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. BES research provides the foundations to develop new clean energy technologies, to mitigate the climate and environmental impacts of energy generation/use, 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 clean energy future. The Basic Energy Sciences Advisory Committee (BESAC) report, "A Remarkable Return on Investment in Fundamental Research,"[w] provides key examples of major technological, commercial, and national security impacts, including clean energy technologies, 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—to answer some of the most challenging science questions and to provide insights on the scientific basis for energy technologies. The above noted BESAC report recounts the central role of these shared resources as a key to U.S. scientific and industrial leadership. In response to the COVID pandemic, BES facilities were at the forefront of the research efforts to understand the virus and to provide therapeutics to combat it. 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 of accomplishment begins with rigorous community-based processes for conceptualization, planning, and execution in construction of facilities that continues in performance assessment for operating facilities.

Key to exploiting scientific discoveries for future clean 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. Materials will need to be more functional than today's energy materials, and new chemical processes will require ever-increasing control at the level of electronic structure and dynamics. 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 have been experimentally realized. 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 clean energy innovations and economic prosperity.

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

Highlights of the FY 2023 Request

The BES FY 2023 Request of $2,420.4 million is an increase of $175.4 million, or 7.8 percent, above the FY 2021 Enacted level. The Request focuses resources on 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 2023 Request are summarized below.

<u>Research</u>

The Request supports for a new research modality of Energy Earthshot Research Centers, which will work toward the stretch goals of the DOE Energy Earthshots and will provide a solid bridge between SC and the DOE energy technology offices. The Request continues funding for the Energy Frontier Research Centers (EFRCs), supports the Batteries and Energy Storage Energy Innovation Hub recompetition, and continues the Fuels from Sunlight Hub awards and the National Quantum Information Science (QIS) Research Centers (NQISRCs). In part through increased funding for the Established Program to Stimulate Competitive Research (EPSCoR), the Reaching a New Energy Sciences Workforce (RENEW) initiative, and the new Funding for Accelerated, Inclusive Research (FAIR) initiative, BES will build stronger programs with underrepresented institutions and regions, including investing in a more diverse and inclusive workforce in order to address environmental justice issues.

Core research priorities in the FY 2023 Request include:

- Clean Energy: BES will continue to support clean energy research that leads to reduced impacts from climate change. The United States and the world face profound challenges due to climate change with a narrow window of opportunity to pursue action to avoid the most catastrophic impacts. As part of the Department's efforts to prioritize R&D investments that advance understanding of climate change and the development of mitigation and adaptation solutions, BES will increase research to provide understanding and foundations for clean energy, with investments across the entire portfolio to accelerate innovation to reduce impacts resulting from climate change while advancing clean energy technologies and infrastructure. A few examples:
    - Direct air capture of carbon dioxide: Designing high-selectivity, high-capacity, and high-throughput chemical separations and materials;
    - Hydrogen, Solar: Foundational science to enable carbon-neutral processes for the production, storage, and use of hydrogen in energy and industrial applications; improved conversion of solar energy to useful energy and fuels, such as hydrogen by water splitting; and
    - Energy Storage: New materials and chemistries for next-generation electrical and thermal energy storage.
- SC Energy Earthshots Initiative: In addition to core clean energy research, this initiative includes support for Energy Earthshot Research Centers (EERCs), a new research modality. Engaging both SC and the energy technology offices, EERCs will address key research challenges at the interface between currently supported basic research and applied research and development activities, to bridge the R&D gap. These challenges are vital to realizing the stretch goals of the DOE Energy Earthshots.
- Critical Materials/Minerals: Critical materials and minerals, including rare earth and platinum-group elements, are vital to the Nation's security and economic prosperity, as well as applications for clean energy and energy storage. In BES, the Request continues support for research to advance our understanding of fundamental properties of these materials, to identify methodologies to reduce their use and to discover substitutes, and to enhance extraction, chemical processing and separation science for rare earths and platinum-group elements.
- Fundamental Science to Transform Advanced Manufacturing: BES increases investments in fundamental science underpinning advanced manufacturing, partnering across SC, with thrusts in circular, clean, low-carbon, and scalable synthesis and processing; transformational operando characterization; multiscale models and tools; and co-design of materials, processes, and products for functionality and use. Research continues on transformative chemistry, materials, and biology for next-generation industries and next-generation tools for elucidating relevant mechanisms for these processes.

- Microelectronics: Also related to Advanced Manufacturing, BES continues its investment in microelectronics with a focus on materials, chemistry, and fundamental device science. BES partners with SC programs to continue support for 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.
- Artificial Intelligence and Machine Learning (AI/ML): The Request increases investments in data science and AI/ML to accelerate fundamental research for the discovery of new chemical mechanisms and material systems with exceptional properties and function and to apply these techniques for effective user facility operations and interpretation of massive data sets.
- Exascale Computing Initiative (ECI): 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.
- Advanced Computing: Partnering with ASCR, BES invests in cost-effective computational, networking, and storage capabilities to transform the national laboratories into an integrated open innovation ecosystem of capabilities, facilities, instruments, and expertise connected via advanced networks and enabling software.
- Biopreparedness Research Virtual Environment (BRaVE): In support of the activity, which brings DOE laboratories together to tackle problems of pressing national importance, BES research will continue developing and expanding capabilities at user facilities for responsiveness to biological threats and development of advanced instrumentation and expertise to address these research challenges.
- Quantum Information Science (QIS): In support of the National Quantum Initiative, NQISRCs established in FY 2020 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.
- Accelerator Science and Technology Initiative: Accelerator R&D is a core capability, which SC stewards for the Nation. Continued 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.
- Reaching a New Energy Sciences Workforce (RENEW): BES increases support for the SC-wide RENEW initiative that leverages SC's world-unique national laboratories, user facilities, and other research infrastructures to provide undergraduate and graduate training opportunities for students and academic institutions not currently well represented in the U.S. S&T ecosystem.
- Funding for Accelerated, Inclusive Research (FAIR): The FAIR initiative will provide focused investment on enhancing research on clean energy, climate, and related topics at minority serving institutions, including attention to underserved and environmental justice regions. The activities will improve the capability of MSIs to perform and propose competitive research and will build beneficial relationships between MSIs and DOE national laboratories and facilities.
- Accelerate Innovation in Emerging Technologies: The Accelerate initiative will support scientific research to accelerate the transition of science advances to energy technologies. The goal is to drive scientific discovery to sustainable production of new technologies across the innovation continuum, to provide experiences in working across this continuum for the workforce needed for industries of the future, and to meet the nation's needs for abundant clean energy, a sustainable environment, and national security.

<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), Stanford Synchrotron Radiation Lightsource (SSRL), and Linac Coherent Light Source (LCLS) will continue operations and are supported at approximately 90 percent of optimum, the funding level required for normal operations based on a 2018 baseline. Both BES-supported neutron sources, the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR), will be operational in FY 2023 and funded at approximately 90 percent of optimum. The Request provides funding for the five Nanoscale Science Research Centers (NSRCs) at approximately 90 percent of optimal.

Projects

The Request provides continuing 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), Second Target Station (STS), and Cryomodule Repair and Maintenance Facility (CRMF) projects. The FY 2023 Request also continues two Major Item of Equipment projects: NSLS-II Experimental Tools-II (NEXT-II) and NSRC Recapitalization. Finally, the Request provides Other Project Costs (OPC) to begin planning for the NSLS-II Experimental Tools-III (NEXT-III) and High Flux Isotope Reactor Pressure Vessel Replacement (HFIR-PVR) projects.

Basic Energy Sciences
FY 2023 Research Initiatives

Basic Energy Sciences supports the following FY 2023 Research Initiatives.

(dollars in thousands)

	FY 2021 Enacted	FY 2022 Annualized CR	FY 2023 Request	FY 2023 Request vs FY 2021 Enacted
Accelerate Innovations in Emerging Technologies	–	–	15,000	+15,000
Accelerator Science and Technology Initiative	5,000	5,000	12,000	+7,000
Advanced Computing	–	–	10,000	+10,000
Artificial Intelligence and Machine Learning	20,000	20,000	29,000	+9,000
Biopreparedness Research Virtual Environment (BRaVE)	–	–	21,500	+21,500
Critical Materials/Minerals	17,000	17,000	25,000	+8,000
Exascale Computing	26,000	26,000	26,000	–
Fundamental Science to Transform Advanced Manufacturing	–	–	20,000	+20,000
Funding for Accelerated, Inclusive Research (FAIR)	–	–	20,000	+20,000
Microelectronics	15,000	15,000	30,000	+15,000
Quantum Information Science	92,050	92,050	102,000	+9,950
Reaching a New Energy Sciences Workforce (RENEW)	–	–	10,000	+10,000
Revolutionizing Polymers Upcycling	8,250	8,250	8,250	–
SC Energy Earthshots	–	–	104,250	+104,250
Total, Research Initiatives	**183,300**	**183,300**	**433,000**	**+249,700**

Basic Energy Sciences
Funding

(dollars in thousands)

	FY 2021 Enacted	FY 2022 Annualized CR	FY 2023 Request	FY 2023 Request vs FY 2021 Enacted
Basic Energy Sciences				
Scattering and Instrumentation Sciences Research	74,031	78,191	101,963	+27,932
Condensed Matter and Materials Physics Research	170,200	176,864	202,538	+32,338
Materials Discovery, Design, and Synthesis Research	71,189	74,644	98,958	+27,769
Established Program To Stimulate Competitive Research EPSCoR	25,000	25,000	35,000	+10,000
Energy Frontier Research Centers - Materials	57,500	57,500	64,678	+7,178
Energy Earthshot Research Centers - Materials	–	–	25,000	+25,000
Materials Sciences and Engineering - Energy Innovation Hubs	24,088	24,088	25,000	+912
Computational Materials Sciences	13,000	13,000	13,492	+492
Total, Materials Sciences and Engineering	**435,008**	**449,287**	**566,629**	**+131,621**
Fundamental Interactions Research	107,904	112,033	122,939	+15,035
Chemical Transformations Research	112,292	117,752	136,919	+24,627
Photochemistry and Biochemistry Research	82,589	84,321	132,925	+50,336
Energy Frontier Research Centers - Chemical	57,500	57,500	64,678	+7,178
Energy Earthshot Research Centers - Chemical	–	–	25,000	+25,000
Chemical Sciences, Geosciences, and Biosciences - Energy Innovation Hubs	20,000	20,000	20,758	+758
Chemical Sciences, Geosciences, and Biosciences - General Plant Projects	1,000	1,000	1,000	–
Computational Chemical Sciences	13,000	13,000	13,492	+492
Total, Chemical Sciences, Geosciences, and Biosciences	**394,285**	**405,606**	**517,711**	**+123,426**

(dollars in thousands)

	FY 2021 Enacted	FY 2022 Annualized CR	FY 2023 Request	FY 2023 Request vs FY 2021 Enacted
X-Ray Light Sources	525,000	552,900	509,425	-15,575
High-Flux Neutron Sources	292,000	295,000	280,754	-11,246
Nanoscale Science Research Centers	139,000	152,500	134,754	-4,246
Other Project Costs	19,000	14,300	17,500	-1,500
Major Items of Equipment	10,500	30,000	50,000	+39,500
Scientific User Facilities, Research	41,207	41,207	50,466	+9,259
Total, Scientific User Facilities (SUF)	**1,026,707**	**1,085,907**	**1,042,899**	**+16,192**
Subtotal, Basic Energy Sciences	**1,856,000**	**1,940,800**	**2,127,239**	**+271,239**
Construction				
21-SC-10, Cryomodule Repair & Maintenance Facility, (CRMF), SLAC	1,000	1,000	10,000	+9,000
19-SC-14, Second Target Station (STS), ORNL	29,000	32,000	32,000	+3,000
18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL	160,000	101,000	9,200	-150,800
18-SC-11, Spallation Neutron Source Proton Power Upgrade (PPU), ORNL	52,000	17,000	17,000	-35,000
18-SC-12, Advanced Light Source Upgrade (ALS-U), LBNL	62,000	75,100	135,000	+73,000
18-SC-13, Linac Coherent Light Source-II-High Energy (LCLS-II-HE), SLAC	52,000	50,000	90,000	+38,000
13-SC-10 - Linac Coherent Light Source-II (LCLS-II), SLAC	33,000	28,100	–	-33,000
Subtotal, Construction	**389,000**	**304,200**	**293,200**	**-95,800**
Total, Basic Energy Sciences	**2,245,000**	**2,245,000**	**2,420,439**	**+175,439**

SBIR/STTR funding:

- FY 2021 Enacted: SBIR $56,592,000 and STTR $7,963,000
- FY 2022 Annualized CR: SBIR $59,161,000 and STTR $8,328,000
- FY 2023 Request: SBIR $63,747,000 and STTR $8,965,000

Basic Energy Sciences
Explanation of Major Changes

	(dollars in thousands) FY 2023 Request vs FY 2021 Enacted
Materials Sciences and Engineering	**+$131,621**
Research will continue to support fundamental scientific opportunities for materials innovations, including those identified in recent BESAC and Basic Research Needs workshop reports. Research priorities include clean energy (e.g., hydrogen, direct air capture of carbon dioxide, energy storage), climate science, critical materials/minerals, exascale (computational materials sciences), data science and AI/ML, advanced computing, advanced manufacturing, microelectronics, BRaVE, QIS, strategic accelerator technology, and RENEW. The Request also includes funding for continued support of the EFRCs, recompetition of the Batteries and Energy Storage Energy Innovation Hub, continuation of the NQISRCs, and the Established Program to Stimulate Competitive Research (EPSCoR). The Request includes funding for the new Energy Earthshot Research Centers and the FAIR and Accelerate initiatives.	
Chemical Sciences, Geosciences, and Biosciences	**+$123,426**
Research will continue to support fundamental scientific opportunities for innovations in chemistry, geosciences and biosciences, including those identified in recent BESAC, Basic Research Needs, and Roundtable workshop reports. Research priorities include clean energy (e.g., energy efficient, sustainable cycles for carbon and hydrogen, and direct air capture of carbon dioxide), climate science, critical materials/minerals, exascale (computational chemical sciences), data science and AI/ML, advanced computing, advanced manufacturing (including polymer upcycling), microelectronics, QIS, and RENEW. The Request also includes funding for continued support of the EFRCs, the Fuels from Sunlight Hub awards, and the NQISRCs. The Request includes funding for the new Energy Earthshot Research Centers and the FAIR and Accelerate initiatives.	
Scientific User Facilities (SUF)	**+$16,192**
The Advanced Light Source (ALS), Advanced Photon Source (APS), National Synchrotron Light Source-II (NSLS-II), Stanford Synchrotron Radiation Lightsource (SSRL), and Linac Coherent Light Source (LCLS) user facilities will operate at approximately 90 percent of optimum, the funding level required for normal operations based on a 2018 baseline. Both BES-supported neutron sources, the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR), will operate at approximately 90 percent of optimum. These facilities will support the BRaVE initiative to maintain capabilities to tackle biological threats. The Request supports all five NSRCs at approximately 90 percent of optimum with funding for continued QIS-related tools development. Research priorities include accelerator science and technology, expansion of instrumentation and expertise for biopreparedness, and applications of data science and AI/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, and provides Other Project Costs (OPC) to begin planning for the NSLS-II Experimental Tools-III (NEXT-III) and High Flux Isotope Reactor Pressure Vessel Replacement (HFIR-PVR) projects.	

	(dollars in thousands) FY 2023 Request vs FY 2021 Enacted
Construction	**-$95,800**
The Request provides continuing support for the Advanced Photon Source-Upgrade (APS-U), the Advanced Light Source Upgrade (ALS-U), the Linac Coherent Light Source-II High Energy (LCLS-II-HE), the SNS Proton Power Upgrade (PPU), the SNS Second Target Station (STS), and the Cryomodule Repair and Maintenance Facility at SLAC.	
Total, Basic Energy Sciences	**+$175,439**

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, as elaborated below. 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 has robust interactions with DOE technology offices through formal and informal coordination activities. Formal coordination includes the Science and Energy Technology Teams (SETTs) that draw on expertise and capabilities stewarded by multiple DOE offices to address forefront energy challenges. For example, BES participates in the Hydrogen SETT, engaging in activities to advance the Hydrogen Energy Earthshot (launched in 2021) aimed at accelerating breakthroughs of more abundant, affordable, and reliable clean energy solutions within the decade.[x] BES also contributes to the Carbon Dioxide Removal SETT and the Carbon Negative Earthshot to address the challenge of long-term removal of carbon dioxide from the atmosphere using a variety of approaches including direct air capture, and the Energy Storage SETT and Long Duration Storage Earthshot to accelerate the development, commercialization, and utilization of next-generation energy storage technologies. BES is also participating in planning for additional Earthshots and crosscutting energy technology areas. In the FY 2023 Request, BES participates in the new SC Energy Earthshots initiative, including the new research modality of Energy Earthshot Research Centers. These Centers will be jointly planned by SC and the DOE energy technology offices, to work toward the stretch goals of the Earthshots by addressing key research challenges at the interface between currently supported basic research and applied research and development activities. Historically, co-siting of research by BES and DOE energy 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 this integration of basic and applied research.

Informal coordination includes participation of BES program managers in regularly scheduled intra-departmental meetings for information exchange and coordination on solicitations, program reviews, and project selections. These interactions cover a broad range of topics including biofuels derived from biomass; solar energy utilization, including solar fuels; critical minerals/materials; advanced nuclear energy systems; vehicle technologies; biotechnology; and fundamental science to transform advanced manufacturing and industrial processes. These activities facilitate cooperation and coordination between BES and the DOE energy technology offices and defense programs. Additionally, DOE technology office personnel participate in reviews of BES research, and BES personnel participate in reviews of research funded by the technology offices.

Program Accomplishments
Mastering energy efficiency for clean energy processes in electricity, fuels, storage, and carbon capture.
The clean energy future requires efficient processes for energy generation, energy storage, and decarbonization. Recent research has made important steps that can lead to a wide range of efficient technologies.

- Photoinduced charge transfer plays a central role in conversion of light energy into electricity and fuels. Researchers used femtosecond time-resolved X-ray photoemission spectroscopy on an organic system to discover a new mechanism that produces charge carriers from excitations by low-energy photons. This provides new options to efficiently harness light energy for photovoltaic or solar fuels applications.
- Electrochemical processes provide energy-efficient approaches to split water into hydrogen, a carbon-neutral fuel, and oxygen. Platinum group elements—critical elements with limited domestic supply—are commonly used as catalysts to speed up the rate of hydrogen production. Scientists demonstrated that earth-abundant elements can be incorporated in metal–organic frameworks, a porous material, to tune their electrocatalytic properties and yield rates of hydrogen production comparable to those with platinum group elements.
- The stability of interfaces is critical to the performance of many energy storage systems. Cryogenic electron microscopy and cryogenic focused ion beam enabled the characterization of the interface between Li metal and lithium

[x] https://www.energy.gov/eere/fuelcells/hydrogen-shot.

phosphorous oxynitride. The structural and chemical information leads to a robust understanding of the stability of these interfaces and can be extended to study other solid-solid interfaces.

- The ocean contains a lot of carbon dioxide as bicarbonate ions that increases as CO_2 in the air increases. The higher CO_2 concentration in the ocean provides an opportunity for easier CO_2 capture. Scientists recently demonstrated that electrochemical CO_2 capture from ocean water at 70 percent efficiency can be efficiently directly coupled with chemical conversion to CO with 95 percent Faradaic efficiency.

Sustainable, low-carbon, and scalable approaches to transform manufacturing.
The key chemicals and materials of the clean energy future must be produced, synthesized, and extracted by efficient, scalable methods that are sustainable over time in an environmentally sensitive way. Researchers have made significant progress with ammonia production, upcycling of plastics, synthesis science, and extraction of rare earths.

- Nitrogenase enzymes catalyze the conversion of nitrogen and water to ammonia at ambient conditions. In contrast, multistep industrial processes produce ammonia from nitrogen and fossil feedstocks at elevated temperatures and pressures. Researchers coupled the enzyme to an inorganic component that controlled electron transfer, allowing greater insight into the catalytic mechanism. The study demonstrated that hydrogen and ammonia production compete and provided mechanistic insight for development of new catalysts and bio-inorganic hybrids for low-carbon ammonia production.
- Researchers have developed energy-efficient approaches to convert polymers, the primary components of plastics, into valuable products that give a second life to single-use plastics. In one approach, the mechanistic understanding allowed tuning of a dual catalyst to promote low-temperature (under $250^{o}C$) conversion of polyethylene to fuels with few byproducts. In another approach, earth-abundant zirconium catalysts coupled with an aluminum reactant allowed conversion of polymers to fatty alcohols that can be used as surfactants.
- Real-time observations and computational modeling of the synthesis of solid-state ceramics yielded a new, simplified model to precisely guide and accelerate this process. Solid-state ceramics are critical for clean energy technologies such as solar cells and batteries, but their preparation is extremely slow and problematic because the process passes through many intermediate states. This computational model explains how to control and accelerate the multistep process and enabled formation of a classic superconducting ceramic 25 times faster than the traditional approach.
- Rare-earth elements—critical materials for modern technology—are difficult to separate from each other because they have similar chemical properties. Scientists have demonstrated an electrochemical approach that forces some of the elements into different oxidation states, making separation possible by means of specially designed extractant molecules. The typical multistep process is reduced to a cleaner, more energy-efficient and scalable single step.
- Crystals made from colloids are valuable in a wide range of applications such as batteries, sensors, and solar cells, but making these crystals with desired properties is quite challenging. A new, robust approach for directing assembly of crystals with desired geometry and properties avoids costly and complex chemical surface engineering and allows tuning properties for new uses. This new method creates precise regions of discrete chemical and physical properties on the surface of particles followed by selective interactions to correctly direct crystal formation.

Materials and chemical sciences enable advances in quantum-based science and technology, and quantum computing enables advances in materials and chemical sciences.
Recent research underscores the two-way relationship between BES-supported science domains and quantum information science. Advances span the areas of molecules for gate operations, understanding of correlated quantum errors, particles for logical operations, and efficient energy computations.

- Scientists studying photovoltaics for light harvesting in molecular crystals uncovered design principles for the light-driven generation and manipulation of long-lived, correlated spin states. A combination of predictive modeling of excited state dynamics, targeted chemical synthesis of molecular systems, and sophisticated time-resolved spectroscopy enabled the discovery of coupled molecules with spin entangled pair states, which could serve as the basis of molecular platforms to perform optically initialized gate operations in quantum information systems operating at room temperature.
- The central challenge in building a quantum computer is error correction. Currently error correction relies on the assumption that errors are not correlated between different quantum bits (or qubits) in the system. Experimental and

modeling research has revealed the existence of correlated errors in multi-qubit superconducting circuits. The data are compatible with absorption in the qubit substrate of cosmic ray muons and gamma rays, giving rise to correlated charge fluctuations in neighboring qubits. These results have major implications for proposed fault tolerant quantum computing and will inform the design of robust next-generation superconducting qubit arrays.

- Researchers have established new experimental evidence of quantum objects called "anyons" that arise from the collective behavior of electrons in two dimensions and were first predicted decades ago. It is also anticipated that a many-anyon system can serve as the basis for quantum computing. Unlike for more well-known particles, moving anyons around each other in solids causes them to acquire a phase factor that can be used to perform logical gate operations on a qubit. As researchers moved anyons in their experimental system they directly observed the expected phase change.
- Quantum computing techniques provide a means to address insurmountable computational barriers for simulating quantum systems on classical computers. Unfortunately, as the number of quantum circuits increases for progressively larger calculations, the opportunity for error also increases. Researchers have demonstrated a mathematical concept known as "connected moments" to compute the total energy of a molecular system using fewer quantum circuits, allowing the equivalent of a full-scale quantum calculation with more modest resources, while also reducing errors.

Confronted by the COVID-19 pandemic, BES user facilities shifted to remote access and conducted research that was instrumental in combating the disease.
BES light sources, neutron sources, and Nanoscale Science Research Centers adapted quickly to changed modes of operation and made key contributions to understanding of the virus, development of vaccines and therapeutics, and fabrication of vital materials.

- User facilities rapidly shifted to remote access and mail-in of material samples in March 2020 to support critical research, mostly devoted to combating the pandemic. Representative topical areas included macromolecular crystallography to study atomic-scale interactions of viral proteins with drug candidates and human proteins, solution state analysis of large and transient macromolecular assemblies, observation of cellular infection, and characterization of respirator filter materials to aid manufacturing.
- More than 700 unique users from more than 125 groups (including most major Pharma companies), using approximately 55 different beamlines at BES light sources and neutron sources, determined more than 450 structures of SARS-CoV-2 proteins with or without potential antivirals or antibodies, leading to more than 80 peer-reviewed publications as of August 2021.
- A decade of studies at APS and SSRL on spike proteins were key to the rapid development and effectiveness of all three SARS-CoV-2 vaccines currently in use in the United States. Furthermore, Pfizer scientists used NSLS-II to research certain structural properties of their vaccine.
- In terms of drug discovery, ALS protein crystallography capabilities supported a large collaboration led by the University of Washington and VIR Biotechnology, which has developed a COVID-19 therapeutic, Sotrovimab, that recently received FDA Emergency Use Authorization. Glaxo-Smith-Kline is now a major ALS partner as the drug approaches commercialization. More candidate drugs developed through research at BES light sources are in clinical trials.
- The Nanoscale Science Research Centers supported research to understand the virus and develop novel detection methods (fast, nanotechnology-based portable diagnostics sensors), synthesize custom nanoparticles for vaccine encapsulation and delivery, improve effectiveness of personal protective equipment (masks, nanoparticle-based antiviral coatings), and develop epidemiological models to predict virus spread.

BES user facilities maintain and enhance their leadership at the cutting edge of research.
From Nobel Prize discoveries to development of new capabilities to engagement of young scientists, BES user facilities stand at the forefront of cutting-edge science.

- The hard x-ray protein crystallography beam lines in ALS Sector 8 contributed strongly to Jennifer Doudna's 2020 Chemistry Nobel Prize-winning discovery of how a protein, known as CRISPR-Cas9, protects bacteria from viral infections. Her lab's structural biology research at ALS enabled fundamental understanding of the molecular basis for the ways in which RNA molecules affect the flow of genetic information in cells.

- The X-ray laser-enhanced attosecond pulse generation (XLEAP) system at LCLS has been upgraded to deliver isolated attosecond (billionths of a billionth of a second) pulses with unprecedented bandwidth to several user experiments. Fulfilling the important goal of time-resolved pump/probe experiments, two-color (frequency) sub-femtosecond (millionth of a billionth of a second) pulses, with sub-femtosecond timing control, were successfully delivered to users.
- The new generation of storage rings and high-repetition-rate free electron lasers requires unprecedented accuracy of optical elements, in order to preserve the ultra-high brightness and coherent flux that these sources will produce. Water-cooled solutions have reached the end of their development potential, and so cryo-optics are the logical next step forward. New cryo-optics experiments being carried out at the BES scientific user facilities are expected to be a mainstay of all high-power coherent beamlines in the future.
- A data science algorithm was developed to model the charge distribution in pixeled X-ray sensors. The model will achieve ultimate X-ray coordinate resolution and will enable the NSLS-II Soft Inelastic Scattering beamline to reach its best possible energy resolution. Undergraduate students from Alaska to the local area contributed to the project under the Science Undergraduate Laboratory Internships program, which encourages undergraduates and recent graduates to pursue science, technology, engineering, and mathematics careers by providing research experiences at the DOE laboratories.

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 clean energy technologies. The Basic Energy Sciences Advisory Committee (BESAC) report on transformative opportunities for discovery science, coupled with the Basic Research Needs workshop reports on energy technologies and roundtable reports, 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 and control of materials synthesis, behavior, and performance that will enable solutions to wide-ranging clean 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, theoretical, computational, and instrumentation research that will enable the predictive design and discovery of new materials with novel structures, functions, and properties.

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

- **Scattering and Instrumentation Sciences Research**—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 Research**—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 Research**—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 Request continues the highest-priority fundamental research that supports the DOE mission, including research that will advance the foundational knowledge necessary to accelerate innovation to reduce impacts resulting from climate change while advancing clean energy technologies and infrastructure. The portfolio emphasizes understanding of how to direct and control energy flow in materials systems over multiple time (femtoseconds to seconds) and length (nanoscale to mesoscale and beyond) scales, and translation of this understanding to prediction of material behavior, transformations, and processes in challenging real-world systems. This will establish a foundational knowledge base for future advanced, clean energy technologies and advanced manufacturing processes, including extremes in temperature, pressure, stress, photon and radiation flux, electromagnetic fields, and chemical exposures. To maintain leadership in materials discovery, the research supported by this subprogram explores new frontiers of 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, chemical, and biological sciences to explore new approaches to novel materials design and advanced manufacturing, including understanding to enable polymer upcycling to higher-value molecular systems. In clean energy-related research, there is a growing emphasis on carbon dioxide removal, including direct capture of carbon dioxide from the air. Other topics in clean energy include a focus on low-carbon hydrogen research and long-duration energy storage. Also, critical materials and minerals research will provide foundational knowledge to enable secure and sustainable supply chains for key clean energy technologies.

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 quantum information science (QIS). Materials science for microelectronics will provide the needed advances for future computing, sensors, detectors, and communication that are critical for national priorities in clean energy and for leadership in advanced research over a wide range of fields. An increasingly important aspect of materials research is the use of data science techniques to enhance the utility of both theoretical and experimental data for predictive design and discovery of materials. As an essential element of this research, this subprogram supports 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.

In addition to a diverse portfolio of single-investigator and small-group research projects, this subprogram supports Computational Materials Sciences, Energy Frontier Research Centers (EFRCs), the Batteries and Energy Storage Hub, SC National Quantum Information Science Research Centers (NQISRCs), in partnership with other SC programs, and, new in FY 2023, Energy Earthshot Research Centers (in partnership with Advanced Scientific Computing Research (ASCR) and Biological and Environmental Research (BER) and with DOE energy technology offices). These research modalities support multi-investigator, multi-disciplinary research focused on forefront scientific challenges in support of the DOE clean energy mission. This subprogram also includes the DOE Established Program to Stimulate Competitive Research (EPSCoR). The DOE EPSCoR program will strengthen investments in early-stage clean energy and climate research for U.S. states and territories that do not historically have large federally-supported academic research programs, expanding DOE research opportunities to a broad and diverse scientific community. This subprogram also supports the Reaching a New Energy Sciences Workforce (RENEW) initiative to provide undergraduate and graduate training opportunities for students and academic institutions not currently well represented in the U.S. S&T ecosystem, such as Minority Serving Institutions (MSIs), individuals from groups historically underrepresented in STEM, and students from communities disproportionately affected by social, economic, and health burdens of the energy system and from EPSCoR jurisdictions.

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 about the relationship among structure, dynamics, and properties, generating scientific knowledge that is foundational to the BES mission. 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 NQISRCs. This program is focused on open questions in materials science and physics, but these characterization tools are broadly applicable to other fields including chemistry, biology, and geoscience, and can be a key component in preparedness for biological threats.

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 link the microscopic and macroscopic properties of energy materials. Included is 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, as is the development and application of cryogenic electron microscopy for challenges in physical sciences. For example, to aid in the design of transformational new materials for clean energy technologies such as batteries, *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). Advances in cryogenic microscopy will support the BRaVE initiative since this instrumentation is heavily used to characterize biological threats. Information from these characterization tools is the foundation for the creation of new materials that have extraordinary tolerance and can function in extreme environments without property degradation. This activity supports the Accelerate initiative, which will support scientific research to accelerate the transition of science advances to energy technologies and the Funding for Accelerated, Inclusive Research (FAIR) initiative which will provide focused investment on enhancing research on clean energy, climate, and related topics at minority serving institutions, including attention to underserved and environmental justice communities.

Condensed Matter and Materials Physics Research
This activity supports fundamental experimental and theoretical research to discover, understand, and control novel phenomena in solid materials, generating scientific knowledge that is foundational to the BES mission. These electronic, magnetic, optical, thermal, and structural materials make up the infrastructure for clean energy technologies and innovations to reduce climate change impacts, as well as accelerator and detector technologies for SC facilities. Also supported is research to understand the role of rare earth and other critical materials in determining functionality, so that they can be reduced or eliminated from key energy technology supply chains.

Experimental research in this program emphasizes discovery and characterization of materials' properties that have the potential to be exploited for new technological functionalities. Complementary theoretical research aims to explain such properties across a broad range of length and time scales. Theoretical research also includes development and integration of predictive theory and modeling for discovery of materials with targeted properties. Advanced computational and data science techniques (including artificial intelligence and machine learning) are increasingly enabling knowledge to be extracted from large materials databases of theoretical calculations and experimental measurements. This program also supports the development of such databases as well as the computational tools that can take advantage of them.

This program continues to emphasize understanding and control of quantum materials whose properties result from interactions of the constituent electrons with each other, the atomic lattice, or light. Investigations include bulk materials as well as 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 electronic, magnetic, and optical properties relevant to energy-efficient microelectronics and quantum information science (QIS). The focus on QIS research couples experimental and theoretical expertise in quantum materials with prototypes of quantum structures that can be used to study the science of device functionality and performance.

Activities also emphasize research to understand how materials respond to temperature, light, radiation, corrosive chemicals, and other environmental conditions. This includes electrical and optical properties of materials related to solar energy as well as the effects of defects on electronic properties, strength, deformation, and failure over a wide range of length and time scales. In FY 2023, these activities will support the SC Energy Earthshots initiative. A recent focus is on extending knowledge of radiation effects to enable predictive capabilities for the extreme environments expected in future nuclear reactors and accelerators for SC facilities.

In FY 2023, BES will continue to partner with other SC programs to support the NQISRCs initiated in FY 2020. These centers focus on a set of QIS applications and cross-cutting topics that span the development space that will impact SC programs, including sensors, communication, quantum emulators/simulators, and enabling technologies that will pave the path to exploit quantum computing in the longer term. Research supported by this program will include theory of materials for quantum applications in computing, communication, and sensing; device science for next-generation QIS systems, including interface science and modeling of materials performance; and synthesis, fabrication, and characterization of quantum materials, including integration into novel device architectures to explore QIS functionality.

In partnership with the Advanced Scientific Computing Research (ASCR), High Energy Physics (HEP), Fusion Energy Sciences (FES), and Nuclear Physics (NP) programs, BES will continue activities begun in FY 2021 to support multi-disciplinary basic research to accelerate the advancement of microelectronic technologies in a co-design innovation ecosystem, as called for by the Basic Research Needs for Microelectronics report.[y] Among the challenges is discovery science that can lead to low-power microelectronics for edge computing as well as for exascale computers and beyond. Such computing capabilities will be necessary to analyze the vast volumes of data that will be generated by future SC facilities. Similarly, transforming power electronics and the electricity grid into a modern, agile, resilient, and energy-efficient system requires improvements in advanced microelectronics materials, and their integration within a co-design framework.

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

Materials Discovery, Design, and Synthesis Research

The discovery and development of new materials has long been recognized as the engine that drives science frontiers, technology innovations, and advanced manufacturing. 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 and design 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, generating scientific knowledge that is foundational to the BES mission, including clean energy and reduction of impacts resulting from climate change. In FY 2023, these activities will support the SC Energy Earthshots initiative.

The BESAC report on transformative opportunities for discovery science reinforced the importance of the continued growth of synthesis science, recognizing the opportunity to realize targeted functionality in materials by controlling the synthesis and assembly of hierarchical architectures and beyond equilibrium matter. In FY 2023 this program will continue to apply materials discovery and synthesis research to understand the unique properties of rare earth and other critical materials and minerals, with the goal of reducing their use. New research directions will be inspired by BES reports related to advanced manufacturing, including polymer upcycling. Understanding of synthesis science will enable design of new systems that are easier to efficiently convert into similar products with comparable or enhanced complexity, functionality, and value. Emphasis will include advancing the basic science of advanced manufacturing through innovative approaches for scalable assembly and integration of predictive modeling with characterization tools tuned to advanced manufacturing scale, complexity, and speed.

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. Major research directions include the controlled synthesis and assembly of nanoscale materials into functional materials with desired properties; 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 academic 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 and world-class national laboratories managed by the DOE. This research leverages DOE national user facilities and takes 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 in the EPSCoR jurisdictions. The FY 2023 program will focus on implementation awards for larger teams and will consider renewals of the FY 2021 awards as well as proposals for new teams. The technical scope will include a focus on clean energy research and climate science, expanding these important research communities and supporting the Energy Earthshot initiative. The program supports early career scientists from EPSCoR jurisdictions on an annual basis and provides complementary support for research grants to eligible institutions.

<u>Energy Frontier Research Centers</u>
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 and gas separation; quantum materials and quantum information science; microelectronics; and materials for future nuclear energy and waste storage. After twelve years of research activity, the program has produced an impressive breadth of scientific accomplishments, including over 14,000 peer-reviewed journal publications.

BES 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. 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 scientific meetings of the EFRC researchers biennially.

In FY 2023, BES will continue EFRC research efforts through awards made in FY 2020 and FY 2022. Scientific emphasis includes research directions identified in recent strategic planning activities, such as investments in clean energy research, climate science, and low-carbon manufacturing.

<u>Energy Earthshot Research Centers</u>
The EERC program is a new modality of research to be launched in FY 2023, building on the success of the Energy Frontier Research Centers. Like the EFRCs, EERCs will bring together multi-investigator, multi-disciplinary teams to perform energy-relevant research with a scope and complexity beyond what is possible in standard single-investigator or small-group awards. Beyond the scope of the EFRCs, EERCs will address the gap between basic research and the applied research and development activities to facilitate the exchange of knowledge between SC and the DOE energy technology offices, which is key to realizing the stretch goals of the Energy Earthshots. EERCs will support team awards involving academic, national lab, and industrial researchers with joint planning by SC and energy technology offices, establishing a new era of cross-office research cooperation. The funding will focus efforts directly at the interface, ensuring that directed fundamental research and capabilities at SC user facilities tackle the most challenging barriers identified in the applied research and development activities.

Existing DOE Energy Earthshots include the Hydrogen Shot, the Long Duration Storage Shot, and the Carbon Negative Shot. Additional topics are under consideration for future announcements. From a science perspective, many research gaps for the Energy Earthshots crosscut all topics and will provide a foundation for other energy technology challenges, including biotechnology, critical minerals/materials, energy-water, subsurface science (including geothermal research), and materials and chemical processes under extreme conditions for nuclear applications. These gaps require multiscale computational and modeling tools, new artificial intelligence and machine learning technologies, real-time characterization, including in extreme environments, and development of the scientific base to co-design processes and systems rather than individual materials, chemistries, and components. EERCs will leverage individual Center research to cross-fertilize the ideas that emerge in one topical area to benefit others with similar challenges accelerating the science, as well as the technologies.

In FY 2023, the Request supports a Funding Opportunity Announcement (FOA) to be released by the Office of Science (BES, Advanced Scientific Computing Research, and Biological and Environmental Research), in coordination with the DOE energy technology offices, for the initial cohort of Energy Earthshot Research Centers. Emphasis will be on the current Earthshot topics and those announced by DOE prior to release of the FOA.

Energy Innovation Hubs

The Joint Center for Energy Storage Research (JCESR), the Batteries and Energy Storage Hub, 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 identified critical scientific gaps to serve as a foundation for the research. The research directions are consistent with the priorities established in the 2017 BES workshop report *Basic Research Needs for Next Generation Electrical Energy Storage*[z] including discovery science for exploration of new battery chemistries and materials with novel functionality. JCESR is focusing on advances that 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 proving critical 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 are being 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, impactful research. In FY 2022, JCESR will receive the tenth and final year of funding, which will support research activities through much of FY 2023. In FY 2023, BES plans to issue a Funding Opportunity Announcement to openly recompete the Batteries and Energy Storage Hub program.

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 physical 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 or functionalities, and in turn, create new advanced, innovative technologies. Given the importance of materials to virtually all technologies, including clean energy, computational materials sciences are critical for American competitiveness in advanced manufacturing and global leadership in innovation.

This paradigm shift will accelerate the design of revolutionary materials to enable the Nation's energy and quantum information security, tackle the climate challenge, and enhance economic competitiveness. 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 or quantum materials with new functionalities. This research is performed by small groups and fully integrated teams. Large teams combine the skills of experts in materials theory, modeling, computation, synthesis, characterization, and fabrication. The research includes development of new ab initio theory,

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

contributing the generated data to databases, as well as advanced characterization and controlled synthesis to validate the computational predictions. It uses the unique world-leading tools and instruments at DOE's user facilities. The computational codes will use DOE's leadership computational facilities and be positioned to take advantage of today's petascale and tomorrow's exascale high-performance computers. This will result in open source, robust, validated, user-friendly software that captures the essential physics of relevant materials systems. The goal is the use of these codes and generated 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 small and large team modalities. Management reviews by a peer review panel are held in the first year of the award for large teams. Mid-term peer reviews are held to assess scientific progress, with regular teleconferences, annual progress reports, and active oversight by BES throughout the performance period. In FY 2023, the funding associated with the four-year awards in FY 2019 will be recompeted for both renewal and new awards.

Activities and Explanation of Changes

(dollars in thousands)

FY 2021 Enacted		FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Materials Sciences and Engineering	**$435,008**	**$566,629**	**+$131,621**
Scattering and Instrumentation Sciences Research	$74,031	$101,963	+$27,932
Funding continues 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 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 focuses on innovation that will enable assessment of new regimes not amenable to current characterization approaches.		The Request will continue to focus on the development and use of advanced characterization tools to address the most challenging fundamental questions in materials science, including quantum behavior and properties. The use of multiscale and multimodal techniques to extract information on multiple length and time scales is a growing emphasis, as is the development and application of cryogenic microscopy techniques to answer open questions in physical sciences. Advanced instrumentation research can be applied to diverse national priorities, including QIS, clean energy science, advanced manufacturing, and preparedness for biological threats. The Request supports the RENEW, FAIR, and Accelerate initiatives.	Funding will emphasize the advancement of novel measurement techniques and application of the tools to a broad range of science challenges, from quantum phenomena in energy materials to soft materials. Expanded investments will include the FAIR and Accelerate initiatives, a focus on basic research related to clean energy and advanced manufacturing, and on research opportunities for underrepresented communities and institutions.

(dollars in thousands)

FY 2021 Enacted	FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Condensed Matter and Materials Physics Research $170,200	$202,538	+$32,338
Funding continues to support research to understand, 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 provides continued support for the QIS Centers established in FY 2020. Investments 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. Support increases for investigations of 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 includes AI/ML for data-driven science to enhance materials discovery.	The Request will continue to emphasize the understanding and control of the fundamental properties of materials that are central to their functionality in a wide range of clean energy-relevant technologies, including critical materials/minerals, and for reduction of climate change impacts. Exploration of quantum materials remains a high priority, and particularly the role that these materials play in microelectronics, accelerators, and the broad emerging field of QIS. The program will continue to partner with other SC program offices to support the NQISRCs that were initiated in FY 2020. Additional investments will support the SC Energy Earthshots initiative, including the response of materials to environmental conditions, such as temperature, light, corrosive chemicals, and radiation, particularly in the context of future clean energy technologies.	Funding will continue to enhance clean energy and climate research, critical materials/minerals as well as materials in high-radiation environments including future accelerators. Efforts will also support the development and integration of computational and data science tools to enable scientific discovery. Expanded investments will include support for the SC Energy Earthshots initiative and a focus on research opportunities for underrepresented communities and institutions.

(dollars in thousands)

FY 2021 Enacted	FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Materials Discovery, Design, and Synthesis Research $71,189	$98,958	+$27,769
Funding continues for 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 is 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 emphasizes new approaches to replace or minimize the use of critical and rare earth materials in energy-relevant technologies.	The Request will continue support for the design, discovery, and synthesis of novel forms of matter with desired properties and functionalities with an emphasis on advancing the fundamental science relevant to future low-carbon manufacturing and reduction of climate change impacts, including innovative approaches to scalable assembly and integration of characterization and predictive modeling. Research will continue to explore science-based solutions to materials criticality. Research on bio-mimetic and biology-inspired materials is relevant to energy technologies as well as other national priorities such as preparedness for and response to biological threats. Additional investments in these topical areas will focus on support for the SC Energy Earthshots initiative.	The scientific focus will continue to evolve in response to research directions identified in recent strategic planning activities, such as the 2020 Basic Research Needs Workshop for Transformative Manufacturing. Expanded investments will include a focus on basic research related to clean energy, climate, and advanced manufacturing, on support for the SC Energy Earthshots initiative, and on research opportunities for underrepresented communities and institutions.

(dollars in thousands)

FY 2021 Enacted	FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Established Program to Stimulate Competitive Research (EPSCoR) $25,000	$35,000	+$10,000
Funding continues 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 emphasizes implementation awards, larger multiple principal investigator grants that develop research capabilities in EPSCoR jurisdictions. The FY 2021 funding opportunity solicits both renewals of FY 2019 awards and new proposals. Investment continues 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 R&D, including research that underpins DOE energy technology programs, the SC Energy Earthshots initiative, and innovations for climate science. Following the previous year's focus on State-National Laboratory Partnership awards, FY 2023 will emphasize Implementation Awards to larger multiple investigator teams that develop research capabilities in EPSCoR jurisdictions. The FY 2023 funding opportunity will consider new and renewal 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 will focus on implementation awards to develop research capabilities in EPSCoR jurisdictions, including clean energy, climate science, and low-carbon manufacturing research. Expanded investments will emphasize climate science and the SC Energy Earthshots initiative. Teams will be encouraged to include institutions serving underrepresented and minority communities. EPSCoR will participate in the SC-wide RENEW and FAIR initiatives to provide training and research opportunities for students and academic institutions not currently well represented in the U.S. S&T ecosystem.

(dollars in thousands)

FY 2021 Enacted	FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Energy Frontier Research Centers $57,500	$64,678	+$7,178
Funding provides 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.	The Request will provide the fourth year of support for the four-year EFRC awards that were made in FY 2020 and the second year of support for awards that were made in FY 2022.	Technical emphasis for the EFRC program will continue to include research directions identified in recent strategic planning activities and aligned with program priorities, including research related to clean energy and low-carbon manufacturing.
Energy Earthshot Research Centers $ —	$25,000	+$25,000
No funding.	The Request will support a Funding Opportunity Announcement (FOA) to be released by the Office of Science (BES, ASCR, BER), in coordination with the DOE Technology Offices, for the initial cohort of Energy Earthshot Research Centers (EERCs). EERCs will bring together the multi-investigator, multi-disciplinary teams necessary to perform energy-relevant research that bridges the gap between basic research and applied research and development activities. They will emphasize the innovations at the basic-applied interface required to advance the current Energy Earthshot topics and those announced by DOE prior to release of the FOA.	The Request will initiate this new activity.

(dollars in thousands)

FY 2021 Enacted	FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Energy Innovation Hubs $24,088	$25,000	+$912
Funding continues 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 continues 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 closely integrates theory, simulation, and experimentation to elucidate the impact of coupled phenomena and enable predictive design of new materials for batteries.	The Request will support an open re-competition of the Batteries and Energy Storage Hub program.	Funding will support the initiation of one or more new Batteries and Energy Storage Hub projects.
Computational Materials Sciences $13,000	$13,492	+$492
Funding continues to support 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 utilizes leadership class computers and will be made available to the broad research community. The codes incorporate frameworks suited for future exascale computer systems.	The Request will continue research that focuses on development of computational codes and associated experimental and computational databases for the predictive design of functional materials. The research includes development of new ab initio theory, populating databases, and advanced characterization and controlled synthesis to validate the computational predictions. The goal is open source, validated software that uses today's DOE's leadership computational facilities and is poised to take advantage of tomorrow's exascale high-performance computers. BES plans to issue a Funding Opportunity Announcement in FY 2023 to recompete awards made in FY 2019.	Funding will continue to support research in ongoing awards as well as potential new and renewal awards resulting from an FY 2023 Funding Opportunity Announcement.

Note:

- *Funding for the subprogram above, includes 3.65 percent of research and development (R&D) funding for the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) Programs.*

Basic Energy Sciences
Chemical Sciences, Geosciences, and Biosciences

Description

Development of innovative clean energy technologies relies on understanding and ultimately controlling transformations of energy among forms and conversions of matter across multiple scales starting at the atomic level. 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, separations, and light-driven chemical transformations. The research addresses how physical and chemical phenomena at the scales of electrons, atoms, and molecules control complex and collective behavior of macroscopic-scale energy and matter conversion systems. At the most fundamental level, research to understand quantum mechanical behavior is rapidly evolving into the ability to control and direct such behavior to achieve desired outcomes. Fundamental knowledge developed through this subprogram can extend the new era of control science to tailor chemical transformations with atomic and molecular precision. The challenge is to achieve predictive understanding of complex chemical, geochemical, and biochemical systems at the same level of detail now known for simpler molecular systems.

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

- **Fundamental Interactions Research**—Discover the foundational factors controlling chemical reactivity and dynamics in gas and condensed phases, and at interfaces, based on understanding quantum interactions among photons, electrons, atoms, and molecules.
- **Chemical Transformations Research**—Understand and control the mechanisms of chemical catalysis, synthesis, separation, stabilization, and transport in complex chemical and subsurface systems, from atomic to geologic scales.
- **Photochemistry and Biochemistry Research**—Elucidate the molecular mechanisms of the capture of light energy and its conversion into electrical and chemical energy through biological and chemical pathways.

The Request continues the highest-priority fundamental research, including support of research to advance scientific understanding and accelerate innovation that can reduce impacts that contribute to climate change while advancing clean energy technologies and infrastructure. Support will continue for research to discover chemical processes for low-carbon, efficient, and circular approaches to advanced manufacturing including chemical upcycling of polymers. Related research emphasizes the chemistry, separations, and substitutions of critical elements important for reducing the dependence on critical materials and minerals while promoting innovative and robust manufacturing supply chains. Fundamental biochemistry will develop models and datasets for discovery of principles to enable biomimetic and biohybrid clean energy systems. Research focused on molecular science will enable new microelectronics and increase understanding of the phenomena relevant to QIS and quantum computing. Bringing simulation and experiments together, integration of data science and computational chemistry will provide the needed tools and infrastructure for shared data repositories.

Five synergistic, foundational research themes are at the intersections of multiple research focus areas in this portfolio. Ultrafast Chemistry probes electron and atom dynamics to understand energy and chemical conversions. Chemistry at Complex Interfaces advances understanding of how interfacial dynamics and structural and functional disorder influence chemical phenomena. Charge Transport and Reactivity explores how charge dynamics contribute to energy flow and chemical conversions. Reaction Pathways in Diverse Environments discovers the influence of nonequilibrium, heterogeneous, nanoscale, and extreme environments on complex reaction mechanisms. Chemistry in Aqueous Environments addresses water's unique properties and the role it plays in energy and chemical conversions.

The subprogram supports a diverse portfolio of research efforts including single investigators, small groups, and larger multi-investigator, cross-disciplinary teams—through EFRCs, the Fuels from Sunlight Energy Innovation Hub program, Computational Chemical Sciences, Data Science, and QIS—to advance foundational science that can enable clean energy technologies. The subprogram also partners across SC to support the NQISRCs that were established in FY 2020 and, new in FY 2023, Energy Earthshot Research Centers (in partnership with Advanced Scientific Computing Research (ASCR) and Biological and Environmental Research (BER) and with DOE energy technology offices). This subprogram also supports the RENEW initiative to provide undergraduate and graduate training opportunities for students and academic institutions not currently well represented in the U.S. S&T ecosystem; the FAIR initiative focused investment on enhancing research on clean energy, climate, and related topics at minority serving institutions; and the Accelerate initiative for scientific research to accelerate the transition of science advances to energy technologies.

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, in condensed phases, and at interfaces. This activity provides leadership for ultrafast chemistry, supporting research that advances ultrafast tools and approaches and their application to probe and control chemical processes. Research supports theory and computation for accurate and efficient descriptions of molecular reactions and chemical dynamics. These efforts provide the foundational knowledge and the state-of-the-art experimental and computational tools necessary to advance the subprogram's research activities and the BES mission, including clean energy approaches that can reduce impacts contributing to climate change.

The principal research thrusts in this activity are atomic, molecular, and optical sciences (AMOS), gas phase chemical physics (GPCP), condensed phase and interfacial molecular science (CPIMS), and computational and theoretical chemistry (CTC). AMOS research emphasizes the fundamental interactions of atoms and molecules with electrons and photons, to characterize and control their behavior. Novel attosecond sources, x-ray free electron laser sources such as the LCLS-II, and ultrafast electron diffraction are used to image the ultrafast dynamics of electrons and charge transport. CPIMS research emphasizes foundational research at the boundary of chemistry and physics, pursuing a molecular-level understanding of chemical, physical, and electron- and photon-driven processes in liquids and at interfaces. Experimental, theoretical, and computational investigations in the condensed phase and at interfaces elucidate the molecular-scale chemical and physical properties and interactions that govern condensed phase structure and dynamics. The GPCP program supports research on fundamental gas-phase chemical processes important in energy applications. Research in this program explores chemical reactivity, kinetics, and dynamics in the gas phase at the level of electrons, atoms, molecules, and nanoparticles. The CTC program supports development, improvement, and integration of new and existing theoretical and massively parallel computational or data-driven strategies for the accurate and efficient prediction or simulation of processes and mechanisms. Research in this area is crucial to utilize emerging exascale computing facilities and to optimize use of existing leadership class computers, leveraging U.S. leadership in the development of open-source computational chemistry codes and databases. In the context of the NQISRCs, this research also lays the groundwork for applications of future quantum computers to computational quantum chemistry.

In FY 2023, BES, in partnership with other SC programs, will continue support for the multi-disciplinary multi-institutional QIS centers, initiated in FY 2020. The NQISRCs will focus on a set of QIS applications or cross-cutting topics including innovative research on sensors, quantum emulators/simulators, and enabling technologies that will pave the path to exploit quantum computing in the longer term. Research initiated in FY 2021 in microelectronics will continue with a focus on unraveling complex mechanisms of chemical reactions at interfaces to inform the design and synthesis of new materials.[aa] The Fundamental Interactions activity will continue to advance data science and computational approaches for chemical sciences with a focus on integration of databases and computational chemistry tools for the generation of scientific knowledge that is foundational to the BES mission.

Chemical Transformations Research

This activity seeks fundamental knowledge of chemical reactivity, matter and charge transport, and chemical separation and stabilization processes that are foundational for developing future clean energy and advanced manufacturing technologies, and for innovations to mitigate or adapt to climate change. Core research areas include catalysis science, separation science, heavy element chemistry, and geosciences. The research entails use of ultrafast spectroscopy to follow transient species during reactions; advances the understanding of charge transport and reactivity, which determine the kinetics of electrocatalytic, separations, and geochemical processes; explores the influence of complex interfaces on chemical transformations; develops the mechanistic insight needed to control reaction pathways in diverse catalytic, separation, and geological environments; and develops understanding of chemistry in subsurface and aqueous systems important in sustainable chemical processes.

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

Catalysis science research is focused on understanding reaction mechanisms, precise synthesis, *operando* characterization, manipulation of catalytic active sites and their environments, and control of reaction conditions for efficiency and selectivity. A primary goal is the molecular-level control of chemical transformations relevant to the sustainable conversion of energy resources, with emphasis on thermal and electrochemical conversions. Separation science research seeks to understand and ultimately predict and control the atomic and molecular interactions and energy exchanges determining the efficiency and viability of chemical separations, with emphasis on critical elements and atmospheric CO_2. The major focus is to advance discovery of principles and predictive design of future chemical separation approaches with improved efficiencies. Heavy element chemistry provides foundational knowledge on the influence of complex environments, such as multiple phases and extreme conditions of temperature and radiation, on the dynamic behavior of actinide compounds. A primary goal is to advance understanding of the unique chemistry of f-electron systems that is required to design new ligands for actinide and rare-earth separations processes, to predict the chemical evolution of actinides in nuclear wastes and next-generation reactors, and to improve models of actinide environmental transport. Geosciences research provides the fundamental science underlying the subsurface chemistry and physics of natural substances under extreme conditions of pressure or confined environments. Areas of emphasis include the molecular-level understanding of phase equilibria, reaction mechanisms and rates associated with aqueous geochemical processes, the distribution and accumulation of elements in the earth upper mantle, and a mechanistic understanding of the origins of subsurface physical properties and the response of earth materials subject to chemo-mechanical stress.

In FY 2023, this activity will continue to support efforts central to transformative approaches to advanced manufacturing,[bb] including predictive design of catalytic and separations processes for circular use of natural and synthetic resources with atom and energy efficiency, as exemplified by polymer upcycling.[cc] In support of the Energy Earthshot initiative, this activity will increase focus on discovery and design of sustainable cycles for carbon and hydrogen, by means of enhanced carbon separation from dilute as well as concentrated sources and clean energy cycles of hydrogen generation, storage, and use. Also supporting the Energy Earthshot initiative, research will increase the fundamental knowledge of subsurface processes across spatial and temporal scales—such as mineralization, crack propagation, and rock fracture—that is critical for developing innovative clean energy technologies for the subsurface. Support will also continue for research to address challenges in critical materials with focus on novel approaches for resource identification and extraction, selective separation, and substitution and use of critical elements. Research will continue to investigate the unique quantum phenomena enabled by f-electron elements, including rare earth elements and actinides. The use of data science and AI/ML approaches will continue to be emphasized in research across the portfolio to accelerate the generation and propagation of scientific knowledge that is foundational to the BES mission.

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. Research explores the dynamic mechanisms of charge transport and reactivity that advances understanding of absorption, transfer, and conversion of energy across spatial and temporal scales and on redox interconversion of small molecules (e.g., carbon dioxide/methane, nitrogen/ammonia, and protons/hydrogen). Studies of ultrafast chemistry and photo-driven quantum coherence probe the short time-scales critical in natural photosynthesis and artificial molecular systems and can provide insights into the role of quantum phenomena in chemical and biochemical reactions. Research expands understanding of the influence of complex interfaces and aqueous environments on the dynamics and function of enzymes, natural and artificial membranes, and nano- to meso-scale structures. The resulting mechanistic understanding can inspire new strategies to control reaction pathways critical for clean energy conversions and for innovations to reduce impacts resulting from climate change.

This activity integrates multidisciplinary research at the interface of chemistry, physics, and biology. Research of biological systems provides insights for understanding and enhancing man-made chemical systems. In a reciprocal manner, studies of chemical (non-biological) systems provide insights on the dynamics and reactivity underlying biochemical processes. Research in natural photosynthesis advances knowledge of biological mechanisms of solar energy capture and conversion and can inspire development of bio-hybrid, biomimetic, and artificial photosynthetic systems for clean energy production.

[bb] https://science.osti.gov/-/media/bes/pdf/reports/2020/Transformative_Mfg_Brochure.pdf

[cc] https://science.osti.gov/-/media/bes/pdf/reports/2020/Chemical_Upcycling_Polymers.pdf

Studies of complex multielectron redox reactions, electron bifurcation, and quantum phenomena in biological systems can suggest innovative approaches to energy conversion and storage strategies for clean energy technologies. Complementary research on the elementary steps of light absorption, charge separation, and charge transport of solar energy conversion in man-made systems provides foundational knowledge for the use of solar energy for carbon-neutral fuel production and electricity generation. Research also addresses fundamental effects resulting from ionizing radiation to understand chemical reactions in extreme environments and to provide insights for remediation, fuel-cycle separation, and design of nuclear reactors.

In FY 2023, research will continue to establish a molecular-level understanding of biochemical and photochemical processes. Efforts will build on BES biochemistry and biophysics research to discover and design chemical processes and complex structures that can enable innovations for clean energy technologies, advanced manufacturing and microelectronics, such as bio-inspired, biohybrid, and biomimetic systems with desired functions and properties. Studies of photo-driven quantum coherence in natural photosynthesis and artificial molecular systems will continue with the goal of developing new strategies for efficient solar energy use. Research will also address challenges of reducing the use of critical and rare earth elements in light absorbers and catalysts for clean energy. Efforts across this research portfolio will continue to generate foundational knowledge critical to the BES mission. In support of the Energy Earthshot initiative, this activity will increase support for research to identify new approaches for harnessing solar energy for chemical conversions, providing knowledge that could enable carbon-neutral hydrogen technologies and advance strategies for other solar fuels. This activity supports the new Accelerate initiative that targets scientific research to accelerate the transition of science advances to energy technologies. This activity provides support for the ongoing SC-wide RENEW initiative and for the new FAIR initiative to build stronger programs at underrepresented institutions, including those in underserved and environmental justice communities, with a focus on enhancing research on clean energy, climate, and related topics.

Energy Frontier Research Centers

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 processes for improved electrochemical conversion and storage of energy; the understanding of catalytic chemistry and biochemistry that are foundational for fuels, chemicals, separations, and polymer upcycling; interdependent energy-water issues; quantum information science; future nuclear energy and the chemistry of waste processing; and advanced interrogation and characterization of the earth's subsurface. After twelve years of research activity, the program has produced an impressive breadth of scientific accomplishments, including over 14,000 peer-reviewed journal publications.

BES 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. Each EFRC undergoes a review of its management structure and approach in the first year of the award and a mid-term assessment by outside experts 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.

In FY 2023 BES will continue EFRC research efforts through awards made in FY 2020 and FY 2022. Scientific emphasis includes research directions identified in recent strategic planning activities such as investments in clean energy research, climate science, and low-carbon manufacturing.

Energy Earthshot Research Centers

The EERC program is a new modality of research to be launched in FY 2023, building on the success of the Energy Frontier Research Centers. Like the EFRCs, EERCs will bring together multi-investigator, multi-disciplinary teams to perform energy-relevant research with a scope and complexity beyond what is possible in standard single-investigator or small-group awards. Beyond the scope of the EFRCs, EERCs will address the gap between basic research and the applied research and development activities to facilitate the exchange of knowledge between SC and the DOE energy technology offices, which is key to realizing the stretch goals of the Energy Earthshots. EERCs will support team awards involving academic, national lab, and industrial researchers with joint planning by SC and energy technology offices, establishing a new era of cross-office research cooperation. The funding will focus efforts directly at the interface, ensuring that directed fundamental research and capabilities at SC user facilities tackle the most challenging barriers identified in the applied research and development activities.

Existing DOE Energy Earthshots include the Hydrogen Shot, the Long Duration Storage Shot, and the Carbon Negative Shot. Additional topics are under consideration for future announcements. From a science perspective, many research gaps for the Energy Earthshots crosscut all topics and will provide a foundation for other energy technology challenges, including biotechnology, critical minerals/materials, energy-water, subsurface science (including geothermal research), and materials and chemical processes under extreme conditions for nuclear applications. These gaps require multiscale computational and modeling tools, new artificial intelligence and machine learning technologies, real-time characterization, including in extreme environments, and development of the scientific base to co-design processes and systems rather than individual materials, chemistries, and components. EERCs will leverage individual Center research to cross-fertilize the ideas that emerge in one topical area to benefit others with similar challenges—accelerating the science, as well as the technologies.

In FY 2023, the Request supports a Funding Opportunity Announcement (FOA) to be released by the Office of Science (BES, ASCR, and BER), in coordination with the DOE energy technology offices, for the initial cohort of Energy Earthshot Research Centers. Emphasis will be on the current Earthshot topics and those announced by DOE prior to release of the FOA.

Energy Innovation Hubs

The two multi-investigator, cross-disciplinary solar fuels research awards for the Fuels from Sunlight Hub program build on the unique accomplishments of the first Fuels from Sunlight Hub and address both new directions and long-standing challenges in the use of solar energy, water, and carbon dioxide as the only inputs for fuels production for clean energy. The FY 2023 Request will continue support for these fundamental research efforts that target innovative solutions to key scientific challenges for solar fuels (as identified in the strategic planning report from the Roundtable on Liquid Solar Fuels), including how to overcome degradation mechanisms to increase durability of solar fuel-generating components and systems, design catalytic microenvironments to selectively produce energy-rich solar fuels, take advantage of the direct coupling of light-driven phenomena and chemical processes to improve component and system performance, and tailor complex phenomena that interact and affect function of integrated multicomponent assemblies for solar fuels production.[dd]

BES uses a variety of methods to regularly assess the progress of the awards, including annual progress reports, regular phone calls with the Directors, periodic Directors' meetings to ensure coordination and communication, and on-site visits and reviews. Each award undergoes a review of its management structure and approach in the first year and beginning in the second year will have an annual peer review of research progress against its scientific goals.

[dd] https://science.osti.gov/-/media/bes/pdf/reports/2020/Liquid_Solar_Fuels_Report.pdf

Computational Chemical Sciences

The computational chemical sciences program (CCS) supports basic research to develop validated, open-source codes and associated experimental/computational databases for modeling and simulation of complex chemical processes and phenomena that allow full use of emerging exascale and future planned DOE leadership-class computing capabilities. BES launched CCS research awards in FY 2017 and additional awards were initiated in FY 2018. The FY 2023 support will continue awards from FY 2021 and FY 2022. This research supports a publicly accessible website[ee] of open source, robust, validated, user-friendly software that captures the essential physics and chemistry of relevant chemical systems. The goal is use of these codes/data by the broader research community and by industry to dramatically accelerate chemical research in the U.S.

BES uses a variety of methods to regularly assess the progress of the CCS awards, including annual progress reports, regular phone calls with the Directors, and periodic meetings of funded activities to ensure coordination and communication. Large team awards undergo a review of management structure and approach in the first year and a mid-term review by outside experts to evaluate scientific progress compared to the project's scientific goals.

General Plant Projects

General Plant Projects 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.

[ee] https://ccs-psi.org/

Activities and Explanation of Changes

(dollars in thousands)

FY 2021 Enacted		FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Chemical Sciences, Geosciences, and Biosciences	**$394,285**	**$517,711**	**+$123,426**
Fundamental Interactions Research	$107,904	$122,939	+$15,035
Funding continues to develop forefront ultrafast approaches, with emphasis on the use of x-ray free electron lasers, including LCLS and its upgrades. Gas-phase research continues studies of how reactive intermediates in heterogeneous environments impact reaction pathways, and quantum phenomena underlying QIS in tailored molecules. Research extends 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 increases with the aim of understanding the energy and chemical conversion mechanisms for clean-energy applications and of designing and synthesizing new materials relevant to microelectronics. This activity continues to develop advanced theoretical and computational approaches that can be scaled to operate on exascale computers. Development of AI/ML methods increases to enable novel data science approaches for knowledge discovery. Research emphasizes efforts to drive advances in the application of quantum information science for understanding and exploiting quantum phenomena in chemical systems. This activity provides continuing support for the QIS Research Centers established in FY 2020.		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 impact reaction pathways. Continued emphasis will be placed on quantum phenomena underlying QIS, such as coherence and entanglement. Research will expand efforts to understand and control chemical processes and quantum phenomena at the molecular level. In FY 2023 research will emphasize understanding and control of interfacial chemical conversion mechanisms for clean energy applications and 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 data science methods will increase to enable novel approaches for knowledge discovery. This activity provides continued support for the NQISRCs established in FY 2020.	Technical emphasis will include new efforts to unravel the fundamental mechanisms of energy and chemical conversions underlying clean energy applications, to understand and exploit quantum phenomena important for QIS, and to understand and control interfacial chemical reactions that can enable new materials for microelectronics. Support will continue for the development of advanced theoretical and computational approaches, with focus on integration of data science and computational chemistry tools for the generation of scientific knowledge that is foundational to the BES mission. Investments will continue a focus on clean energy research in underrepresented communities and institutions.

(dollars in thousands)

FY 2021 Enacted	FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Chemical Transformations Research $112,292	$136,919	+$24,627
Funding continues 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 important in clean-energy applications and chemical upcycling of polymers. Separation science research continues to focus on novel approaches to separate complex chemical mixtures with high efficiency, with increased focus on separation of carbon dioxide from dilute mixtures. Geosciences research continues 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 continues to deepen understanding of actinide speciation and reactivity, fundamental theories of f-electron systems, and approaches to synthesize and separate actinide compounds. Research on the chemistry of rare earth elements, including heavy elements such as lanthanides, focuses on understanding their reactivity to limit their use in catalytic processes, their interactions and chemical processes in multiphase systems relevant to separations, and their behavior in rare-earth containing minerals that are relevant to extraction in geological environments.	The Request will continue supporting fundamental research to understand catalytic mechanisms for thermo- and electro-chemical conversions important in clean energy and advanced manufacturing technologies, including chemical upcycling of polymers, and in innovations to reduce climate change impacts. Separation science research will continue to focus on innovative mechanisms for high-efficiency processes, including reactive and electro-separations, and novel solvents. Heavy element research will continue to deepen understanding of actinide speciation and reactivity and fundamental theories of f-electron systems. Geosciences research will continue to elucidate subsurface phenomena, such as mineralization and rock fracture propagation under extreme subsurface conditions. Areas for increased emphasis include atomically precise synthesis of new catalysts and studies of chemical processes required to develop clean energy technologies: multiscale phenomena in extreme and constrained environments in the subsurface; separations and extraction of rare earth elements from complex and dilute mixtures; and alternative approaches that reduce use of critical elements.	Funding will emphasize research on catalysis and separation science research for studies of the chemistry of rare earth and platinum-group elements to enable improved extraction, separation, substitution, and reduction in use; for development of innovative approaches to sustainable, energy-efficient carbon and hydrogen cycles; and for reduction of climate change impacts. Support will continue for research to provide the foundational knowledge needed for advanced manufacturing. The use of data science and AI/ML approaches will continue to be emphasized in research across the portfolio to accelerate the generation and sharing of scientific knowledge and its impact in clean energy technologies. Expanded investment will include support for the SC Energy Earthshots initiative and a focus on clean energy research in underrepresented communities and institutions.

(dollars in thousands)

FY 2021 Enacted	FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Photochemistry and Biochemistry Research $82,589	$132,925	+$50,336
Funding continues 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 provide fundamental knowledge to guide the design of new clean-energy systems. Funding increases 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, informs bioinspired design of catalysts and reaction pathways, for instance to guide new approaches for clean-energy applications and polymer upcycling. Research on metal uptake and use by biological systems informs bio-inspired separation processes. Studies also increase understanding of how rare elements can be minimized in photo-absorbers and catalysts for solar fuels. Advances in solar fuels 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 address the relationship between quantum phenomena and the efficiency and fidelity of energy transfer and conversion.	The Request will continue support of core research to understand physical, chemical, biophysical, and biochemical processes of light energy capture and conversion. Studies of light absorption, energy transfer, charge transport, separation processes, and photocatalysis will provide fundamental insights that can lead to innovations in the design of new clean energy systems and processes and in reduction of climate change impacts. Study of biochemical processes and structures will provide a foundation for bio-inspired, biohybrid, and biomimetic systems with desired functions and properties, including design of efficient catalysts and reaction pathways. Solar fuels research will continue to address the molecular mechanisms of photon capture, charge transport, product selectivity and separation from non-target molecules, and the reduction of critical elements in photoabsorbers and catalysts. Biological and chemical studies will investigate how quantum phenomena affect energy conversion efficiency and fidelity. The Request supports the SC Energy Earthshots, FAIR, RENEW, and Accelerate initiatives.	Technical emphasis will include research that targets fundamental science for innovation in clean energy technologies and in reduction of climate change impacts through increased knowledge of fundamental biochemical, chemical, and biophysical principles; bio-inspired design and development of biomimetic and biohybrid energy systems and processes; and the discovery and understanding of mechanisms and processes of energy capture and conversion in both natural and artificial systems. Expanded investment will include the SC Energy Earthshots, FAIR, and Accelerate initiatives, and a focus on clean energy research in underrepresented communities and institutions.

(dollars in thousands)

FY 2021 Enacted	FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Energy Frontier Research Centers $57,500	$64,678	+$7,178
Funding provides 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.	The Request will provide the final year of support for four-year EFRC awards that were made in FY 2020 and the second year of support for awards that were made in FY 2022.	Technical emphasis for the EFRC program will continue to include research directions identified in recent strategic planning activities and aligned with program priorities, including research related to clean energy and low-carbon manufacturing.
Energy Earthshot Research Centers $ —	$25,000	+$25,000
No funding.	The Request will support a Funding Opportunity Announcement (FOA) to be released by the Office of Science (BES, ASCR, BER), in coordination with the DOE Technology Offices, for the initial cohort of Energy Earthshot Research Centers (EERCs). EERCs will bring together the multi-investigator, multi-disciplinary teams necessary to perform energy-relevant research that bridges the gap between basic research and applied research and development activities. They will emphasize the innovations at the basic-applied interface required to advance the current SC Energy Earthshot topics and those announced by DOE prior to release of the FOA.	Funding will support this new activity in FY 2023.

(dollars in thousands)

FY 2021 Enacted	FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Energy Innovation Hubs $20,000	$20,758	+$758
Funding continues 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 continues 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 into principles for solar energy capture and conversion into liquid fuels. Efforts that integrate experiment and theory and couple high-throughput experimentation with artificial intelligence continue to be emphasized.	The Request will continue support of fundamental research to address both long-standing and emerging new scientific challenges for solar fuels generation. Research will continue to focus on innovative artificial photosynthesis approaches to generate liquid fuels using only sunlight, carbon dioxide, and water as inputs. Experiment and theory are integrated for the design of processes, components, and systems for selective, stable, and efficient liquid solar fuels production for clean energy.	Funding will continue support for prior year awards in priority research areas.

(dollars in thousands)

FY 2021 Enacted	FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Computational Chemical Sciences $13,000	$13,492	+$492
Funding continues 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 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.	The Request will continue CCS awards made in FY 2021 and FY 2022, with ongoing research to develop public, open-source codes for future exascale computer platforms.	Funding will continue support for prior year awards in priority research areas.
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.

Note:

- *Funding for the subprogram above, includes 3.65 percent of research and development (R&D) funding for the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) Programs.*

Basic Energy Sciences
Scientific User Facilities (SUF)

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 a wide diversity of universities, industry, and government laboratories to advance a broad 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 electrons, x-rays, 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 facilities, 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 with improved computational and data analysis infrastructure, improved nanoscience 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 data science 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 instrument) to save the highest-value data from user experiments.

The BES user 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 and delivery systems 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.

In FY 2019, more than 16,000 scientists and engineers in many fields of science and technology used BES scientific facilities. Due to the COVID-19 pandemic, BES scientific user facilities were under curtailed user operations, available mainly through remote access for the majority of the instruments during the second half of FY 2020 and all of FY 2021. Additional funds provided through the CARES Act supported extraordinary operations of the light and neutron sources and nanoscale science research centers for COVID-specific research during curtailed operations. The BES facilities supported over 12,500 users in FY 2020 and over 11,300 users in FY 2021. Light sources and neutron sources were able to provide critical support to the development of potential therapeutic drugs and vaccines through structural studies of the proteins of the SARS CoV-2 virus, which causes COVID-19. All of the user facilities contributed to other COVID-19 activities, including research on masks, characterization of novel manufacturing for medical equipment, and delivery of therapeutics. The BES facilities will continue to support ongoing research efforts to combat COVID-19 and evolve the tools and expertise needed for future public health challenges. In FY 2023, continued support for biological threats at the light and neutron sources is included in the Biopreparedness Research Virtual Environment (BRaVE) initiative.

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 their 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 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. Facility upgrade projects are underway for the APS, ALS, and LCLS to ensure ongoing world leadership for these facilities.

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. In FY 2023, NEXT-III will receive Other Project Costs support for planning of the next cadre of beamlines.

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 uniquely distinguished via isotope substitution experiments, for example substitution of deuterium for hydrogen 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 instruments for inelastic scattering, small angle scattering, powder and single crystal diffraction, neutron imaging, and engineering diffraction.

The Spallation Neutron Source (SNS) at ORNL uses a different 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, cascades of 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 large suite of capabilities for high and low temperature, high magnetic field, and high-pressure sample environment equipment is available for the instruments. 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.

Current construction projects at SNS focus on maintaining world-leadership for neutron scattering. In addition, for FY 2023 Other Project Costs are requested to initiate planning for replacement of the aging HFIR pressure vessel.

Nanoscale Science Research Centers

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 while they interact with their physical and chemical environments. 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 Nanoscale Science Research Centers (NSRCs) focus on interdisciplinary discovery research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. Distinct from the x-ray and neutron sources, NSRCs comprise of a suite of smaller unique tools and expert scientific staff. The five NSRCs 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 and scanning probe microscopy; and nanostructure fabrication and integration. Selected thematic areas include catalysis, electronic materials, nanoscale photonics, and soft and biological materials. The centers are typically near BES facilities for x-rays or neutrons, or near SC-supported computation facilities, which complement and leverage each other's capabilities. These custom-designed laboratories contain clean rooms, nanofabrication resources, one-of-a-kind signature instruments, and other instruments generally available only at major user facilities. The NSRC electron and scanning probe microscopy capabilities provide superior atomic-scale spatial resolution and simultaneously obtain structural, chemical, and other types of information from sub-nanometer regions at short time scales. They house one of the highest resolution electron microscopes in the world. Data science approaches are enabling large and fast data acquisition, real-time analysis, and autonomous experiments. Operating funds enable cutting-edge research, provide technical support, and administer the user program at these facilities, which serve academic, government, and industry researchers with access determined through external peer review of user proposals.

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 comprises 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 NSRC core facilities, additional beamlines for the NSLS II, 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 that is specific to BES facility needs and directions. BES coordinates with the SC Office of Accelerator R&D and Production on crosscutting research and technology areas. Accelerator research is the cornerstone for the development of new technologies that will improve performance of accelerator-based light sources and neutron scattering facilities, in support of the Accelerator Science and Technology Initiative. 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 the most advanced Artificial Intelligence (AI)/Machine Learning (ML) 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 BES 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 supports training in the field of particle beams and their associated accelerator applications. This activity will support the Reaching a New Energy Sciences Workforce (RENEW) initiative to provide undergraduate and graduate training opportunities for students and academic institutions not currently well represented in the U.S. S&T ecosystem, such as Minority Serving Institutions (MSIs), individuals from groups historically underrepresented in STEM, and students from communities disproportionately affected by social, economic, and health burdens of the energy system, and from the Established Program to Stimulate Competitive Research (EPSCoR) jurisdictions. This activity will also support the BRaVE initiative, which brings DOE laboratories together to tackle problems of pressing national importance, BES research will continue developing and maintaining capabilities at user facilities related to biotechnology for responsiveness to biological threats and development of advanced instrumentation to address these research challenges.

Activities and Explanation of Changes

(dollars in thousands)

FY 2021 Enacted		FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Scientific User Facilities (SUF)	**$1,026,707**	**$1,042,899**	**+$16,192**
X-Ray Light Sources	$525,000	$509,425	-$15,575
The funding supports operations at five BES light sources (LCLS, APS, ALS, NSLS-II, and SSRL).		The Request will support operations at five BES light sources (LCLS, APS, ALS, NSLS-II, and SSRL).	Funding will support LCLS, APS, ALS, NSLS-II and SSRL operations at 90 percent of optimal, the level for normal operations based on FY 2018 baseline. Facilities will optimize operational support, prioritizing staff support for users, including development of capabilities under the BRaVE initiative.
High-Flux Neutron Sources	$292,000	$280,754	-$11,246
The funding supports operations at SNS and HFIR.		The Request will support operations at SNS and HFIR.	Funding will support operations for SNS and HFIR at approximately 90 percent of optimal, the level for normal operations based on FY 2018 baseline. Facilities will optimize operational support, prioritizing staff support for users, including development of capabilities under the BRaVE initiative.
Nanoscale Science Research Centers	$139,000	$134,754	-$4,246
The funding supports operations for the five NSRCs (CFN, CNM, CNMS, TMF, and CINT). The NSRCs continue to develop nanoscience and QIS-related research infrastructure and capabilities for materials synthesis, device fabrication, metrology, modeling and simulation.		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 at approximately 90 percent of optimal, the level for normal operations based on FY 2018 baseline, including support to develop QIS-related research infrastructure and capabilities. Facilities will optimize operational support, prioritizing staff support for users.

(dollars in thousands)

FY 2021 Enacted	FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Other Project Costs $19,000	$17,500	-$1,500
Other Project Costs continue for the LCLS-II-HE project at SLAC National Accelerator Laboratory, PPU at Oak Ridge National Laboratory, Second Target Station project at Oak Ridge National Laboratory, and the Cryomodule Repair and Maintenance Facility (CRMF) project at SLAC.	The Request will support Other Project Costs for the LCLS-II-HE project at SLAC, the Second Target Station project at ORNL, the Advanced Photon Source Upgrade (APS-U) project at ANL, and the Cryomodule Repair and Maintenance Facility (CRMF) project at SLAC. The Request also initiates OPC for the High Flux Isotope Reactor Pressure Vessel Replacement (HFIR-PVR) project at ORNL and the National Synchrotron Light Source-II (NSLS-II) Experimental Tools-III (NEXT-III) project at BNL.	Funding will support the initiation of planning for the HFIR-PVR project at ORNL and the NSLS-II NEXT-III project at BNL. OPC will support preliminary project plans for these activities.
Major Items of Equipment $10,500	$50,000	+$39,500
The funding supports 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 also continues with R&D, design, engineering, prototyping, other supporting activities, and possible procurements. The project received CD-1/3A approval on 4/15/2021.	The Request will continue the beamline project for NSLS-II (NEXT-II) at BNL and the recapitalization project for the NSRCs. Both projects are planning for CD-2/3 approval early in FY 2022.	Funding will support the baseline funding profiles for the NEXT-II and NSRC Recapitalization MIE projects.

(dollars in thousands)

FY 2021 Enacted	FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Research $41,207	$50,466	+$9,259
The funding supports 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.	The Request will support high-priority research activities for advanced seeded FEL schemes that provide several orders of magnitude performance enhancement, detectors with high read out rate, optics that can handle high heat load and preserve the coherent wave front, and applications of data science 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. In addition, research will expand to include enabling capabilities for response to biological threats.	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 data science methods and tools to address data and information challenges at the BES user facilities, including accelerator optimization, control, prognostics, and experiment automation and real time data analysis. Funding will support the BRaVE initiative to enable facility capabilities for responsiveness to biological threats. Investment will include research in underrepresented communities and institutions.

Note:

- *Funding for the subprogram above, includes 3.65 percent of research and development (R&D) funding for the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) Programs.*

Basic Energy Sciences
Construction

Description

Accelerator-based x-ray light sources, accelerator-based pulsed neutron sources, and reactor-based neutron sources are essential user facilities that enable critical DOE mission-driven science, including research in support of clean energy, as well as research in response to national priorities such as the COVID-19 pandemic. 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.

21-SC-10, Cryomodule Repair & Maintenance Facility (CRMF), SLAC

The CRMF project will provide a much needed capability to maintain, repair, and test superconducting radiofrequency (SRF) accelerator components. These components include but are not limited to superconducting RF cavities and cryomodules that make up the new superconducting accelerator being constructed by the LCLS-II and LCLS-II-HE projects, high brightness electron injectors, and superconducting undulators. 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 25,000 gross square foot building to contain the necessary equipment. The building will need a concrete shielded enclosure for cryomodule testing, a control room, a vertical test stand area for testing SRF cavities and components, supplied with cryogenic refrigeration and a 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 6, 2019, with a current TPC range of $70,000,000–$98,000,000. A combined CD-1/3A is projected for 2Q FY 2023.

19-SC-14, Second Target Station (STS), ORNL

The STS project will expand SNS capabilities for neutron scattering research by exploiting part of the higher SNS accelerator proton beam 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 beam power density 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 15 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-1, Approve Alternative Selection and Cost Range, on November 23, 2020, which established the approved TPC range of $1,800,000,000–$3,000,000,000 and CD-2, Approve Performance Baseline, is expected 2Q FY 2025.

18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL

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 x-ray brightness and coherent flux. At least seven new x-ray beamlines will be installed and several existing beamlines will be upgraded to take advantage of the enhanced x-ray properties. APS-U will ensure that the APS remains a world leader in hard x-ray science. The project received 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, projected in 2Q FY 2026.

18-SC-11, Spallation Neutron Source Proton Power Upgrade (PPU), ORNL

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 by fabricating and installing seven new superconducting radio frequency (SRF) cryomodules and supporting RF equipment, upgrade the first target station to accommodate beam power up to 2 MW, and deliver a 2 MW-qualified target. 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. The improved target performance at the increased beam power of 2 MW is enabled by the addition of a new gas injection system and a redesigned mercury target vessel. The project received CD-3, Approve Start of Construction, on October 6, 2020, with a Total Project Cost (TPC) of $271,567,000 and CD-4, Approve Project Completion, expected in 4Q FY 2028.

18-SC-12, Advanced Light Source Upgrade (ALS-U), LBNL

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 project received CD-2, Approve Performance Baseline, on April 2, 2021, with a Total Project Cost (TPC) of $590,000,000 and CD-3, Approve Start of Construction, is expected in 1Q of FY 2023.

18-SC-13, Linac Coherent Light Source-II-High Energy (LCLS-II-HE), SLAC

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-3A, Approve Long Lead Procurements, on May 12, 2020, with the TPC range of $290,000,000–$480,000,000. Between CD-3A and the current budget process, the TPC estimate has increased to $660,000,000 as a result of a maturing design effort that identified additional costs across the project scope, added scope for a new superconducting electron source, and increased the project’s contingency to address several future risks. The LCLS-II-HE project continues to assess the impact of COVID-19 on the project’s cost and schedule. A combined CD-2/3 approval is projected for 4Q FY 2023 and CD-4 is projected for 2Q FY 2031.

Activities and Explanation of Changes

(dollars in thousands)

FY 2021 Enacted		FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
Construction	**$389,000**	**$293,200**	**-$95,800**
21-SC-10, Cryomodule Repair & Maintenance Facility (CRMF), SLAC	$1,000	$10,000	+$9,000
Funding supports conducting a conceptual design and an Analysis of Alternatives to determine a revised cost range for the project at SLAC. Engineering and design activities may begin.		The Request will continue the initial design effort and initiate long-lead procurements and site preparations for civil construction upon associated CD approvals. CD-1/3A is projected for 2Q FY 2023.	Funding will advance progress on the CRMF project.
19-SC-14, Second Target Station (STS), ORNL	$29,000	$32,000	+$3,000
Funding continues to support planning, R&D, and engineering activities to assist in maturing the project preliminary design, scope, cost, schedule and key performance parameters with emphasis on advancing the accelerator, target, instrument, controls, and conventional civil construction subsystems.		The project will continue the activities of planning, R&D, and engineering to mature the project's preliminary design, scope, cost, schedule, and key performance parameters.	Funding will advance progress on the STS project.

(dollars in thousands)

FY 2021 Enacted	FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL $160,000	$9,200	-$150,800
Funding continues to support advancing the final designs, engineering, prototyping, testing, fabrication, procurement of baseline and spare hardware, integration, and installation for the storage ring and experimental facilities, and site preparation and civil construction associated with the long beamlines.	The Request will support ongoing construction activities to include civil construction associated with the long beamline building. Dark time for installation is projected to begin 2Q FY 2023.	Funding will advance progress on the APS-U project. The APS-U current baseline (from the CD-2 approval) does not include potential COVID impacts that could increase the baseline cost and extend the schedule; this situation is being carefully monitored.
18-SC-11, Spallation Neutron Source Proton Power Upgrade (PPU), ORNL $52,000	$17,000	-$35,000
Funding continues to support R&D, engineering, prototyping, design, testing, fabrication, procurement of baseline and spare hardware, component integration and installation, and civil construction. Advancing the target R&D, engineering, design, and prototyping in conjunction with SNS operations target improvement plans will be a high priority.	The project will support the installation of additional cryomodules and related radiofrequency systems, operation of the second PPU test target at increased power levels, and construction of the tunnel stub that will facilitate connection to the future Second Target Station.	Funding will advance progress on the PPU project.
18-SC-12, Advanced Light Source Upgrade (ALS-U), LBNL $62,000	$135,000	+$73,000
Funding continues to support engineering, design, R&D prototyping and long lead procurements of construction items and other tasks as required.	The project will continue to advance construction activities making progress towards CD-3, projected for 1Q FY 2023.	Funding will advance progress on the ALS-U project.

(dollars in thousands)

FY 2021 Enacted	FY 2023 Request	Explanation of Changes FY 2023 Request vs FY 2021 Enacted
18-SC-13, Linac Coherent Light Source-II-High Energy (LCLS-II-HE), SLAC $52,000	$90,000	+$38,000
Funding continues to support engineering, design, R&D prototyping, and long lead procurements of construction items as authorized along with other tasks as required.	Funding will support engineering, design, R&D prototyping, continuing long lead procurements of construction items and preparation of the project baseline. Other tasks as required. A combined CD-2/3 approval is projected for 4Q FY 2023 and CD-4 is projected for 2Q FY 2031.	Funding will advance progress on the LCLS-II-HE project.
13-SC-10 - Linac Coherent Light Source-II (LCLS-II), SLAC $33,000	$ —	-$33,000
Funding continues to support installation of all remaining major accelerator and x-ray systems and equipment commissioning activities.	No funding is requested in FY 2023.	Final funding for LCLS-II was requested in FY 2022.

Basic Energy Sciences
Capital Summary

(dollars in thousands)

	Total	Prior Years	FY 2021 Enacted	FY 2022 Annualized CR	FY 2023 Request	FY 2023 Request vs FY 2021 Enacted
Capital Operating Expenses						
Capital Equipment	N/A	N/A	46,950	65,800	69,500	+22,550
Minor Construction Activities						
General Plant Projects	N/A	N/A	10,000	1,740	15,652	+5,652
Accelerator Improvement Projects	N/A	N/A	30,539	24,431	39,958	+9,419
Total, Capital Operating Expenses	**N/A**	**N/A**	**87,489**	**91,971**	**125,110**	**+37,621**

Capital Equipment

(dollars in thousands)

	Total	Prior Years	FY 2021 Enacted	FY 2022 Annualized CR	FY 2023 Request	FY 2023 Request vs FY 2021 Enacted
Capital Equipment						
Major Items of Equipment						
Scientific User Facilities (SUF)						
NSLS-II Experimental Tools-II (NEXT-II), BNL	87,283	3,283	5,500	15,000	25,000	+19,500
NSRC Recapitalization	74,150	4,150	5,000	15,000	25,000	+20,000
Total, MIEs	N/A	N/A	10,500	30,000	50,000	+39,500
Total, Non-MIE Capital Equipment	N/A	N/A	36,450	35,800	19,500	-16,950
Total, Capital Equipment	**N/A**	**N/A**	**46,950**	**65,800**	**69,500**	**+22,550**

Note:

- *GPP activities less than $5M include design and construction for additions and/or improvements to land, buildings, replacements or addition to roads, and general area improvements. AIP activities less than $5M include minor construction at an existing accelerator facility.*

Minor Construction Activities

(dollars in thousands)

	Total	Prior Years	FY 2021 Enacted	FY 2022 Annualized CR	FY 2023 Request	FY 2023 Request vs FY 2021 Enacted
General Plant Projects (GPP)						
GPPs (greater than or equal to $5M and less than $20M)						
HFIR Guide Hall Extension	18,000	–	9,000	740	8,260	-740
SNS Sample Environment Building	5,392	–	–	–	5,392	+5,392
Total GPPs (greater than or equal to $5M and less than $20M)	N/A	N/A	9,000	740	13,652	+4,652
Total GPPs less than $5M	N/A	N/A	1,000	1,000	2,000	+1,000
Total, General Plant Projects (GPP)	**N/A**	**N/A**	**10,000**	**1,740**	**15,652**	**+5,652**
Accelerator Improvement Projects (AIP)						
AIPs (greater than or equal to $5M and less than $20M)						
Spallation Neutron Source Cold Box-Engineering	10,000	–	–	–	10,000	+10,000
Spare Cold Box for RF Cryoplant	5,200	–	5,200	–	–	-5,200
Cold Source Helium Refrigerator System	9,339	–	9,339	–	–	-9,339
Moderator Test Stand (SNS)	6,250	–	–	6,250	–	–
Transmitter #4 (NSLS-II)	5,100	–	–	–	5,100	+5,100
HFIR Beamline SANTA	6,700	–	–	–	6,700	+6,700
Total AIPs (greater than or equal to $5M and less than $20M)	N/A	N/A	14,539	6,250	21,800	+7,261
Total AIPs less than $5M	N/A	N/A	16,000	18,181	18,158	+2,158
Total, Accelerator Improvement Projects (AIP)	**N/A**	**N/A**	**30,539**	**24,431**	**39,958**	**+9,419**
Total, Minor Construction Activities	**N/A**	**N/A**	**40,539**	**26,171**	**55,610**	**+15,071**

Note:

- *The Total funding for the HFIR Guide Hall Extension GPP project is $9,000,000. This project, originally requested in FY 2021, has been delayed. Design efforts will be fully funded in FY 2022 ($740,000) and the remaining funds are requested in FY 2023 ($8,260,000).*

Basic Energy Sciences
Major Items of Equipment Description(s)

Scientific User Facilities (SUF) MIEs:

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

The NEXT-II project will 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-2, Approve Performance Baseline, and CD-3, Approve Start of Construction, on October 13, 2021. The approved total project cost is $94,500,000. The FY 2023 Request of $25,000,000 will continue R&D, prototyping, other supporting activities, and construction/equipment procurements. The project is planning for CD-4 approval early in FY 2027.

Nanoscale Science Research Center (NSRC) Recapitalization Project

The NSRCs started early operations in 2006-2007 and now, over a decade later, instrumentation recapitalization is needed 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 a combined CD-1, Approve Alternative Selection and Cost Range, and CD-3A, Approve Long-Lead Procurements, on April 15, 2021. The current total project cost range is $70,000,000 to $95,000,000 with a point estimate of $80,000,000. The FY 2023 Request of $25,000,000 will continue R&D, design, engineering, prototyping, other supporting activities, and construction/equipment procurements. The project is planning for CD-2/3 approval in FY 2022.

Basic Energy Sciences
Construction Projects Summary

(dollars in thousands)

	Total	Prior Years	FY 2021 Enacted	FY 2022 Annualized CR	FY 2023 Request	FY 2023 Request vs FY 2021 Enacted
21-SC-10, Cryomodule Repair & Maintenance Facility (CRMF), SLAC						
Total Estimated Cost (TEC)	90,300	–	1,000	1,000	10,000	+9,000
Other Project Cost (OPC)	3,700	–	1,000	2,000	–	-1,000
Total Project Cost (TPC)	**94,000**	**–**	**2,000**	**3,000**	**10,000**	**+8,000**
19-SC-14, Spallation Neutron Source Second Target Station (STS), ORNL						
Total Estimated Cost (TEC)	2,143,000	21,000	29,000	32,000	32,000	+3,000
Other Project Cost (OPC)	99,000	32,805	13,000	–	5,000	-8,000
Total Project Cost (TPC)	**2,242,000**	**53,805**	**42,000**	**32,000**	**37,000**	**-5,000**
18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL						
Total Estimated Cost (TEC)	796,500	529,800	156,500	101,000	9,200	-147,300
Other Project Cost (OPC)	18,500	8,500	–	5,000	5,000	+5,000
Total Project Cost (TPC)	**815,000**	**538,300**	**156,500**	**106,000**	**14,200**	**-142,300**
18-SC-11, Spallation Neutron Source Proton Power Upgrade (PPU), ORNL						
Total Estimated Cost (TEC)	257,769	156,000	52,000	17,000	17,000	-35,000
Other Project Cost (OPC)	13,798	10,798	3,000	–	–	-3,000
Total Project Cost (TPC)	**271,567**	**166,798**	**55,000**	**17,000**	**17,000**	**-38,000**

(dollars in thousands)

	Total	Prior Years	FY 2021 Enacted	FY 2022 Annualized CR	FY 2023 Request	FY 2023 Request vs FY 2021 Enacted
18-SC-12, Advanced Light Source Upgrade (ALS-U), LBNL						
Total Estimated Cost (TEC)	562,000	136,000	62,000	75,100	135,000	+73,000
Other Project Cost (OPC)	28,000	28,000	–	–	–	–
Total Project Cost (TPC)	**590,000**	**164,000**	**62,000**	**75,100**	**135,000**	**+73,000**
18-SC-13, Linac Coherent Light Source-II-High Energy (LCLS-II-HE), SLAC						
Total Estimated Cost (TEC)	628,000	73,157	55,500	50,000	90,000	+34,500
Other Project Cost (OPC)	32,000	12,000	2,000	3,000	4,000	+2,000
Total Project Cost (TPC)	**660,000**	**85,157**	**57,500**	**53,000**	**94,000**	**+36,500**
13-SC-10, Linac Coherent Light Source II (LCLS-II), SLAC						
Total Estimated Cost (TEC)	1,080,200	1,016,299	35,801	28,100	–	-35,801
Other Project Cost (OPC)	56,200	51,900	–	4,300	–	–
Total Project Cost (TPC)	**1,136,400**	**1,068,199**	**35,801**	**32,400**	**–**	**-35,801**
Total, Construction						
Total Estimated Cost (TEC)	**N/A**	**N/A**	**391,801**	**304,200**	**293,200**	**-98,601**
Other Project Cost (OPC)	**N/A**	**N/A**	**19,000**	**14,300**	**14,000**	**-5,000**
Total Project Cost (TPC)	**N/A**	**N/A**	**410,801**	**318,500**	**307,200**	**-103,601**

Note:

- *The FY 2021 Enacted amounts in the table above include reprogramming of funds from the APS-U project (-$3,500,000) to the LCLS-II-HE project (+$3,500,000) and the LCLS-II project (+$2,801,000). In the table above, the FY 2023 President's Request does not reflect OPC funding to begin planning for the NSLS-II Experimental Tools-III (NEXT-III) and High Flux Isotope Reactor Pressure Vessel Replacement (HFIR-PVR) line-item construction projects.*

Basic Energy Sciences
Funding Summary

(dollars in thousands)

	FY 2021 Enacted	FY 2022 Annualized CR	FY 2023 Request	FY 2023 Request vs FY 2021 Enacted
Research	869,500	895,100	1,133,806	+264,306
Facility Operations	956,000	1,000,400	924,933	-31,067
Projects				
Line Item Construction (LIC)	408,000	318,500	310,700	-97,300
Major Items of Equipment (MIE)	10,500	30,000	50,000	+39,500
Total, Projects	**418,500**	**348,500**	**360,700**	**-57,800**
Other	1,000	1,000	1,000	–
Total, Basic Energy Sciences	**2,245,000**	**2,245,000**	**2,420,439**	**+175,439**

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.

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 2021 Enacted	FY 2021 Current	FY 2022 Annualized CR	FY 2023 Request	FY 2023 Request vs FY 2021 Enacted
Scientific User Facilities - Type A					
Advanced Light Source	**68,908**	**66,669**	**72,908**	**66,914**	**-1,994**
Number of Users	1,800	1,159	1,400	1,200	-600
Achieved Operating Hours	–	3,002	–	–	–
Planned Operating Hours	3,168	3,168	3,300	2,952	-216
Optimal Hours	3,400	3,400	3,400	3,280	-120
Percent of Optimal Hours	93.2%	88.3%	97.1%	90.0%	-3.2%
Advanced Photon Source	**142,158**	**137,388**	**151,258**	**138,387**	**-3,771**
Number of Users	4,300	3,686	4,000	2,700	-1,600
Achieved Operating Hours	–	4,836	–	–	–
Planned Operating Hours	5,000	5,000	3,980	2,790	-2,210
Optimal Hours	5,000	5,000	4,100	3,100	-1,900
Percent of Optimal Hours	100.0%	96.7%	97.1%	90.0%	-10.0%
National Synchrotron Light Source II	**118,647**	**114,752**	**122,647**	**114,743**	**-3,904**
Number of Users	1,300	1,022	1,600	1,450	+150
Achieved Operating Hours	–	4,484	–	–	–
Planned Operating Hours	4,500	4,500	4,850	4,500	–
Optimal Hours	4,800	4,800	5,000	5,000	+200
Percent of Optimal Hours	93.8%	93.4%	97.0%	90.0%	-3.8%

(dollars in thousands)

	FY 2021 Enacted	FY 2021 Current	FY 2022 Annualized CR	FY 2023 Request	FY 2023 Request vs FY 2021 Enacted
Stanford Synchrotron Radiation Light Source	**44,544**	**43,191**	**49,344**	**43,957**	**-587**
Number of Users	950	1,030	1,350	1,150	+200
Achieved Operating Hours	–	4,915	–	–	–
Planned Operating Hours	5,020	5,020	5,050	4,500	-520
Optimal Hours	5,400	5,400	5,200	5,000	-400
Percent of Optimal Hours	93.0%	91.0%	97.1%	90.0%	-3.0%
Linac Coherent Light Source	**150,743**	**146,478**	**156,743**	**145,424**	**-5,319**
Number of Users	800	720	800	850	+50
Achieved Operating Hours	–	4,499	–	–	–
Planned Operating Hours	4,500	4,500	4,560	4,950	+450
Optimal Hours	4,600	4,600	4,700	5,500	+900
Percent of Optimal Hours	97.8%	97.8%	97.0%	90.0%	-7.8%
Spallation Neutron Source	**183,532**	**177,006**	**185,032**	**178,847**	**-4,685**
Number of Users	730	483	800	420	-310
Achieved Operating Hours	–	4,501	–	–	–
Planned Operating Hours	4,600	4,600	4,350	2,430	-2,170
Optimal Hours	4,900	4,900	4,600	2,700	-2,200
Percent of Optimal Hours	93.9%	91.9%	94.6%	90.0%	-3.9%
High Flux Isotope Reactor	**108,468**	**105,278**	**109,968**	**101,907**	**-6,561**
Number of Users	500	202	560	350	-150
Achieved Operating Hours	–	3,295	–	–	–
Planned Operating Hours	3,100	3,100	3,900	2,520	-580
Optimal Hours	3,300	3,300	4,000	2,800	-500
Percent of Optimal Hours	93.9%	99.8%	97.5%	90.0%	-3.9%

(dollars in thousands)

	FY 2021 Enacted	FY 2021 Current	FY 2022 Annualized CR	FY 2023 Request	FY 2023 Request vs FY 2021 Enacted
Scientific User Facilities - Type B					
Center for Nanoscale Materials	**28,275**	**28,261**	**31,239**	**27,024**	**-1,251**
Number of Users	500	428	480	450	-50
Center for Functional Nanomaterials	**25,113**	**24,296**	**27,913**	**25,424**	**+311**
Number of Users	500	571	520	490	-10
Molecular Foundry	**32,162**	**30,931**	**34,296**	**30,743**	**-1,419**
Number of Users	700	654	750	700	–
Center for Nanophase Materials Sciences	**28,131**	**26,662**	**30,931**	**26,889**	**-1,242**
Number of Users	500	656	580	550	+50
Center for Integrated Nanotechnologies	**25,319**	**23,920**	**28,121**	**24,674**	**-645**
Number of Users	600	721	660	625	+25
Total, Facilities	**956,000**	**924,832**	**1,000,400**	**924,933**	**-31,067**
Number of Users	13,180	11,332	13,500	10,935	-2,245
Achieved Operating Hours	–	29,532	–	–	–
Planned Operating Hours	29,888	29,888	29,990	24,642	-5,246
Optimal Hours	31,400	31,400	31,000	27,380	-4,020

Note:

- *Achieved Operating Hours and Unscheduled Downtime Hours will only be reflected in the Congressional budget cycle which provides actuals.*

Basic Energy Sciences
Scientific Employment

	FY 2021 Enacted	FY 2022 Annualized CR	FY 2023 Request	FY 2023 Request vs FY 2021 Enacted
Number of Permanent Ph.Ds (FTEs)	4,860	4,990	5,670	+810
Number of Postdoctoral Associates (FTEs)	1,340	1,400	1,680	+340
Number of Graduate Students (FTEs)	2,090	2,180	2,670	+580
Number of Other Scientific Employment (FTEs)	3,050	3,100	3,310	+260
Total Scientific Employment (FTEs)	**11,340**	**11,670**	**13,330**	**+1,990**

Note:
- *Other Scientific Employment (FTEs) includes technicians, engineers, computer professionals and other support staff.*

21-SC-10, Cryomodule Repair & Maintenance Facility (CRMF), SLAC
SLAC National Accelerator Laboratory
Project is for Design and Construction

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

Summary

The FY 2023 Request for the Cryomodule Repair and Maintenance Facility (CRMF) project at SLAC National Accelerator Laboratory is $10,000,000 of Total Estimated Cost (TEC) funding. This project has a preliminary Total Project Cost (TPC) range of $70,000,000 to $98,000,000. These cost ranges encompass the most feasible preliminary alternatives at this time. The current preliminary TPC estimate for this project is $94,000,000.

Significant Changes

CRMF was initiated in FY 2021. The most recent DOE Order 413.3B approved Critical Decision (CD) is CD-0, Approve Mission Need, approved on December 6, 2019. This Construction Project Data Sheet (CPDS) is an update of the FY 2022 CPDS and does not include a new start for FY 2023.

FY 2021 funding launched the alternatives analysis and conceptual design activities required for CD-1. The FY 2022 Request continues the analysis of alternatives and matures the conceptual design with expertise from an architectural and engineering (AE) firm. The FY 2023 Request will support planning, engineering, design, R&D, prototyping, long-lead procurements, site preparations for civil construction, and preparing for CD-1 combined with CD-3A long-lead procurements for the cryoplant.

A Federal Project Director, certified to Level I, has been assigned to this project.

Critical Milestone History

Fiscal Year	CD-0	Conceptual Design Complete	CD-1	CD-2	Final Design Complete	CD-3	D&D Complete	CD-4
FY 2021	12/6/19	1Q FY 2021	1Q FY 2021	1Q FY 2022	4Q FY 2022	1Q FY 2023	N/A	1Q FY 2027
FY 2022	12/6/19	4Q FY 2022	4Q FY 2022	4Q FY 2023	2Q FY 2024	2Q FY 2024	N/A	4Q FY 2028
FY 2023	12/6/19	1Q FY 2023	2Q FY 2023	1Q FY 2025	4Q FY 2024	1Q FY 2025	N/A	4Q 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

Fiscal Year	Performance Baseline Validation	CD-3A
FY 2021	4Q FY 2021	1Q FY 2022
FY 2022	4Q FY 2023	4Q FY 2023
FY 2023	4Q FY 2024	2Q FY 2023

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

Project Cost History

(dollars in thousands)

Fiscal Year	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, Total	TPC
FY 2021	4,000	66,000	70,000	10,000	10,000	80,000
FY 2022	7,000	81,000	88,000	10,000	10,000	98,000
FY 2023	5,600	84,700	90,300	3,700	3,700	94,000

Note:

- *This project has not received CD-2 approval; therefore, funding estimates are preliminary.*

2. Project Scope and Justification

Scope

The preliminary scope of the CRMF project is to construct a building to support the repair, maintenance, and testing of superconducting radiofrequency (SRF) accelerator components. These components may include but are not limited to SRF cavities and cryomodules, future capabilities for high brightness electron injectors, and superconducting undulators. The requirements will be refined as the project matures. The initial concept includes a building with a concrete shielded enclosure for cryomodule testing, a control room, a vertical test stand area for testing SRF cavities and components, supplied with cryogenic refrigeration and a distribution box, cryomodules handling 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 includes the potential for later installation of a dedicated SRF electron injector development and test area, which requires extending the envisioned building length by 30 feet, a 40 mega-electronvolt (MeV) SRF linac to provide the equipment and diagnostics necessary for an integrated injector test stand, and equipment to refurbish and test the niobium SRF cavities. The project is pre-CD-2; the scope included in the alternative selection and cost range will be refined at CD-1.

Justification

SC, through the two current BES construction projects, LCLS-II and LCLS-II-HE, is making over a $1,800,000,000 capital investment in an 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 20-23 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. FNAL and TJNAF produce the cryomodules making use of specialized fabrication, assembly, and test capabilities available there. To make any repairs, the facilities must currently send the cryomodules 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, during construction of the LCLS-II facility it was determined that cryomodules could be damaged during transportation; transportation of cryomodules for repairs during operations would pose a risk to reliable facility operations. This approach also assumed that either FNAL or TJNAF would have the maintenance capabilities available when needed. 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 is designed to meet these challenges and will provide the capability to repair, maintain, and test SRF accelerator components, primarily 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.

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 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	19,000 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 (TEC)			
FY 2021	1,000	1,000	–
FY 2022	1,000	1,000	–
FY 2023	3,600	3,600	3,000
Outyears	–	–	2,600
Total, Design (TEC)	**5,600**	**5,600**	**5,600**
Construction (TEC)			
FY 2023	6,400	6,400	4,000
Outyears	78,300	78,300	80,700
Total, Construction (TEC)	**84,700**	**84,700**	**84,700**
Total Estimated Cost (TEC)			
FY 2021	1,000	1,000	–
FY 2022	1,000	1,000	–
FY 2023	10,000	10,000	7,000
Outyears	78,300	78,300	83,300
Total, TEC	**90,300**	**90,300**	**90,300**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Other Project Cost (OPC)			
FY 2021	1,000	1,000	59
FY 2022	2,000	2,000	800
FY 2023	–	–	1,000
Outyears	700	700	1,841
Total, OPC	**3,700**	**3,700**	**3,700**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Project Cost (TPC)			
FY 2021	2,000	2,000	59
FY 2022	3,000	3,000	800
FY 2023	10,000	10,000	8,000
Outyears	79,000	79,000	85,141
Total, TPC	**94,000**	**94,000**	**94,000**

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design	4,000	5,650	**N/A**
Design - Contingency	1,600	1,350	**N/A**
Total, Design (TEC)	**5,600**	**7,000**	**N/A**
Site Preparation	8,800	8,000	**N/A**
Equipment	26,160	7,400	**N/A**
Other Construction	25,500	46,850	**N/A**
Construction - Contingency	24,240	18,750	**N/A**
Total, Construction (TEC)	**84,700**	**81,000**	**N/A**
Total, TEC	**90,300**	**88,000**	**N/A**
Contingency, TEC	*25,840*	*20,100*	***N/A***
Other Project Cost (OPC)			
Conceptual Planning	500	500	**N/A**
Conceptual Design	1,700	5,500	**N/A**
Start-up	500	1,500	**N/A**
OPC - Contingency	1,000	2,500	**N/A**
Total, Except D&D (OPC)	**3,700**	**10,000**	**N/A**
Total, OPC	**3,700**	**10,000**	**N/A**
Contingency, OPC	*1,000*	*2,500*	***N/A***
Total, TPC	**94,000**	**98,000**	**N/A**
Total, Contingency (TEC+OPC)	***26,840***	***22,600***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Fiscal Year	Type	Prior Years	FY 2021	FY 2022	FY 2023	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
FY 2022	TEC	—	1,000	1,000	—	86,000	88,000
	OPC	—	1,000	2,000	—	7,000	10,000
	TPC	—	2,000	3,000	—	93,000	98,000
FY 2023	TEC	—	1,000	1,000	10,000	78,300	90,300
	OPC	—	1,000	2,000	—	700	3,700
	TPC	—	2,000	3,000	10,000	79,000	94,000

Note:

- *This project has not received CD-2 approval; therefore, funding estimates are preliminary.*

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	FY 2028
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	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, Maintenance and Repair	5,500	5,500	286,000	137,500

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 18,600 to 25,000 gross square feet building may be constructed as part of this project.

8. Acquisition Approach

The CRMF Project will be sited at the SLAC National Accelerator Laboratory and is being acquired under the existing DOE Management and Operations contract.

SLAC is preparing a Conceptual Design Report for the CRMF project and has the required project management systems in place to execute the project.

Preliminary cost estimates 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 and/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 (STS), ORNL
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 2023 Request for Second Target Station (STS) project is $32,000,000 of Total Estimated Cost (TEC) funding and $5,000,000 of Other Project Costs (OPC) funding. This project has a preliminary Total Project Cost (TPC) range of $1,800,000,000 to $3,000,000,000. This cost range encompasses the most feasible preliminary alternatives. The current preliminary TPC estimate is $2,242,000,000.

Significant Changes
STS was initiated in FY 2019. The most recent DOE Order 413.3B approved Critical Decision (CD) is CD-1, Approve Alternative Selection and Cost Range, approved on November 23, 2020. This Construction Project Data Sheet (CPDS) is an update of the FY 2022 CPDS and does not include a new start for FY 2023.

In FY 2021, the project received CD-1 and continued planning, R&D, design, engineering, and other activities required to advance the STS project toward CD-2. The focus was maturing the accelerator, target, instrument, controls, and conventional civil construction subsystems. A commercial Architect/Engineer (AE) firm was contracted to assist in advancing the planning, engineering, and design. Proposals from scientific community teams for world-class instrument concepts were reviewed and eight were selected for inclusion in the project planning. In FY 2022, the project continues planning, R&D, and engineering to assist in maturing the project design, scope, cost, schedule and key performance parameters with continued emphasis on advancing the accelerator, target, instrument, controls, and conventional civil construction subsystems.
FY 2023 funds will support advancing the highest priority R&D and design activities including the proton accelerator extraction magnets and power supplies, proton beam window, and neutron optics systems, the Target and Moderator Reflector assemblies, the Bunker Shielding and components, design of the Integrated Control Systems and the design of the machine and personnel protection systems. Due to the extension of the project duration beyond initial projections, the project and program are evaluating the best approach to deliver threshold performance.

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 2020	1/7/09	2Q FY 2022	2Q FY 2022	2Q FY 2023	2Q FY 2025	2Q FY 2024	N/A	4Q FY 2031
FY 2021	1/7/09	2Q FY 2021	2Q FY 2021	3Q FY 2024	3Q FY 2026	3Q FY 2025	N/A	2Q FY 2032
FY 2022	1/7/09	4/30/21	11/23/20	2Q FY 2025	4Q FY 2029	2Q FY 2025	N/A	2Q FY 2037
FY 2023	1/7/09	4/30/21	11/23/20	2Q FY 2025	4Q FY 2029	2Q FY 2025	N/A	2Q FY 2037

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, Total	TPC
FY 2020	65,500	1,138,500	1,204,000	45,300	45,300	1,249,300
FY 2021	65,500	1,158,200	1,223,700	45,300	45,300	1,269,000
FY 2022	333,000	1,810,000	2,143,000	99,000	99,000	2,242,000
FY 2023	332,757	1,810,243	2,143,000	99,000	99,000	2,242,000

Note:
- *This project has not received CD-2 approval; therefore, funding estimates are preliminary.*

2. Project Scope and Justification

Scope
To address the gap in advanced neutron sources and instrumentation, the STS project will design, build, install, and test the equipment necessary to provide the four primary elements of the new Spallation Neutron Source (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 Key Performance Parameters (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 350,000 ft^2 of new buildings, making conventional facility construction a major contributor to project costs.

Justification
The Basic Energy Sciences (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 in part 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 Oak Ridge National Laboratory (ORNL), the SNS has been fulfilling this need. In accordance with the 1996 Basic Energy Sciences Advisory Committee (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 a proton beam that is highly concentrated to produce a very high-density beam of protons that strikes a rotating solid tungsten target. The produced neutron beam illuminates moderators located above and below the target that will feed up to 22 experimental beamlines (eight within the STS project scope) with neutron beams 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, requested separately, will double the power of the SNS accelerator complex to 2.8 MW so that STS can use one out of every four proton pulses to produce cold neutron beams with the highest peak brightness 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, which currently operates at 60 Hz, but will operate at 45 pulses/second when STS is operating) 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 fourth 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 eight best-in-class instruments, 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 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
Demonstrate independent control of the proton beam on the two target stations	Operate beam to FTS at 45 pulses/s, with no beam to STS. Operate beam to STS at 15 Hz, with no beam to FTS. Operate with beam to both target stations 45 pulses/s at FTS and 15 Hz at STS	Operate beam to FTS at 45 pulses/s, with no beam to STS. Operate beam to STS at 15 Hz, with no beam to FTS. Operate with beam to both target stations 45 pulses/s at FTS and 15 Hz at STS
Demonstrate proton beam power on STS at 15 Hz	100 kW beam power	700 kW beam power
Measure STS neutron brightness	peak brightness of 2 x 10^{13}n/cm^2/sr/Å/s at 5 Å	peak brightness of 2 x 10^{14}n/cm^2/sr/Å/s at 5 Å
Beamlines transitioned to operations	8 beamlines successfully passed the integrated functional testing per the transition to operations parameters acceptance criteria	≥ 8 beamlines successfully passed the integrated functional testing per the transition to operations parameters acceptance criteria

3. Financial Schedule

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
Design (TEC)			
FY 2019	1,000	1,000	–
FY 2020	20,000	20,000	–
FY 2021	29,000	29,000	20,360
FY 2022	32,000	32,000	46,000
FY 2023	32,000	32,000	45,000
Outyears	218,757	218,757	221,397
Total, Design (TEC)	**332,757**	**332,757**	**332,757**
Construction (TEC)			
Outyears	1,810,243	1,810,243	1,810,243
Total, Construction (TEC)	**1,810,243**	**1,810,243**	**1,810,243**
Total Estimated Cost (TEC)			
FY 2019	1,000	1,000	–
FY 2020	20,000	20,000	–
FY 2021	29,000	29,000	20,360
FY 2022	32,000	32,000	46,000
FY 2023	32,000	32,000	45,000
Outyears	2,029,000	2,029,000	2,031,640
Total, TEC	**2,143,000**	**2,143,000**	**2,143,000**

(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	10,917
FY 2021	13,000	13,000	5,916
FY 2022	–	–	10,353
FY 2023	5,000	5,000	5,769
Outyears	48,195	48,195	53,646
Total, OPC	**99,000**	**99,000**	**99,000**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
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	10,917
FY 2021	42,000	42,000	26,276
FY 2022	32,000	32,000	56,353
FY 2023	37,000	37,000	50,769
Outyears	2,077,195	2,077,195	2,085,286
Total, TPC	**2,242,000**	**2,242,000**	**2,242,000**

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design	258,000	256,500	**N/A**
Design - Contingency	74,757	76,500	**N/A**
Total, Design (TEC)	**332,757**	**333,000**	**N/A**
Construction	1,290,000	1,291,500	**N/A**
Construction - Contingency	520,243	518,500	**N/A**
Total, Construction (TEC)	**1,810,243**	**1,810,000**	**N/A**
Total, TEC	**2,143,000**	**2,143,000**	**N/A**
Contingency, TEC	*595,000*	*595,000*	***N/A***
Other Project Cost (OPC)			
R&D	22,875	22,875	**N/A**
Conceptual Design	24,750	24,750	**N/A**
Start-up	20,250	20,250	**N/A**
OPC - Contingency	31,125	31,125	**N/A**
Total, Except D&D (OPC)	**99,000**	**99,000**	**N/A**
Total, OPC	**99,000**	**99,000**	**N/A**
Contingency, OPC	*31,125*	*31,125*	***N/A***
Total, TPC	**2,242,000**	**2,242,000**	**N/A**
Total, Contingency (TEC+OPC)	***626,125***	***626,125***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Fiscal Year	Type	Prior Years	FY 2021	FY 2022	FY 2023	Outyears	Total
FY 2020	TEC	2,000	—	—	—	1,202,000	1,204,000
	OPC	11,500	—	—	—	33,800	45,300
	TPC	13,500	—	—	—	1,235,800	1,249,300
FY 2021	TEC	21,000	1,000	—	—	1,201,700	1,223,700
	OPC	32,805	1,000	—	—	11,495	45,300
	TPC	53,805	2,000	—	—	1,213,195	1,269,000
FY 2022	TEC	21,000	29,000	32,000	—	2,061,000	2,143,000
	OPC	32,805	13,000	—	—	53,195	99,000
	TPC	53,805	42,000	32,000	—	2,114,195	2,242,000
FY 2023	TEC	21,000	29,000	32,000	32,000	2,029,000	2,143,000
	OPC	32,805	13,000	—	5,000	48,195	99,000
	TPC	53,805	42,000	32,000	37,000	2,077,195	2,242,000

Note:

- *This project has not received CD-2 approval; therefore, funding estimates are preliminary.*

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	FY 2037
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	FY 2062

Related Funding Requirements
(dollars in thousands)

	Annual Costs		Life Cycle Costs	
	Previous Total Estimate	Current Total Estimate	Previous Total Estimate	Current Total Estimate
Operations, Maintenance and Repair	59,000	59,000	1,475,000	1,475,000

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.

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	~350,000
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"	~350,000
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

Based on the DOE determination at CD-1, ORNL is acquiring the STS project under the existing DOE Management and Operations (M&O) contract.

The M&O contractor prepared a Conceptual 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 design and procure the key technical subsystem components. Some technical system designs will require research and development activities. Preliminary cost estimates for most of these systems are based on operating experience of SNS and vendor estimates, while some first-of-a-kind systems are based on expert judgement. 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 are being exploited fully in planning and executing STS.

18-SC-10, Advanced Photon Source Upgrade (APS-U), ANL
Argonne National Laboratory
Project is for Design and Construction

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

Summary

The FY 2023 Request for the Advanced Photon Source-Upgrade (APS-U) project is $9,200,000 of Total Estimated Cost (TEC) funding and $5,000,000 of Other Project Costs (OPC) funding. The project has a Total Project Cost (TPC) of $815,000,000.

Significant Changes

The APS-U became a line item project in FY 2018. The most recent approved DOE Order 413.3B critical decision is CD-3, *Approve Start of Construction*, which was approved on July 25, 2019. CD-4, *Approve Project Completion*, is projected for 2Q FY 2026. This Construction Project Data Sheet (CPDS) is an update of the FY 2022 CPDS and does not include a new start for FY 2023. There are no significant changes.

FY 2021 funding enabled the advancement of the storage ring and experimental facilities final design, engineering, prototyping, testing, fabrication, procurement of baseline and spare hardware, integration, and installation, and enabled site preparation and civil construction activities for the Long Beamline Building (LBB). The project received and inspected hardware for the storage ring and experimental facilities and advanced the integrated magnet module assembly. FY 2022 funding emphasizes fabrication, procurement, acceptance testing, integration and assembly, and preparing all items for installation in FY 2023. Civil construction for the LBB and final design will be completed. The FY 2023 Request activities emphasize system integration, testing, and assembly in preparation for the storage ring removal and installation during the experimental dark time, tentatively scheduled to begin in April 2023.

To date, the project encountered delays in its progress and has required use of both cost and schedule contingency. The COVID-19 pandemic continues to affect personnel, cause supply chain delays in deliveries, and increase costs for procurements/subcontracts. The project and program are carefully monitoring progress and contingency, with options under active evaluation in the event of unacceptable costs/schedule impacts.

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 2018	4/22/10	9/18/15	2/4/16	1Q FY 2019	2Q FY 2020	4Q FY 2019	N/A	1Q FY 2026
FY 2019	4/22/10	9/18/15	2/4/16	2Q FY 2019	4Q FY 2021	1Q FY 2020	N/A	2Q FY 2026
FY 2020	4/22/10	9/18/15	2/4/16	12/9/18	1Q FY 2022	1Q FY 2020	N/A	2Q FY 2026
FY 2021	4/22/10	9/18/15	2/4/16	12/9/18	1Q FY 2022	7/25/19	N/A	2Q FY 2026
FY 2022	4/22/10	9/18/15	2/4/16	12/9/18	1Q FY 2022	7/25/19	N/A	2Q FY 2026
FY 2023	4/22/10	9/18/15	2/4/16	12/9/18	4Q 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 Start of Operations or Project Closeout

Fiscal Year	Performance Baseline Validation	CD-3A	CD-3B
FY 2018	1Q FY 2019	8/30/12	10/6/16
FY 2019	2Q FY 2019	8/30/12	10/6/16
FY 2020	12/9/18	8/30/12	10/6/16
FY 2021	12/9/18	8/30/12	10/6/16
FY 2022	12/9/18	8/30/12	10/6/16
FY 2023	12/9/18	8/30/12	10/6/16

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, Total	TPC
FY 2018	157,015	561,985	719,000	51,000	51,000	770,000
FY 2019	167,000	590,100	757,100	12,900	12,900	770,000
FY 2020	162,825	633,675	796,500	18,500	18,500	815,000
FY 2021	190,425	606,075	796,500	18,500	18,500	815,000
FY 2022	189,638	606,862	796,500	18,500	18,500	815,000
FY 2023	210,867	585,633	796,500	18,500	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, up to 500 times brighter than the present APS. The project's scope includes a new very low emittance multi-bend achromat (MBA) lattice storage ring in the existing tunnel, new permanent magnet and superconducting insertion devices optimized for brightness and flux, 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 high energy, hard x-ray light source technology. The six giga-electronvolt (GeV), very low emittance European Synchrotron Radiation Facility-Extremely Brilliant Source (ESRF-EBS) in France came on line in 2020; China initiated construction of the High Energy Photon Source (HEPS) in Beijing, a six GeV hard x-ray synchrotron light source, planned to come on line in 2026; the six GeV PETRA-IV extremely low emittance storage ring at DESY in Hamburg, and SPring-8-II in Japan are well into campaigns of major upgrades of beamlines and are also incorporating technological advancements in accelerator science to enhance performance for hard x-ray energies (>20 keV).

The APS upgrade will provide a world-class hard x-ray synchrotron radiation facility, with up to 500 times increased brightness and coherent flux over the current APS and will be a unique asset in the U.S. portfolio of scientific user facilities. The APS-U is a critical and cost-effective next step in the photon science strategy that will keep the U.S. at the forefront of scientific research, combining with other facilities to give the U.S. a complementary set of storage ring and free-electron laser x-ray light sources.

The high-brightness, high-energy penetrating hard x-rays will provide a unique scientific capability directly relevant to probing real-world materials and applications in energy, the environment, new and improved materials, and biological studies. The APS upgrade 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]	> 1×10^{20}	1×10^{22}
Brightness @ 60 keV[1]	> 1×10^{19}	1×10^{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 (TEC)			
FY 2012	19,200	19,200	9,095
FY 2013	15,000	15,000	17,825
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	26,000	26,000	23,829
FY 2019	14,650	14,650	23,985
FY 2020	22,988	22,988	28,486
FY 2021	18,200	18,200	23,059
FY 2022	3,029	3,029	5,515
Total, Design (TEC)	**210,867**	**210,867**	**210,867**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Construction (TEC)			
FY 2012	800	800	–
FY 2013	5,000	5,000	3,391
FY 2014	2,985	2,985	4,534
FY 2015	–	–	573
FY 2017	7,715	7,715	389
FY 2018	67,000	67,000	6,307
FY 2019	113,150	113,150	24,425
FY 2020	143,512	143,512	55,859
FY 2021	138,300	138,300	125,595
FY 2022	97,971	97,971	179,778
FY 2023	9,200	9,200	147,517
Outyears	–	–	37,265
Total, Construction (TEC)	**585,633**	**585,633**	**585,633**
Total Estimated Cost (TEC)			
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	93,000	93,000	30,136
FY 2019	127,800	127,800	48,410
FY 2020	166,500	166,500	84,345
FY 2021	156,500	156,500	148,654
FY 2022	101,000	101,000	185,293
FY 2023	9,200	9,200	147,517
Outyears	–	–	37,265
Total, TEC	**796,500**	**796,500**	**796,500**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Other Project Cost (OPC)			
FY 2010	1,000	1,000	587
FY 2011	7,500	7,500	3,696
FY 2012	–	–	4,217
FY 2022	5,000	5,000	–
FY 2023	5,000	5,000	5,748
Outyears	–	–	4,252
Total, OPC	**18,500**	**18,500**	**18,500**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Project Cost (TPC)			
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	93,000	93,000	30,136
FY 2019	127,800	127,800	48,410
FY 2020	166,500	166,500	84,345
FY 2021	156,500	156,500	148,654
FY 2022	106,000	106,000	185,293
FY 2023	14,200	14,200	153,265
Outyears	–	–	41,517
Total, TPC	**815,000**	**815,000**	**815,000**

Note:

– *In FY 2021, the Office of Science (SC) reprogrammed $2,200,000 of FY 2019 funds, $3,500,000 of FY 2020 funds, and $3,500,000 of FY 2021 funds to the LCLS-II-HE project at SLAC. The FY 2019, FY 2020, and FY 2021 Budget Authority in the table above reflects the reprogrammings. The funds for FY 2023 are required to maintain the project profile.*

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design	209,868	187,921	166,962
Design - Contingency	999	1,717	9,696
Total, Design (TEC)	**210,867**	**189,638**	**176,658**
Equipment	503,727	478,809	465,180
Other Construction	17,000	17,000	17,000
Construction - Contingency	64,906	111,053	137,662
Total, Construction (TEC)	**585,633**	**606,862**	**619,842**
Total, TEC	**796,500**	**796,500**	**796,500**
Contingency, TEC	*65,905*	*112,770*	*147,358*
Other Project Cost (OPC)			
Conceptual Planning	1,000	1,000	1,000
Conceptual Design	7,500	7,500	7,500
Start-up	8,662	7,570	7,100
OPC - Contingency	1,338	2,430	2,900
Total, Except D&D (OPC)	**18,500**	**18,500**	**18,500**
Total, OPC	**18,500**	**18,500**	**18,500**
Contingency, OPC	*1,338*	*2,430*	*2,900*
Total, TPC	**815,000**	**815,000**	**815,000**
Total, Contingency (TEC+OPC)	***67,243***	***115,200***	***150,258***

5. **Schedule of Appropriations Requests**

(dollars in thousands)

Fiscal Year	Type	Prior Years	FY 2021	FY 2022	FY 2023	Outyears	Total
FY 2018	TEC	162,500	—	—	—	556,500	719,000
	OPC	8,500	—	—	—	42,500	51,000
	TPC	171,000	—	—	—	599,000	770,000
FY 2019	TEC	222,500	—	—	—	534,600	757,100
	OPC	8,500	—	—	—	4,400	12,900
	TPC	231,000	—	—	—	539,000	770,000
FY 2020	TEC	515,500	—	—	—	281,000	796,500
	OPC	8,500	—	—	—	10,000	18,500
	TPC	524,000	—	—	—	291,000	815,000
FY 2021	TEC	535,500	150,000	—	—	111,000	796,500
	OPC	8,500	—	—	—	10,000	18,500
	TPC	544,000	150,000	—	—	121,000	815,000
FY 2022	TEC	533,300	160,000	101,000	—	2,200	796,500
	OPC	8,500	—	5,000	—	5,000	18,500
	TPC	541,800	160,000	106,000	—	7,200	815,000
FY 2023	TEC	529,800	156,500	101,000	9,200	—	796,500
	OPC	8,500	—	5,000	5,000	—	18,500
	TPC	538,300	156,500	106,000	14,200	—	815,000

Note:

– *In FY 2021, the Office of Science (SC) reprogrammed $2,200,000 of FY 2019 funds, $3,500,000 of FY 2020 funds, and $3,500,000 of FY 2021 funds to the LCLS-II-HE project at SLAC. The FY 2023 Request in the table above reflects the reprogrammings. The funds for FY 2023 are required to maintain the project profile.*

6. **Related Operations and Maintenance Funding Requirements**

Start of Operation or Beneficial Occupancy	FY 2026
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	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, Maintenance and Repair	18,000	18,000	450,000	450,000

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

7. D&D Information

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

	Square Feet
New area being constructed by this project at ANL	24,000-25,000
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"	24,000-25,000
Area of D&D in this project at ANL	—
Area at other sites to be transferred, sold, and/or D&D outside the project, including area previously "banked"	—
Total area eliminated	—

The gross square feet of the LBB is approximately 25,000, which will house two APS-U beamlines extending beyond the current APS experimental facilities and the support laboratories. This includes the square feet for the Activated Materials Laboratory, funded by the Office of Nuclear Energy.

8. Acquisition Approach

ANL is acquiring 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 has 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 Environment, Safety and Health (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 is procuring 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 is 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 is evaluated through the annual laboratory performance appraisal process.

18-SC-11, Spallation Neutron Source Proton Power Upgrade (PPU), ORNL
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 2023 Request for the Proton Power Upgrade (PPU) project is $17,000,000 of Total Estimated Cost (TEC) funding. The Total Project Cost (TPC) is $271,567,000.

Significant Changes
PPU was initiated in FY 2018. The most recent DOE Order 413.3B approved Critical Decision (CD) is a combined CD-2, Approve Performance Baseline and CD-3, Approve Start of Construction, approved on October 6, 2020. CD-4, Approve Project Completion, is anticipated in 4Q FY 2028. This Construction Project Data Sheet (CPDS) is an update of the FY 2022 CPDS and does not include a new start for FY 2023.

In FY 2021, the project continued R&D, engineering, prototyping, preliminary and final design, testing, fabrication, procurement of baseline and spare hardware, and component integration and installation and civil construction, focusing on initial target procurement, initial cryomodule production, and continued RF equipment procurement, and initiated equipment installation in the klystron gallery. In FY 2022, the project will prioritize the remaining activities of R&D, engineering, prototyping, final design, testing, fabrication, procurement of baseline and spare hardware, component integration and installation, and civil construction site preparation, with priority on continuing RF equipment installation in the klystron gallery, cryomodule assembly, first complete cryomodule receipt, installation of the first two cryomodules in the accelerator, and advancing the target knowledge base by running the first PPU test target during SNS operations. In FY 2023, the project will operate the second PPU test target at increased power levels; install two additional cryomodules and related radiofrequency systems, begin first target station upgrades to support high-flow target gas injection; and start construction of the tunnel stub that will facilitate connection to the future Second Target Station.

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 2020	1/7/09	8/1/17	4/4/18	2Q FY 2021	4Q FY 2022	3Q FY 2022	N/A	3Q FY 2027
FY 2021	1/7/09	8/1/17	4/4/18	2Q FY 2021	4Q FY 2022	2Q FY 2021	N/A	3Q FY 2027
FY 2022	1/7/09	8/1/17	4/4/18	10/6/20	1Q FY 2023	10/6/20	N/A	4Q FY 2028
FY 2023	1/7/09	8/1/17	4/4/18	10/6/20	2Q FY 2022	10/6/20	N/A	4Q 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

Fiscal Year	Performance Baseline Validation	CD-3A	CD-3B
FY 2020	2Q FY 2021	10/5/18	2Q FY 2020
FY 2021	2Q FY 2021	10/5/18	9/3/19
FY 2022	10/6/20	10/5/18	9/3/19
FY 2023	10/6/20	10/5/18	9/3/19

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, Total	TPC
FY 2020	27,300	210,000	237,300	12,700	12,700	250,000
FY 2021	46,700	189,502	236,202	13,798	13,798	250,000
FY 2022	40,000	217,802	257,802	13,798	13,798	271,600
FY 2023	45,300	212,469	257,769	13,798	13,798	271,567

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.

Justification

The Basic Energy Sciences (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 in part by operating large-scale user facilities consisting of a complementary set of intense x-ray 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 Oak Ridge National Laboratory (ORNL) in 2007, currently fulfills the need. The SNS was designed to be upgradeable so as to maintain its position of scientific leadership in the future, in accordance with the 1996 Basic Energy Sciences Advisory Committee (BESAC) (Russell Panel) Report recommendation, and many technical margins were built into the SNS systems to facilitate a power upgrade into the 2 - 4 MW range with the ability to extract some of that power to a second target station.

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

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

Key Performance Parameters (KPPs)

The Threshold KPPs, represent the minimum acceptable performance that the project must achieve. Achievement of the Threshold KPPs will be a prerequisite for approval of CD-4, Project Completion. The Objective KPPs represent the desired project performance.

Performance Measure	Threshold	Objective
Beam power on target	1.7 MW at 1.25 giga-electron volts (GeV)	2.0 MW at 1.3 GeV
Beam energy	1.25 GeV	1.3 GeV
Target reliability lifetime without target failure	1,250 hours at 1.7 MW	1,250 hours at 2.0 MW
Stored beam intensity in ring	≥ 1.6×10^{14} protons at 1.25 GeV	≥ 2.24×10^{14} protons at 1.3 GeV

3. Financial Schedule

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Estimated Cost (TEC)			
Design (TEC)			
FY 2018	5,000	5,000	2,655
FY 2019	16,000	16,000	13,109
FY 2020	14,700	14,700	12,510
FY 2021	9,600	9,600	11,746
FY 2022	–	–	3,700
FY 2023	–	–	1,000
Outyears	–	–	580
Total, Design (TEC)	**45,300**	**45,300**	**45,300**
Construction (TEC)			
FY 2018	31,000	31,000	1,794
FY 2019	44,000	44,000	8,018
FY 2020	45,300	45,300	28,564
FY 2021	42,400	42,400	41,249
FY 2022	17,000	17,000	65,000
FY 2023	17,000	17,000	48,000
Outyears	15,769	15,769	19,844
Total, Construction (TEC)	**212,469**	**212,469**	**212,469**
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	41,074
FY 2021	52,000	52,000	52,995
FY 2022	17,000	17,000	68,700
FY 2023	17,000	17,000	49,000
Outyears	15,769	15,769	20,424
Total, TEC	**257,769**	**257,769**	**257,769**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
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	–	–	92
FY 2021	3,000	3,000	111
FY 2022	–	–	650
FY 2023	–	–	1,800
Outyears	–	–	1,534
Total, OPC	**13,798**	**13,798**	**13,798**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
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	41,166
FY 2021	55,000	55,000	53,106
FY 2022	17,000	17,000	69,350
FY 2023	17,000	17,000	50,800
Outyears	15,769	15,769	21,958
Total, TPC	**271,567**	**271,567**	**271,567**

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design	36,960	32,000	32,000
Design - Contingency	8,340	8,000	8,000
Total, Design (TEC)	**45,300**	**40,000**	**40,000**
Construction	168,502	163,452	163,466
Construction - Contingency	43,967	54,350	54,303
Total, Construction (TEC)	**212,469**	**217,802**	**217,769**
Total, TEC	**257,769**	**257,802**	**257,769**
Contingency, TEC	*52,307*	*62,350*	*62,303*
Other Project Cost (OPC)			
R&D	2,408	2,408	2,408
Conceptual Design	7,250	7,250	7,250
Other OPC Costs	3,480	3,480	3,480
OPC - Contingency	660	660	660
Total, Except D&D (OPC)	**13,798**	**13,798**	**13,798**
Total, OPC	**13,798**	**13,798**	**13,798**
Contingency, OPC	*660*	*660*	*660*
Total, TPC	**271,567**	**271,600**	**271,567**
Total, Contingency (TEC+OPC)	***52,967***	***63,010***	***62,963***

5. **Schedule of Appropriations Requests**

(dollars in thousands)

Fiscal Year	Type	Prior Years	FY 2021	FY 2022	FY 2023	Outyears	Total
FY 2020	TEC	101,000	—	—	—	136,300	237,300
	OPC	10,300	—	—	—	2,400	12,700
	TPC	111,300	—	—	—	138,700	250,000
FY 2021	TEC	156,000	5,000	—	—	75,202	236,202
	OPC	10,798	3,000	—	—	—	13,798
	TPC	166,798	8,000	—	—	75,202	250,000
FY 2022	TEC	156,000	52,000	17,000	—	32,802	257,802
	OPC	10,798	3,000	—	—	—	13,798
	TPC	166,798	55,000	17,000	—	32,802	271,600
FY 2023	TEC	156,000	52,000	17,000	17,000	15,769	257,769
	OPC	10,798	3,000	—	—	—	13,798
	TPC	166,798	55,000	17,000	17,000	15,769	271,567

6. **Related Operations and Maintenance Funding Requirements**

Start of Operation or Beneficial Occupancy	FY 2028
Expected Useful Life	40 years
Expected Future Start of D&D of this capital asset	FY 2068

Related Funding Requirements
(dollars in thousands)

	Annual Costs		Life Cycle Costs	
	Previous Total Estimate	**Current Total Estimate**	**Previous Total Estimate**	**Current Total Estimate**
Operations, Maintenance and Repair	9,325	9,325	373,000	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

Based on the DOE determination at CD-1, the PPU project is being 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 is partnering with other laboratories for design and procurement of key technical subsystem components. Some technical system designs will require research and development activities. 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 have been sought and are being applied as appropriate 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 (ALS-U), LBNL
Lawrence Berkeley National Laboratory
Project is for Design and Construction

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

Summary

The FY 2023 Request for the Advanced Light Source Upgrade (ALS-U) project is $135,000,000 of Total Estimated Cost (TEC) funding. The project has a Total Project Cost (TPC) of $590,000,000.

Significant Changes

The ALS-U was initiated in FY 2018. The most recent DOE Order 413.3B approved Critical Decision (CD) is CD-2, Approve Performance Baseline, approved on April 2, 2021. This Construction Project Data Sheet (CPDS) is an update of the FY 2022 CPDS and does not include a new start for FY 2023.

FY 2021 funding continued support of planning, engineering, design, R&D, prototyping activities, and long-lead procurements. FY 2022 funding continues support of planning, engineering, design, R&D, prototyping, and procurements of both long-lead components for the accumulator ring installation as well as start of major procurements for the storage ring systems and components. In addition, FY 2022 funding will support advancing the design for the radiation shielding and required seismic upgrades. FY 2023 funding will continue support of planning, engineering, design, R&D, prototyping, testing, and procurements with an emphasis on accumulator, beamline, insertion device, and storage ring procurements and continue installation of the accumulator ring in the ALS tunnel.

As final design and long-lead time procurements progress, COVID-19 impacts have required use of both cost and schedule contingency. The COVID-19 pandemic continues to affect personnel, cause supply chain delays in deliveries, and increase costs for staff/procurements/subcontracts. The project and program are carefully monitoring progress, cost estimates, and contingency, with options under active evaluation in the event of unacceptable cost/schedule impacts.

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	9/27/16	4/30/18	9/21/18	2Q FY 2021	4Q FY 2021	1Q FY 2022	N/A	2Q FY 2028
FY 2022	9/27/16	4/30/18	9/21/18	4/2/21	2Q FY 2022	3Q FY 2022	N/A	4Q FY 2029
FY 2023	9/27/16	4/30/18	9/21/18	4/2/21	4Q FY 2022	1Q FY 2023	N/A	4Q 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
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	4Q FY 2020	4Q FY 2020
FY 2020	2Q FY 2021	4Q FY 2019
FY 2021	2Q FY 2021	12/19/19
FY 2022	4/2/21	12/19/19
FY 2023	4/2/21	12/19/19

CD-3A – Approve Long-Lead Procurements scope included the equipment required for the electron accumulator ring.

Project Cost History

(dollars in thousands)

Fiscal Year	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, Total	TPC
FY 2019	39,000	243,000	282,000	38,000	38,000	320,000
FY 2020	89,750	248,250	338,000	30,000	30,000	368,000
FY 2021	89,750	290,450	380,200	30,000	30,000	410,200
FY 2022	135,711	426,289	562,000	28,000	28,000	590,000
FY 2023	134,340	427,660	562,000	28,000	28,000	590,000

2. Project Scope and Justification

Scope

The ALS-U project will upgrade the existing ALS facility by replacing the existing electron storage ring with a new electron storage ring based on a multi-bend achromat (MBA) lattice design to provide a soft x-ray source that is orders of magnitude 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 inner shield wall to enable on- and off-axis, swap-out injection and extraction into and from the new storage ring 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 two new undulator beamlines that are optimized for the novel science made possible by the beam's new high coherent flux. The project intends to reuse the existing building, utilities, electron gun, linac, and booster synchrotron equipment currently at ALS. Prior to CD-2, the scope was increased to include radiation shielding and safety-mandated seismic structural upgrades to the ALS facility. 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 but not above that. NSLS-II is somewhat lower in brightness than the new Swedish light source, MAX-IV, which began user operations in 2017 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 the 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 is possible with LCLS-II 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 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 x 10^{19}	≥ 2 x 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 (TEC)			
FY 2018	16,000	16,000	–
FY 2019	35,000	35,000	22,054
FY 2020	29,770	29,770	30,386
FY 2021	33,570	33,570	32,775
FY 2022	20,000	20,000	28,947
FY 2023	–	–	14,681
Outyears	–	–	5,497
Total, Design (TEC)	**134,340**	**134,340**	**134,340**
Construction (TEC)			
FY 2019	25,000	25,000	–
FY 2020	30,230	30,230	6,260
FY 2021	28,430	28,430	12,415
FY 2022	55,100	55,100	31,211
FY 2023	135,000	135,000	123,604
Outyears	153,900	153,900	254,170
Total, Construction (TEC)	**427,660**	**427,660**	**427,660**
Total Estimated Cost (TEC)			
FY 2018	16,000	16,000	–
FY 2019	60,000	60,000	22,054
FY 2020	60,000	60,000	36,646
FY 2021	62,000	62,000	45,190
FY 2022	75,100	75,100	60,158
FY 2023	135,000	135,000	138,285
Outyears	153,900	153,900	259,667
Total, TEC	**562,000**	**562,000**	**562,000**

(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	3,262
Outyears	–	–	4,440
Total, OPC	**28,000**	**28,000**	**28,000**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
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	39,908
FY 2021	62,000	62,000	45,190
FY 2022	75,100	75,100	60,158
FY 2023	135,000	135,000	138,285
Outyears	153,900	153,900	264,107
Total, TPC	**590,000**	**590,000**	**590,000**

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design	101,098	95,702	92,967
Design - Contingency	33,242	40,009	38,778
Total, Design (TEC)	**134,340**	**135,711**	**131,745**
Construction	150,093	N/A	142,165
Equipment	171,743	300,615	161,449
Construction - Contingency	105,824	125,674	126,641
Total, Construction (TEC)	**427,660**	**426,289**	**430,255**
Total, TEC	**562,000**	**562,000**	**562,000**
Contingency, TEC	*139,066*	*165,683*	*165,419*
Other Project Cost (OPC)			
R&D	4,971	8,200	8,241
Conceptual Planning	2,000	2,000	2,000
Conceptual Design	12,100	12,100	12,100
Start-up	2,000	2,000	2,000
OPC - Contingency	6,929	3,700	3,659
Total, Except D&D (OPC)	**28,000**	**28,000**	**28,000**
Total, OPC	**28,000**	**28,000**	**28,000**
Contingency, OPC	*6,929*	*3,700*	*3,659*
Total, TPC	**590,000**	**590,000**	**590,000**
Total, Contingency (TEC+OPC)	***145,995***	***169,383***	***169,078***

5. Schedule of Appropriations Requests

(dollars in thousands)

Fiscal Year	Type	Prior Years	FY 2021	FY 2022	FY 2023	Outyears	Total
FY 2019	TEC	10,000	—	—	—	272,000	282,000
	OPC	12,000	—	—	—	26,000	38,000
	TPC	22,000	—	—	—	298,000	320,000
FY 2020	TEC	89,000	—	—	—	249,000	338,000
	OPC	28,000	—	—	—	2,000	30,000
	TPC	117,000	—	—	—	251,000	368,000
FY 2021	TEC	136,000	13,000	—	—	231,200	380,200
	OPC	28,000	—	—	—	2,000	30,000
	TPC	164,000	13,000	—	—	233,200	410,200
FY 2022	TEC	136,000	62,000	75,100	—	288,900	562,000
	OPC	28,000	—	—	—	—	28,000
	TPC	164,000	62,000	75,100	—	288,900	590,000
FY 2023	TEC	136,000	62,000	75,100	135,000	153,900	562,000
	OPC	28,000	—	—	—	—	28,000
	TPC	164,000	62,000	75,100	135,000	153,900	590,000

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	FY 2029
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	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, Maintenance and Repair	—	—	—	—

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

Based on the DOE determination at CD-1, Lawrence Berkeley National Laboratory (LBNL) is acquiring the ALS-U project under the existing DOE Management and Operations (M&O) contract.

The ALS-U project 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. 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 are being competitively bid and awarded based on best value to the government. The M&O contractor's performance is being evaluated through the annual laboratory performance appraisal process.

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

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

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

Summary

The FY 2023 Request for the Linac Coherent Light Source-II High Energy (LCLS-II-HE) project is $90,000,000 of Total Estimated Cost (TEC) funding and $4,000,000 of Other Project Costs (OPC) funding. This project at CD-1 established a preliminary Total Project Cost (TPC) range of $290,000,000 to $480,000,000. This cost range encompassed the most feasible preliminary alternatives at CD-1. Pending CD-2 reviews, the project's TPC estimate is likely to exceed the current level of $660,000,000, and could approach $710,000,000 when COVID-driven cost and schedule increases are included.

Significant Changes

The LCLS-II-HE project was initiated in FY 2019. The most recent DOE Order 413.3B approved Critical Decision (CD) is CD-3A, Approve Long-Lead Procurements, which was approved on May 12, 2020. The LCLS-II-HE project is continuing to assess the impact of COVID-19 on the project's cost, schedule, and project milestones. The combined CD-2/3 approval is projected for 4Q FY 2023 and CD-4 is now projected for 2Q FY 2031. This Construction Project Data Sheet (CPDS) is an update of the FY 2022 CPDS and does not include a new start for FY 2023.

FY 2021 funding continued engineering, design, R&D, prototyping, and long-lead procurements of construction items. FY 2022 funding supports engineering, design, R&D, prototyping, continuing long-lead procurements, and advancing the preliminary and final designs. Priority activities include initiating the low emittance injector design and cryomodule production at the partner labs. FY 2023 funding will continue engineering, design, R&D, prototyping, long-lead procurements, low emittance injector designs, cryomodule production at the partner labs, and preparations for baselining the project, and will start prototype gun production.

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	12/15/16	3/23/18	9/21/18	2Q FY 2023	1Q FY 2023	2Q FY 2023	N/A	1Q FY 2029
FY 2022	12/15/16	3/23/18	9/21/18	4Q FY 2022	3Q FY 2022	4Q FY 2022	N/A	2Q FY 2030
FY 2023	12/15/16	3/23/18	9/21/18	4Q FY 2023	3Q FY 2025	4Q FY 2023	N/A	2Q FY 2031

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

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	2Q FY 2023	2Q FY 2020
FY 2022	4Q FY 2022	5/12/20
FY 2023	4Q FY 2023	5/12/20

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

<u>Project Cost History</u>

(dollars in thousands)

Fiscal Year	TEC, Design	TEC, Construction	TEC, Total	OPC, Except D&D	OPC, Total	TPC
FY 2019	34,000	266,000	300,000	20,000	20,000	320,000
FY 2020	34,000	314,000	348,000	20,000	20,000	368,000
FY 2021	34,000	374,000	408,000	20,000	20,000	428,000
FY 2022	39,000	589,000	628,000	32,000	32,000	660,000
FY 2023	39,000	589,000	628,000	32,000	32,000	660,000

2. Project Scope and Justification

<u>Scope</u>

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, generated by a superconducting electron source, 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. Additional scope is being considered to address several risks associated with the linac performance, operation reliability and scientific mission capability.

<u>Justification</u>

The leadership position of LCLS-II will be challenged by the European x-ray free electron laser (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- 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 2022–2024 is the first step to address this capability gap. LCLS-II will be the premier 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 fully address the capability gaps and 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 (TEC)			
FY 2018	2,000	2,000	–
FY 2019	10,000	10,000	130
FY 2020	8,000	8,000	2,884
FY 2021	8,000	8,000	9,554
FY 2022	6,000	6,000	15,000
FY 2023	3,000	3,000	4,000
Outyears	2,000	2,000	7,432
Total, Design (TEC)	**39,000**	**39,000**	**39,000**
Construction (TEC)			
FY 2018	6,000	6,000	–
FY 2019	15,200	15,200	4,270
FY 2020	31,957	31,957	19,620
FY 2021	47,500	47,500	41,497
FY 2022	44,000	44,000	50,000
FY 2023	87,000	87,000	75,000
Outyears	357,343	357,343	398,613
Total, Construction (TEC)	**589,000**	**589,000**	**589,000**
Total Estimated Cost (TEC)			
FY 2018	8,000	8,000	–
FY 2019	25,200	25,200	4,400
FY 2020	39,957	39,957	22,504
FY 2021	55,500	55,500	51,051
FY 2022	50,000	50,000	65,000
FY 2023	90,000	90,000	79,000
Outyears	359,343	359,343	406,045
Total, TEC	**628,000**	**628,000**	**628,000**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
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	4,081
FY 2021	2,000	2,000	1,507
FY 2022	3,000	3,000	4,000
FY 2023	4,000	4,000	2,500
Outyears	11,000	11,000	16,680
Total, OPC	**32,000**	**32,000**	**32,000**

(dollars in thousands)

	Budget Authority (Appropriations)	Obligations	Costs
Total Project Cost (TPC)			
FY 2018	10,000	10,000	1,191
FY 2019	31,200	31,200	6,441
FY 2020	43,957	43,957	26,585
FY 2021	57,500	57,500	52,558
FY 2022	53,000	53,000	69,000
FY 2023	94,000	94,000	81,500
Outyears	370,343	370,343	422,725
Total, TPC	**660,000**	**660,000**	**660,000**

Note:

– *In FY 2021, the Office of Science reprogrammed $19,343,211.24 of prior year funds from this project to support the LCLS-II project at SLAC. The Prior Year Budget Authority in the table above reflects this reprogramming. Also in FY 2021, a total of $10,000,000 in current year and prior year funding was reprogrammed to the LCLS-II-HE project and additional funds are included in the outyears to maintain the project profile.*

4. Details of Project Cost Estimate

(dollars in thousands)

	Current Total Estimate	Previous Total Estimate	Original Validated Baseline
Total Estimated Cost (TEC)			
Design	35,000	35,000	**N/A**
Design - Contingency	4,000	4,000	**N/A**
Total, Design (TEC)	**39,000**	**39,000**	**N/A**
Construction	33,000	N/A	**N/A**
Site Preparation	9,000	8,000	**N/A**
Equipment	468,000	410,000	**N/A**
Other Construction	N/A	29,000	**N/A**
Construction - Contingency	79,000	142,000	**N/A**
Total, Construction (TEC)	**589,000**	**589,000**	**N/A**
Total, TEC	**628,000**	**628,000**	**N/A**
Contingency, TEC	*83,000*	*146,000*	***N/A***
Other Project Cost (OPC)			
R&D	15,000	12,000	**N/A**
Conceptual Planning	2,000	2,000	**N/A**
Conceptual Design	2,000	2,000	**N/A**
Start-up	8,000	8,000	**N/A**
OPC - Contingency	5,000	8,000	**N/A**
Total, Except D&D (OPC)	**32,000**	**32,000**	**N/A**
Total, OPC	**32,000**	**32,000**	**N/A**
Contingency, OPC	*5,000*	*8,000*	***N/A***
Total, TPC	**660,000**	**660,000**	**N/A**
Total, Contingency (TEC+OPC)	***88,000***	***154,000***	***N/A***

5. Schedule of Appropriations Requests

(dollars in thousands)

Fiscal Year	Type	Prior Years	FY 2021	FY 2022	FY 2023	Outyears	Total
FY 2019	TEC	5,000	—	—	—	295,000	300,000
	OPC	2,000	—	—	—	18,000	20,000
	TPC	7,000	—	—	—	313,000	320,000
FY 2020	TEC	50,000	—	—	—	298,000	348,000
	OPC	12,000	—	—	—	8,000	20,000
	TPC	62,000	—	—	—	306,000	368,000
FY 2021	TEC	86,000	14,000	—	—	308,000	408,000
	OPC	12,000	2,000	—	—	6,000	20,000
	TPC	98,000	16,000	—	—	314,000	428,000
FY 2022	TEC	66,657	52,000	50,000	—	459,343	628,000
	OPC	12,000	2,000	3,000	—	15,000	32,000
	TPC	78,657	54,000	53,000	—	474,343	660,000
FY 2023	TEC	73,157	55,500	50,000	90,000	359,343	628,000
	OPC	12,000	2,000	3,000	4,000	11,000	32,000
	TPC	85,157	57,500	53,000	94,000	370,343	660,000

Note:

– *In FY 2021, the Office of Science reprogrammed $19,343,211.24 of prior year funds from this project to support the LCLS-II project at SLAC. The Prior Year Budget Authority in the table above reflects this reprogramming. Also in FY 2021, a total of $10,000,000 in current year and prior year funding was reprogrammed to the LCLS-II-HE project and additional funds are included in the outyears to maintain the project profile.*

6. Related Operations and Maintenance Funding Requirements

Start of Operation or Beneficial Occupancy	FY 2031
Expected Useful Life	25 years
Expected Future Start of D&D of this capital asset	FY 2056

Related Funding Requirements
(dollars in thousands)

	Annual Costs		Life Cycle Costs	
	Previous Total Estimate	**Current Total Estimate**	**Previous Total Estimate**	**Current Total Estimate**
Operations, Maintenance and Repair	21,500	21,500	537,500	537,500

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

Based on the DOE determination at CD-1, SLAC National Accelerator Laboratory is acquiring the LCLS-II-HE project under the existing DOE Management and Operations (M&O) contract.

SLAC has completed a Conceptual Design Report for the LCLS-II-HE project and is in the preliminary design phase, identifying 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 operating and are maintained as a SLAC-wide resource.

SLAC is partnering with other laboratories for design and procurement of key technical subsystem components. Technical system designs 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 is fully exploiting 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 are exploited fully in planning and executing LCLS-II-HE.