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 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; rather 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.

Highlights of the FY 2021 Request
The BES FY 2021 Request of $1,935,673,000 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 2021 Request are summarized below.

<u>Research</u>
The Request continues funding for the Energy Frontier Research Centers (EFRCs), the Batteries and Energy Storage Energy Innovation Hub, and the Fuels from Sunlight Energy Innovation Hub. Core research priorities in the FY 2021 Request include:

- Critical materials: Critical materials, including rare earth elements, are vital to the Nation's security and economic prosperity. In BES, the Request increases support for research to advance our understanding of fundamental properties

[a] https://science.osti.gov/~/media/bes/pdf/BESat40/BES_at_40.pdf

of these materials, identify methodologies to reduce their use and to discover substitutes, and enhance chemical processing and separation science for rare earths.

- Artificial Intelligence (AI) and Machine Learning (ML) for data-driven science: The Request increases investments in AI methods and ML tools to accelerate fundamental research for the discovery of new chemical mechanisms and material systems with exceptional properties and function.
- Exascale computing: 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.
- Microelectronics: BES increases its investment in microelectronics with a focus on materials, chemistry, and fundamental device science. BES will partner with Advanced Scientific Computing Research (ASCR), High Energy Physics (HEP), and Fusion Energy Sciences (FES) to support multi-disciplinary microelectronics research to accelerate the advancement of microelectronic technologies in a co-design innovation ecosystem in which materials, chemistries, devices, systems, architectures, algorithms, and software are developed in a closely integrated fashion.
- Next-generation biology: There is a significant opportunity to cross-fertilize and leverage discoveries and approaches across the biological, physical, and computational sciences to develop bio-inspired, biohybrid and biomimetic systems. Areas of focus include neuromorphic computing, programmable biomaterials and biocatalysts, and next-generation tools for characterization of chemical, biological, biomaterial, and biohybrid systems.
- Polymer upcycling: Fundamental research can provide the foundational knowledge for polymer upcycling, that is, the selective deconstruction of the polymers that constitute plastics, followed by reassembly into high-value chemicals, fuels, or materials in a repeating cycle. Areas of focus include transformative chemistry and biology for polymer upcycling, design of next-generation polymeric materials, and next-generation tools for elucidating chemical and biological mechanisms.
- Quantum information science (QIS): In support of the National Quantum Initiative, SC QIS Center(s) established in FY 2020 will constitute an interdisciplinary partnership among SC programs. This partnership complements a robust core research portfolio stewarded by the individual SC programs to create the ecosystem across universities, national laboratories, and industry that is needed to advance developments in QIS and related technology.
- Strategic accelerator technology: Accelerator R&D is a core capability, which SC stewards for the Nation. Support for this initiative will allow the U.S. to continue to provide the world's most comprehensive and advanced accelerator-based facilities for scientific research, and to continue to attract and train the workforce needed to design and operate these facilities.

<u>Facility Operations</u>

In the Scientific User Facilities subprogram, BES maintains a balanced suite of complementary tools. 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 91 percent of optimum. The Linac Coherent Light Source (LCLS) operations continue at 97 percent of optimum. Both BES-supported neutron sources, the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR), will be operational in FY 2021 and funded at approximately 91 percent of optimum. The Request provides funding for the five Nanoscale Science Research Centers (NSRCs) for continued QIS-related tools development.

<u>Projects</u>

The Request provides continued support for the Advanced Photon Source Upgrade (APS-U), Advanced Light Source Upgrade (ALS-U), Linac Coherent Light Source-II High Energy (LCLS-II-HE), Proton Power Upgrade (PPU), and Second Target Station (STS) projects. The FY 2021 Request includes one new construction project, the Cryomodule Repair and Maintenance Facility (CRMF). The FY 2021 Request also continues two Major Item of Equipment projects: NSLS-II Experimental Tools-II (NEXT-II) and NSRC Recapitalization.

FY 2021 Research Initiatives

Basic Energy Sciences supports the following FY 2021 Research Initiatives.

	(dollars in thousands)			
	FY 2019 Enacted	**FY 2020 Enacted**	**FY 2021 Request**	**FY 2021 Request vs FY 2020 Enacted**
New Research Initiatives				
Next Generation Biology Initiative	—	—	3,750	+3,750
Rare Earth / Separation Science Initiative	—	—	25,000	+25,000
Revolutionizing Polymer Upcycling	—	—	8,250	+8,250
Strategic Accelerator Technology Initiative	—	—	6,250	+6,250
Total, New Research Initiatives	**—**	**—**	**43,250**	**+43,250**
Ongoing Research Initiatives				
Artificial Intelligence and Machine Learning	3,214	10,000	20,000	+10,000
Exascale Computing Initiative	26,000	26,000	26,000	—
Microelectronics Innovation	—	5,000	30,000	+25,000
Quantum Information Science	49,517	72,270	72,270	—
Total, Ongoing Research Initiatives	**78,731**	**113,270**	**148,270**	**+35,000**

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Funding

(dollars in thousands)

	FY 2019 Enacted	FY 2020 Enacted	FY 2021 Request	FY 2021 Request vs FY 2020 Enacted
Materials Sciences and Engineering				
Scattering and Instrumentation Sciences Research	71,235	71,235	65,205	-6,030
Condensed Matter and Materials Physics Research	132,463	144,963	166,875	+21,912
Materials Discovery, Design, and Synthesis Research	65,443	65,443	67,489	+2,046
Established Program to Stimulate Competitive Research (EPSCoR)	19,270	24,088	7,001	-17,087
Energy Frontier Research Centers (EFRCs)	55,800	57,500	57,500	—
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	15,165	15,197	+32
Total, Materials Sciences and Engineering	**395,744**	**415,482**	**416,355**	**+873**
Chemical Sciences, Geosciences, and Biosciences				
Fundamental Interactions Research	89,067	101,567	99,611	-1,956
Chemical Transformations Research	97,836	97,836	101,385	+3,549
Photochemistry and Biochemistry Research	75,724	75,724	67,413	-8,311
Energy Frontier Research Centers (EFRCs)	54,200	57,500	57,500	—
Energy Innovation Hubs—Fuels from Sunlight	15,000	20,000	20,000	—
Computational Chemical Sciences (CCS)	13,000	13,000	13,000	—
General Plant Projects (GPP)	1,000	1,000	1,000	—
SBIR/STTR	13,063	13,851	13,596	-255
Total, Chemical Sciences, Geosciences, and Biosciences	**358,890**	**380,478**	**373,505**	**-6,973**

(dollars in thousands)

	FY 2019 Enacted	FY 2020 Enacted	FY 2021 Request	FY 2021 Request vs FY 2020 Enacted
Scientific User Facilities				
X-Ray Light Sources	505,000	518,791	494,830	-23,961
High-Flux Neutron Sources	282,000	289,701	260,088	-29,613
Nanoscale Science Research Centers (NSRCs)	135,000	138,687	129,938	-8,749
Other Project Costs	19,100	23,000	7,000	-16,000
Major Items of Equipment	—	10,500	2,000	-8,500
Research	29,457	39,879	36,206	-3,673
SBIR/STTR	32,509	36,482	31,751	-4,731
Total, Scientific User Facilities	**1,003,066**	**1,057,040**	**961,813**	**-95,227**
Subtotal, Basic Energy Sciences	**1,757,700**	**1,853,000**	**1,751,673**	**-101,327**
Construction				
21-SC-10 Cryomodule Repair & Maintenace Facility (CRMF)	—	—	1,000	+1,000
19-SC-14 Second Target Station (STS), ORNL	1,000	20,000	1,000	-19,000
18-SC-10 Advanced Photon Source Upgrade (APS-U), ANL	130,000	170,000	150,000	-20,000
18-SC-11 Spallation Neutron Source Proton Power Upgrade (PPU), ORNL	60,000	60,000	5,000	-55,000
18-SC-12 Advanced Light Source Upgrade (ALS-U), LBNL	60,000	60,000	13,000	-47,000
18-SC-13 Linac Coherent Light Source-II-High Energy (LCLS-II-HE), SLAC	28,000	50,000	14,000	-36,000
13-SC-10 Linac Coherent Light Source-II (LCLS-II), SLAC	129,300	—	—	—
Total, Construction	**408,300**	**360,000**	**184,000**	**-176,000**
Total, Basic Energy Sciences	**2,166,000**	**2,213,000**	**1,935,673**	**-277,327**

SBIR/STTR funding:

- FY 2019 Enacted: SBIR $52,617,000 and STTR $7,400,000
- FY 2020 Enacted: SBIR $57,423,000 and STTR $8,075,000
- FY 2021 Request: SBIR $53,080,000 and STTR $7,464,000

Basic Energy Sciences
Explanation of Major Changes

	(dollars in thousands) **FY 2021 Request vs FY 2020 Enacted**
Materials Sciences and Engineering Research will continue to support fundamental scientific opportunities, including those identified in recent BESAC and Basic Research Needs workshop reports. Research priorities include critical materials, computational materials sciences, AI/ML for data-driven science, next-generation microelectronics, QIS, and strategic accelerator technology. The Request also includes funding for continued support of the EFRCs and the Batteries and Energy Storage Energy Innovation Hub.	**+873**
Chemical Sciences, Geosciences, and Biosciences Research will continue to support fundamental scientific opportunities, including those identified in recent BESAC, Basic Research Needs, and Roundtable workshop reports. Research priorities include critical materials, computational chemical sciences, AI/ML for data-driven science, next-generation biology, next-generation microelectronics, polymer upcycling, and QIS. The Request also includes funding for continued support of the EFRCs and the Fuels from Sunlight Energy Innovation Hub.	**-6,973**
Scientific User Facilities The Advanced Light Source (ALS), Advanced Photon Source (APS), National Synchrotron Light Source-II (NSLS-II), and the Stanford Synchrotron Radiation Lightsource (SSRL) user facilities will operate at approximately 91 percent of optimum. The Linac Coherent Light Source (LCLS) operations continue at 97 percent of optimum. Both BES-supported neutron sources, the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR), will operate at approximately 91 percent of optimum. The Request continues to support all five NSRCs, with funding for continued QIS-related tools development. Research priorities include strategic accelerator technology and applications of AI methods and ML techniques to accelerator optimization, control, prognostics, and data analysis. The Request also continues two major items of equipment: the NEXT-II beamline project for NSLS-II and the NSRC recapitalization project.	**-95,227**
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. The Request includes one new project, a Cryomodule Repair and Maintenance Facility.	**-176,000**
Total, Basic Energy Sciences	**-277,327**

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 polymer upcycling; biofuels derived from biomass; solar energy utilization, including solar fuels; energy storage; advanced nuclear energy systems; vehicle technologies; and improving efficiencies in manufacturing and industrial processes. 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 DOE national laboratory system plays a crucial role in achieving integration of basic and applied research.

Program Accomplishments
Harnessing quantum phenomena to accelerate discovery in QIS.
Novel approaches to exploit quantum mechanical phenomena in quantum devices, such as quantum computers and quantum sensors, hold the promise of providing unprecedented insight into the origins of material functionalities and chemical processes.

- Researchers discovered a new superconductor composed of a single layer of iron selenide on a strontium titanate substrate. Generally, superconductors do not respond to light. However, for this new superconductor, ultrafast laser (or low power, ultra violet) pulses can be used to increase the temperature at which the material becomes superconducting from 24 to 30 Kelvin. This superconducting state persisted for days, but could be reversed by high voltage pulses. This newly discovered, photo-induced superconductivity effect is being explored for novel quantum devices.
- Scientists reported the first demonstration of electrically tunable superconductivity in a device composed of three atomically thin (2D) layers of graphene sandwiched between 2D layers of boron nitride to form a repeating pattern called a moiré superlattice. Application of an electric field changes the electron density in the graphene layers, allowing highly controllable switching between electrically insulating and superconducting states in a single sample. The device can be used to study the interplay between atoms and electrons in exotic new materials with potential use in quantum computation and related electronics.
- A new quantum algorithm for simulating molecules was developed, which reduces quantum hardware requirements by allowing the quantum computer to determine its own circuit automatically and algorithmically customized for each molecule being simulated. This is an important step toward simulating more complicated and larger molecules on today's noisy, intermediate-scale quantum computers.

Precision science to discover, understand, and control chemical processes and materials.
Advanced synthesis and characterization techniques are used to explore chemical and physical behaviors to enable understanding and control of their functionality for energy-relevant and information applications.

- Researchers explained how single-atom catalysts affect the stability of reaction intermediates in important energy-relevant transformations, resulting in more efficient and selective catalysts. These recent advances not only validate the utilization of these catalysts for fundamental structure-reactivity relationship studies, but also indicate their untapped potential to manipulate chemical reactions.

- Researchers demonstrated that optically transparent and electrically conductive functional materials can be rapidly fabricated from polymer templates with exquisite microstructural organization using a chemical synthesis technique called sequential infiltration synthesis. Materials synthesized by these methods have been applied to important applications in lithography, oil sorption, protein separations, and optical coatings.
- Resilient and flexible borophene holds promise for fabricating atomically thin electronic devices. However, only nanoscale phase domains had been produced, preventing detailed analyses and device fabrication. Scientists used advanced electron microscopy techniques to directly visualize and verify that use of a copper substrate formed much larger single-crystal domains. The large crystals of this previously unknown borophene phase are expected to allow electrons to move through the structure quickly, which is crucial for developing flexible electronic devices.

Learning from biology to inspire new approaches to advanced energy technologies.
The development of energy technologies critically depends on discovery and creation of new chemical processes and high-performance materials with functions and properties exceeding those currently available. Biological systems provide inspiration for new approaches to manipulate matter, energy, entropy, and information across multiple length scales.

- Researchers discovered a new class of material that absorbs and fixes atmospheric carbon dioxide to grow and self-repair using incident sunlight. In a cascade of reactions, the prototype material uses embedded chloroplasts extracted from plants to capture carbon through photosynthetically produced sugars (glucose). Ultimately, these sugars are transformed into a continuously regenerating, expanding, and densifying polymer matrix capable of self-repair.
- In photosynthesis, solar energy is used to extract and use electrons from water and to make energy-dense compounds from carbon dioxide. In plants, the combination of two protein complexes, Photosystems I and II, is required to accomplish this energy-intensive process with high efficiency. Researchers found that these natural membrane-bound proteins can self-assemble with synthetic cobalt or nickel catalysts and use light to make hydrogen gas, suggesting natural/synthetic hybrid systems could be used for solar fuel production.
- Industry relies on high temperature and pressure to convert nitrogen into ammonia, a key component in fertilizers. In nature, the nitrogenase enzyme performs this same chemistry at room temperature and pressure. Replicating this feat at an industrial scale would help reduce energy costs and global carbon emissions. Using computational and experimental methods, scientists discovered that biology couples the production of hydrogen, which releases energy, with cleaving nitrogen, which requires energy, enabling the enzyme to convert nitrogen to ammonia efficiently. These results provide new insights for design of synthetic catalysts for ammonia synthesis.

Data science to advance discovery in basic energy sciences.
AI/ML techniques are enabling researchers to identify reaction pathways, predict physical and chemical properties, and design new chemicals and materials. Development and application of machine learning algorithms can be limited by the availability of extensive databases of experimental and simulated data and the throughput by which data can be generated. New, interpretable data models are helping to accelerate scientific discovery.

- Researchers coupled data infrastructure to high throughput experimentation to yield the world's largest database of materials experiments. Using the extensive database, they created a model that predicts the optical absorption spectrum from a material's image and vice versa. Light absorption characteristics of photocatalysts and photoelectrodes have been difficult to predict, but this result advances ML for discovery and characterization of these materials for energy conversion.
- Tectonic faults slip in various manners, ranging from ordinary earthquakes to slow slip events. Using new machine learning techniques trained on laboratory data, researchers discovered a new geophysical signal in the Cascadia subduction zone in the Pacific Northwest. This signal occurs as a continuously broadcasting low-amplitude tremor that precisely relates to the fault displacement rate throughout the slow slip cycle. These insights may prove useful in determining if and how a slow slip may couple to or evolve into a major earthquake.
- The Materials Project at Lawrence Berkeley National Laboratory has been a leader in producing material property databases and is now developing software to evaluate electronic and mechanical properties from such data. Recent applications include calculations of hundreds of electronic surface parameters, the largest database of such properties. Machine learning algorithms were developed to accelerate the optimization of two-dimensional layered materials for next generation electronics. Experimental data and calculations were combined for high throughput screening of transparent conductors for next generation optoelectronics.

New techniques and capabilities at BES facilities.
Advances in tools and instruments often drive scientific discovery. Recent developments and upgrades at the scientific user facilities provide users with cutting-edge capabilities for ground-breaking science.

- The Dynamic Diffraction Direct Detector (4D Camera) at the Molecular Foundry achieved an unprecedented 87,000 frames per second. This is 60 times faster than previous high speed electron detectors. The detector enables real-time contrast ptychographic imaging. This new capability is a breakthrough in nanoscale strain mapping and quantification of materials using scanning electron diffraction imaging methods at high resolution.
- An advanced nano-diffraction capability developed at the National Synchrotron Light Source-II is able to obtain strain mapping with a few nanometer resolution for microprocessors with complex 3D structure. This capability is a critical research tool for next-generation microelectronics.
- The upgraded WAND diffractometer at the High Flux Isotope Reactor provides wide angle coverage and high flux, useful for monitoring in-situ material synthesis under complex environment and stroboscopic measurements of ferroelectric switching. This capability will help identify new routes for the synthesis of advanced energy materials that are difficult to synthesize.

BES user facilities help industry advance the technology frontiers.
In FY 2019, more than 600 industrial users conducted experiments at the BES scientific user facilities using the advanced instrumentation and methods available to test, probe, and develop their technologies.

- A team of Molecular Foundry scientists and Dow Chemical users developed a method to apply pulsed-electron beams to image a beam-sensitive material with atomic resolution. This is the first time that beam-sensitive and air-sensitive magnesium chloride has been studied with atomic resolution. The new technique could be used to study other soft materials and could aid the development of sustainable plastics.
- Neutron diffraction at SNS provided important information on the chemical reactions during the “batch to glass” (sand, alumina, and additives to glass) process in real time at 1400 degrees Celsius. This information will be useful to build new models that will improve production processes and decrease the amount of time required to bring new and more durable types of glasses for commercial applications (e.g., car windows, screens on electronic devices, etc.) and to improve the efficiency and reliability of the glass manufacturing processes.
- Center for Functional Nanomaterials staff worked with users from the Toyota Research Institute and Michigan State University to study the mechanism of rechargeable batteries with magnesium metal anodes. Experiments revealed that the combination of a highly functional solid electrolyte interphase at the anode and magnesium nanocrystals formed during operation are key to improved performance. Magnesium has five times more volumetric energy storage density compared to graphite anodes used in commercial lithium-ion batteries.

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, polymer upcycling, 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 and extreme conditions.
- **Condensed Matter and Materials Physics**—Understanding the foundations of material functionality and behavior including electronic, thermal, optical, mechanical, and rare-earth properties, the impact of extreme environments, and 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 approaches learned from biological systems, that limit the use of rare earth and other critical materials, and that enable more effective polymer chemistries.

The portfolio emphasizes understanding of how to direct and control energy flow in materials systems over multiple time (from femtoseconds to seconds) and length (from the nanoscale to mesoscale) scales, 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, accelerator technologies, and most industrial settings. To maintain leadership in materials discovery, the research that this subprogram supports explores new frontiers of unpredicted, emergent materials behavior; utilization of nanoscale control; and materials systems that are metastable or far from equilibrium. This research includes investigation of the interfaces between physical and biological sciences to explore new approaches to novel materials design. A growing emphasis in materials chemistry is understanding and novel approaches to enable polymer recycling to higher value molecular systems. Also essential is the 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. An increasingly important aspect of materials research is the use of AI/ML 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. The subprogram also supports, in partnership with other SC programs, SC QIS Centers beginning in FY 2020. 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 has been a finding in several of the Basic Research Needs reports. 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, including the use of cryogenic environments to evaluate properties only occurring at these temperatures and to learn about processes and interfaces in materials that are damaged by the probes used to characterize them. 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 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. New materials are increasingly critical to advance accelerator technologies, including magnets, optics, sensors, and detectors.

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 understanding is critical in the search for ways to reduce or eliminate the need for rare earth and other critical materials in energy-relevant technologies.

This activity also emphasizes research to understand how materials respond to their environments, including the influence of temperature, electromagnetic fields, radiation, corrosive chemicals, and other extreme conditions. 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. Research in this area 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 theories used to describe material properties across a broad range of length and time scales, from the atomic scale to the macroscale where the influence of size, shape, and composition is not adequately understood. In addition, current theories fail to describe the time evolution of these properties from femtoseconds to seconds and to much longer time scales. 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 AI/ML 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. BES is establishing research priorities and its unique role in this critical field through community engagement in roundtable discussions, interactions with other SC programs, and at the interagency level. 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. Quantum materials are also important for next-generation microelectronics and accelerator technologies, including magnets, detectors, and sensors.

This activity includes the SC QIS Centers, which 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[a] and the Roundtable on Opportunities for Basic Research for Next-Generation Quantum Systems[b], 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.

[a] https://science.osti.gov/-/media/bes/pdf/reports/2016/BRNQM_rpt_Final_12-09-2016.pdf
[b] https://science.osti.gov/-/media/bes/pdf/reports/2018/Quantum_systems.pdf

In FY 2021, BES, in partnership with other SC programs, will continue support for the multi-disciplinary multi-institutional QIS center(s), selected through a merit review process in FY 2020. The SC QIS centers will focus on a set of QIS applications or cross-cutting topics that collectively cover the development space that may impact SC Programs, including work on sensors, quantum emulators/simulators and enabling technologies that will pave the path to exploit quantum computing in the longer term.

This activity also contributes to microelectronics research, including basic research to accelerate the advancement of microelectronic technologies in a co-design innovation ecosystem. Computing systems encompassing new materials, devices, architectures, algorithms, and software are needed to maintain the continued upward trajectory in performance that Moore's law scaling has historically provided. Optimization must occur at every level of computing and power microelectronics systems, and co-design principles are essential to meet the future needs of SC and the nation. Among the challenges is discovery science that can lead to microelectronics for exascale computers and beyond with a small footprint and low power utilization. Such high performance computation will be necessary for analyzing and managing the vast amount of data that will be generated by future SC facilities to enable new discoveries. Furthermore, transforming power electronics and the electricity grid into a modern, agile, resilient, and energy-efficient system requires advances in new microelectronics materials, and their integration within a co-design framework. In FY 2021, BES will partner with ASCR, HEP, and FES to support multi-disciplinary microelectronics research. Informed by community strategic planning efforts including the Basic Research Needs for Microelectronics report, key technical areas will include materials, chemistry, and fundamental device science; component integration, architecture, and algorithms; and next-generation tools for synthesis, fabrication, and characterization of devices and systems.

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. BES will enhance this program in FY 2021 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. New research directions will be inspired by the roundtable report on upcycling of polymers, the molecules that make-up plastics. Understanding of the synthesis process will enable design of new systems that are easier to recycle into similar products with comparable complexity and value.

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 biology-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 DOE'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 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 FY 2021 program will focus on implementation awards for larger teams and will consider renewals of the FY 2019 awards as well as proposals for new teams. 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 ten years of research activity, the program has produced an impressive breadth of scientific accomplishments, including over 11,600 peer-reviewed journal publications.

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

Energy Innovation Hubs—Batteries and Energy Storage
The Joint Center for Energy Storage Research (JCESR) focuses on 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, 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*/*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 accelerate the design of new functional materials.

BES manages the computational materials science research activities using the approaches developed 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

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[a] https://science.osti.gov/-/media/bes/pdf/reports/2017/BRN_NGEES_rpt.pdf

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

(dollars in thousands)

FY 2020 Enacted		FY 2021 Request	Explanation of Changes FY 2021 Request vs FY 2020 Enacted
Materials Sciences and Engineering	**$415,482**	**$416,355**	**+$873**
Scattering and Instrumentation Sciences Research	$71,235	$65,205	-$6,030
Funding continues 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.		The Request will continue to push the frontiers of instrumentation and techniques needed to understand materials properties and enable materials discovery, including quantum phenomena, materials behavior in extreme energy-related environments, and multidimensional phenomena (requiring simultaneous assessment crossing space, time, and chemical evolution). Investments will emphasize hypothesis driven research with x-ray free electron lasers, imaging with coherent x-rays, advanced neutron scattering probes of interfaces and soft materials, cryogenic electron microscopy probes, and multimodal techniques that combine probes. Research will focus on innovation that will enable assessment of new regimes not amenable to current characterization approaches.	Funding emphasizes forefront R&D of novel techniques to understand quantum phenomena and soft materials, including cryogenic techniques.

(dollars in thousands)

FY 2020 Enacted		FY 2021 Request	Explanation of Changes FY 2021 Request vs FY 2020 Enacted
Condensed Matter and Materials Physics Research	$144,963	$166,875	+$21,912
Funding continues 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. 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 other SC Program Offices to establish at least one multi-disciplinary multi-institutional QIS center, which will be selected through a merit reviewed process conducted 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 SC Programs and include work on sensors, quantum emulators/ simulators and enabling technologies that will pave the path to exploit quantum computing in the longer term.		The Request will continue to support research to understand, better design, and discover new quantum materials, and to advance the theory needed to understand quantum phenomena. Included is a specific focus on research to support QIS and related systems. This activity will provide continued support for the QIS Centers established in FY 2020. The Request will also continue to establish the science base for next generation optical and electronic materials, including a new emphasis on materials for next generation microelectronics and for accelerator magnets, optics, and detectors. The Request increases support to investigate the unique properties associated with rare earth and critical materials to identify opportunities for substitutions and reduced use of these elements in energy relevant technologies. Theory and modeling research will include AI/ML for data-driven science to enhance materials discovery.	Funding emphasizes new tools and approaches to accelerate the discovery of new materials that will reduce or eliminate the use of rare earth elements while retaining their unique functionality for energy relevant technologies. Activities include enhancement of AI/ML techniques to better use data from both experiments and calculations. In addition, the increase will support a new focus on the science needed to provide the materials required for next generation microelectronics and for accelerator magnets, optics, detectors, and sensors.

(dollars in thousands)

FY 2020 Enacted	FY 2021 Request	Explanation of Changes FY 2021 Request vs FY 2020 Enacted
Materials Discovery, Design, and Synthesis Research $65,443	$67,489	+$2,046
Funding continues 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.	The Request will continue research on innovative synthesis and discovery of materials through scientific understanding of the basic chemical and physical phenomena, and science-based utilization of biological concepts. Support will be maintained for investigation of fundamental dynamics and kinetics of synthesis and self-assembly over multiple length and timescales, including the role of defects and interfaces. Research will emphasize new approaches to replace or minimize the use of critical and rare earth materials.	The increase will support additional investment in research to better understand synthesis approaches and materials discovery to enable rare earth substitution and reduced use of critical materials, utilizing synthetic advances in related fields and predictive theory, modeling, and data mining/AI to accelerate progress.
Established Program to Stimulate Competitive Research (EPSCoR) $24,088	$7,001	-$17,087
Funding continues 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.	The Request will continue to support early stage science, including research that underpins DOE energy technology programs. Following the previous year's focus on state-lab partnership awards, FY 2021 will emphasize implementation awards, larger multiple principal investigator grants that develop research capabilities in EPSCoR jurisdictions. The FY 2021 funding opportunity will consider both renewals of FY 2019 awards and new proposals. Investment will continue in early career research faculty from EPSCoR designated jurisdictions and in co-investment with other programs for awards to eligible institutions.	Funding focuses on implementation awards that facilitate larger team awards for the development of research capabilities.

(dollars in thousands)

FY 2020 Enacted		FY 2021 Request		Explanation of Changes FY 2021 Request vs FY 2020 Enacted	
Energy Frontier Research Centers (EFRCs)	$57,500		$57,500		$—
Funding continues to support four-year EFRC awards that were made in FY 2018. In addition, FY 2020 funds support a solicitation that will recompete the four-year EFRC awards made in FY 2016, which focused on science relevant to DOE’s environmental management mission, and make new awards that are responsive to recent BES strategic planning workshop reports, including use-inspired science relevant to advanced microelectronics, QIS, and polymer upcycling.		The Request will provide the fourth year of support for four-year EFRC awards that were made in FY 2018 and the second year of support for four-year EFRC awards that were made in FY 2020.		No changes.	
Energy Innovation Hubs—Batteries and Energy Storage	$24,088		$24,088		$—
Funding continues 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 impact of coupled phenomena and for predictive design of new materials for batteries.		The Request will continue the prior year’s focus, based on the renewal of the JCESR Hub in FY 2018. Early stage research for next generation electrical energy storage for the grid and vehicles will continue to emphasize understanding the fundamentals of electrochemistry (transport, solvation, evolution of chemistries and materials during charge/ discharge) and discovery of the coupled factors that govern performance. The research will closely integrate theory, simulation, and experimentation to elucidate the impact of coupled phenomena and enable predictive design of new materials for batteries.		No changes.	

(dollars in thousands)

FY 2020 Enacted		FY 2021 Request	Explanation of Changes FY 2021 Request vs FY 2020 Enacted
Computational Materials Sciences	$13,000	$13,000	$—
Funding continues research on current Computational Materials Sciences (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 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 incorporate frameworks suited for future exascale computer systems.	No changes.
SBIR/STTR	$15,165	$15,197	+$32
In FY 2020, SBIR/STTR funding will be set at 3.65 percent of non-capital funding.		In FY 2021, SBIR/STTR funding will be set at 3.65 percent of non-capital funding.	The SBIR/STTR funding will be consistent with the BES total budget.

Basic Energy Sciences
Chemical Sciences, Geosciences, and Biosciences

Description

Transformations of energy among forms, and rearrangements of matter across multiple scales, starting at the atomic level, 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 transformations. 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 quantum mechanical behavior 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 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 Fuels from Sunlight Energy Innovation Hub, Computational Chemical Sciences, data science, and QIS—to focus on forefront scientific challenges that relate to the DOE energy mission. The subprogram also supports, in partnership with other SC programs, SC QIS Centers beginning in FY 2020.

The 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; conversions of increasingly complex chemical systems such as polymers and mixed feedstocks; and the use of AI/ML for data-driven science.

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 their behavior. 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 LCLS are used to image the dynamics of electrons and charge transport. Chemical physics research builds from the AMOS foundation by examining the reactivity of molecules whose chemistry is profoundly affected by the environment, such as 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 chemistry 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 the 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 of 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,[a] 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 2021, BES, in partnership with other SC programs, will continue support for the multi-disciplinary multi-institutional QIS center(s), selected through a merit review process in FY 2020. The SC QIS centers will focus on a set of QIS applications or cross-cutting topics that collectively cover the development space that may impact SC Programs, including work on sensors, quantum emulators/simulators and enabling technologies that will pave the path to exploit quantum computing in the longer term.

This activity also supports microelectronics research, including basic research to accelerate the advancement of microelectronic technologies in a co-design innovation ecosystem. Computing systems encompassing new materials, devices, architectures, algorithms, and software will be needed to maintain the continued upward trajectory in performance that Moore's law scaling has historically provided. Optimization must occur at every level of computing and power microelectronics systems, and co-design principles will be essential to meet the future needs of DOE-SC and the nation. Among the challenges is discovery science that can lead to microelectronics for exascale computers and beyond with a small footprint and low power utilization. Such high performance computation will be necessary for analyzing and managing the vast amount of data that will be generated by future DOE-SC facilities to enable new discoveries. Furthermore, advances in new microelectronics materials, and their integration within a co-design framework, are required to transform power electronics and the electricity grid into a modern, agile, resilient, and energy-efficient system. In FY 2021, BES will partner with ASCR, HEP, and FES to support multi-disciplinary microelectronics research. Informed by community strategic planning efforts including the Basic Research Needs for Microelectronics report,[b] key technical areas will include materials, chemistry, and device physics; component integration, architecture, and algorithms; and next-generation tools for synthesis, fabrication, and characterization of devices and systems.

Chemical Transformations Research

This activity advances the knowledge of chemical reactivity, matter transport, and chemical separation and stabilization processes to provide foundational knowledge in core research areas – catalysis science, separation science, heavy element chemistry and geosciences – that are critical for developing the next generation of energy applications. The research uses tools from Ultrafast Chemistry to identify transient species during reactions and refine theories of reactivity; advance understanding of Charge Transport and Reactivity important in electrocatalytic, electroseparations, and geochemical redox processes; explore Chemistry at Complex Interfaces in catalytic, geochemical and separation systems; and develop understanding of Chemistry in Aqueous Environments that play important roles in geochemical transformations and chemical separations, including heavy elements. 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 activity includes the development and application of theoretical, computational and data analytics methods to achieve a deeper understanding of reaction pathways in complex systems and design new molecules and materials (e.g., catalysts and membranes) that enable control over chemical processes.

Chemical Transformations Research comprises four core areas: Catalysis Science, Separation Science, Heavy Element Chemistry, and Geosciences. Catalysis science research emphasizes understanding of reaction mechanisms, precise synthesis, *operando* characterization and manipulation of catalytic active sites and their environments, and control of reaction conditions for optimized efficiency and selectivity. A primary goal is the molecular-level control of chemical transformations relevant to the sustainable conversion of energy resources, with a focus on thermal and electrochemical conversions of complex feedstocks, including synthetic polymers and mixed hydrocarbons and carbohydrates. Separation science research seeks to understand and ultimately predict and control the atomic and molecular interactions and energy exchanges determining the efficiency of chemical separations. The major focus is to advance discovery of principles driving

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[a] https://science.osti.gov/bes/Community-Resources/Reports

[b] https://science.osti.gov/-/media/bes/pdf/reports/2019/BRN_Microelectronics_rpt.pdf

separation processes and predictive design of future chemical separation processes that demand less energy, as well as media with the desired chemical and transport properties. Emphasis is placed on extracting actinides and rare earth elements and efficiently separating gas, liquid, and solid mixtures. Heavy element chemistry provides foundational knowledge on the influence of complex environments, such as liquid-solid and liquid-liquid interfaces, and extreme conditions, such as temperature and radiation, on the dynamic and kinetic behavior of actinide compounds in these environments. A primary goal is to gain an understanding of the unique chemistry of f-electron systems that is required to design new ligands and processes for actinide separations processes, predict the chemical evolution of actinides in nuclear wastes and next-generation reactors, and improve models of actinide environmental transport. 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). Areas of emphasis include the molecular-level understanding of phase equilibria, reaction mechanisms and rates associated with aqueous geochemical processes, and a mechanistic understanding of the origins of subsurface physical properties and the response of earth materials associated with processes such as chemo-mechanical stress corrosion and strain localization. This knowledge will advance abilities to model and predict phenomena such as subsurface migration, mineralization, crack propagation and subsurface fracture that occur over multiple scales of time and space.

This activity supports efforts central to revolutionizing polymer upcycling and to addressing challenges in critical materials, rare earth elements, and separation science. As identified by the BES strategic planning report from the Roundtable on Chemical Upcycling of Polymers,[a] fundamental research can provide the foundational knowledge needed to enable polymer upcycling—the selective deconstruction of polymers that make up plastic followed by reassembly into high-value chemicals, fuels, or materials. Research opportunities include transformative chemistry and biology for chemical conversion and upcycling of polymers, design of next generation polymers and polymeric materials, and next generation tools for determining chemical and biochemical mechanisms with potential benefit for polymer upcycling. Research will build upon this activity's efforts in catalysis science and separation science to develop efficient, selective processes for polymer deconstruction and reconstruction, including the upcycling of complex mixtures of polymeric materials. Rare earth elements provide enhanced performance and new materials functionality based on their rich electronic properties. Research opportunities includes the discovery, design, and synthesis of new materials and processes that limit the use of rare earths, and separation science to enhance recovery of rare earth elements from both minerals and recycled materials. Research will build on this activity's efforts in heavy element chemistry, geosciences, separation science, and catalysis science for understanding the chemistry and physics of f-electron systems to advance the predictive design of controlled molecular and material structures; for understanding the interactions of solutions with interfaces, including mineral interfaces, to provide foundational knowledge needed to advance separations of rare earth elements from critical minerals and recycled materials; and the design of new catalysts that limit the use of rare earths and noble metals.

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 and can foster the development of bioinspired, biomimetic, and biohybrid energy systems.

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 such as 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, including those in Ultrafast Chemistry, are used to investigate quantum phenomena in natural and artificial systems; these 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 on the synthesis, dynamics, and function of natural and artificial

[a] https://science.osti.gov/-/media/bes/pdf/BESat40/Polymer_Upcycling_Brochure.pdf

membranes and nano- to meso-scale structures increases knowledge of both Chemistry at Complex Interfaces and Chemistry in Aqueous Environments. Multidisciplinary studies of the structural, functional and mechanistic properties of enzymes, enzyme systems, and energy-relevant biological reactions advance understanding of Reaction Pathways in Diverse Environments and identify principles important for catalyst function, selectivity, and stability.

The biosciences research supported under this activity sits at the interface between chemistry/physics and biology. This multidisciplinary integration enables research in biological systems to provide insights for understanding and enhancing man-made chemical systems while, in a reciprocal manner, studies of chemical (non-biological) systems provide insights into the dynamics and chemical reactivity underlying biochemical processes. Research in natural photosynthesis advances knowledge of biological mechanisms of solar energy capture and conversion and encompasses 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 photosynthetic proteins, membranes and cellular compartments. The mechanistic understanding of natural photosynthesis can inspire development of bio-hybrid, biomimetic, and artificial photosynthetic systems for solar fuels production and inform 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 reactions and pathways related to energy capture, conversion, and storage in natural systems, including complex multielectron redox reactions, electron transfer and bifurcation, metal uptake and use, 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 biological systems will identify principles for the design of highly selective and efficient catalysts, for instance, for ammonia synthesis or polymer conversion; the control of electron flow to achieve desired metabolic products; and the design of next-generation energy conversion technologies. Complementary research on solar energy conversion in 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. Research also addresses the 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 the extreme environments 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.

Research focused on molecular-level understanding of biochemical processes advances SC's Next-Generation Biology initiative. New efforts in this activity will build on BES biochemistry and biophysics research to discover and design chemical processes and complex structures that can enable development of bio-inspired, biohybrid, and biomimetic energy systems with desired functions and properties. Studies will target the molecular-level mechanisms nature uses to control complex chemical conversions, including error-correcting and defect-managing mechanisms, and to manage information and signal transduction in complex hierarchical systems. Research will also continue to develop new approaches for dynamic and in-situ imaging and characterization, including capabilities at SC facilities, and computational tools for understanding complex assembly and other biochemical processes.

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 ten years of research activity, the program has produced an impressive breadth of scientific accomplishments, including over 11,600 peer-reviewed journal publications.

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

Energy Innovation Hubs—Fuels from Sunlight

Based on competitive merit review, new multi-investigator, cross-disciplinary solar fuels research awards will be initiated in FY 2020 to address both emerging new directions and long-standing challenges in the use of solar energy, water, and carbon dioxide as the only inputs for fuels production. The FY 2021 Request will continue support for this early-stage fundamental research on solar fuels generation that is building on the unique accomplishments of the first Fuels from Sunlight Hub and is addressing key scientific challenges identified by the strategic planning report from the Roundtable on Liquid Solar Fuels.[a]

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 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. The FY 2017 awards will be recompeted in FY 2021. 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 U.S.

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.

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[a] https://science.osti.gov/-/media/bes/pdf/reports/2020/Solar_Fuels_Brochure.pdf

General Plant Projects (GPP)
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.

Activities and Explanation of Changes

(dollars in thousands)

FY 2020 Enacted		FY 2021 Request	Explanation of Changes FY 2021 Request vs FY 2020 Enacted
Chemical Sciences, Geosciences, and Biosciences	**$380,478**	**$373,505**	**-$6,973**
Fundamental Interactions Research	$101,567	$99,611	-$1,956
Funding continues to develop forefront ultrafast approaches to study and control energy flow and bond rearrangements in gas-phase, condensed phase and interfacial chemical phenomena. Gas-phase research continues studies of reaction pathways in heterogeneous environments and expands to examine quantum phenomena in tailored molecules. Research efforts extend to understand and control chemical and quantum phenomena in increasingly complex multiphase environments. Understanding, leading to control of interfacial reactivity, informs the design and synthesis of new materials relevant to microelectronics. This activity continues to develop advanced theoretical and computational approaches, including AI/ML for data-driven science, that will operate on future exascale computers, and to drive advances in the application of quantum computing for molecular calculations. BES will partner with other SC Program Offices to establish at least one multi-disciplinary multi-institutional QIS center, which will be selected through a merit reviewed process conducted 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 SC Programs and include work on sensors, quantum emulators/ simulators and enabling technologies that will pave the path to exploit quantum computing in the longer term.		The Request will continue to develop forefront ultrafast approaches, with emphasis on the use of x-ray free electron lasers, including LCLS and its upgrades. Gas-phase research will continue studies of how reactive intermediates in heterogeneous environments impact reaction pathways, and quantum phenomena underlying QIS, 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. Research to understand and control interfacial chemical reactions will increase with the aim of designing and synthesizing new materials relevant to microelectronics. This activity will continue to develop advanced theoretical and computational approaches that can be scaled to operate on exascale computers. Development of AI/ML methods will increase to enable novel data science approaches for knowledge discovery. Research will emphasize efforts to drive advances in the application of quantum information science for understanding and exploiting quantum phenomena in chemical systems. This activity provides continued support for the QIS Centers established in FY 2020.	Funding will emphasize new efforts to understand and control interfacial chemical reactions that can enable new materials for microelectronics and will support research in studies of quantum phenomena important for QIS and the impact of molecular environments on these phenomena. Support will continue the development of advanced theoretical and computational approaches, with increased emphasis on the development and application of AI/ML methods that will enable novel data science approaches for knowledge discovery.

(dollars in thousands)

FY 2020 Enacted		FY 2021 Request	Explanation of Changes FY 2021 Request vs FY 2020 Enacted
Chemical Transformations Research	$97,836	$101,385	+$3,549
Funding continues to support predictive fundamental research on the design and synthesis of novel catalysts to efficiently convert chemical feedstocks, including hydrocarbons, biomass, and synthetic polymers, to high-value fuels and chemicals. Fundamental studies 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 continues on innovative approaches for separating chemical mixtures with emphasis on 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. Support continues to understand 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. Heavy element research continues to expand the knowledge of the chemistry of actinide reactivity, bonding, synthesis, and separation, supports training in nuclear chemistry, and advances theoretical methods to accurately describe the chemistry of f-electron systems.		The Request will continue support for fundamental research to understand mechanisms of catalysis and to predict, design, and synthesize novel catalysts and bioinspired metal complexes with enhanced performance for thermo- and electro-chemical conversions, with an increased emphasis on chemical upcycling of polymers. Separation science research will continue to focus on novel approaches to separate complex chemical mixtures with high efficiency, with a new emphasis on separations processes, including reactive separations that will facilitate the chemical upcycling of polymers. Geosciences research will continue to elucidate subsurface phenomena, such as mineral nucleation, and rock fracture propagation, with an emphasis on the intersection of geochemical and geophysical processes under extreme subsurface conditions. Heavy element research will continue to deepen understanding of actinide speciation and reactivity, fundamental theories of f-electron systems, and approaches to synthesize and separate actinide compounds. New efforts on the chemistry of rare earth elements, including heavy elements such as lanthanides, will focus on understanding their reactivity to limit their use in catalytic processes, their interactions and chemical processes in multiphase systems relevant to separations from complex mixtures, and their behavior in rare-earth containing minerals, particularly the interaction of these minerals with aqueous solutions, that are relevant to extraction in geological environments.	Funding will emphasize atomically precise synthesis and control of new catalytic and chemically active functions; understanding multiscale phenomena in extreme and constrained environments; and developing integrated computational and data science approaches to predict multiscale and multiphysics processes. Support will increase for research on catalysis and separations, including reactive separations, for chemical upcycling of polymers. Increased emphasis on the chemistry of rare earths will include selective separations from solutions, dynamics and reactivity at mineral-water interfaces during extraction and recovery, utilization of the f-electron properties of rare-earth elements, and understanding the promotor properties of rare-earth elements used for catalysis.

(dollars in thousands)

FY 2020 Enacted	FY 2021 Request	Explanation of Changes FY 2021 Request vs FY 2020 Enacted
Photochemistry and Biochemistry Research $75,724	$67,413	-$8,311
Funding continues 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 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 advance solar fuels research as well as provide insights into quantum phenomena in energy transfer. Research on biocatalysis continues 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 continue as well as studies of reactivity across complex interfaces, in aqueous environments, and under dynamic conditions.	The Request will continue to support fundamental research that emphasizes an understanding of the physical, chemical, and biochemical processes of light energy capture and conversion in biological and chemical systems. Studies of light absorption, energy transfer, charge transport and separation, separations processes, and photocatalysis in both natural and artificial systems will provide fundamental knowledge to guide the design of new energy systems. The Request will increase focus on biochemical processes and complex structures that can enable development of bio-inspired, biohybrid, and biomimetic energy systems with desired functions and properties. Research on molecular mechanisms of biocatalysis, revealed by studies of enzyme structure and function, multi-electron redox reactions, and electron bifurcation, will inform bioinspired design of catalysts and reaction pathways, for instance to guide new approaches for polymer upcycling. Research on metal uptake and use by biological systems will inform bio-inspired separation processes. Studies will also increase understanding of how rare elements can be minimized in photo-absorbers and catalysts for solar fuels. Advances in solar fuels will continue via research on molecular mechanisms of photon capture, electron transfer, and product selectivity and separation from non-target molecules. Studies of light energy capture will address the relationship between quantum phenomena and the efficiency and fidelity of energy transfer and conversion.	Funding will emphasize charge transport, energy transfer, light harvesting, separations, photo- and biocatalytic mechanisms, self-assembly/repair of complex structures, and excited-state dynamics of processes important for energy capture and conversion in biological and chemical systems. Such research will place an increased emphasis on fundamental principles for bioinspired design and development of biomimetic and biohybrid energy systems and processes.

(dollars in thousands)

FY 2020 Enacted	FY 2021 Request	Explanation of Changes FY 2021 Request vs FY 2020 Enacted
Energy Frontier Research Centers (EFRCs) $57,500	$57,500	$ —
Funding continues to support four-year EFRC awards that were made in FY 2018. In addition, FY 2020 funds will support a solicitation that will recompete the four-year EFRC awards made in FY 2016, which focused on science relevant to DOE's environmental management mission, and make new awards that are responsive to recent BES strategic planning workshop reports, including use-inspired science relevant to advanced microelectronics, QIS, and polymer upcycling.	The Request will provide the fourth year of support for four-year EFRC awards that were made in FY 2018 and the second year of support for four-year EFRC awards that were made in FY 2020.	No changes.
Energy Innovation Hubs—Fuels from Sunlight $20,000	$20,000	$ —
Funding supports early-stage fundamental research on solar fuels generation that builds on the unique capabilities and accomplishments of the Joint Center for Artificial Photosynthesis. New awards of multi-investigator, cross-disciplinary solar fuels research solicited in the FY 2020 recompetition will continue to address emerging new directions as well as long-standing challenges in this transformational area of energy science. Research focuses on tackling forefront, fundamental scientific challenges for generating fuels using only sunlight, carbon dioxide, and water as inputs. Advances in this area also benefit from consideration of photodriven generation of fuels from molecules other than carbon dioxide. The research capitalizes 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 Request will continue to support early-stage fundamental research on solar fuels generation to address both emerging new directions and long-standing scientific challenges in this area of energy science. Research will continue to focus on generating fuels using only sunlight, carbon dioxide, and water as inputs. However, photodriven generation of fuels from molecules other than carbon dioxide can also provide important new insights and may be supported to reveal principles for solar energy capture and conversion into liquid fuels. Efforts that integrate experiment and theory and couple high-throughput experimentation with artificial intelligence will continue to be emphasized.	No changes.

(dollars in thousands)

FY 2020 Enacted		FY 2021 Request	Explanation of Changes FY 2021 Request vs FY 2020 Enacted
Computational Chemical Sciences	$13,000	$13,000	$—
Funding continues the Computational Chemical Sciences (CCS) awards made in FY 2017 and FY 2018, with ongoing focus on developing public, open source codes for future exascale computer platforms.		The Request will continue CCS awards made in FY 2018, with ongoing focus on developing public, open source codes for future exascale computer platforms. In addition, FY 2021 funds will support a recompetition of CCS awards made in FY 2017, and make awards for development of new theoretical and computational approaches and open source codes in areas relevant to directions identified in BES strategic planning workshop reports.	Funding will support priority research areas for CCS awards as identified in BES strategic planning workshop reports
General Plant Projects	$1,000	$1,000	$ —
Funding supports minor facility improvements at Ames Laboratory.		The Request will support minor facility improvements at Ames Laboratory.	No changes.
SBIR/STTR	$13,851	$13,596	-$255
In FY 2020, SBIR/STTR funding will be set at 3.65 percent of non-capital funding.		In FY 2021, SBIR/STTR funding will be set at 3.65 percent of non-capital funding.	The SBIR/STTR funding will be consistent with the BES total budget.

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 unique tools to thousands of researchers from universities, industry, and government laboratories 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, researchers 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. Keeping BES accelerator-based facilities at the forefront requires continued, transformative advances in accelerator science and technology. Strategic investments in high-brightness electron injectors, superconducting undulators with strong focusing, and high gradient superconducting cavities will have the most impactful benefits. X-ray free electron laser (FEL) oscillators offer the most near-future attainable advances in x-ray science capabilities, requiring additional research efforts in x-ray resonant cavities and high heat-load diamond materials. Research in seeded FEL schemes for full coherent x-rays, and attosecond electron and x-ray pulse generation are critical for multi-terawatt FEL amplifiers required by single-particle imaging.

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 online 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. Applications of AI/ML methods and tools are being implemented in new software and hardware to help address these data and information challenges and needs. Challenges include speeding up high-fidelity simulations for online models, fast tuning in high-dimensional space, anomaly/breakout detection, 'virtual diagnostics' that can operate at high repetition rates, and sophisticated compression/rejection data pipelines operating at the 'edge' (next to the detector) to save the highest value data from user experiments.

In FY 2019, more than 16,000 scientists and engineers in many fields of science and technology used BES scientific facilities. These facilities provide unique capabilities to the scientific community and industry and are a critical component of maintaining U.S. leadership in the physical sciences. Collectively, these user facilities and enabling tools contribute to important research results that span the continuum from basic to applied research and embrace the full range of scientific and technological endeavors, including chemistry, physics, geology, materials science, environmental science, biology, and biomedical science. These capabilities enable scientific insights that can lead to the discovery and design of advanced materials and novel chemical processes with broad societal impacts, from energy applications to information technologies and biopharmaceutical discoveries. The advances enabled by these facilities extend from energy-efficient catalysts to spin-based electronics and new drugs for cancer therapy. For approved, peer-reviewed projects, operating time is available at no cost to researchers who intend to publish their results in the open literature.

X-Ray Light Sources

X-rays are an essential tool for studying the structure of matter and have long been used to peer into material through which visible light cannot penetrate. Today's light source facilities produce x-rays that are billions of times brighter than medical x-rays. Scientists use these highly focused, intense beams of x-rays to reveal the identity and arrangement of atoms in a wide range of materials. The tiny wavelength of x-rays allows us to see things that visible light cannot resolve, such as the arrangement of atoms in metals, semiconductors, biological molecules, and other materials. The fundamental tenet of materials research is that structure determines function. The practical corollary that converts materials research from an intellectual exercise into a foundation of our modern technology-driven economy is that structure can be manipulated to construct materials with 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 seven 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 was started in FY 2020 to 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, isotope production, 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 such as mercury. 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 world-leading instruments include very high resolution inelastic and quasi-elastic scattering capabilities, powder and single crystal diffraction, polarized and unpolarized beam reflectometry, and spin echo and small angle scattering spectrometers. A full suite of high and low temperature, high magnetic field, and high pressure sample environment equipment is available on each instrument. All the SNS instruments are in high demand by researchers world-wide in a range of disciplines from biology to materials sciences and condensed matter physics.

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

The NSRCs focus on interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. They are a different class of facility than the x-ray and neutron sources, as NSRCs are 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 are used 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 development 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 manipulations to reduce the cost and complexity and improve performance of next generation FELs, and development of intense laser-based terahertz (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

(dollars in thousands)

FY 2020 Enacted		FY 2021 Request	Explanation of Changes FY 2021 Request vs FY 2020 Enacted
Scientific User Facilities	**$1,057,040**	**$961,813**	**-$95,227**
X-Ray Light Sources	$518,791	$494,830	-$23,961
Funding supports LCLS operations, which resume in the third quarter of FY 2020 upon completion of installation of LCLS-II accelerator components. All light source facilities will operate at approximately 100 percent of optimal.		The Request will support operations at five BES light sources (LCLS, APS, ALS, NSLS-II, and SSRL).	Funding will support LCLS operations at 97 percent of optimal. The remaining light source facilities will operate at approximately 91 percent of optimal.
High-Flux Neutron Sources	$289,701	$260,088	-$29,613
Funding supports SNS and HFIR operations. These facilities will operate at 100 percent of optimal.		The Request will support operations at SNS and HFIR.	Funding will support operations for SNS and HFIR at approximately 91 percent of optimal.
Nanoscale Science Research Centers	$138,687	$129,938	-$8,749
Funding supports operations of five NSRCs, with funding for nanoscience, QIS research, and related development of synthesis and characterization tools.		The Request will provide funding for five NSRCs (CFN, CNM, CNMS, TMF, and CINT). The NSRCs will continue to develop nanoscience and QIS-related research infrastructure and capabilities for materials synthesis, device fabrication, metrology, modeling and simulation.	Funding will support operations for the five NSRCs as well as QIS-related research infrastructure and capabilities.
Other Project Costs	$23,000	$7,000	-$16,000
Funding supports Other Project Costs for the LCLS-II-HE project at SLAC National Accelerator Laboratory, ALS-U at Lawrence Berkeley National Laboratory, and the Second Target Station at Oak Ridge National Laboratory.		The Request will support Other Project Costs for the LCLS-II-HE project at SLAC National Accelerator Laboratory, PPU at Oak Ridge National Laboratory, and the Second Target Station project at Oak Ridge National Laboratory. The Request initiates the Cryomodule Repair and Maintenance Facility (CRMF) project.	Other Project Costs follow project plans.

(dollars in thousands)

FY 2020 Enacted		FY 2021 Request	Explanation of Changes FY 2021 Request vs FY 2020 Enacted
Major Items of Equipment	$10,500	$2,000	-$8,500
Funding initiates a beamline project for NSLS-II (NEXT-II) at Brookhaven National Laboratory and will support conceptual designs of new beamlines. The FY 2020 Enacted budget also initiates a recapitalization project for the NSRCs and will support planning and design activities in preparation for CD-1, along with possible procurements.		The Request will continue the beamline project for NSLS-II (NEXT-II) at Brookhaven National Laboratory. Design work for NEXT-II will continue along with R&D, prototyping, other supporting activities, and possible long lead procurements. The recapitalization project for the NSRCs will also continue with R&D, design, engineering, prototyping, other supporting activities, and possible procurements.	Funding will support the NEXT-II and NSRC Recapitalization MIE projects.
Research	$39,879	$36,206	-$3,673
Funding supports high-priority research activities for detectors and optics instrumentation and applications of machine learning techniques to accelerator optimization, control, prognostics, and data analysis.		The Request will support high-priority research activities for advanced seeded FEL schemes that provide several orders of magnitude performance enhancement, detectors and optics instrumentation and applications of machine learning techniques to accelerator optimization, control, prognostics, and data analysis. Research will emphasize transformative advances in accelerator science and technology that lead to significant improvements in very high brightness and high current electron sources and in high intensity proton sources.	Funding will support investment in future accelerator technologies to continue to provide the world's most comprehensive and advanced accelerator-based facilities for scientific research. Funding will also continue the development of AI/ML methods and tools to address data and information challenges at the BES user facilities, including accelerator optimization, control, prognostics, and data analysis.
SBIR/STTR	$36,482	$31,751	-$4,731
In FY 2020, SBIR/STTR funding will be set at 3.65 percent of non-capital funding.		In FY 2021, SBIR/STTR funding will be set at 3.65 percent of non-capital funding.	The SBIR/STTR funding will be consistent with the BES total budget.

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.

<u>Advanced Photon Source Upgrade (APS-U)</u>

The 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-3, Approve Start of Construction, on July 25, 2019, with a Total Project Cost (TPC) of $815,000,000 and CD-4, Approve Project Completion, in 2Q FY 2026.

<u>Advanced Light Source Upgrade (ALS-U)</u>

The ALS-U project will upgrade the existing ALS facility by replacing the existing electron storage ring with a new electron storage ring based on a multi-bend achromat lattice design, which will provide a soft x-ray source that is up to 1000 times brighter 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-3A, Approve Long Lead Procurements, on December 19, 2019. The current TPC range is $330,000,000 - $495,000,000.

<u>Linac Coherent Light Source-II-HE (LCLS-II-HE)</u>

The LCLS-II-HE project will increase the energy of the superconducting linac currently under construction as part of the LCLS-II project from 4 giga-electronvolts (GeV) to 8 GeV and thereby expand the high repetition rate operation (1 million pulses per second) of this unique facility 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. The current TPC range is $290,000,000 - $480,000,000.

<u>Proton Power Upgrade (PPU)</u>

The PPU project will double the proton beam power capability of the Spallation Neutron Source (SNS) from 1.4 megawatts (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 CD-3B, Approve Long Lead Procurements, on September 3, 2019. The current TPC range is $184,000,000 - $320,000,000.

<u>Second Target Station (STS)</u>

The 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 project received CD-0, Approve Mission Need, on January 7, 2009. The current TPC range is $800,000,000 - $1,500,000,000.

Cryomodule Repair and Maintenance Facility (CRMF)
The CRMF project will provide a much needed capability to maintain, repair, and test superconducting radiofrequency (SRF) accelerator components, including SRF cryomodules that make up the new superconducting accelerator being constructed by the LCLS-II and LCLS-II-HE projects. The facility will provide for the full disassembly and repair of the SRF cryomodule; the ability to disassemble, clean, and reassemble the SRF cavities and cavity string; testing capabilities for the full cryomodule; and separate testing capabilities for individual SRF cavities. To accomplish this, the project is envisioned to require a 19,000 to 23,000 gross square foot building to contain the necessary equipment. The building will need a concrete shielded enclosure for cryomodule testing, a control room, vertical test stand area for testing SRF cavities and components, a cryogen distribution box which is connected to a source of liquid helium and will distribute liquid helium within the CRMF building, cryomodule fixtures used to insert and remove the cold mass from the cryomodule vacuum vessel, a cleanroom partitioned into class 10 and class 1000 areas, a loading and cryomodule preparation area, storage areas, and a 15 ton bridge crane for moving equipment from one area to another within the building. The project received CD-0, Approve Mission Need, on December 5, 2019. The current TPC range is $70,000,000 - $98,000,000.

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 percent 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

(dollars in thousands)

FY 2020 Enacted		FY 2021 Request		Explanation of Changes FY 2021 Request vs FY 2020 Enacted
Construction	**$360,000**		**$184,000**	**-$176,000**
21-SC-10, Cryomodule Repair and Maintenance Facility (CRMF), SLAC	$—		$1,000	+$1,000
No funds were requested in FY 2020.		The Request will support conducting an Analysis of Alternatives to determine the project site and the basic parameters on which to base a conceptual design. Engineering and design activities may begin.		This is the initial request for the CRMF project.
19-SC-14, Second Target Station (STS), ORNL	$20,000		$1,000	-$19,000
Funding supports continued planning, targeted R&D and engineering design, and other activities required to advance the STS project. Construction funds will be executed after the appropriate critical decision approvals are received.		The Request will continue planning, R&D, and engineering activities to assist in maturing the project design, scope, cost, schedule and key performance parameters.		Funding will support the STS project.
18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL	$170,000		$150,000	-$20,000
Funding supports 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 will support advancing the final engineering designs, engineering, prototyping, testing, fabrication, procurement, integration, and installation for the storage ring and experimental facilities, and further site preparation and civil construction associated with the long beamlines.		Funding will support the APS-U project.

(dollars in thousands)

FY 2020 Enacted		FY 2021 Request		Explanation of Changes FY 2021 Request vs FY 2020 Enacted	
18-SC-11, Spallation Neutron Source Proton Power Upgrade (PPU), ORNL	$60,000		$5,000		-$55,000
Funding supports R&D, engineering, prototyping, preliminary and final design, testing, fabrication, procurement, component integration and installation, and other activities required to advance the PPU project.		The Request will continue support of R&D, engineering, prototyping, preliminary and final designs, testing, fabrication, procurement, component integration and installation, and civil construction site preparation. Advancing the target R&D, engineering, design, and prototyping in conjunction with SNS operations target improvement plans will be a high priority.		Funding will support the PPU project.	
18-SC-12, Advanced Light Source Upgrade (ALS-U), LBNL	$60,000		$13,000		-$47,000
Funding supports planning, engineering, design, R&D, equipment prototyping, testing, and other activities to advance the ALS-U project.		The Request will continue support of engineering, design, R&D prototyping and long lead procurements of construction items.		Funding will support the ALS-U project.	
18-SC-13, Linac Coherent Light Source-II High Energy (LCLS-II-HE), SLAC	$50,000		$14,000		-$36,000
Funding supports planning, engineering, design, R&D, equipment prototyping, testing, and other activities required to advance the LCLS-II-HE project.		The Request will continue engineering, design, R&D prototyping, and long lead procurements of construction items.		Funding will support the LCLS-II-HE project.	

Basic Energy Sciences
Capital Summary

(dollars in thousands)

	Total	Prior Years	FY 2019 Enacted	FY 2020 Enacted	FY 2021 Request	FY 2021 Request vs FY 2020 Enacted
Capital Operating Expenses						
Capital Equipment	N/A	N/A	76,610	46,825	35,325	-11,500
Minor Construction Activities						
General Plant Projects (GPP)	N/A	N/A	3,000	1,000	1,000	—
Accelerator Improvement Projects (AIP)	N/A	N/A	48,045	10,700	56,612	+45,912
Total, Capital Operating Expenses	**N/A**	**N/A**	**127,655**	**58,525**	**92,937**	**+34,412**

Capital Equipment

(dollars in thousands)

	Total	Prior Years	FY 2019 Enacted	FY 2020 Enacted	FY 2021 Request	FY 2021 Request vs FY 2020 Enacted
Capital Equipment						
Major Items of Equipment						
Scientific User Facilities						
NSLS-II Experimental Tools-II (NEXT-II), BNL	80,000	—	—	5,500	1,000	-4,500
NSRC Recapitalization	80,000	—	—	5,000	1,000	-4,000
Total, MIEs	N/A	N/A	—	10,500	2,000	-8,500
Total, Non-MIE Capital Equipment	N/A	N/A	76,610	36,325	33,325	-3,000
Total, Capital Equipment	**N/A**	**N/A**	**76,610**	**46,825**	**35,325**	**-11,500**

Minor Construction Activities

(dollars in thousands)

	Total	Prior Years	FY 2019 Enacted	FY 2020 Enacted	FY 2021 Request	FY 2021 Request vs FY 2020 Enacted
General Plant Projects (GPP)						
Total GPPs less than $5M[a]	N/A	N/A	3,000	1,000	1,000	—
Total, General Plant Projects (GPP)	**N/A**	**N/A**	**3,000**	**1,000**	**1,000**	**—**
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	—	—	—
DISCOVER, Spallation Neutron Source, ORNL	18,500	N/A	—	—	18,500	+18,500
Full Scale SCL Chemistry Upgrade, Spallation Neutron Source, ORNL	5,000	N/A	—	—	5,000	+5,000
Guide Hall Extension, High Flux Isotope Reactor, ORNL	9,000	N/A	—	—	9,000	+9,000
Storage Ring HVAC System Upgrade, Advanced Light Source, LBNL	6,900	N/A	650[b]	6,250[b]	—	-6,250
Copper to Soft Xray, Linac Coherent Light Source, SLAC	7,664	N/A	7,664[b]	—	—	—
3rd Harmonic Cavity, National Synchrotron Light Source-II, BNL	8,760	N/A	—	—	8,760	+8,760
3rd RF Cavity, National Synchrotron Light Source-II, BNL	9,300	5,100	4,200[b]	—	—	—
Total, AIPs (greater than or equal to $5M and less than $20M)	N/A	N/A	25,914	6,250	41,260	+35,010
Total, AIPs less than $5M[c]	N/A	N/A	22,131	4,450	15,352	+10,902
Total, Accelerator Improvement Projects (AIP)	**N/A**	**N/A**	**48,045**	**10,700**	**56,612**	**+45,912**
Total, Minor Construction Activities	**N/A**	**N/A**	**51,045**	**11,700**	**57,612**	**+45,912**

[a] GPP activities less than $5 million include design and construction for additions and/or improvements to land, buildings, replacements or additions to roads, and general area improvements.
[b] Funding was not previously included in the FY 2020 Request because it was not required to be disclosed as minor construction project.
[c] AIP activities less than $5 million include minor construction at an existing accelerator facility.

Basic Energy Sciences
Major Items of Equipment Description(s)

Scientific User Facilities MIEs:

NSLS-II Experimental Tools-II (NEXT-II) Project

The NEXT-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 project received CD-0, Approve Mission Need, on December 19, 2018. The current total project cost range is $40,000,000 to $80,000,000. The FY 2021 Request of $1,000,000 will continue R&D, prototyping, other supporting activities, and possible long lead procurements.

Nanoscale Science Research Center (NSRC) Recapitalization Project

The 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 project received CD-0, Approve Mission Need, on December 19, 2018. The current total project cost range is $50,000,000 to $90,000,000. The FY 2021 Request of $1,000,000 will continue R&D, design, engineering, prototyping, other supporting activities, and possible procurements.

Basic Energy Sciences
Construction Projects Summary

(dollars in thousands)

	Total	Prior Years	FY 2019 Enacted	FY 2020 Enacted	FY 2021 Request	FY 2021 Request vs FY 2020 Enacted
21-SC-10, Cryomodule Repair and Maintenance Facility (CRMF)						
TEC	70,000	—	—	—	1,000	+1,000
OPC	10,000	—	—	—	1,000	+1,000
TPC	**80,000**	**—**	**—**	**—**	**2,000**	**+2,000**
19-SC-14, Second Target Station (STS), ORNL						
TEC	1,223,700	—	1,000	20,000	1,000	-19,000
OPC	45,300	10,805	5,000	17,000	1,000	-16,000
TPC	**1,269,000**	**10,805**	**6,000**	**37,000**	**2,000**	**-35,000**
18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL						
TEC	796,500	235,500	130,000	170,000	150,000	-20,000
OPC	18,500	8,500	—	—	—	—
TPC	**815,000**	**244,000**[a]	**130,000**	**170,000**	**150,000**	**-20,000**
18-SC-11, Proton Power Upgrade (PPU), ORNL						
TEC	236,202	36,000	60,000	60,000	5,000	-55,000
OPC	13,798	10,798	—	—	3,000	+3,000
TPC	**250,000**	**46,798**	**60,000**	**60,000**	**8,000**	**-52,000**
18-SC-12, Advanced Light Source Upgrade (ALS-U), LBNL						
TEC	380,200	16,000	60,000	60,000	13,000	-47,000
OPC	30,000	24,000	2,000	2,000	—	-2,000
TPC	**410,200**	**40,000**	**62,000**	**62,000**	**13,000**	**-49,000**

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

(dollars in thousands)

	Total	Prior Years	FY 2019 Enacted	FY 2020 Enacted	FY 2021 Request	FY 2021 Request vs FY 2020 Enacted
18-SC-13, Linac Coherent Light Source-II-HE (LCLS-II-HE), SLAC						
TEC	408,000	8,000	28,000	50,000	14,000	-36,000
OPC	20,000	2,000	6,000	4,000	2,000	-2,000
TPC	**428,000**	**10,000**	**34,000**	**54,000**	**16,000**	**-38,000**
13-SC-10, Linac Coherent Light Source-II (LCLS-II), SLAC						
TEC	993,100	863,800	129,300	—	—	—
OPC	51,900	45,800	6,100	—	—	—
TPC	**1,045,000**	**909,600**[a]	**135,400**	**—**	**—**	**—**
Total, Construction						
TEC	**4,107,702**	**1,159,300**	**408,300**	**360,000**	**184,000**	**-176,000**
OPC	**189,498**	**101,903**	**19,100**	**23,000**	**7,000**	**-16,000**
TPC	**4,297,200**	**1,261,203**	**427,400**	**383,000**	**191,000**	**-192,000**

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

Basic Energy Sciences
Funding Summary

(dollars in thousands)

	FY 2019 Enacted	FY 2020 Enacted	FY 2021 Request	FY 2021 Request vs FY 2020 Enacted
Research	815,600	871,321	856,817	-14,504
Facility Operations	922,000	947,179	884,856	-62,323
Projects				
Major Items of Equipment	—	10,500	2,000	-8,500
Construction	427,400	383,000	191,000	-192,000
Total, Projects	427,400	393,500	193,000	-200,500
Other[a]	1,000	1,000	1,000	—
Total, Basic Energy Sciences	**2,166,000**	**2,213,000**	**1,935,673**	**-277,327**

[a] 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 for TYPE A facilities:

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 2019 Enacted	FY 2019 Current	FY 2020 Enacted	FY 2021 Request	FY 2021 Request vs FY 2020 Enacted
TYPE A FACILITIES					
Advanced Light Source	**$66,283**	**$66,583**	**$68,093**	**$63,842**	**-$4,251**
Number of users	2,000	2,171	1,800	1,500	-300
Achieved operating hours	N/A	4,468	N/A	N/A	N/A
Planned operating hours	4,700	4,700	3,880	3,750	-130
Optimal hours	4,700	4,700	3,880[a]	4,100	+220
Percent optimal hours	100%	95.1%	100%	91.5%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A

[a] Optimal hours decreased for maintenance and the PG&E Public Safety Power Shutoffs.

(dollars in thousands)

	FY 2019 Enacted	FY 2019 Current	FY 2020 Enacted	FY 2021 Request	FY 2021 Request vs FY 2020 Enacted
Advanced Photon Source	**$136,743**	**$138,743**	**$140,477**	**$131,708**	**-$8,769**
Number of users	5,700	5,426	4,900	4,700	-200
Achieved operating hours	N/A	4,909	N/A	N/A	N/A
Planned operating hours	5,000	5,000	5,000	4,550	-450
Optimal hours	5,000	5,000	5,000	5,000	—
Percent optimal hours	100%	98.2%	100%	91.0%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A
National Synchrotron Light Source-II, BNL	**$114,127**	**$114,277**	**117,244**	**$109,925**	**-$7,319**
Number of users	1,600	1,755	1,700	1,500	-200
Achieved operating hours	N/A	4,863	N/A	N/A	N/A
Planned operating hours	5,000	5,000	5,000	4,550	-450
Optimal hours	5,000	5,000	5,000	5,000	—
Percent optimal hours	100%	97.3%	100%	91.0%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A
Stanford Synchrotron Radiation Lightsource	**$42,847**	**$43,497**	**$44,017**	**$41,268**	**-$2,749**
Number of users	1,650	1,761	1,500	1,400	-100
Achieved operating hours	N/A	5,004	N/A	N/A	N/A
Planned operating hours	5,070	5,070	5,090	4,900	-190
Optimal hours	5,070	5,070	5,090	5,400	-310
Percent optimal hours	100%	98.7%	100%	90.7%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A
Linac Coherent Light Source	**$145,000**	**$150,400**	**$148,960**	**$148,087**	**-$873**
Number of users	300	529	500	800	+300
Achieved operating hours	N/A	1,512	N/A	N/A	N/A
Planned operating hours	1,600	1,600	2,500	4,480	+1,980
Optimal hours	1,600[a]	1,600	2,500	4,600	+2,100
Percent optimal hours	100%	94.5%	100%	97.4%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A

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

(dollars in thousands)

	FY 2019 Enacted	FY 2019 Current	FY 2020 Enacted	FY 2021 Request	FY 2021 Request vs FY 2020 Enacted
Spallation Neutron Source	**$205,714**	**$206,214**	**$187,048**	**$165,588**	**-$21,460**
Number of users	800	758	800	730	-70
Achieved operating hours	N/A	3,771	N/A	N/A	N/A
Planned operating hours	4,900	4,900	4,600	4,550	-50
Optimal hours	4,900	4,900	4,600	5,000	+400
Percent optimal hours	100%	77.0%	100%	91.0%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A
High Flux Isotope Reactor	**$76,286**	**$76,286**	**$102,653**	**$94,500**	**-$8,153**
Number of users	560	—	520	500	-20
Achieved operating hours	N/A	3[a]	N/A	N/A	N/A
Planned operating hours	4,000	4,000	3,900	3,650	-250
Optimal hours	4,000	4,000	3,900	4,000	+100
Percent optimal hours	100%	0.1%	100%	91.3%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A
TYPE B FACILITIES					
Center for Nanoscale Materials	**$27,704**	**$27,704**	**$28,461**	**$26,665**	**-$1,796**
Number of users	600	599	530	500	-30
Center for Functional Nanomaterials	**$24,148**	**$24,148**	**$24,807**	**$23,243**	**-$1,564**
Number of users	580	593	510	500	-10
Molecular Foundry	**$31,237**	**$31,987**	**$32,090**	**$30,065**	**-$2,025**
Number of users	700	1,011	800	700	-100
Center for Nanophase Materials Sciences	**$27,078**	**$27,078**	**$27,818**	**$26,063**	**-$1,755**
Number of users	600	653	630	600	-30
Center for Integrated Nanotechnologies	**$24,833**	**$24,833**	**$25,511**	**$23,902**	**-$1,609**
Number of users	600	860	700	600	-100

[a] HFIR was shut down in Q1 FY 2019 due to a fuel element failure. A corrective action plan was implemented and HFIR restarted in November 2019.

(dollars in thousands)

	FY 2019 Enacted	FY 2019 Current	FY 2020 Enacted	FY 2021 Request	FY 2021 Request vs FY 2020 Enacted
Total Facilities	**$922,000**	**$931,750**	**$947,179**	**$884,856**	**-$62,323**
Number of users	15,690	16,116	14,890	14,030	-860
Achieved operating hours	N/A	24,530	N/A	N/A	N/A
Planned operating hours	30,270	30,270	29,970	30,430	-460
Optimal hours	30,270	30,270	29,970	33,100	+3,130
Percent optimal hours[a]	100%	82.2%	100%	92.3%	N/A
Unscheduled downtime hours	<10%	<10%	<10%	<10%	N/A

[a] For total facilities only, this is a "funding weighted" calculation FOR ONLY TYPE A facilities: $\frac{\sum_{1}^{n}[(\%\text{OH for facility n}) \times (\text{funding for facility n operations})]}{\text{Total funding for all facility operations}}$

Basic Energy Sciences
Scientific Employment

	FY 2019 Enacted	FY 2020 Enacted	FY 2021 Request	FY 2021 Request vs FY 2020 Enacted
Number of permanent Ph.D.'s (FTEs)	4,800	4,950	4,680	-270
Number of postdoctoral associates (FTEs)	1,310	1,370	1,310	-60
Number of graduate students (FTEs)	2,050	2,140	2,060	-80
Other scientific employment (FTEs) [a]	3,030	3,100	2,890	-210

[a] Includes technicians, engineers, computer professionals and other support staff.

21-SC-10, Cryomodule Repair and Maintenance Facility
Project is for Design and Construction

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

Summary

The FY 2021 Request for the Cryomodule Repair and Maintenance Facility (CRMF) project is $2,000,000, including $1,000,000 in Total Estimated Cost (TEC) funds and $1,000,000 in Other Project Costs (OPC) funds. The most recent DOE Order 413.3B approved Critical Decision (CD) is CD-0 (Approve Mission Need), approved on December 5, 2019. The notional Total Project Cost (TPC) range, approved at CD-0 is $70,000,000 - $98,000,000 based on a point estimate of $80,000,000.

Significant Changes

This a new Construction Project Data Sheet (CPDS) and CRMF is a new start for FY 2021.

In FY 2020, SLAC National Accelerator Laboratory (SLAC) recognized a critical need for a facility capable of repairing and maintaining the cryomodules being installed through the Linac Coherent Light Source-II (LCLS-II) and LCLS-II High Energy (LCLS-II-HE) construction projects. SLAC developed and submitted a proposal for the CRMF to Basic Energy Sciences for consideration. The proposal was sent out to an independent group of experts in the field of superconducting radiofrequency science and superconducting linac construction for review and comment. The proposal was well received by the experts, and based on their support, BES developed a Mission Need Statement document as required to support CD-0, Approve Mission Need. The FY 2021 Request will support conducting an Analysis of Alternatives to determine the project site and the basic design parameters on which to base a conceptual design. Depending on progress and appropriate CD approvals, some of the FY 2021 Request funding may be used for engineering and design activities.

A Federal Project Director will be assigned to this project prior to CD-1.

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 2021[a]	12/05/2019	1Q FY 2021	1Q FY 2021	1Q FY 2022	4Q FY 2022	1Q FY 2023	N/A	1Q 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
FY 2021[a]	4Q FY 2021	1Q FY 2022

CD-3A – Approve Long-Lead Procurements: As the project planning and design matures, long lead procurement may be requested in FY 2022 to mitigate cost and schedule risk to the project.

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

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 2021[a]	4,000	66,000	70,000	10,000	N/A	10,000	80,000

2. Project Scope and Justification

Scope

The preliminary scope of the CRMF project is to construct a building to contain the necessary equipment to maintain, repair, and test superconducting radiofrequency (SRF) accelerator components. The building will need a concrete shielded enclosure for cryomodule testing, a control room, vertical test stand area for testing SRF cavities and components, a cryogen distribution box which is connected to a source of liquid helium and will distribute liquid helium within the CRMF building, cryomodule fixtures used to insert and remove the cold mass from the cryomodule vacuum vessel, a cleanroom partitioned into class 10 and class 1000 areas, a loading and cryomodule preparation area, storage areas, and a 15 ton bridge crane for moving equipment from one area to another within the building.

Optional scope to be considered and included in the preliminary scope includes a stand-alone cryoplant that would provide a source of liquid helium (if one is not available at the selected site), a dedicated SRF injector test area which requires extending the envisioned building length by 30 feet, and a 40 mega-electronvolt (MeV) SRF linac to provide the equipment and diagnostics necessary for an integrated injector test stand.

Justification

SC, through the two current BES construction projects, LCLS-II and LCLS-II-HE, is making over a $1,400,000,000 capital investment in a SRF linac at SLAC to support the science mission of DOE. The LCLS-II project is providing a 4 GeV SRF-based linear accelerator capable of providing 1 megahertz (MHz) electron pulses to create a free electron, x-ray laser. This machine contains 35 SRF cryomodules to accelerate the electrons to 4 GeV. The LCLS-II-HE will increase the energy of the LCLS-II linac to 8 GeV by providing an additional 20 SRF cryomodules of a similar design to the LCLS-II ones, but operating at a higher accelerating gradient. SLAC has partnered with Fermi National Accelerator Laboratory (FNAL) and the Thomas Jefferson National Accelerator Facility (TJNAF) to provide the accelerating cryomodules. The cryomodules are produced at FNAL and TJNAF making use of specialized fabrication, assembly, and test capabilities available there. To make any repairs, the cryomodules must currently be sent back to either FNAL or TJNAF at an increased risk of damage, cost, and schedule delays.

The initial assumption was that cryomodules could be shipped back to the partner laboratories as needed for maintenance at a rate of 1 to 2 cryomodules per year. However, cryomodules could be damaged during transportation, posing a risk to facility operations. This approach also assumes that either FNAL or TJNAF would have the maintenance capabilities available when needed. Recently, TFNAF has agreed to manufacture cryomodules for an accelerator upgrade to the Spallation Neutron Source linac and the production facilities at FNAL will produce cryomodules for the Proton Improvement Plan-II (PIP-II) linac upgrade at FNAL. At this time, the two partner laboratories have informed SLAC that they will need 6 to 12 months of advance notice to schedule maintenance or repairs to the SLAC hardware.

The proposed CRMF will provide the capability to maintain, repair, and test SRF accelerator components, the primary one being the SRF cryomodules that make up the new superconducting accelerator being constructed by the LCLS-II and LCLS-II-HE construction projects. The facility will provide for the full disassembly and repair of the SRF cryomodule; the ability to disassemble, clean, and reassemble the SRF cavities and cavity string; testing capabilities for the full cryomodule; and separate testing capabilities for individual SRF cavities.

[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 photon energy range for LCLS-II-HE could be extended by lowering the emittance of the electron injector which requires an R&D effort. Progress in this area at SLAC has been hindered by lack of an appropriate research and development facility with testing capabilities. This needed R&D effort is currently being performed at LBNL and ANL in partnership with SLAC. The CRMF project could provide this needed support to SLAC when constructed.

Prior to CD-1, SC will conduct an Analysis of Alternatives that, among other things, will examine the cost benefits of having a dedicated CRMF facility at SLAC versus relying on partner laboratories or others to provide this capability. The risk in schedule and operations in terms of cost of having the facility sited somewhere other than SLAC will be included in this cost analysis. SC will also evaluate the proposed project scope as part of the Analysis of Alternatives required for CD-1 approval.

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 Key Performance Parameters (KPPs) are preliminary and may change as the project continues towards CD-2. At CD-2 approval, the KPPs will be baselined. The Threshold KPPs represent the minimum acceptable performance that the project must achieve. The Objective KPPs represent the desired project performance. Achievement of the Threshold KPPs will be a prerequisite for approval of CD-4, Project Completion.

Performance Measure	Threshold	Objective
Conventional Facilities Building Area	22,000 gross square feet	25,000 gross square feet
Electron Beam Energy	50 MeV	128 MeV
Cryogenic Cooling Capacity at 2K	100 Watts	250 Watts

3. Financial Schedule

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
Design			
FY 2021	1,000	1,000	1,000
Outyears	3,000	3,000	3,000
Total, Design	4,000	4,000	4,000
Construction			
Outyears	66,000	66,000	66,000
Total, Construction	66,000	66,000	66,000
Total Estimated Cost (TEC)			
FY 2021	1,000	1,000	1,000
Outyears	69,000	69,000	69,000
Total, TEC	**70,000**	**70,000**	**70,000**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Other Project Cost (OPC)			
FY 2021	1,000	1,000	1,000
Outyears	9,000	9,000	9,000
Total, OPC	**10,000**	**10,000**	**10,000**
Total Project Cost (TPC)			
FY 2021	2,000	2,000	2,000
Outyears	78,000	78,000	78,000
Total, TPC[a]	**80,000**	**80,000**	**80,000**

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design			
Design	3,500	N/A	N/A
Contingency	500	N/A	N/A
Total, Design	4,000	N/A	N/A
Construction			
Site Preparation	1,000	N/A	N/A
Equipment	35,000	N/A	N/A
Other Construction	15,500	N/A	N/A
Contingency	14,500	N/A	N/A
Total, Construction	66,000	N/A	N/A
Total, TEC	**70,000**	**N/A**	**N/A**
Contingency, TEC	*15,000*	*N/A*	*N/A*

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

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Other Project Cost (OPC)			
OPC except D&D			
R&D	1,000	N/A	N/A
Conceptual Planning	1,000	N/A	N/A
Conceptual Design	2,000	N/A	N/A
Start-Up	3,000	N/A	N/A
Contingency	3,000	N/A	N/A
Total, OPC	**10,000**	**N/A**	**N/A**
Contingency, OPC	*3,000*	*N/A*	*N/A*
Total Project Cost	**80,000**	**N/A**	**N/A**
Total, Contingency (TEC+OPC)	***18,000***	***N/A***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2021	Outyears	Total
FY 2021	TEC	—	1,000	69,000	70,000
	OPC	—	1,000	9,000	10,000
	TPC	—	2,000	78,000	80,000

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	FY 2027
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	FY 2052

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	5,500	N/A	286,000

Additional operations and maintenance costs are expected above the estimated costs to operate the LCLS-II facility. The estimate will be updated and additional details will be provided after CD-1, Approve Alternate Selection and Cost Range.

7. D&D Information

At this stage of project planning and development, SC anticipates that a new 19,000 to 23,000 gsf building may be constructed as part of this project.

8. Acquisition Approach

DOE has not determined the site of the CRMF project. If the selected site is a national laboratory, then the project would be acquired under the existing DOE Management and Operations contract for that laboratory.

The selected site will prepare a Conceptual Design Report for the CRMF project and demonstrate that they have the required project management systems in place to execute the project.

The selected organization 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 similar facilities at other national laboratories, to the extent practicable. The project will fully exploit recent cost data from similar operating facilities in planning and budgeting. SLAC or partner laboratory staff may assist with completing the design of the technical systems. The selected contractor or subcontracted vendors with the necessary capabilities will fabricate technical equipment. All subcontracts will be competitively bid and awarded based on best value to the government.

Lessons learned from other SC projects and other similar facilities will be exploited fully in planning and executing CRMF.

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 2021 Request for Second Target Station (STS) project is $2,000,000, including $1,000,000 in Total Estimated Cost (TEC) funds and $1,000,000 in Other Project Costs (OPC) funds. 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 Construction Project Data Sheet (CPDS) is an update of the FY 2020 CPDS and does not include a new start for FY 2021. There are no significant changes.

In FY 2019, the project advanced the planning, research and development (R&D), and conceptual design and conducted technical design reviews for the major systems (target, instruments, controls, accelerator, and conventional facilities). In FY 2020, the project continues planning, R&D, design, engineering, and other activities required to advance the STS project toward CD-1. The focus will be on project planning and initiation activities such as refining the initial cost estimates and refining the scope definitions, key performance parameters, and TPC range. In FY 2021, the project will continue the FY 2020 activities of planning, R&D, and engineering to assist in maturing the project design, scope, cost, schedule and key performance parameters.

A Federal Project Director, certified to level II, 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 2020	1/07/09	2Q FY 2022	2Q FY 2022	2Q FY 2023	2Q FY 2025	2Q FY 2024	N/A	4Q FY 2031
FY 2021[a]	1/07/09	2Q FY 2021	2Q FY 2021	3Q FY 2024	3Q FY 2026	3Q FY 2025	N/A	2Q FY 2032

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	65,500	1,138,500	1,204,000	45,300	N/A	45,300	1,249,300
FY 2021[a]	65,500	1,158,200	1,223,700	45,300	N/A	45,300	1,269,000

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

2. Project Scope and Justification

Scope

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 will be located in unoccupied space east of the existing first target station (FTS). The project requires approximately 380,000 ft^2 of new buildings, making conventional facility construction a major contributor to project costs.

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 community conducted numerous studies since the 1970's that have established the scientific justification and need for a very high-intensity pulsed neutron source in the U.S. Since 2007, when it began its user program at ORNL, the SNS has been fulfilling this need. In accordance with the 1996 BESAC (Russell Panel) Report recommendation, SNS has many technical margins built into its systems to facilitate a power upgrade into the 2-4 megawatt (MW) range to maintain its position of scientific leadership in the future.

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." ORNL held four workshops 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 STS will feature 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 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 Key Performance Parameters (KPPs) are preliminary and may change as the project continues towards CD-2. At CD-2 approval, the KPPs will be baselined. The Threshold KPPs represent the minimum acceptable performance that the project must achieve. The Objective KPPs represent the desired project performance. Achievement of the Threshold KPPs will be a prerequisite for approval of CD-4, Project Completion.

Performance Measure	Threshold	Objective
Beam power on target	0.25 MW at 1.3 giga-electronvolts (GeV)	0.7 MW at 1.3 GeV
Beam energy	1.3 GeV	1.3 GeV
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	20,000	20,000	2,000
FY 2021	1,000	1,000	17,500
Outyears	43,500	43,500	46,000
Total, Design	65,500	65,500	65,500
Construction			
Outyears	1,158,200	1,158,200	1,158,200
Total, Construction	1,158,200	1,158,200	1,158,200
Total Estimated Cost (TEC)			
FY 2019	1,000	1,000	—
FY 2020	20,000	20,000	2,000
FY 2021	1,000	1,000	17,500
Outyears	1,201,700	1,201,700	1,204,200
Total, TEC	**1,223,700**	**1,223,700**	**1,223,700**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Other Project Cost (OPC)			
FY 2016	5,941	5,941	3,069
FY 2017	62	62	2,818
FY 2018	4,802	4,802	250
FY 2019	5,000	5,000	6,262
FY 2020	17,000	17,000	17,400
FY 2021	1,000	1,000	2,950
Outyears	11,495	11,495	12,551
Total, OPC	**45,300**	**45,300**	**45,300**
Total Project Cost (TPC)			
FY 2016	5,941	5,941	3,069
FY 2017	62	62	2,818
FY 2018	4,802	4,802	250
FY 2019	6,000	6,000	6,262
FY 2020	37,000	37,000	19,400
FY 2021	2,000	2,000	20,450
Outyears	1,213,195	1,213,195	1,216,751
Total, TPC[a]	**1,269,000**	**1,269,000**	**1,269,000**

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design			
Design	48,500	48,500	N/A
Contingency	17,000	17,000	N/A
Total, Design	65,500	65,500	N/A
Construction			
Construction	864,700	845,000	N/A
Contingency	293,500	293,500	N/A
Total, Construction	1,158,200	1,138,500	N/A
Total, TEC	**1,223,700**	**1,204,000**	**N/A**
Contingency, TEC	*310,500*	*310,500*	*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
Other Project Cost (OPC)			
OPC except D&D			
R&D	4,502	1,500	N/A
Conceptual Design	20,852	18,375	N/A
Start-Up	8,621	14,100	N/A
Contingency	11,325	11,325	N/A
Total, OPC	**45,300**	**45,300**	**N/A**
Contingency, OPC	*11,325*	*11,325*	*N/A*
Total Project Cost[a]	**1,269,000**	**1,249,300**	**N/A**
Total, Contingency (TEC+OPC)	***321,825***	***321,825***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2019[b]	FY 2020	FY 2021	Outyears	Total
FY 2020	TEC	—	1,000	1,000	1,000	1,201,000	1,204,000
	OPC	6,500	5,000	—	1,000	32,800	45,300
	TPC	6,500	6,000	1,000	2,000	1,233,800	1,249,300
FY 2021	TEC	—	1,000	20,000	1,000	1,201,700	1,223,700
	OPC	10,805	5,000	17,000	1,000	11,495	45,300
	TPC	10,805	6,000	37,000	2,000	1,213,195	1,269,000

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	2Q FY 2032
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	2Q FY 2057

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] The project is pre-CD-2; the estimated cost and schedule shown are preliminary. Construction will not be executed without appropriate CD approvals.
[b] 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 ORNL will acquire the STS project under the existing DOE Management and Operations (M&O) contract.

The M&O contractor prepared a Technical Design Report for the STS project and identified key design activities, requirements, and high-risk subsystem components 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. ORNL, partner laboratory staff, and/or vendors will complete design of the technical systems. Vendors and/or partner labs with the necessary capabilities will fabricate the technical equipment. ORNL will competitively bid and award all subcontracts based on best value to the government. The M&O contractor's performance will be evaluated through the annual laboratory performance appraisal process.

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 2021 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-3 (Approve Start of Construction), was approved on July 25, 2019, with a Total Project Cost (TPC) of $815,000,000 and CD-4, Approve Project Completion, in 2Q FY 2026.

Significant Changes

This Construction Project Data Sheet (CPDS) is an update of the FY 2020 CPDS and does not include a new start for FY 2021. There are no significant changes.

In FY 2019, APS-U completed the majority of equipment prototyping and development work and awarded most of the contracts for accelerator magnets, support structures, power supplies, vacuum chambers, experimental systems, front ends, and insertion devices needed to maintain the project schedule. Deliveries of the production first articles are arriving for receiving inspection and are successfully passing acceptance testing. FY 2020 funding enables the advancement of the storage ring and experimental facilities final design, engineering, prototyping, testing, fabrication, procurement, integration and installation, and site preparation for the long beamlines. The project will complete the final design of the long beamline building, lease off-site space for storage, assembly and receiving, and start practicing integrated module assembly. The FY 2021 Request will support ongoing FY 2020 activities to advance the final designs, engineering, prototyping, testing, fabrication, procurement, integration, and installation for the storage ring and experimental facilities. Further site preparation and civil construction associated with the long beamlines will occur. System integration, test, and assembly in preparation for the storage ring removal and installation during the experimental dark time will be a high priority.

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	4/22/10	9/18/15	2/04/16	1Q FY 2019	2Q FY 2020	4Q FY 2019	N/A	1Q FY 2026
FY 2019	4/22/10	9/18/15	2/04/16	2Q FY 2019	4Q FY 2021	1Q FY 2020	N/A	2Q FY 2026
FY 2020	4/22/10	9/18/15	2/04/16	12/09/18	1Q FY 2022	1Q FY 2020	N/A	2Q FY 2026
FY 2021	4/22/10	9/18/15	2/04/16	12/09/18	1Q FY 2022	7/25/19	N/A	2Q FY 2026

CD-0 – Approve Mission Need for a construction project with a conceptual scope and cost range
Conceptual Design Complete – Actual date the conceptual design was completed (if applicable)
CD-1 – Approve Alternative Selection and Cost Range
CD-2 – Approve Performance Baseline
Final Design Complete – Estimated/Actual date the project design will be/was 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	8/30/12	10/06/16
FY 2019	2Q FY 2019	8/30/12	10/06/16
FY 2020	12/09/18	8/30/12	10/06/16
FY 2021	12/09/18	8/30/12	10/06/16

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
FY 2021	190,425	606,075	796,500	18,500	N/A	18,500	815,000

2. Project Scope and Justification

Scope

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's scope includes constructing a new storage ring, incorporating an multi-bend achromat (MBA) lattice utilizing the existing tunnel, new insertion devices optimized for brightness and flux, superconducting undulators for selected beamlines, new or upgraded front-ends, and any required modifications to the linac, booster, and radiofrequency systems. 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.

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 will provide the nation's researchers with a world-class scientific user facility for mission-focused research and advanced 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 to 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 six giga-electronvolt (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. The MBA lattice will provide 100 to 1000 times increased brightness and coherent flux. 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.

By building capability on the existing APS facility at 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.

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.

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. The Objective KPPs represent the desired project performance. Achievement of the Threshold KPPs is a prerequisite for approval of CD-4, Project Completion.

Performance Measure	Threshold	Objective
Storage Ring Energy	> 5.7 GeV, with systems installed for 6 GeV operation	6 GeV
Beam Current	≥ 25 milliamps (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	9,095
FY 2013	15,000	15,000	17,825

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
FY 2014	17,015	17,015	12,889
FY 2015	20,000	20,000	19,782
FY 2016	20,000	20,000	22,529
FY 2017	34,785	34,785	23,873
FY 2018	—	—	15,991
FY 2019	—	—	4,016
Total, MIE funding	126,000	126,000	126,000
Line item funding			
FY 2018	26,000	26,000	7,838
FY 2019	14,650	14,650	22,340
FY 2020	21,000	21,000	29,420
FY 2021	2,775	2,775	4,827
Total, Line item funding	64,425	64,425	64,425
Total, Design	190,425	190,425	190,425
Construction			
MIE funding			
FY 2012	800	800	—
FY 2013	5,000	5,000	3,391
FY 2014	2,985	2,985	4,534
FY 2015	—	—	573
FY 2016	—	—	—
FY 2017	7,715	7,715	389
FY 2018	—	—	4,222
FY 2019	—	—	3,391
Total, MIE funding	16,500	16,500	16,500
Line item funding			
FY 2018	67,000	67,000	2,085
FY 2019	115,350	115,350	18,638
FY 2020	149,000	149,000	153,950
FY 2021	147,225	147,225	217,075
Outyears	111,000	111,000	197,827
Total, Line item funding	589,575	589,575	589,575
Total, Construction	606,075	606,075	606,075

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (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	24,262
FY 2018	—	—	20,213
FY 2019	—	—	7,407
Total, MIE funding	142,500	142,500	142,500
Line item funding			
FY 2018	93,000	93,000	9,923
FY 2019	130,000	130,000	40,978
FY 2020	170,000	170,000	183,370
FY 2021	150,000	150,000	221,902
Outyears	111,000	111,000	197,827
Total, Line item 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 funding			
Outyears	10,000	10,000	10,000
Total, Line item funding	10,000	10,000	10,000
Total, OPC	**18,500**	**18,500**	**18,500**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Project Cost (TPC)			
MIE funding			
FY 2010	1,000	1,000	587
FY 2011	7,500	7,500	3,696
FY 2012	20,000	20,000	13,312
FY 2013	20,000	20,000	21,216
FY 2014	20,000	20,000	17,423
FY 2015	20,000	20,000	20,355
FY 2016	20,000	20,000	22,529
FY 2017	42,500	42,500	24,262
FY 2018	—	—	20,213
FY 2019	—	—	7,407
Total, MIE funding	151,000	151,000	151,000
Line item funding			
FY 2018	93,000	93,000	9,923
FY 2019	130,000	130,000	40,978
FY 2020	170,000	170,000	183,370
FY 2021	150,000	150,000	221,902
Outyears	121,000	121,000	207,827
Total, Line item 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	182,825	146,825	166,962
Contingency	7,600	16,000	9,696
Total, Design	190,425	162,825	176,658

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Construction			
Equipment	461,675	483,575	465,180
Other Construction	17,000	15,000	17,000
Contingency	127,400	135,100	137,662
Total, Construction	606,075	633,675	619,842
Total, TEC	**796,500**	**796,500**	**796,500**
Contingency, TEC	*135,000*	*151,100*	*147,358*
Other Project Cost (OPC)			
OPC except D&D			
Conceptual Planning	1,000	1,000	1,000
Conceptual Design	7,500	7,500	7,500
Start-Up	7,100	7,800	7,100
Contingency	2,900	2,200	2,900
Total, OPC	**18,500**	**18,500**	**18,500**
Contingency, OPC	*2,900*	*2,200*	*2,900*
Total Project Cost	**815,000**	**815,000**	**815,000**
Total, Contingency (TEC+OPC)	***137,900***	***153,300***	***150,258***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2019	FY 2020	FY 2021	Outyears	Total
FY 2018	TEC	162,500	81,772	152,419	160,000	162,309	719,000
	OPC	8,500	—	—	5,000	37,500	51,000
	TPC	171,000	81,772	152,419	165,000	199,809	770,000
FY 2019	TEC	162,500	60,000	150,000	159,780	224,820	757,100
	OPC	8,500	—	—	—	4,400	12,900
	TPC	171,000	60,000	150,000	159,780	229,220	770,000
FY 2020	TEC	235,500	130,000	150,000	160,000	121,000	796,500
	OPC	8,500	—	—	5,000	5,000	18,500
	TPC	244,000	130,000	150,000	165,000	126,000	815,000
FY 2021	TEC	235,500	130,000	170,000	150,000	111,000	796,500
	OPC	8,500	—	—	—	10,000	18,500
	TPC	244,000	130,000	170,000	150,000	121,000	815,000

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	2Q FY 2026
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	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 will be updated as the project is executed.

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 ANL	26,000-28,000
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"	26,000-28,000
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

ANL will acquire the APS-U project under the existing DOE Management and Operations (M&O) contract between DOE and UChicago Argonne, LLC. 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 radiofrequency 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. ANL will procure these items through competitive bids based on a 'best value' basis from a variety of sources, depending on the item, and 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. The M&O contractor's performance will be evaluated through the annual laboratory performance appraisal process.

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

Summary

The FY 2021 Request for the Proton Power Upgrade (PPU) project is $8,000,000, including $5,000,000 in Total Estimated Cost (TEC) funds and $3,000,000 in Other Project Costs (OPC) funds. The most recent DOE O 413.3B approved Critical Decision (CD) is CD-3B (Approve Long Lead Procurements), approved on September 3, 2019. The preliminary Total Project Cost (TPC) range, based on early concepts under consideration, is $184,000,000 - $320,000,000.

Significant Changes

This Construction Project Data Sheet (CPDS) is an update of the FY 2020 CPDS and does not include a new start for FY 2021. There are no significant changes.

In FY 2019, the project continued R&D, design, engineering, prototyping, preliminary and final design, long-lead procurement, and activities aimed at further advancing the target performance in coordination with Spallation Neutron Source (SNS) operations target management. Additional long lead procurement authority (CD-3B), approved in late FY 2019 and executed in FY 2020, will advance the klystron gallery buildout, radiofrequency (RF) procurements, and cryomodule hardware procurements and assembly. In FY 2020, the project will continue R&D, engineering, prototyping, preliminary and final design, testing, fabrication, procurement, and component integration and installation. Target R&D, engineering, design, and prototyping to improve performance and reliability will also continue. In FY 2021, the project will prioritize these continuing activities of R&D, engineering, prototyping, preliminary and final design, testing, fabrication, procurement, component integration and installation, and civil construction site preparation. Advancing the target R&D, engineering, design, and prototyping in conjunction with SNS operations target improvement plans will be a high priority.

A Federal Project Director, certified to level I, 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 2020	1/07/09	8/01/17	4/04/18	2Q FY 2021	4Q FY 2022	3Q FY 2022	N/A	3Q FY 2027
FY 2021[a]	1/07/09	8/01/17	4/04/18	2Q FY 2021	4Q FY 2022	2Q FY 2021	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

[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	CD-3B
FY 2020	2Q FY 2021	10/05/18	2Q FY 2020
FY 2021[a]	2Q FY 2021	10/05/18	9/03/19

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.

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	27,300	210,000	237,300	12,700	N/A	12,700	250,000
FY 2021[a]	46,700	189,502	236,202	13,798	N/A	13,798	250,000

2. Project Scope and Justification

Scope

The PPU project will design, build, install, and test the equipment necessary to double the accelerator power from 1.4 megawatts (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 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.

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 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 to 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

[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 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 two neutron scattering facilities in the BES portfolio, the High Flux Isotope Reactor (HFIR) and the SNS, are both sited at 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.

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 and cavitation 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.

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 Key Performance Parameters (KPPs) are preliminary and may change as the project continues towards CD-2. At CD-2 approval, the KPPs will be baselined. The Threshold KPPs represent the minimum acceptable performance that the project must achieve. The Objective KPPs represent the desired project performance. Achievement of the Threshold KPPs will be a prerequisite for approval of CD-4, Project Completion.

Performance Measure	Threshold	Objective
Beam power on target	1.7 MW at 1.25 giga-electronvolts (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	≥ 2.24x1014 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	16,000	16,000	12,647
FY 2020	20,700	20,700	17,640
FY 2021	5,000	5,000	8,060
Outyears	—	—	5,698
Total, Design	46,700	46,700	46,700

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Construction			
FY 2018	31,000	31,000	1,794
FY 2019	44,000	44,000	8,480
FY 2020	39,300	39,300	86,000
FY 2021	—	—	18,026
Outyears	75,202	75,202	75,202
Total, Construction	189,502	189,502	189,502
Total Estimated Cost (TEC)			
FY 2018	36,000	36,000	4,449
FY 2019	60,000	60,000	21,127
FY 2020	60,000	60,000	103,640
FY 2021	5,000	5,000	26,086
Outyears	75,202	75,202	80,900
Total, TEC	**236,202**	**236,202**	**236,202**
Other Project Cost (OPC)			
FY 2016	4,059	4,059	1,267
FY 2017	6,739	6,739	3,773
FY 2018	—	—	3,004
FY 2019	—	—	1,567
FY 2020	—	—	1,187
FY 2021	3,000	3,000	1,830
Outyears	—	—	1,170
Total, OPC	**13,798**	**13,798**	**13,798**
Total Project Cost (TPC)			
FY 2016	4,059	4,059	1,267
FY 2017	6,739	6,739	3,773
FY 2018	36,000	36,000	7,453
FY 2019	60,000	60,000	22,694
FY 2020	60,000	60,000	104,827
FY 2021	8,000	8,000	27,916
Outyears	75,202	75,202	82,070
Total, TPC	**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	38,800	20,800	N/A
Contingency	7,900	6,500	N/A
Total, Design	46,700	27,300	N/A
Construction			
Construction	137,702	156,000	N/A
Contingency	51,800	54,000	N/A
Total, Construction	189,502	210,000	N/A
Total, TEC	**236,202**	**237,300**	**N/A**
Contingency, TEC	*59,700*	*60,500*	N/A
Other Project Cost (OPC)			
OPC except D&D			
R&D	2,800	2,500	N/A
Conceptual Design	6,498	5,225	N/A
Other OPC Costs	1,300	1,800	N/A
Contingency	3,200	3,175	N/A
Total, OPC	**13,798**	**12,700**	**N/A**
Contingency, OPC	*3,200*	*3,175*	*N/A*
Total Project Cost	**250,000**	**250,000**	**N/A**
Total, Contingency (TEC+OPC)	***62,900***	***63,675***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2019[a]	FY 2020	FY 2021	Outyears	Total
FY 2020	TEC	36,000	60,000	5,000	30,000	106,300	237,300
	OPC	10,300	—	—	—	2,400	12,700
	TPC	46,300	60,000	5,000	30,000	108,700	250,000
FY 2021	TEC	36,000	60,000	60,000	5,000	75,202	236,202
	OPC	10,798	—	—	3,000	—	13,798
	TPC	46,798	60,000	60,000	8,000	75,202	250,000

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

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	3Q FY 2027
Expected Useful Life	40 years
Expected Future Start of D&D of this capital asset	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

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.

The M&O contractor has completed a Conceptual Design Report for the PPU project and identified key design activities, requirements, and high-risk subsystem components 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. ORNL, partner laboratory staff, and/or vendors will complete the design of the technical systems. Vendors and/or partner labs with the necessary capabilities will fabricate technical equipment. 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. The M&O contractor's performance will be evaluated through the annual laboratory performance appraisal process.

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 2021 Request for the Advanced Light Source Upgrade (ALS-U) project is $13,000,000. The most recent DOE Order 413.3B approved Critical Decision (CD) is CD-3A (Approve Long Lead Procurements), approved December 19, 2019. 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 2020 CPDS and does not include a new start for FY 2021.

The project TPC estimate increased to $410,200,000 at the approval of CD-3A and the Project Completion Date (CD-4) remains at 2Q FY 2028. The TPC estimate increase resulted from a maturing design effort for the project which identified additional costs in the project office, accelerator systems, beamlines, and removal and installation elements. Cost increases resulted from the addition of scope to reduce risks, correction of labor estimates, and updating of equipment costs resulting from design improvements.

In FY 2019, the project continued planning, engineering, design, research and development (R&D), and prototyping activities. FY 2020 funding continues the support of planning, engineering, design, and R&D prototyping activities, and initiates long lead procurements. FY 2021 funding will continue support of engineering, design, R&D prototyping, and long lead procurements of construction items. Authorization of full construction activities is anticipated for late in FY 2021 or early FY 2022.

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	9/27/16	4Q FY 2019	4Q FY 2019	4Q FY 2020	4Q FY 2022	4Q FY 2021	N/A	4Q FY 2026
FY 2020	9/27/16	4/30/18	9/21/18	2Q FY 2021	4Q FY 2021	1Q FY 2022	N/A	2Q FY 2028
FY 2021[a]	9/27/16	4/30/18	9/21/18	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 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	2Q FY 2021	4Q FY 2019
FY 2021[a]	2Q FY 2021	12/19/19

CD-3A – Approve Long-Lead Procurements: As the project planning and design matures, long lead procurement may be requested in FY 2020 to mitigate cost and schedule risk of 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	89,750	248,250	338,000	30,000	N/A	30,000	368,000
FY 2021[a]	89,750	290,450	380,200	30,000	N/A	30,000	410,200

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 (approximately 50-2,000 electronvolts [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 (approximately 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, BES operates advanced ring-based light sources that produce soft x-rays. The 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

[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.

but not above that. NSLS-II is somewhat lower in brightness than the new Swedish light source, MAX-IV, which is currently under commissioning and represents the first use of a MBA lattice design in a light source facility. Neither NSLS-II nor ALS make use of the newer MBA lattice design. 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 APS-U and 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, which is under construction at ANL, 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, which is under construction at SLAC, 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 existing ALS is a 1.9 GeV storage ring operating at 500 milliamps (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 $500,000,000 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.*

Key Performance Parameters (KPPs)

The Key Performance Parameters (KPPs) are preliminary and may change as the project continues towards CD-2. At CD-2 approval, the KPPs will be baselined. The Threshold KPPs represent the minimum acceptable performance that the project must achieve. The Objective KPPs represent the desired project performance. Achievement of the Threshold KPPs will be a prerequisite for approval of CD-4, Project Completion.

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]	> 2×10^{19}	≥ 2×10^{21}
New MBA Beamlines	2	≥ 2

[1]Units = photons/sec/0.1% BW/mm2/mrad2

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	22,054
FY 2020	10,000	10,000	27,946
FY 2021	13,000	13,000	24,000
Outyears	15,750	15,750	15,750
Total, Design	89,750	89,750	89,750
Construction			
FY 2019	25,000	25,000	—
FY 2020	50,000	50,000	50,000
FY 2021	—	—	22,000
Outyears	215,450	215,450	218,450
Total, Construction	290,450	290,450	290,450
Total Estimated Cost (TEC)			
FY 2018	16,000	16,000	—
FY 2019	60,000	60,000	22,054
FY 2020	60,000	60,000	77,946
FY 2021	13,000	13,000	46,000
Outyears	231,200	231,200	234,200
Total, TEC	**380,200**	**380,200**	**380,200**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Other Project Cost (OPC)			
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	1,863
FY 2020	2,000	2,000	5,607
FY 2021	—	—	—
Outyears	2,000	2,000	4,095
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
FY 2019	62,000	62,000	23,917
FY 2020	62,000	62,000	83,553
FY 2021	13,000	13,000	46,000
Outyears	233,200	233,200	238,295
Total, TPC[a]	**410,200**	**410,200**	**410,200**

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	69,800	N/A
Contingency	19,950	19,950	N/A
Total, Design	89,750	89,750	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
Construction			
Site Preparation	—	—	N/A
Equipment	230,400	188,500	N/A
Other Construction	—	—	N/A
Contingency	60,050	59,750	N/A
Total, Construction	290,450	248,250	N/A
Total, TEC	**380,200**	**338,000**	**N/A**
Contingency, TEC	*80,000*	*79,700*	*N/A*
Other Project Cost (OPC)			
OPC except D&D			
Conceptual Planning	2,000	2,000	N/A
Conceptual Design	12,100	12,100	N/A
Research and Development	8,000	8,000	N/A
Start-Up	2,000	1,200	N/A
Contingency	5,900	6,700	N/A
Total, OPC	**30,000**	**30,000**	**N/A**
Contingency, OPC	*5,900*	*6,700*	*N/A*
Total Project Cost	**410,200**	**368,000**	**N/A**
Total, Contingency (TEC+OPC)	***85,900***	***86,400***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years	FY 2019	FY 2020	FY 2021	Outyears	Total
FY 2019	TEC	—	10,000	26,540	32,640	212,820	282,000
	OPC	10,000	2,000	5,000	—	21,000	38,000
	TPC	10,000	12,000	31,540	32,640	233,820	320,000
FY 2020	TEC	16,000	60,000	13,000	68,000	181,000	338,000
	OPC	24,000	2,000	2,000	—	2,000	30,000
	TPC	40,000	62,000	15,000	68,000	183,000	368,000
FY 2021	TEC	16,000	60,000	60,000	13,000	231,200	380,200
	OPC	24,000	2,000	2,000	—	2,000	30,000
	TPC	40,000	62,000	62,000	13,000	233,200	410,200

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	2Q FY 2028
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	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	—

7. D&D Information

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

8. Acquisition Approach

DOE has determined that the Lawrence Berkeley National Laboratory (LBNL) will acquire the ALS-U project under the existing DOE Management and Operations (M&O) contract.

LBNL has prepared a Conceptual Design Report for the ALS-U project and identified key design activities, requirements, and high-risk subsystem components 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. Planning and budgeting for the project will exploit recent cost data from similar projects. LBNL or partner laboratory staff will complete the design of the technical systems. 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. The M&O contractor’s performance will be evaluated through the annual laboratory performance appraisal process.

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

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 2021 Request for the Linac Coherent Light Source-II High Energy (LCLS-II-HE) project is $16,000,000, including $14,000,000 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 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 2020 CPDS and does not include a new start for FY 2021.

The project underwent a successful Independent Project Review by the Office of Science in November 2019 to request approval of CD-3A, Approve Long Lead Procurements. The CD-3A approval is anticipated in the 2Q FY 2020. The project's Total Project Cost (TPC) estimate increased to $428,000,000 at the time of the CD-3A review. The Project Completion Date (CD-4) remains at 1Q FY 2029. The TPC estimate increase resulted from a maturing design effort that identified additional costs across the project scope and an increase in the project's contingency to address several future risks. Two major risks centered on the ability to operate the LCLS-II cryomodules above their design accelerating gradient and for the LCLS-II-HE cryomodules to meet their design operating gradient which is significantly higher than previously achieved. The R&D program in progress for the LCLS-II-HE cryomodules is showing promise but is not yet complete. The performance of the LCLS-II cryomodules will not be known until sometime in FY 2020 when the LCLS-II project begins the accelerator commissioning. Both risks can be mitigated by adding additional cryomodules to the project.

In FY 2019, the project continued planning, engineering, design, R&D, and prototyping activities. The project initiated an R&D program aimed at further advancing the performance of the superconducting radio frequency (RF) cavities, which has shown promise on meeting the technological goals required. FY 2020 funding continues the support of planning, engineering, design, R&D prototyping, and long lead procurements, as appropriate. FY 2021 funding will continue engineering, design, R&D prototyping, and long lead procurements of construction items.

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	12/15/16	3Q FY 2019	1Q FY 2019	1Q FY 2021	1Q FY 2023	2Q FY 2022	N/A	2Q FY 2026
FY 2020	12/15/16	3/23/18	9/21/18	2Q FY 2023	1Q FY 2023	2Q FY 2023	N/A	1Q FY 2028
FY 2021[a]	12/15/16	3/23/18	9/21/18	2Q FY 2023	1Q FY 2023	2Q FY 2023	N/A	1Q FY 2029

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

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

D&D Complete – Completion of D&D work
CD-4 – Approve Start of Operations or Project Closeout

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

CD-3A – Approve Long-Lead Procurements for cryomodule associated parts and equipment.

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	34,000	314,000	348,000	20,000	N/A	20,000	368,000
FY 2021[a]	34,000	374,000	408,000	20,000	N/A	20,000	428,000

2. Project Scope and Justification

Scope

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

Justification

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

There is also 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

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

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, 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 megahertz (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.

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 Key Performance Parameters (KPPs) are preliminary and may change as the project continues towards CD-2. At CD-2 approval, the KPPs will be baselined. The Threshold KPPs represent the minimum acceptable performance that the project must achieve. The Objective KPPs represent the desired project performance. Achievement of the Threshold KPPs will be a prerequisite for approval of CD-4, Project Completion.

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	4,400
FY 2020	6,000	6,000	11,600
FY 2021	6,000	6,000	8,000
Outyears	10,000	10,000	10,000
Total, Design	34,000	34,000	34,000
Construction			
FY 2018	6,000	6,000	—
FY 2019	18,000	18,000	—
FY 2020	44,000	44,000	64,000
FY 2021	8,000	8,000	12,000
Outyears	298,000	298,000	298,000
Total, Construction	374,000	374,000	374,000
Total Estimated Cost (TEC)			
FY 2018	8,000	8,000	—
FY 2019	28,000	28,000	4,400
FY 2020	50,000	50,000	75,600
FY 2021	14,000	14,000	20,000
Outyears	308,000	308,000	308,000
Total, TEC	**408,000**	**408,000**	**408,000**
Other Project Cost (OPC)			
FY 2018	2,000	2,000	1,191
FY 2019	6,000	6,000	2,041
FY 2020	4,000	4,000	7,959
FY 2021	2,000	2,000	2,809
Outyears	6,000	6,000	6,000
Total, OPC	**20,000**	**20,000**	**20,000**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Project Cost (TPC)			
FY 2018	10,000	10,000	1,191
FY 2019	34,000	34,000	6,441
FY 2020	54,000	54,000	83,559
FY 2021	16,000	16,000	22,809
Outyears	314,000	314,000	314,000
Total, TPC[a]	**428,000**	**428,000**	**428,000**

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	250,700	236,000	N/A
Other Construction	9,000	9,000	N/A
Contingency	111,300	66,000	N/A
Total, Construction	374,000	314,000	N/A
Total, TEC	**408,000**	**348,000**	**N/A**
Contingency, TEC	*114,800*	*69,500*	*N/A*

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

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Other Project Cost (OPC)			
OPC except D&D			
R&D	4,000	4,000	N/A
Conceptual Planning	1,500	1,500	N/A
Conceptual Design	2,000	2,000	N/A
Start-Up	6,500	6,500	N/A
Contingency	6,000	6,000	N/A
Total, OPC	**20,000**	**20,000**	**N/A**
Contingency, OPC	*6,000*	*6,000*	*N/A*
Total Project Cost	**428,000**	**368,000**	**N/A**
Total, Contingency (TEC+OPC)	***120,800***	***75,500***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Request Year	Type	Prior Years[a]	FY 2019	FY 2020	FY 2021	Outyears	Total
FY 2019	TEC	—	5,000	20,060	25,000	249,940	300,000
	OPC	—	2,000	4,000	—	14,000	20,000
	TPC	—	7,000	24,060	25,000	263,940	320,000
FY 2020	TEC	8,000	28,000	14,000	60,000	238,000	348,000
	OPC	2,000	6,000	4,000	—	8,000	20,000
	TPC	10,000	34,000	18,000	60,000	246,000	368,000
FY 2021	TEC	8,000	28,000	50,000	14,000	308,000	408,000
	OPC	2,000	6,000	4,000	2,000	6,000	20,000
	TPC	10,000	34,000	54,000	16,000	314,000	428,000

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	1Q FY 2029
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	1Q FY 2054

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] 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, SC anticipates that there will be no new area being constructed in the construction project.

8. Acquisition Approach

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

SLAC has prepared a Conceptual Design Report for the LCLS-II-HE project and identified key design activities, requirements, and high-risk subsystem components 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. The M&O contractor will fully exploit recent cost data in planning and budgeting for the project. SLAC or partner laboratory staff will complete the design of the technical systems. SLAC or subcontracted vendors with the necessary capabilities will fabricate the technical equipment. All subcontracts will be competitively bid and awarded based on best value to the government. The M&O contractor's performance will be evaluated through the annual laboratory performance appraisal process.

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