in FY 2016 and FY 2018.	The Request will continue to support four-year EFRC awards that were made in FY 2018. In addition, FY 2020 funds will support a recompetition of the four-year EFRC awards made in FY 2016, which focused on science relevant to DOE's environmental management mission. Finally, the request will support a solicitation for new EFRCs that are responsive to recent BES strategic planning workshop reports, including use-inspired science relevant to advanced microelectronics and QIS.	Additional funds in FY 2020 will be used to expand the EFRC portfolio in topical areas of the highest priority to DOE, including microelectronics and QIS.
Energy Innovation Hubs—Fuels from Sunlight $15,000,000	$20,000,000	+$5,000,000
The FY 2019 Enacted budget continues to support JCAP's fundamental research on the science of carbon dioxide reduction.	The Request will support early-stage fundamental research on solar fuels generation that builds on JCAP's unique capabilities and accomplishments to date. A competition will be held to solicit new awards of multi-investigator, cross-disciplinary solar fuels research to address emerging new directions as well as long-standing challenges in this transformational area of energy science. Research will focus on tackling forefront, fundamental scientific challenges for generating fuels using only sunlight, carbon dioxide, and water as inputs. Advances in this area will also benefit from consideration of photodriven generation of fuels from molecules other than CO_2. The research will capitalize on unique capabilities and accomplishments developed to date to elucidate scientific principles for light energy capture and conversion into chemical bonds by integrating experiment and theory, including coupling high-throughput experimentation with artificial intelligence to accelerate progress.	The highest priorities in fundamental solar fuels generation research will be supported, building on capabilities and accomplishments developed by the former Fuels from Sunlight Hub, JCAP. Additional funding will expand fundamental research efforts in challenging aspects of solar fuels generation with a particular emphasis on photo-electrocatalysis for CO_2. The focus remains on use of only sunlight, carbon dioxide, and water as inputs for fuel production; however, new insights may be gained from studies of photodriven conversion of other molecules to fuels.

FY 2019 Enacted		FY 2020 Request	Explanation of Changes FY 2020 Request vs FY 2019 Enacted
Computational Chemical Sciences	$13,000,000	$13,000,000	$—
The FY 2019 Enacted budget continues to support Computational Chemical Sciences (CCS) awards that were made in FY 2017 and any new awards in complementary research areas made in FY 2018.		The Request will continue the CCS awards, with ongoing focus on developing public, open source codes for future exascale computer platforms.	No changes.
General Plant Projects	$1,000,000	$1,000,000	$—
The FY 2019 Enacted budget supports minor facility improvements at Ames Laboratory.		The Request will support minor facility improvements at Ames Laboratory.	No changes.
SBIR/STTR	$13,063,000	$12,498,000	-$565,000
In FY 2019, SBIR/STTR funding is set at 3.65% of non-capital funding.		In FY 2020, SBIR/STTR funding will be set at 3.65% of non-capital funding.	Funding changes are the direct result of decreases in 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.

The twelve BES scientific user facilities provide the nation with the most comprehensive and advanced x-ray, neutron, and electron based experimental tools enabling fundamental discovery science. Hundreds of experiments are conducted simultaneously around the clock generating vast quantities of raw experimental data that must be stored, transported, and then analyzed to convert the raw data into information to unlock the answers to important scientific questions. Managing the collection, transport and analysis of data at the BES facilities is a growing challenge as new facilities come on line with expanded scientific capabilities coupled together with advances in detector technology. Over the next decade, the data volume, and the computational power to process the data, is expected to grow by several orders of magnitude. Artificial intelligence and machine learning will bring new software and hardware advances to help address these data and information challenges.

In FY 2018, the BES scientific facilities were used by more than 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 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.

Since completing construction of NSLS-II in FY 2015, BES has invested in the scientific research capabilities at this advanced light source facility by building specialized experimental stations or “beamlines.” The initial suite of 7 beamlines has expanded to the current 28 beamlines with room for at least 30 more. In order to adopt the most up-to-date technologies and to provide the most advanced capabilities, BES plans a phased approach to new beamlines at NSLS-II, as was done for the other light sources in the BES portfolio. The NSLS-II Experimental Tools-II (NEXT-II) major item of equipment (MIE) project proposed in the FY 2020 request will provide three best-in-class beamlines to support the needs of the U.S. research community. These beamlines will focus on the techniques of coherent diffraction imaging, soft x-ray spectromicroscopy, and nanoscale probes of electronic excitations.

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

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

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

The Spallation Neutron Source (SNS) at ORNL uses another approach for generating neutron beams where an accelerator generates protons that strike a heavy-metal target. As a result of the impact, neutrons are produced in a process known as spallation. The SNS 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.

Nanoscale Science Research Centers (NSRCs)

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

The NSRCs focus on interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. They are a different class of facility than the x-ray and neutron sources, as NSRCs are comprised of a suite of smaller unique tools and expert scientific staff rather than based on a large accelerator or reactor. 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 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. The NSRCs will continue to develop nanoscience and QIS-related research infrastructure and capabilities for materials synthesis, device 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.

Other Project Costs

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.

Major Items of Equipment

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 and capabilities.

Research

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. As the complexity of accelerators and the performance requirements continue to grow the need for more dynamic and adaptive control systems becomes essential. Particle accelerators are complicated interconnected machines and ideal for applications of artificial intelligence and machine learning algorithms to improve performance optimization, rapid recovery of fault conditions and prognostics to anticipate problems. 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.

Activities and Explanation of Changes

FY 2019 Enacted		FY 2020 Request	Explanation of Changes FY 2020 Request vs FY 2019 Enacted
Scientific User Facilities	**$1,003,066,000**	**$942,433,000**	**-$60,633,000**
X-Ray Light Sources	$505,000,000	$484,514,000	-$20,486,000
The FY 2019 Enacted budget continues LCLS operations 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 continue at 100% of optimum.		The Request supports LCLS operations, which will resume in the second quarter of FY 2020 upon completion of installation of LCLS-II accelerator components. The remaining light source facilities will operate at approximately 87% of optimal.	The funding will support operations at five BES light sources (LCLS, APS, ALS, NSLS-II, and SSRL).
High-Flux Neutron Sources	$282,000,000	$254,665,000	-$27,335,000
The FY 2019 Enacted budget continues support for SNS and HFIR operations at 100% of optimum.		The Request provides funding for SNS and HFIR. These facilities will operate at approximately 87% of optimal.	The funding will support operations for SNS and HFIR.
Nanoscale Science Research Centers	$135,000,000	$127,229,000	-$7,771,000
The FY 2019 Enacted budget supports all five NSRCs, with part of the funding designated for tool development for QIS.		The Request provides funding for five BES Nanoscale Science Research Centers, with funding for nanoscience, QIS research, and related development of synthesis and characterization tools.	The funding will support operations for the five NSRCs.
Other Project Costs	$19,100,000	$6,000,000	-$13,100,000
The FY 2019 Enacted budget supports the LCLS-II project at SLAC National Accelerator Laboratory, ALS-U at Lawrence Berkeley National Laboratory, LCLS-II-HE at SLAC, and the Second Target Station at ORNL.		The Request will support Other Project Costs for the LCLS-II-HE project at SLAC National Accelerator Laboratory and ALS-U at Lawrence Berkeley National Laboratory.	Other Project Costs decrease in FY 2020 according to the project plans for LCLS-II and ALS-U.

FY 2019 Enacted	FY 2020 Request	Explanation of Changes FY 2020 Request vs FY 2019 Enacted
Major Items of Equipment $—	$2,000,000	+$2,000,000
No MIE funds were appropriated in FY 2019.	The Request includes funds to initiate a beamline project for NSLS-II (NEXT-II) at Brookhaven National Laboratory and will support conceptual designs of new beamlines. The Request also includes MIE funds to initiate a recapitalization project for the NSRCs and will support planning and design activities in preparation for CD-1, along with possible procurements.	The Request initiates two new MIEs: NEXT-II and NSRC Recapitalization project.
Research $29,457,000	$36,118,000	+$6,661,000
The FY 2019 Enacted budget supports 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 was appropriated for these activities in FY 2019.	The Request will support high-priority research activities for detectors and optics instrumentation and applications of machine learning techniques to accelerator optimization, control, prognostics, and data analysis.	The research increase will be used to explore artificial intelligence methods and machine learning techniques for application to accelerator improvements.
SBIR/STTR $32,509,000	$31,907,000	-$602,000
In FY 2019, SBIR/STTR funding is set at 3.65% of non-capital funding.	In FY 2020, SBIR/STTR funding will be set at 3.65% of non-capital funding.	Funding changes are the direct result of decreases in non-capital funding.

Basic Energy Sciences
Construction

Description

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

The **Linac Coherent Light Source-II (LCLS-II)** project will provide a second source of electrons at LCLS by constructing a 4 GeV, high repetition rate, superconducting linear accelerator in addition to adding two new variable gap undulators to generate an unprecedented high-repetition-rate free-electron laser. This new x-ray source will solidify the LCLS complex as the world leader in ultrafast x-ray science for decades to come. 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. The project received approval for CD-2, Approve Performance Baseline, on December 9, 2018, establishing a Total Project Cost (TPC) of $815,000,000 and a CD-4, Project Completion date of March 31, 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. The project received CD-1, Approve Alternative Selection and Cost Range, on September 21, 2018, establishing a cost range of $330,000,000 - $495,000,000 based on a point estimate of $368,000,000 and projected project finish in 2028.

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. The project received CD-1, Approve Alternative Selection and Cost Range, on September 21, 2018, establishing a cost range of $290,000,000 - $480,000,000 based on a point estimate of $368,000,000 and projected project finish in 2028.

The **Proton Power Upgrade (PPU)** project will double the proton beam power capability of the Spallation Neutron Source (SNS) from 1.4 MW to 2.8 MW, upgrade the first target station to accommodate beam power up to 2 MW, and deliver a 2 MW qualified target. PPU will fabricate and install seven new superconducting radio frequency (RF) cryomodules, with supporting RF equipment, in the existing linac tunnel and klystron gallery respectively. Equipment will be upgraded to handle the higher beam current. The ring will be upgraded with minor modifications to the injection and extraction areas. The increased beam power of 2 MW to be provided to the first target station will be enabled by the additional cryomodules, and improved target performance will be enabled by the addition of a new target gas injection system and a redesigned mercury target vessel. The project received approval for CD-1, Approve Alternative Selection and Cost Range, on April 4, 2018. The current TPC range is $184,000,000 - $320,000,000 based on a point estimate of $250,000,000 and a projected project finish in 2027. The project received CD-3A, Approve Long Lead Procurements, approval on October 5, 2018, authorizing long lead and advanced procurements for accelerator components and associated systems.

The **Second Target Station (STS)** project will expand SNS capabilities for neutron scattering research by exploiting part of the higher SNS accelerator proton power (2.8 MW) enabled by the PPU project. The STS will be a complementary pulsed source with a narrow proton beam which increases the proton power density by up to 4.5 times compared to the first target station (FTS). This dense beam of protons, when deposited on a compact, rotating, water-cooled tungsten target will create neutrons through spallation and direct them to high efficiency coupled moderators to produce an order of magnitude higher brightness cold neutrons than were previously achievable. By optimizing the design of the instruments with advanced neutron optics, optimized geometry for 10 Hz operation, and advanced detectors, the detection resolution will be up to two orders of magnitude higher, enabling new research opportunities. The most recent DOE O 413.3B approved CD is CD-0 (Approve Mission Need), approved on January 7, 2009. The current TPC range is $800,000,000 - $1,500,000,000.

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 CD-2, Approve Performance Baseline, which are reproduced in the construction project data sheet.

Activities and Explanation of Changes

FY 2019 Enacted		FY 2020 Request	Explanation of Changes FY 2020 Request vs FY 2019 Enacted
Construction	**$408,300,000**	**$183,000,000**	**-$225,300,000**
19-SC-14, Second Target Station (STS), ORNL	$1,000,000	$1,000,000	$—
The FY 2019 Enacted budget supports planning, targeted R&D and engineering design, and other activities required to advance the STS project.		The Request will support continued planning, targeted R&D and engineering design, and other activities required to advance the STS project using Other Project Costs funds appropriated in prior years. Construction funds will be executed after the appropriate critical decision approvals are received.	The Request continues funding for the STS project.
18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL	$130,000,000	$150,000,000	+$20,000,000
The FY 2019 Enacted budget supports targeted R&D, engineering design, equipment prototyping, testing, fabrication, site preparation, installation, and long lead and advance procurements.		The Request will support targeted R&D, engineering design, equipment prototyping, testing, fabrication, site preparation, installation, long lead and advanced procurements, and other activities required to advance the APS-U project.	The Request continues funding for the APS-U project.
18-SC-11, Spallation Neutron Source Proton Power Upgrade (PPU), ORNL	$60,000,000	$5,000,000	-$55,000,000
The FY 2019 Enacted budget supports R&D, engineering, prototyping, preliminary and final design, long-lead procurement, and other activities required to advance the PPU project.		The Request will support R&D, engineering, prototyping, preliminary and final design, long-lead procurement, and other activities required to advance the PPU project.	The Request continues funding for the PPU project.
18-SC-12, Advanced Light Source Upgrade (ALS-U), LBNL	$60,000,000	$13,000,000	-$47,000,000
The FY 2019 Enacted budget supports R&D, engineering design, equipment prototyping, testing, and other activities required to advance the ALS-U project.		The Request will support planning, engineering design, R&D, equipment prototyping, testing, and other activities to advance the ALS-U project.	The Request continues funding for the ALS-U project.

FY 2019 Enacted	FY 2020 Request	Explanation of Changes FY 2020 Request vs FY 2019 Enacted
18-SC-13, Linac Coherent Light Source-II High Energy (LCLS-II-HE), SLAC $28,000,000	$14,000,000	-$14,000,000
The FY 2019 Enacted budget supports R&D, engineering design, equipment prototyping, testing, and other activities required to advance the LCLS-II-HE project.	The Request will support planning, engineering design, R&D, equipment prototyping, testing, and other activities required to advance the LCLS-II-HE project.	The Request continues funding for the LCLS-II-HE project.
13-SC-10, Linac Coherent Light Source-II (LCLS-II), SLAC $129,300,000	$—	-$129,300,000
The FY 2019 Enacted budget supports 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.	No funding is requested for FY 2020. FY 2019 was the last year of funding for LCLS-II. The project will continue with construction activities towards an early completion in FY 2020 – FY 2021.	Final funding was provided in FY 2019.

Basic Energy Sciences
Capital Summary

	(dollars in thousands)					
	Total	Prior Years	FY 2018 Enacted	FY 2019 Enacted	FY 2020 Request	FY 2020 Request vs FY 2019 Enacted
Capital Operating Expenses Summary						
Capital Equipment	N/A	N/A	48,831	76,610	38,755	-37,855
Minor Construction Activities						
General Plant Projects (GPP)	N/A	N/A	1,000	3,000	1,000	-2,000
Accelerator Improvement Projects (AIP)	N/A	N/A	9,950	33,800	29,500	-4,300
Total, Capital Operating Expenses	**N/A**	**N/A**	**59,781**	**113,410**	**69,255**	**-44,155**

Capital Equipment

	(dollars in thousands)					
	Total	Prior Years	FY 2018 Enacted	FY 2019 Enacted	FY 2020 Request	FY 2020 Request vs FY 2019 Enacted
Capital Equipment						
Major Items of Equipment (MIE)						
NSLS-II Experimental Tools-II (NEXT-II), BNL	60,000	—	—	—	1,000	+1,000
NSRC Recapitalization	60,000	—	—	—	1,000	+1,000
Total MIEs	N/A	N/A	—	—	2,000	+2,000
Total Non-MIE Capital Equipment	N/A	N/A	48,831	76,610	36,755	-39,855
Total, Capital Equipment	**N/A**	**N/A**	**48,831**	**76,610**	**38,755**	**-37,855**

Minor Construction Activities

	(dollars in thousands)					
	Total	Prior Years	FY 2018 Enacted	FY 2019 Enacted	FY 2020 Request	FY 2020 Request vs FY 2019 Enacted
General Plant Projects (GPP)						
GPP less than $5M[a]	N/A	N/A	1,000	3,000	1,000	-2,000
Total, GPP	**N/A**	**N/A**	**1,000**	**3,000**	**1,000**	**-2,000**

[a] GPP activities less than $5M include design and construction for additions and/or improvements to land, buildings, replacements or additions to roads, and general area improvements.

	(dollars in thousands)					
	Total	**Prior Years**	**FY 2018 Enacted**	**FY 2019 Enacted**	**FY 2020 Request**	**FY 2020 Request vs FY 2019 Enacted**
Accelerator Improvement Projects (AIP)						
Greater than or Equal to $5M and less than $20M						
VENUS, Spallation Neutron Source, ORNL	13,400	N/A	—	13,400	—	-13,400
DISCOVER, Spallation Neutron Source, ORNL	18,500	N/A	—	—	18,500	+18,500
Total AIPs (great than or equal to $5M and less than $20M)	N/A	N/A	—	13,400	18,500	+5,100
Total AIPs less than $5M[a]	N/A	N/A	9,950	20,400	11,000	-9,400
Total, Accelerator Improvement Projects	N/A	N/A	9,950	33,800	29,500	-4,300
Total, Minor Construction Activities	**N/A**	**N/A**	**10,950**	**36,800**	**30,500**	**-6,300**

[a] AIP activities less than $5M include minor construction at an existing accelerator facility.

Basic Energy Science
Major Item of Equipment Description(s)

Scientific User Facilities MIEs:
The *NSLS-II Experimental Tools-II (NEXT-II) Project:* The NSLS-II Experimental Tools-II project proposes to add three world-class beamlines to the NSLS-II Facility as part of a phased buildout of beamlines to provide advances in scientific capabilities for the soft x-ray user community. These beamlines will focus on the techniques of coherent diffraction imaging, soft x-ray spectromicroscopy, and nanoscale probes of electronic excitations. The preliminary notional cost range for this project is $40M to $60M. The preliminary total project cost (TPC) point estimate is $60M based on a project finish in FY 2026.

The *NSRC Recapitalization Project*: The Nanoscale Science Research Centers (NSRCs) started early operations in 2006-2007 and now, a decade later, they need to recapitalize their instrumentation to continue to perform cutting edge science to support and accelerate advances in the fields of nanoscience, materials, chemistry, and biology. The recapitalization will also provide essential support for quantum information science and systems. The preliminary notional cost range for this project is $50M to $90M. The preliminary TPC point estimate is $60M based on a project finish in FY 2026.

Basic Energy Sciences
Construction Projects Summary

(dollars in thousands)

	Total	Prior Years	FY 2018 Enacted	FY 2019 Enacted	FY 2020 Request	FY 2020 Request vs FY 2019 Enacted
19-SC-14, Second Target Station (STS), ORNL						
TEC	1,204,000	—	—	1,000	1,000	—
OPC	45,300	—	—	5,000	—	-5,000
TPC	**1,249,300**	—	—	**6,000**	**1,000**	-5,000
18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL						
TEC	815,000	—	93,000	130,000	150,000	+20,000
OPC	—	—	—	—	—	—
TPC	**815,000**	—[a]	**93,000**	**130,000**	**150,000**	**+20,000**
18-SC-11, Proton Power Upgrade (PPU), ORNL						
TEC	250,000	—	36,000	60,000	5,000	-55,000
OPC	—	—	—	—	—	—
TPC	**250,000**	—	**36,000**	**60,000**	**5,000**	**-55,000**
18-SC-12, Advanced Light Source Upgrade (ALS-U), LBNL						
TEC	338,000	—	16,000	60,000	13,000	-47,000
OPC	30,000	10,000	14,000	2,000	2,000	—
TPC	**368,000**	**10,000**	**30,000**	**62,000**	**15,000**	**-47,000**
18-SC-13, Linac Coherent Light Source-II-HE (LCLS-II-HE), SLAC						
TEC	348,000	—	8,000	28,000	14,000	-14,000
OPC	20,000	—	2,000	6,000	4,000	-2,000
TPC	**368,000**	—	**10,000**	**34,000**	**18,000**	**-16,000**

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

(dollars in thousands)

	Total	Prior Years	FY 2018 Enacted	FY 2019 Enacted	FY 2020 Request	FY 2020 Request vs FY 2019 Enacted
13-SC-10, Linac Coherent Light Source-II (LCLS-II), SLAC						
TEC	993,100	671,700	192,100	129,300	—	-129,300
OPC	51,900	37,900	7,900	6,100	—	-6,100
TPC	**1,045,000**	**709,600**[a]	**200,000**	**135,400**	—	**-135,400**
Total, Construction						
TEC	N/A	N/A	345,100	408,300	183,000	-225,300
OPC	N/A	N/A	23,900	19,100	6,000	-13,100
TPC	**N/A**	**N/A**	**369,000**	**427,400**	**189,000**	**-238,400**

Funding Summary

(dollars in thousands)

	FY 2018 Enacted	FY 2019 Enacted	FY 2020 Request	FY 2020 Request vs FY 2019 Enacted
Research	821,403	815,600	799,877	-15,723
Facility Operations	898,597	922,000	866,408	-55,592
Projects	369,000	427,400	191,000	-236,400
Other[b]	1,000	1,000	1,000	—
Total, Basic Energy Sciences	**2,090,000**	**2,166,000**	**1,858,285**	**-307,715**

[a] LCLS-II received $85,600,000 in FY 2010-FY 2013 as an MIE.
[b] Includes non-Facility related GPP.

Basic Energy Sciences
Scientific User Facility Operations

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.

(dollars in thousands)

	FY 2018 Enacted	FY 2018 Current	FY 2019 Enacted	FY 2020 Request	FY 2020 Request vs FY 2019 Enacted
TYPE A FACILITIES					
Advanced Light Source	**$64,606**	**$64,606**	**$66,283**	**$62,511**	**-$3,772**
Number of Users	2,066	2,066	2,000	1,800	-200
Achieved operating hours	N/A	5,228	N/A	N/A	N/A
Planned operating hours	5,100	5,100	4,700	4,600	-100
Optimal hours	5,300	5,300	4,700[a]	5,300	+600
Percent optimal hours	96.2%	98.6%	100.0%	86.8%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A

[a] Optimal hours decreased for scheduled maintenance.

(dollars in thousands)

	FY 2018 Enacted	FY 2018 Current	FY 2019 Enacted	FY 2020 Request	FY 2020 Request vs FY 2019 Enacted
Advanced Photon Source	**$133,285**	**$133,285**	**$136,743**	**$128,962**	**-$7,781**
Number of Users	5,704	5,704	5,700	4,900	-800
Achieved operating hours	N/A	4,883	N/A	N/A	N/A
Planned operating hours	5,000	5,000	5,000	4,350	-650
Optimal hours	5,000	5,000	5,000	5,000	—
Percent optimal hours	100.0%	97.7%	100.0%	87.0%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A
National Synchrotron Light Source-II, BNL	**$111,241**	**$111,241**	**$114,127**	**$107,633**	**-$6,494**
Number of Users	1,364	1,364	1,600	1,350	-250
Achieved operating hours	N/A	4,589	N/A	N/A	N/A
Planned operating hours	4,750	4,750	5,000	4,350	-650
Optimal hours	5,000	5,000	5,000	5,000	—
Percent optimal hours	95.0%	91.8%	100.0%	87.0%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A
Stanford Synchrotron Radiation Lightsource	**$41,763**	**$41,763**	**$42,847**	**$40,408**	**-$2,439**
Number of Users	1,752	1,752	1,650	1,500	-150
Achieved operating hours	N/A	5,076	N/A	N/A	N/A
Planned operating hours	5,200	5,200	5,070	4,700	-370
Optimal hours	5,400	5,400	5,070[a]	5,400	330
Percent optimal hours	96.3%	94.0%	100.0%	87.0%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A
Linac Coherent Light Source	**$138,008**	**$138,008**	**$145,000**	**$145,000**	—
Number of Users	937	937	300	500	+200
Achieved operating hours	N/A	4,535	N/A	N/A	N/A
Planned operating hours	4,750	4,750	1,600	2,900	+1,300
Optimal hours	5,000	5,000	1,600[b]	3,000	+1,400
Percent optimal hours	95.0%	90.7%	100.0%	96.7%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A

[a] Optimal hours decreased for scheduled maintenance.
[b] LCLS Optimal hours reduced in preparation for installation activities related to LCLS-II.

(dollars in thousands)

	FY 2018 Enacted	FY 2018 Current	FY 2019 Enacted	FY 2020 Request	FY 2020 Request vs FY 2019 Enacted
Spallation Neutron Source	**$204,098**	**$204,098**	**$205,714**	**$185,774**	**-$19,940**
Number of Users	644	644	800	730	-70
Achieved operating hours	N/A	3,010	N/A	N/A	N/A
Planned operating hours	2,850	2,850	4,900	4,350	-550
Optimal hours	3,000[a]	3,000[a]	4,900	5,000	100
Percent optimal hours	95.0%	100.3%	100.0%	87.0%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A
High Flux Isotope Reactor	**$74,670**	**$74,670**	**$76,286**	**$68,891**	**-$7,395**
Number of Users	561	561	560	500	-60
Achieved operating hours	N/A	4,059	N/A	N/A	N/A
Planned operating hours	3,900	3,900	4,000	3,500	-500
Optimal hours	4,000	4,000	4,000	4,000	—
Percent optimal hours	97.5%	101.5%	100.0%	87.5%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A
Lujan Neutron Scattering Center	**$1,000**	$1,000	—	—	—
Achieved operating hours	N/A	N/A	N/A	N/A	N/A
Planned operating hours	—	—	—	—	—
Optimal hours	—	—	—	—	—
Percent optimal hours	N/A	N/A	N/A	N/A	N/A
Unscheduled downtime hours	N/A	N/A	N/A	N/A	N/A
TYPE B FACILITIES					
Center for Nanoscale Materials	**$26,783**	**$26,783**	**$27,704**	**$26,109**	**-$1,595**
Number of users	608	608	600	530	-70
Center for Functional Nanomaterials	**$22,759**	**$22,759**	**$24,148**	**$22,758**	**-$1,390**
Number of users	581	581	580	510	-70
Molecular Foundry	**$30,184**	**$30,184**	**$31,237**	**$29,438**	**-$1,799**
Number of users	939	939	700	600	-100

(dollars in thousands)

	FY 2018 Enacted	FY 2018 Current	FY 2019 Enacted	FY 2020 Request	FY 2020 Request vs FY 2019 Enacted
Center for Nanophase Materials Sciences	**$26,180**	**$26,180**	**$27,078**	**$25,520**	**-$1,558**
Number of users	640	640	600	530	-70
Center for Integrated Nanotechnologies	**$24,020**	**$24,020**	**$24,833**	**$23,404**	**-$1,429**
Number of users	659	659	600	530	-70
Total, All Facilities	**$898,597**	**$898,597**	**$922,000**	**$866,408**	**-$55,592**
Number of Users	16,455	16,455	15,690	13,980	-1,710
Achieved operating hours	N/A	31,380	N/A	N/A	N/A
Planned operating hours	31,550	31,550	30,270	28,750	-1,520
Optimal hours	32,700	32,700	30,270	32,700	+2,430
Percent of optimal hours	96.3%	96.5%	98.6%	88.9%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A

Scientific Employment

	FY 2018 Enacted	FY 2019 Enacted	FY 2020 Request	FY 2020 Request vs FY 2019 Enacted
Number of permanent Ph.D.'s (FTEs)	4,870	4,800	4,520	-280
Number of postdoctoral associates (FTEs)	1,340	1,310	1,250	-60
Number of graduate students (FTEs)	2,090	2,050	1,960	-90
Other[a]	3,060	3,030	2,820	-210

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

19-SC-14, Second Target Station
Oak Ridge National Laboratory, Oak Ridge, Tennessee
Project is for Design and Construction

1. Summary, Significant Changes, and Schedule and Cost History

Summary

The FY 2020 Request for Second Target Station (STS) project is $1,000,000. The most recent DOE O 413.3B approved Critical Decision (CD) is CD-0 (Approve Mission Need), approved on January 7, 2009. The current Total Project Cost (TPC) range is $800,000,000 - $1,500,000,000.

Significant Changes

This initial construction project data sheet (CPDS) for FY 2020 funding does not include a new start for the budget year.

In FY 2019, the project will advance the planning, research and development, prototyping, and conceptual design. In FY 2020, the project continues planning, targeted R&D and engineering design, and other activities required to advance the STS project using Other Project Costs (OPC) funds appropriated in prior years. FY 2020 construction funds will be executed after the appropriate critical decision (CD) approvals are received.

A Federal Project Director has not yet been assigned to this project.

Critical Milestone History

Fiscal Year	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2020[a]	1/7/2009	2Q FY 2022	2Q FY 2022	2Q FY 2023	2Q FY 2025	2Q FY 2024	N/A	4Q FY 2031

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

Project Cost History

(dollars in thousands)

Fiscal Year	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, D&D	OPC, Total	TPC
FY 2020[a]	65,500	1,138,500	1,204,000	45,300	—	45,300	1,249,300

2. Project Scope and Justification

Scope

The global landscape in neutron scattering science is changing rapidly. To sustain our position at the frontier in materials and chemical characterization, dramatic improvements in experimental capabilities are needed. In particular, upgraded neutron sources are necessary to achieve the Basic Energy Sciences (BES) mission.

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

The 2015 Basic Energy Sciences Advisory Committee report "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science" identified five new transformative opportunities that have the potential to transform many of today's energy-related technologies involving matter and energy. Advances in neutron sources and instrumentation play a direct part in advancing science to achieve those opportunities.

The two neutron scattering facilities in the BES portfolio, the High Flux Isotope Reactor (HFIR) and the SNS are both sited at Oak Ridge National Laboratory (ORNL) and address one of the DOE's key research areas—the use of neutrons and sophisticated instrumentation to probe materials. Many technical margins were built into SNS systems to facilitate a power upgrade to at least 2 MW, with the ability to extract some of that power to a second target station.

To address the gap in advanced neutron sources and instrumentation, the SNS project will design, build, install, and test the equipment necessary to provide the four primary elements of the new SNS facility: the neutron target and moderators; the accelerator systems; the instruments; and the conventional facilities. Costs for acceptance testing, integrated testing, and initial commissioning to demonstrate achievement of the KPPs are included in the STS scope.

The STS features an optimally sized 30 cm^2 proton beam that is concentrated into one-fifth the area of the FTS beam to produce a very high density beam of protons that strikes a 1.1 meter diameter rotating solid tungsten target. The produced neutron beam illuminates three moderators located above and below the target that will feed up to 22 experimental beamlines with neutron energies conditioned for specific instruments. The small-volume cold neutron moderator system is geometrically optimized to deliver higher peak brightness neutrons.

The SNS Proton Power Upgrade (PPU) project will double the power of the SNS accelerator complex to 2.8 MW so that STS can use one out of every six proton pulses to produce cold neutron beams with the highest peak brilliance of any current or projected neutron sources. The high-brightness pulsed source optimized for cold neutron production will operate at 15 Hz (as compared to FTS at 60 Hz) to provide the large time-of-flight intervals corresponding to the broad time and length scales required to characterize complex materials. The project will provide a series of kicker magnets to divert every sixth proton pulse away from the FTS to a new line feeding the STS. Additional magnets will further deflect the beam into the transport line to the new target. A final set of quadrupole magnets will tailor the proton beam shape and distribution to match the compact source design.

An initial set of 22 instrument concepts, developed with input from the user community, are largely built on known and demonstrated technologies but will need some research and development to deliver unprecedented levels of performance. Advanced neutron optics designs are needed for high alignment and stability requirements. The lower repetition rate of STS pushes the chopper design to larger diameter rotating elements with tighter limits on allowed mechanical vibration. The higher peak neutron production of STS will put a greater demand on neutron detector technology.

The STS complex will be located in unoccupied space east of the existing FTS. The project requires approximately 380,000 ft2 of new buildings, making conventional facility construction a major contributor to project costs. The layout can consolidate instruments with beamlines less than 40 m long in a hall adjacent to the STS target building to free up space for the longest beamlines (50% longer than the longest FTS beamline) on the opposite side of the STS target.

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." BES accomplishes its mission by operation of large-scale user facilities consisting of a complementary set of intense x-rays sources, neutron scattering centers, electron beam characterization capabilities, and research centers for nanoscale science.

In the area of neutron science, the scientific justification and need for a very high-intensity pulsed neutron source in the U.S. has been established by numerous studies by the scientific community since the 1970s. This need is currently being fulfilled by the SNS, which began its user program at ORNL in 2007. In accordance with the 1996 BESAC (Russell Panel) Report recommendation, the SNS was designed to be upgradeable so as to maintain its position of scientific leadership in the future, and many technical margins were built into the SNS systems to facilitate a power upgrade into the 2-4 MW range.

An upgraded SNS would enable many advances in the opportunities described in the 2015 BESAC report “Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science.” Four workshops were held to assess the neutron scattering needs in quantum condensed matter, soft matter, biology, and the frontiers in materials discovery. These four areas encompass and directly map to the transformative opportunities identified in the BES Grand Challenges update. Quantum materials map most directly to harnessing coherence in light and matter, while soft matter and biology are aligned primarily with mastering hierarchical architectures and beyond-equilibrium matter, and frontiers in materials discovery explored many of the topics in beyond ideal materials and systems: understanding the critical roles of heterogeneity, interfaces, and disorder. As an example, while neutrons already play an important role in the areas of biology and soft matter, step change improvements in capability will be required to make full use of the unique properties of neutrons to meet challenges in mastering hierarchical architectures and beyond-equilibrium matter and understanding the critical roles of heterogeneity and interfaces. The uniform conclusion from all workshops was that in the areas of science covered, neutrons play a unique and pivotal role in understanding structure and dynamics in materials required to develop future technologies.

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

Key Performance Parameters (KPPs)

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

Performance Measure	Threshold	Objective
Beam power on target	0.25 MW at 1.0 GeV	0.47 MW at 1.3 GeV
Beam energy	1.3 GeV	≥ 1.3 GeV
Target operational lifetime without failure	2,000 hours at 0.25 MW	2,500 hours at 0.5 MW
Proton Beam size	≤ 60 cm^2	30 cm^2
Neutron peak brightness	$1.7x10^{14}$	$3.5x10^{14}$
Number of operating instruments at CD-4	6	8

3. Financial Schedule

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
Design			
FY 2019	1,000	1,000	—
FY 2020	1,000	1,000	—
Outyears	63,500	63,500	65,500
Total, Design	65,500	65,500	65,500
Construction			
Outyears	1,138,500	1,138,500	1,138,500

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total, Construction	1,138,500	1,138,500	1,138,500
Total Estimated Costs (TEC)			
FY 2019	1,000	1,000	—
FY 2020	1,000	1,000	—
Outyears	1,202,000	1,202,000	1,204,000
Total, TEC	**1,204,000**	**1,204,000**	**1,204,000**
Other Project Costs (OPC)			
FY 2016	6,500	6,500	3,069
FY 2017	—	—	2,870
FY 2018	—	—	227
FY 2019	5,000	5,000	4,700
FY 2020	—	—	425
Outyears	33,800	33,800	34,009
Total, OPC	**45,300**	**45,300**	**45,300**
Total Project Costs (TPC)			
FY 2016	6,500	6,500	3,069
FY 2017	—	—	2,870
FY 2018	—	—	227
FY 2019	6,000	6,000	4,700
FY 2020	1,000	1,000	425
Outyears	1,235,800	1,235,800	1,238,009
Total, TPC[a]	**1,249,300**	**1,249,300**	**1,249,300**

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design			
Design	48,500	N/A	N/A
Contingency	17,000	N/A	N/A
Total, Design	65,500	N/A	N/A
Construction			
Construction	845,000	N/A	N/A
Contingency	293,500	N/A	N/A
Total, Construction	1,138,500	N/A	N/A
Total, TEC	**1,204,000**	N/A	N/A
Contingency, TEC	*310,500*	*N/A*	*N/A*
Other Project Cost (OPC)			
OPC except D&D			
R&D	1,500	N/A	N/A

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

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Conceptual Design	18,375	N/A	N/A
Start-Up	14,100	N/A	N/A
Contingency	11,325	N/A	N/A
Total, OPC	**45,300**	N/A	N/A
Contingency, OPC	*11,325*	*N/A*	*N/A*
Total Project Cost[a]	**1,249,300**	**N/A**	**N/A**
Total, Contingency (TEC+OPC)	***321,825***	***N/A***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2018	FY 2019[a]	FY 2020	Outyears	Total
FY 2020	TEC	—	—	1,000	1,000	1,202,000	1,204,000
	OPC	6,500	—	5,000	—	33,800	45,300
	TPC	6,500	—	6,000	1,000	1,235,800	1,249,300

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy (fiscal quarter or date)	4Q FY 2031
Expected Useful Life (number of years)	25
Expected Future Start of D&D of this capital asset (fiscal quarter)	4Q FY 2056

Related Funding Requirements
(dollars in thousands)

	Annual Costs		Life Cycle Costs	
	Previous Total Estimate	Current Total Estimate	Previous Total Estimate	Current Total Estimate
Operations and Maintenance	N/A	45,000	N/A	1,125,000

The numbers presented are the incremental operations and maintenance costs above the existing SNS facility without escalation. The estimate will be updated and additional details will be provided after CD-2, Approve Performance Baseline.

[a] While no funding was requested, Congress appropriated $6,000,000 for STS in FY 2019.

7. 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 ORNL	~380,000
Area of D&D in this project at ORNL	—
Area at ORNL to be transferred, sold, and/or D&D outside the project, including area previously "banked"	~380,000
Area of D&D in this project at other sites	—
Area at other sites to be transferred, sold, and/or D&D outside the project, including area previously "banked"	—
Total area eliminated	—

8. Acquisition Approach

DOE has determined that the STS project will be acquired by ORNL under the existing DOE Management and Operations (M&O) contract.

A Technical Design Report for the STS project has been prepared. Key design activities, requirements, and high-risk subsystem components have been 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 an ORNL-wide resource.

ORNL will partner with other laboratories for design and procurement of key technical subsystem components. Some technical system designs will require research and development activities. Preliminary cost estimates for these systems are based on operating experience of SNS and vendor quotes. Design of the technical systems will be completed by ORNL, partner laboratory staff, and/or vendors. Technical equipment will be fabricated by vendors and/or partner labs 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 STS.

18-SC-10, Advanced Photon Source-Upgrade
Argonne National Laboratory
Project is for Design and Construction

1. Summary, Significant Changes, and Schedule and Cost History

Summary

The FY 2020 Request for the Advanced Photon Source-Upgrade (APS-U) project is $150,000,000. The most recent DOE Order 413.3B approved Critical Decision, CD-2 (Approve Performance Baseline), was approved on December 9, 2018, with a Total Project Cost (TPC) of $815,000,000 and CD-4, Approve Project Completion, in FY 2026.

Significant Changes

This Construction Project Data Sheet (CPDS) is an update of the FY 2019 CPDS and does not include a new start for the budget year. The TPC increased from $770,000,000 to $815,000,000 to meet the mission need of delivering a world-class hard x-ray light source scientific user facility. The APS-U project performed multiple scientific and technical reviews to incorporate the recommendations from the scientific user community. This resulted in additional world-leading scientific instruments being recommended and incorporated into the project scope that will provide new and advanced capabilities, particularly in the areas of coherent scattering, coherent imaging, and high energy microscopy. The project cost and Key Performance Parameters (KPPs) have been updated to include these enhancements that take full advantage of the upgraded APS source and storage ring.

In FY 2018, APS-U procured accelerator, experimental systems, and front end components needed to maintain the project schedule. APS-U awarded contracts for more than half of the storage ring magnets, critical superconducting RF system components, and state of the art beamline optics in addition to key materials for the front ends and undulators as long lead and advanced procurements (LLP/APs). FY 2019 funding completes the majority of equipment prototyping and development work. Engineering design, testing, fabrication, installation, additional LLP/APs, and site preparation for the long beamlines continue. Planned activities for FY 2020 include continuing targeted development, prototyping and finishing associated engineering designs, testing, and fabrication. Receipt, acceptance, and preparation for installation of incoming vendor fabricated components procured as LLP/APs will occur along with initial system integration and assembly. After CD-3, procurements beyond the currently approved LLP/APs will begin. Further site preparation and civil construction associated with the long beamlines will occur.

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

Critical Milestone History

Fiscal Year	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2018	4/22/2010	9/18/2015	2/4/2016	1Q FY 2019	2Q FY 2020	4Q FY 2019	N/A	1Q FY 2026
FY 2019	4/22/2010	9/18/2015	2/4/2016	2Q FY 2019	4Q FY 2021	1Q FY 2020	N/A	2Q FY 2026
FY 2020	4/22/2010	9/18/2015	2/4/2016	12/09/2018	1Q FY 2022	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 or will be completed (if applicable)
CD-1 – Approve Design Scope and Project Cost and Schedule Ranges
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 Project Completion

Fiscal Year	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
FY 2020	12/09/2018	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.

Project Cost History

(dollars in thousands)

Fiscal Year	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	167,000	590,100	757,100	12,900	N/A	12,900	770,000
FY 2020	162,825	633,675	796,500	18,500	N/A	18,500	815,000

2. 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 at Argonne National Laboratory (ANL), 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 light 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 an 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 also 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.

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

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 injection mode with systems installed for 200 mA operation	200 mA in top-up injection mode
Horizontal Emittance	< 130 pm-rad at 25 mA	≤ 42 pm-rad at 200 mA
Brightness @ 20 keV[1]	> 1 x 10^{20}	1 x 10^{22}
Brightness @ 60 keV[1]	> 1 x 10^{19}	1 x 10^{21}
New APS-U Beamlines Transitioned to Operations	7	≥ 9

[1]Units = photons/sec/mm^2/$mrad^2$/0.1% BW

3. **Financial Schedule**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
Design			
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	28,775	28,775	23,098
FY 2018	—	—	12,716
FY 2019	—	—	2,343
Total, MIE funding	119,990	119,990	119,990
Line item construction funding			
FY 2018	32,000	32,000	3,021
FY 2019	7,735	7,735	17,150
FY 2020	3,100	3,100	19,850
FY 2021	—	—	2,814
Total, Line item construction funding	42,835	42,835	42,835
Total, Design	162,825	162,825	162,825
Construction			
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	—	—	677
FY 2016	—	—	—
FY 2017	13,725	13,725	389
FY 2018	—	—	7,497
FY 2019	—	—	5,064
FY 2020	—	—	775
Total, MIE funding	22,510	22,510	22,510
Line item construction funding			
FY 2018	61,000	61,000	6,902
FY 2019	122,265	122,265	127,833
FY 2020	146,900	146,900	171,250
FY 2021	160,000	160,000	161,500
FY 2022	121,000	121,000	126,250
FY 2023	—	—	15,375
FY 2024	—	—	2,055
Total, Line item construction funding	611,165	611,165	611,165
Total, Construction	633,675	633,675	633,675

(dollars in thousands)

	Budget Authority (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	—	—	20,213
FY 2019	—	—	7,407
FY 2020	—	—	775
Total, MIE funding	142,500	142,500	142,500
Line item construction funding			
FY 2018	93,000	93,000	9,923
FY 2019	130,000	130,000	144,983
FY 2020	150,000	150,000	191,100
FY 2021	160,000	160,000	164,314
FY 2022	121,000	121,000	126,250
FY 2023	—	—	15,375
FY 2024	—	—	2,055
Total, Line item construction funding	654,000	654,000	654,000
Total, TEC	**796,500**	**796,500**	**796,500**
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	—	—	4,217
Total MIE funding	8,500	8,500	8,500
Line item construction funding			
FY 2021	5,000	5,000	4,500
FY 2022	5,000	5,000	4,500
FY 2023	—	—	1,000
Total, Line item construction funding	10,000	10,000	10,000
Total, OPC	**18,500**	**18,500**	**18,500**
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

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
FY 2016	20,000	20,000	22,529
FY 2017	42,500	42,500	23,487
FY 2018	—	—	20,213
FY 2019	—	—	7,407
FY 2020	—	—	775
Total, MIE funding	151,000	151,000	151,000
Line item construction funding			
FY 2018	93,000	93,000	9,923
FY 2019	130,000	130,000	144,983
FY 2020	150,000	150,000	191,100
FY 2021	165,000	165,000	168,814
FY 2022	126,000	126,000	130,750
FY 2023	—	—	16,375
FY 2024	—	—	2,055
Total, Line item construction funding	664,000	664,000	664,000
Total, TPC	**815,000**	**815,000**	**815,000**

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design			
Design	146,825	157,150	N/A
Contingency	16,000	9,850	N/A
Total, Design	162,825	167,000	N/A
Construction			
Equipment	483,575	426,420	N/A
Other Construction	15,000	14,680	N/A
Contingency	135,100	149,000	N/A
Total, Construction	633,675	590,100	N/A
Total, TEC	**796,500**	**757,100**	**N/A**
Contingency, TEC	*151,100*	*158,850*	*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	7,800	3,250	N/A
Contingency	2,200	1,150	N/A
Total, OPC	**18,500**	**12,900**	**N/A**
Contingency, OPC	*2,200*	*1,150*	*N/A*
Total Project Cost	**815,000**	**770,000**	**N/A**
Total Contingency (TEC+OPC)	***153,300***	***160,000***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2018	FY 2019	FY 2020	FY 2021	FY 2022	FY 2023	Outyears	Total
FY 2018	TEC	142,500	20,000	81,772	152,419	160,000	82,500	79,809	—	719,000
	OPC	8,500	—	—	—	5,000	27,500	10,000	—	51,000
	TPC	151,000	20,000	81,772	152,419	165,000	110,000	89,809	—	770,000
FY 2019	TEC	142,500	20,000	60,000	150,000	159,780	133,100	91,720	—	757,100
	OPC	8,500	—	—	—	—	2,200	2,200	—	12,900
	TPC	151,000	20,000	60,000	150,000	159,780	135,300	93,920	—	770,000
FY 2020	TEC	142,500	93,000	130,000	150,000	160,000	121,000	—	—	796,500
	OPC	8,500	—	—	—	5,000	5,000	—	—	18,500
	TPC	151,000	93,000	130,000	150,000	165,000	126,000	—	—	815,000

6. 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
(dollars in thousands)

	Annual Costs		Life Cycle Costs	
	Previous Total Estimate	Current Total Estimate	Previous Total Estimate	Current Total Estimate
Operations and Maintenance	N/A	18,000	N/A	450,000

The numbers presented are the incremental operations and maintenance costs above the existing APS facility without escalation. The estimate will be updated as the project is executed.

7. 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	—
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	—
Area at other sites to be transferred, sold, and/or D&D outside the project including area previously "banked"	—
Total area eliminated	—

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

8. Acquisition Approach

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

ANL will have prime responsibility for oversight of all contracts required to execute this project which will include managing the design and construction of the APS-U accelerator incorporating an 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.

18-SC-11, Proton Power Upgrade
Oak Ridge National Laboratory, Oak Ridge, Tennessee
Project is for Design and Construction

1. Summary, Significant Changes, and Schedule and Cost History

<u>**Summary**</u>

The FY 2020 Request for the Proton Power Upgrade (PPU) project is $5,000,000. The most recent DOE O 413.3B approved Critical Decision (CD) is CD-3A (Approve Long Lead Procurements), approved on October 5, 2018. The preliminary Total Project Cost (TPC) range, based on early concepts under consideration, is $184,000,000 - $320,000,000.

<u>**Significant Changes**</u>

Congress first appropriated funds for PPU in FY 2018 and was a new start in that year. This Construction Project Data Sheet (CPDS) for FY 2020 funding does not include a new start for the budget year.

In FY 2018, PPU advanced the technical system designs, including completing the status report on the 2 MW target conceptual design scoping analysis. The project received CD-1 (Approve Alternative Selection and Cost Range) approval on April 4, 2018 for a TPC range of $184,000,000 - $320,000,000. CD-3A (Approve Long Lead Procurements) approval was received on October 5, 2018 for up to $10,505,000 for niobium material, cryomodule cavities, and related cryomodule procurements. No funding was requested for PPU in FY 2019; however, Congress appropriated $60,000,000 in FY 2019, which enables R&D, engineering, prototyping, preliminary and final design, long-lead procurement, and target R&D aimed at further advancing the target performance in coordination with SNS operations target management. In FY 2020, funds will be utilized for R&D, engineering, prototyping, preliminary and final design. Target R&D will continue. Additional long lead procurement authority (CD-3B), if approved, will advance the klystron gallery buildout, RF procurements, and cryomodule hardware procurements and assembly.

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

<u>**Critical Milestone History**</u>

Fiscal Year	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2020[a]	1/7/2009	8/1/2017	4/4/2018	2Q FY 2021	4Q FY 2022	3Q FY 2022	N/A	3Q FY 2027

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

Fiscal Year	Performance Baseline Validation	CD-3A	CD-3B
FY 2020[a]	2Q FY 2021	10/5/2018	2Q FY 2020

CD-3A – Approve Long-Lead Procurements, niobium material, cryomodule cavities, and related cryomodule procurements.
CD-3B – Approve Long-Lead Procurements, klystron gallery buildout, RF procurements, and cryomodule hardware.

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

Project Cost History

(dollars in thousands)

Fiscal Year	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, D&D	OPC, Total	TPC
FY 2020[a]	27,300	210,000	237,300	12,700	N/A	12,700	250,000

2. Project Scope and Justification

Scope

The global landscape in neutron scattering science is changing rapidly. To sustain the U.S.'s position at the frontier in materials and chemical characterization, dramatic improvements in experimental capabilities are needed. In particular, upgraded neutron sources are necessary to achieve the Basic Energy Sciences (BES) mission.

The 2015 Basic Energy Sciences Advisory Committee report "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science" identified five new transformative opportunities that have the potential to transform many of today's energy-related technologies involving matter and energy.b Advances in neutron sources and instrumentation directly play a part in achieving four of those five goals.

The two neutron scattering facilities in the BES portfolio, the High Flux Isotope Reactor (HFIR) and the SNS, are both sited at Oak Ridge National Laboratory (ORNL) and address one of the DOE's key research areas—the use of neutrons and sophisticated instrumentation to probe materials. Many technical margins were built into SNS systems to facilitate a power upgrade to at least 2 MW, with the ability to extract some of that power to a second target station.

To address the gap in advanced neutron sources and instrumentation, the PPU project will design, build, install, and test the equipment necessary to double the accelerator power from 1.4 MW to 2.8 MW, upgrade the existing SNS target system to accommodate beam power up to 2 MW, and deliver a 2 MW qualified target. PPU also includes the provision for a stub-out in the SNS transport line to the existing target to facilitate rapid connection to a new proton beamline. The project also includes modifications to some buildings and services. Costs for acceptance testing, integrated testing, and initial commissioning to demonstrate achievement of the KPPs are included in the PPU scope.

PPU will accomplish the energy upgrade by fabricating and installing seven new superconducting RF cryomodules, with supporting RF equipment, in the existing SNS linac tunnel and klystron gallery. The high voltage converter modulators and klystrons for some of the existing installed RF equipment will be upgraded to handle the higher beam current. The accumulator ring will be upgraded with minor modifications to the injection and extraction areas. A new high volume gas injection system for pressure pulse mitigation in the mercury target and a redesigned mercury target vessel will allow the first target station to handle the increased beam power of 2 MW.

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." BES accomplishes its mission by operating large-scale user facilities consisting of a complementary set of intense x-rays sources, neutron scattering centers, electron beam characterization capabilities, and research centers for nanoscale science.

In the area of neutron science, numerous studies by the scientific community since the 1970s have established the scientific justification and need for a very high-intensity pulsed neutron source in the U.S. The SNS, which began its user program at ORNL in 2007, currently fulfills the need. In accordance with the 1996 BESAC (Russell Panel) Report recommendation, the

[a] The project is pre-CD-2; the estimated cost and schedule shown are preliminary. Construction will not be executed without appropriate CD approvals.
[b] https://science.energy.gov/~/media/bes/besac/pdf/Reports/Challenges_at_the_Frontiers_of_Matter_and_Energy_rpt.pdf

SNS was designed to be upgradeable so as to maintain its position of scientific leadership in the future, and many technical margins were built into the SNS systems to facilitate a power upgrade into the 2-4 MW range.

An upgraded SNS will enable many advances in the opportunities described in the 2015 BESAC report “Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science.” Four workshops were held by ORNL to assess the neutron scattering needs in quantum condensed matter, soft matter, biology, and the frontiers in materials discovery. These four areas encompass and directly map to the transformative opportunities identified in the BES Grand Challenges update. Quantum materials map most directly to harnessing coherence in light and matter, while soft matter and biology align primarily with mastering hierarchical architectures and beyond-equilibrium matter, and frontiers in materials discovery explored many of the topics in beyond ideal materials and systems: understanding the critical roles of heterogeneity, interfaces, and disorder. As an example, while neutrons already play an important role in the areas of biology and soft matter, step change improvements in capability will be required to make full use of the unique properties of neutrons to meet challenges in mastering hierarchical architectures and beyond-equilibrium matter and understanding the critical roles of heterogeneity and interfaces. The uniform conclusion from all workshops was that in the areas of science covered, neutrons play a unique and pivotal role in understanding structure and dynamics in materials required to develop future technologies.

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. If project performance is sustained and funds are available, the project will attain the objective KPPs. The KPPs presented here are preliminary, pre-baseline values. The final key parameters will be established as part of CD-2, Approve Performance Baseline.

Performance Measure	Threshold	Objective
Beam power on target	1.7 MW at 1.25 GeV	2.0 MW at 1.3 GeV
Beam energy	1.25 GeV	1.3 GeV
Target operational time without failure	1,250 hours at 1.7 MW	1,250 hours at 2.0 MW
Stored beam intensity in ring	≥ 1.6×10^{14} protons at 1.25 GeV	≥ 2.24×10^{14} protons at 1.3 GeV
Number of PPU installed cryomodules	6	7

3. Financial Schedule

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
Design			
FY 2018	5,000	5,000	2,655
FY 2019	18,000	18,000	19,400
FY 2020	4,300	4,300	4,450
Outyears	—	—	795
Total, Design	27,300	27,300	27,300
Construction			
FY 2018	31,000	31,000	1,794

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
FY 2019	42,000	42,000	30,600
FY 2020	700	700	34,250
Outyears	136,300	136,300	143,356
Total, Construction	210,000	210,000	210,000
Total Estimated Costs (TEC)			
FY 2018	36,000	36,000	4,449
FY 2019	60,000	60,000	50,000
FY 2020	5,000	5,000	38,700
Outyears	136,300	136,300	144,151
Total, TEC	**237,300**	**237,300**	**237,300**
Other Project Costs (OPC)			
FY 2016	3,500	3,500	1,267
FY 2017	6,800	6,800	3,773
FY 2018	—	—	3,004
FY 2019	—	—	2,256
FY 2020	—	—	—
Outyears	2,400	2,400	2,400
Total, OPC	**12,700**	**12,700**	**12,700**
Total Project Costs (TPC)			
FY 2016	3,500	3,500	1,267
FY 2017	6,800	6,800	3,773
FY 2018	36,000	36,000	7,453
FY 2019	60,000	60,000	52,256
FY 2020	5,000	5,000	38,700
Outyears	138,700	138,700	146,551
Total, TPC[a]	**250,000**	**250,000**	**250,000**

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design			
Design	20,800	N/A	N/A
Contingency	6,500	N/A	N/A
Total, Design	27,300	N/A	N/A
Construction			
Construction	156,000	N/A	N/A
Contingency	54,000	N/A	N/A
Total, Construction	210,000	N/A	N/A
Total, TEC	**237,300**	**N/A**	**N/A**

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

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Contingency, TEC	*60,500*	*N/A*	*N/A*
Other Project Cost (OPC)			
OPC except D&D			
R&D	2,500	N/A	N/A
Conceptual Design	5,225	N/A	N/A
Other OPC Costs	1,800	N/A	N/A
Contingency	3,175	N/A	N/A
Total, OPC	**12,700**	**N/A**	**N/A**
Contingency, OPC	*3,175*	*N/A*	*N/A*
Total Project Cost[a]	**250,000**	**N/A**	**N/A**
Total, Contingency (TEC+OPC)	**63,675**	***N/A***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2018[a]	FY 2019[b]	FY 2020	Outyears	Total
FY 2020	TEC	—	36,000	60,000	5,000	136,300	237,300
	OPC	10,300	—	—	—	2,400	12,700
	TPC	10,300	36,000	60,000	5,000	138,700	250,000

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy (fiscal quarter or date)	3Q FY 2027
Expected Useful Life (number of years)	40
Expected Future Start of D&D of this capital asset (fiscal quarter)	3Q FY 2067

Related Funding Requirements
(dollars in thousands)

	Annual Costs		Life Cycle Costs	
	Previous Total Estimate	Current Total Estimate	Previous Total Estimate	Current Total Estimate
Operations and Maintenance	N/A	9,325	N/A	373,000

The numbers presented are the incremental operations and maintenance costs above the existing SNS facility without escalation. The estimate will be updated and additional details will be provided after CD-2, Approve Performance Baseline.

[a] While no funding was requested, Congress appropriated $36,000,000 for PPU in FY 2018.
[b] While no funding was requested, Congress appropriated $60,000,000 for PPU in FY 2019.

7. 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 ORNL	3,000–4,000
Area of D&D in this project at ORNL	—
Area at ORNL to be transferred, sold, and/or D&D outside the project, including area previously "banked"	3,000–4,000
Area of D&D in this project at other sites	—
Area at other sites to be transferred, sold, and/or D&D outside the project, including area previously "banked"	—
Total area eliminated	—

8. Acquisition Approach

DOE has determined that the PPU project will be acquired by ORNL under the existing DOE Management and Operations (M&O) contract.

A Conceptual Design Report for the PPU project has been completed. Key design activities, requirements, and high-risk subsystem components have been 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 an ORNL-wide resource.

ORNL will partner with other laboratories for design and procurement of key technical subsystem components. Some technical system designs will require research and development activities. Preliminary cost estimates for these systems are based on operating experience of SNS and vendor quotes. Design of the technical systems will be completed by ORNL, partner laboratory staff, and/or vendors. Technical equipment will be fabricated by vendors and/or partner labs 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 PPU.

18-SC-12 Advanced Light Source Upgrade
Lawrence Berkeley National Laboratory
Project is for Design and Construction

1. Summary, Significant Changes, and Schedule and Cost History

Summary

The FY 2020 Request for the Advanced Light Source Upgrade (ALS-U) project is $15,000,000, including $13,000,000 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 Decision (CD) is CD-1 (Approve Alternate Selection and Cost Range), approved September 21, 2018. The preliminary Total Project Cost (TPC) range, based on the reviewed conceptual design, is $330,000,000 - $495,000,000.

Significant Changes

This Construction Project Data Sheet (CPDS) is an update of the FY 2019 CPDS and does not include a new start for FY 2020. The current TPC estimate increased from $320,000,000 to $368,000,000 and the Project Completion Date (CD-4) was extended by nearly two years to 2Q FY 2028. An independent cost review in July 2018 recommended a new TPC range of $330,000,000 - $495,000,000 based on the quality of the cost estimate, and a point estimate of $368,000,000 for the total cost. The increase in the estimated TPC is due to the conceptual design process, which results in design changes, refinement of the engineering cost estimates, and cost escalation. Changes to the planned project funding profile results in the extension of the project completion date.

In FY 2018, ALS-U developed and completed their Conceptual Design and underwent both an Independent Cost Review by DOE's Office of Project Management and an Independent Project Review by SC's Office of Project Assessment in July 2018. The project received CD-1, Approve Alternative Selection and Cost Range, in September 2018. FY 2019 funding continues to support planning, engineering, design, research and development (R&D), prototyping activities and initiate long lead procurements to the extent supported by design maturity. FY 2020 funding will continue the support of planning, engineering, design, and R&D prototyping activities and additional long lead procurements.

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

Critical Milestone History

Fiscal Year	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2019	9/27/2016	4Q FY 2019	4Q FY 2019	4Q FY 2020	4Q FY 2022	4Q FY 2021	N/A	4Q FY 2026
FY 2020[a]	9/27/2016	4/30/2018	9/21/2018	2Q FY 2021	4Q FY 2021	1Q FY 2022	N/A	2Q FY 2028

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 or will be 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

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

Fiscal Year	Performance Baseline Validation	CD-3A
FY 2019	4Q FY 2020	4Q FY 2020
FY 2020[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.

Project Cost History

(dollars in thousands)

Fiscal Year	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, D&D	OPC, Total	TPC
FY 2019	39,000	243,000	282,000	38,000	N/A	38,000	320,000
FY 2020[b]	89,750	248,250	338,000	30,000	N/A	30,000	368,000

2. 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 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

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

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. 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.

Performance Measure	Threshold	Objective
Storage Ring Energy	≥ 1.9 GeV	2.0 GeV
Beam Current	> 25 mA	500 mA
Horizontal Emittance	< 150 pm-rad	< 85 pm-rad
Brightness @ 1 keV[1]	> 2 x 10^{19}	≥ 2 x 10^{21}
New MBA Beamlines	2	≥ 2

[1]Units = photons/sec/0.1% BW/mm^2/$mrad^2$

3. Financial Schedule

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
Design			
FY 2018	16,000	16,000	—
FY 2019	35,000	35,000	30,000
FY 2020	10,000	10,000	20,000
Outyears	28,750	28,750	39,750
Total, Design	89,750	89,750	89,750
Construction			
FY 2019	25,000	25,000	15,000
FY 2020	3,000	3,000	10,000
Outyears	220,250	220,250	223,250
Total, Construction	248,250	248,250	248,250
Total Estimated Costs (TEC)			
FY 2018	16,000	16,000	—
FY 2019	60,000	60,000	45,000
FY 2020	13,000	13,000	30,000
Outyears	249,000	249,000	263,000
Total, TEC	**338,000**	**338,000**	**338,000**
Other Project Costs (OPC)			
OPC except D&D			
FY 2016	5,000	5,000	1,430
FY 2017	5,000	5,000	5,306
FY 2018	14,000	14,000	11,699
FY 2019	2,000	2,000	4,000
FY 2020	2,000	2,000	3,500
Outyears	2,000	2,000	4,065
Total, OPC	30,000	30,000	30,000
Total Project Cost (TPC)			
FY 2016	5,000	5,000	1,430
FY 2017	5,000	5,000	5,306
FY 2018	30,000	30,000	11,699

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
FY 2019	62,000	62,000	49,000
FY 2020	15,000	15,000	33,500
Outyears	251,000	251,000	267,065
Total, TPC[a]	**368,000**	**368,000**	**368,000**

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design			
Design	69,800	30,000	N/A
Contingency	19,950	9,000	N/A
Total, Design	89,750	39,000	N/A
Construction			
Site Preparation	—	5,000	N/A
Equipment	188,500	170,000	N/A
Other Construction	—	—	N/A
Contingency	59,750	68,000	N/A
Total, Construction	248,250	243,000	N/A
Total, TEC	**338,000**	**282,000**	**N/A**
Contingency, TEC	*79,700*	*77,000*	*N/A*
Other Project Cost (OPC)			
OPC except D&D			N/A
Conceptual Planning	2,000	2,000	N/A
Conceptual Design	12,100	12,000	N/A
Research and Development	8,000	10,000	N/A
Start-Up	1,200	6,000	N/A
Contingency	6,700	8,000	N/A
Total, OPC	**30,000**	**38,000**	**N/A**
Contingency, OPC	*6,700*	*8,000*	*N/A*
Total Project Cost[a]	**368,000**	**320,000**	**N/A**
Total, Contingency (TEC+OPC)	***86,400***	***85,000***	***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.

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2018[a]	FY 2019	FY 2020	Outyears	Total
FY 2019	TEC	—	—	10,000	26,540	245,460	282,000
	OPC	10,000	—	2,000	5,000	21,000	38,000
	TPC	10,000	—	12,000	31,540	266,460	320,000
FY 2020	TEC	—	16,000	60,000	13,000	249,000	338,000
	OPC	10,000	14,000	2,000	2,000	2,000	30,000
	TPC	10,000	30,000	62,000	15,000	251,000	368,000

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy (fiscal quarter or date)	2Q FY 2028
Expected Useful Life (number of years)	25
Expected Future Start of D&D of this capital asset (fiscal quarter)	2Q FY 2053

Related Funding Requirements
(dollars in thousands)

	Annual Costs		Life Cycle Costs	
	Previous Total Estimate	Current Total Estimate	Previous Total Estimate	Current Total Estimate
Operations and Maintenance	N/A	—	N/A	—

No additional operations and maintenance costs are expected above the existing ALS facility. The estimate will be updated and additional details will be provided after CD-2, Approve Project Performance Baseline.

7. 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.

8. Preliminary Acquisition Approach

DOE has determined that the ALS-U project will be acquired by the Lawrence Berkeley National Laboratory (LBNL) under the existing DOE Management and Operations contract.

A Conceptual Design Report for the ALS-U project has been prepared. Key design activities, requirements, and high-risk subsystem components have been 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 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] While no funding was requested, Congress appropriated $30,000,000 for ALS-U in FY 2018.

18-SC-13, Linac Coherent Light Source-II High Energy
SLAC National Accelerator Laboratory
Project is for Design and Construction

1. Summary, Significant Changes, and Schedule and Cost History

Summary

The FY 2020 Request for the Linac Coherent Light Source-II High Energy (LCLS-II-HE) project is $18,000,000, including $14,000,000 in Total Estimated Cost (TEC) funds and $4,000,000 in Other Project Costs (OPC) funds. The most recent DOE Order 413.3B approved Critical Decision (CD) is CD-1 (Approve Alternate Selection and Cost Range), approved on September 21, 2018. The preliminary Total Project Cost (TPC) range based on the reviewed conceptual design is $290,000,000 - $480,000,000.

Significant Changes

This Construction Project Data Sheet (CPDS) is an update of the FY 2019 CPDS and does not include a new start for FY 2020. The current Total Project Cost (TPC) estimate increased from $320,000,000 to $368,000,000 and the Project Completion Date (CD-4) was extended by nearly two years to 1Q FY 2028. The independent cost review in June 2018 recommended a new TPC range of $290,000,000 - $480,000,000 based on the quality of the cost estimate, and a point estimate of $368,000,000 for the total cost. The increase in the estimated TPC was due to the conceptual design process which resulted in design changes and refinement of the engineering cost estimates. Changes to the project funding profile resulted in the extension of the project completion date.

In FY 2018, LCLS-II-HE developed and completed their Conceptual Design and underwent both an Independent Cost Review by DOE's Office of Project Management and an Independent Project Review by SC's Office of Project Assessment in June 2018. The project received CD-1, Approve Alternative Selection and Cost Range, in September 2018. The project also initiated a research and development (R&D) program aimed at further advancing the performance of the superconducting radio frequency (RF) cavities. FY 2019 funding supports the continued planning, engineering, design, R&D, prototyping activities, and initiates long lead and/or advanced procurements to the extent supported by design maturity. FY 2020 funding will continue the support of planning, engineering, design, R&D prototyping, and additional long lead procurements, as appropriate.

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

Critical Milestone History

Fiscal Year	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2019	12/15/2016	3Q FY 2019	3Q FY 2019	1Q FY 2021	1Q FY 2023	2Q FY 2022	N/A	2Q FY 2026
FY 2020[a]	12/15/2016	3/23/2018	9/21/2018	2Q FY 2023	1Q FY 2023	2Q FY 2023	N/A	1Q FY 2028

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 or will be 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.

Fiscal Year	Performance Baseline Validation	CD-3A
FY 2019	1Q FY 2021	4Q FY 2019
FY 2020[a]	2Q FY 2023	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.

Project Cost History

(dollars in thousands)

Fiscal Year	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, D&D	OPC, Total	TPC
FY 2019	34,000	266,000	300,000	20,000	N/A	20,000	320,000
FY 2020[a]	34,000	314,000	348,000	20,000	N/A	20,000	368,000

2. 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 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-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.

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

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 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.

Performance Measure	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)	$5x10^{8}$ (50x spontaneous @8 keV)	> 10^{11} @ 8 keV (200 µJ) or > 10^{10} @ 12.8 keV (20 µJ)

3. Financial Schedule

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
Design			
FY 2018	2,000	2,000	—
FY 2019	10,000	10,000	8,000

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
FY 2020	6,000	6,000	8,000
Outyears	16,000	16,000	18,000
Total, Design	34,000	34,000	34,000
Construction			
FY 2018	6,000	6,000	—
FY 2019	18,000	18,000	18,000
FY 2020	8,000	8,000	14,000
Outyears	282,000	282,000	282,000
Total, Construction	314,000	314,000	314,000
Total Estimated Costs (TEC)			
FY 2018	8,000	8,000	—
FY 2019	28,000	28,000	26,000
FY 2020	14,000	14,000	22,000
Outyears	298,000	298,000	300,000
Total, TEC	**348,000**	**348,000**	**348,000**
Other Project Costs (OPC)			
OPC except D&D			
FY 2018	2,000	2,000	1,191
FY 2019	6,000	6,000	6,000
FY 2020	4,000	4,000	4,000
Outyears	8,000	8,000	8,809
Total, OPC	20,000	20,000	20,000
Total Project Cost (TPC)			
FY 2018	10,000	10,000	1,191
FY 2019	34,000	34,000	32,000
FY 2020	18,000	18,000	26,000
Outyears	306,000	306,000	308,809
Total, TPC[a]	**368,000**	**368,000**	**368,000**

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design			
Design	30,500	30,500	N/A
Contingency	3,500	3,500	N/A
Total, Design	34,000	34,000	N/A
Construction			
Site Preparation	3,000	3,000	N/A
Equipment	236,000	182,000	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 Construction	9,000	9,000	N/A
Contingency	66,000	72,000	N/A
Total, Construction	314,000	266,000	N/A
Total, TEC	**348,000**	**300,000**	**N/A**
Contingency, TEC	*69,500*	*75,500*	*N/A*
Other Project Cost (OPC)			
OPC except D&D			
Conceptual Planning	1,500	1,500	N/A
Conceptual Design	2,000	4,000	N/A
Research and Development	4,000	4,000	N/A
Start-Up	6,500	8,000	N/A
Contingency	6,000	2,500	N/A
Total, OPC	**20,000**	**20,000**	**N/A**
Contingency, OPC	*6,000*	*2,500*	*N/A*
Total Project Cost[a]	**368,000**	**320,000**	**N/A**
Total Contingency (TEC+OPC)	***75,500***	***78,000***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2018[b]	FY 2019	FY 2020	Outyears	Total
FY 2019	TEC	—	—	5,000	20,060	274,940	300,000
	OPC	—	—	2,000	4,000	14,000	20,000
	TPC	—	—	7,000	24,060	288,940	320,000
FY 2020	TEC	—	8,000	28,000	14,000	298,000	348,000
	OPC	—	2,000	6,000	4,000	8,000	20,000
	TPC	—	10,000	34,000	18,000	306,000	368,000

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy (fiscal quarter or date)	1Q FY 2028
Expected Useful Life (number of years)	25
Expected Future Start of D&D of this capital asset (fiscal quarter)	1Q FY 2053

Related Funding Requirements
(dollars in thousands)

	Annual Costs		Life Cycle Costs	
	Previous Total Estimate	Current Total Estimate	Previous Total Estimate	Current Total Estimate
Operations and Maintenance	N/A	21,500	N/A	537,500

[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.
[b] While no funding was requested, Congress appropriated $10,000,000 for LCLS-II-HE in FY 2018.

The numbers presented are the incremental operations and maintenance costs above the LCLS-II facility without escalation. The estimate will be updated and additional details will be provided after CD-2, Approve Project Performance Baseline.

7. 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.

8. Acquisition Approach

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

A Conceptual Design Report for the LCLS-II-HE project has been prepared. Key design activities, requirements, and high-risk subsystem components have been 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 will 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.