Office of Science Priority Research Areas for SCGSR Program

Priority Research Areas for SCGSR 2023 Solicitation 1

It is an Eligibility Requirement that applicants to the DOE SCGSR Program must be pursuing graduate research aligned with one or more of the Priority Research Areas for a specific solicitation call. The applicant's proposed SCGSR research project to be conducted at a DOE laboratory must address stated aims in at least one of the priority areas listed for that solicitation.

The priority research areas for SCGSR 2023 Solicitation 1 consist of both convergence research topics of interest to multiple Office of Science (SC) program offices and those primarily from one SC program office. The SC program offices include: Advanced Scientific Computing Research (**ASCR**), Basic Energy Sciences (**BES**), Biological and Environmental Research (**BER**), Fusion Energy Sciences (**FES**), High Energy Physics (**HEP**), Nuclear Physics (**NP**), Isotope R&D and Production (**DOE IP**), and Accelerator R&D and Production (**ARDAP**). A brief overview of the Office of Science SCGSR program is available here, and detailed information about a specific program office can be found at the Office of Science website (https://science.osti.gov/Programs).

Descriptions below are provided to help understand the scope and focus of each priority area for SCGSR 2023 Solicitation 1. Please note: some areas have exclusions**.** Applicants must identify in the online application system which listed priority research area their proposed SCGSR research project is most aligned with. **It is strongly recommended that applicants carefully read the full descriptions of priority areas of consideration and consult with the SCGSR program, if necessary, before making a final selection.** Applications with a proposed research project that does not explicitly address an Office of Science research priority area and/or does not make specific reference to the stated aims of one of the listed areas below will NOT be considered.

I. Convergence Research Topical Areas

Introduction

The call for SCGSR applications on convergence research topics encourages forward-looking ideas, innovative concepts, and exploratory approaches that reflect the DOE Office of Science's emerging areas and strategic priorities through collaboration across existing disciplinary boundaries. Convergence research topics, by nature, bring together people from different academic disciplines and/or different sub-areas represented in the Office of Science, and are formed for achievements possible only through such integration. People from different disciplinary cultures intermingle on, and benefit from, different perspectives, languages, knowledge, theories, methods, and tools, in the pursuit of shared research interests and challenges. Their integration on multiple dimensions and at multiple scales may give birth to new disciplines, frameworks, and approaches that bring about profound, long-lasting impact on multiple communities. For proposed SCGSR research projects, the combination of different talents is expected to be expressly cross-cutting to achieve an advance specifically enabled by transdisciplinary efforts. The basic research team for an SCGSR project consists of a graduate student, the primary graduate thesis advisor, and a collaborating DOE laboratory scientist at the DOE host laboratory. Due to the convergent nature of the research topics in this Section, it is required that the team members come from different disciplinary backgrounds (including different sub-areas represented in the Office of Science), or at least that the graduate student and his/her collaborating DOE laboratory scientist be from different disciplines. Furthermore, it is encouraged to engage other DOE laboratory scientists from different disciplines, as necessary, during the project period and beyond.

Training graduate students at the convergence of multiple- and trans-disciplinary scientific discoveries and communities has been identified as a top priority for U.S. workforce development. Since its inception in 2014, the SCGSR program has demonstrated strength in preparing graduate students for science, technology, engineering, or mathematics (STEM) careers of critical importance to the DOE Office of Science mission through extended graduate research residence at DOE national laboratories and facilities. The inherent inter- and multi-disciplinary nature of the team science culture and world-class scientific facilities at national laboratories nurtures a workforce development ecosystem that readily addresses transdisciplinary research challenges of national importance. The graduate training opportunities in convergence research topical areas at national laboratories are expected to help accelerate graduate students' research and professional growth through access to multiple disciplinary talents and resources, and to prepare graduate students for careers in cutting-edge transdisciplinary research fields.

The Department of Energy's Office of Science supports a broad spectrum of basic research endeavors, from fundamental studies within a single academic discipline to collaborations involving multiple disciplines at both domestic and international scales. The convergence research topical areas shown here represent cross-cutting research themes and shared interests across the Office of Science's research program offices. Each area shown below is associated with research interests from at least two or more Office of Science program offices. SCGSR applications submitted to one of the following convergence research areas must address research topic(s) of interest to at least two of the participating DOE Office of Science's programs for that area, and are subject to evaluation by the relevant program offices. Based on the evaluation of proposed research focus and scope, an SCGSR application selecting one of the convergence research areas may be considered better aligned with one of the non-convergence research areas and be subject to further evaluation in a non-convergence research area under an Office of Science program office in this solicitation. **If applicants are not certain if they should submit an application to a convergence area in this section or a non-convergence area under a single Office of Science's program office, it is recommended to submit the application to the convergence area first.**

The convergence research topical areas for the SCGSR program include:

(a) Microelectronics (Participating Programs: ASCR, BES, HEP, and NP)

The Department of Energy's Office of Science programs have always been at the cutting edge of microelectronics, both as a consumer and as an engine of scientific understanding that has enabled many of the technological breakthroughs adopted by industry. This has driven transformative advances in microelectronics for the challenging demands of DOE's high-performance computing, scientific user facilities, and discovery science experiments. Today, the end of Moore's Law, along with the emergence of new computing and sensing workloads and rapidly expanding data volumes, have resulted in an unprecedented need and opportunity to "redesign" the microelectronics innovation process to continue to satisfy the ever growing demands. In addition, greatly improved microelectronics are needed for the nation's electricity grid if it is to be energy-efficient, resilient to natural phenomena and intentional attack, and agile in adapting to fluctuations in power demand and generation. Sustained and rapid progress in microelectronics science and technology from millivolt to megavolt scales is thus essential if we are to continue pushing the boundaries of science within DOE and, more significantly, to continue to lead the global information and power technology revolution.

In this context, the term "microelectronics" is used broadly to refer to semiconductors and related materials, processing chemistries, design, fabrication, packaging, sensors, devices, integrated circuits, processors, computing paradigms and architectures, modeling and simulation, software tools, and related technologies. To enable continued advances in sensing, computing, communication, networking, and power technologies, a fundamental rethinking is needed of the science behind the materials and chemistries, synthesis and fabrication, device physics, energy efficiency, architectures, algorithms, and software. These advances must be developed collectively in a spirit of co-design, where each scientific discipline informs and engages the other to achieve orders-of-magnitude improvements in system-level performance. Co-design involves multi-disciplinary collaboration that takes into account the interdependencies among material properties, device physics, architectures, and the software stack for developing the microelectronics systems of the future.

Applications should embrace a multi-disciplinary approach to address DOE's microelectronics needs in the areas of computing, instrumentation for scientific user facilities and discovery science experiments, and power grid management.

Relevant topics are outlined in the priority research directions from the Basic Research Needs for Microelectronics Workshop report (https://science.osti.gov/-/media/bes/pdf/reports/2019/BRN_Microelectronics_rpt.pdf).

EXCLUSIONS: Activities that focus on Quantum Information Science or Quantum Computing will NOT be considered.

(b) Data Science (Participating Programs: ASCR, BES, BER, FES, HEP, and NP)

Data science combines computer science, applied mathematics, and statistics with domain science to discover new knowledge from often complex (such as unstructured or heterogenous) data sets generated from experimental and/or computational studies. As part of data science, machine learning and artificial intelligence methods are rapidly evolving and leading to more accurate predictions and trustworthy decisions and actions. Thus, these methods are being applied widely in society. Data science has already had an impact in areas such as the chemical and materials sciences as well as bioinformatics, medicine, drug discovery, systems control, geophysics, astronomy, and particle physics. Many opportunities still remain for data science to accelerate the rate of fundamental discovery.

The DOE SC programs express their interest in receiving applications that focus on innovative applications of modern data science approaches (artificial intelligence, machine learning, deep learning, etc.) and/or approaches to data capture and management that would enable data science for cutting-edge research relevant to the Office of Science. A priority outcome from this research should be increased capture, integration, and use of scientific data relevant to SC research and database interoperability to develop novel, robust, data-driven, hypothesis-based models that lead to improved understanding and advancement of energy research. The proposed research activities, for example, may entail novel data science approaches to enable real-time control of experiments through feedback from predictive simulations and data models, or the unleashing and enhancement of high-value DOE research data in ways that are findable, accessible, interoperable, and reusable (FAIR) by other researchers. Research activities that align with the SC Public Reusable Research (PuRe) Data Resources initiative and engage the data repositories, knowledge bases, and analysis platforms it supports, are encouraged. Use of data models should fill knowledge gaps, correct erroneous predictions based on existing models, extract knowledge from noisy data, and ideally extrapolate beyond the range of the available datasets.

EXCLUSIONS: Quantum computing or quantum systems for quantum information science; 'omics' data and systems biology approaches; applied research, such as design or optimization of instruments, devices, or tools; areas covered already in the topics for ASCR, BES, BER, FES, HEP, and NP.

(c) Conservation Laws and Symmetries (Participating Programs: HEP and NP)

The study of conservation laws and the symmetries of nature is a cross-cutting area at the core of understanding particle physics, nuclear physics, astrophysics, and condensed-matter physics. Symmetries (and their violations) provide convergent themes for our picture of Nature and the Universe, from the smallest constituents of matter through nuclei and condensed-matter systems to astronomical scales. The study of the symmetries of matter and space-time has greatly improved our understanding of their properties and started a hundred years ago with the seminal work of Emmy Noether. Such symmetries or invariants of the system underpin conservation laws, novel states of matter, classical and quantum phase transitions, and the existence of exotic particles. For example, exotic excitations predicted a long time ago in one subfield of physics have been observed in condensed matter physics in the form of quasiparticles. Examples include relativistic Dirac fermions, Weyl fermions, Majorana fermions, Laughlin quasiparticles, skyrmions, and Cooper pairs. Conformal field theories, topology, duality, or emergent gravity in strongly interacting systems offer new descriptions or means to probe and control quantum states at unprecedented accuracy and fidelity. Relevant studies in nuclear and particle physics include searches for breaking of time-reversal symmetry with electric dipole moments of leptons, nucleons, and nuclei, CP-violation in the neutrino sector, and searches for new particles and currents in precision studies of nuclear decays. Research in these areas, both experimental and theoretical, is actively pursued across the convergent disciplines.

EXCLUSIONS: Activities that focus on Quantum Information Science or Quantum Computing will NOT be considered.

(d) Accelerator Science (Participating Programs: ASCR, BES, BER, FES, HEP, NP, DOE IP, and ARDAP)

Today, particle beams from over 30,000 accelerators worldwide play an important role in scientific discovery and in application areas ranging from diagnosing and treating disease to powering industrial processes. To remain competitive for accelerator innovation, a sustained, cross-disciplinary effort on advancing the basic science is required. In 2008, the Department of Energy's Office of Science has launched an initiative to encourage breakthroughs in accelerator science and their translation into applications for the nation's health, prosperity, and security. Moreover, vibrant research areas/topics have been established in multiple research programs under the DOE Office of Science (such as BES, FES, HEP, NP, DOE IP, and ARDAP), and funding has been provided for research and development activities in DOE national laboratories and universities nationwide. Continued U.S. innovation and leadership in basic accelerator research and in the areas of energy, environment and national security, rests on the next generation of accelerator scientists. DOE national laboratories host a comprehensive suite of world-class accelerator facilities and detector laboratories, as well as provide training opportunities that are not always available in a university setting. Applicants are encouraged to take advantage of graduate research and training opportunities at DOE national laboratories in the area of Accelerator Science.

Applications submitted to the convergence research area on Accelerator Science must address research topic(s) of interest to at least two of the participating DOE Office of Science's programs (ASCR, BES, BER, FES, HEP, NP, DOE IP, and ARDAP). Please refer to the description of the non-convergence area/topic on Accelerator/Detector R&D under a single SC program office for specific topics of interest. **If applicants are not certain if they should submit an application to this convergence area or a non-convergence area under a single program office, it is recommended to submit the application to the convergence area on Accelerator Science first.** Applications submitted under the convergence area that are not accepted as a convergence area application will still have the chance to be considered in a non-convergence area/topic on Accelerator/Detector R&D under a single program if the proposed research addresses the interest of that program.

II. Advanced Scientific Computing Research (ASCR)

The Advanced Scientific Computing Research (ASCR) program's mission is to advance applied mathematics and computer science; deliver the most sophisticated computational scientific applications in partnership with disciplinary science; advance computing and networking capabilities; and develop future generations of computing hardware and software tools for science and engineering in partnership with the research community, including U.S. industry.
ASCR supports cross-disciplinary research in which other domains of scientific inquiry may provide the data to provide use-cases for computer scientists and applied mathematicians to devise generalized methods, models, algorithms, and tools. ASCR's interest in these fields is not to solve the specific problems in other scientific domains but to use those challenges to advance the state of the art and increase knowledge in its fields of research.

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Program Website: https://science.osti.gov/ascr/

The priority areas for ASCR include the following:

- Develop mathematical models, methods, and algorithms to accurately describe and predict the behavior of complex systems involving processes that span vastly different time and/or length scales.
- Advance key areas of computer science that:
    - Enable the design and development of extreme scale computing systems and their effective use in the path to scientific discoveries; and

    - Transform extreme scale data from experiments and simulations into scientific insight.
- Advance key areas of computational science and discovery that support the missions of SC through mutually beneficial partnerships.
- Develop and deliver forefront computational, networking and collaboration tools and facilities that enable scientists worldwide to work together to extend the frontiers of science.

The computing resources and high-speed networks required to meet SC needs exceed the state of- the-art by a significant margin. Furthermore, the system software, algorithms, software tools and libraries, programming models and the distributed software environments needed to accelerate scientific discovery through modeling and simulation are often beyond the realm of commercial interest. To establish and maintain DOE's modeling and simulation leadership in scientific areas that are important to its mission, ASCR operates Leadership Computing facilities, a high-performance production computing center, and a high-speed network, implementing a broad base research portfolio in applied mathematics, computer and network sciences, and computational science to solve complex problems on computational resources that are on a trajectory to reach exascale and beyond.

ASCR's research priority areas for SCGSR program include:

(a) Applied Mathematics

This subprogram supports basic research leading to fundamental mathematical advances and computational breakthroughs across DOE and SC missions. Important areas of basic research include:

- novel deterministic or randomized numerical methods for the scalable solution of large-scale, linear and nonlinear systems of equations, including those solution methods that take into consideration the possibilities brought about by future HPC architectures;
- optimization techniques and next-generation solvers;
- numerical methods for modeling multiscale, multiphysics, or multi-component continuous or discrete systems that span a wide range of time and length scales;
- methods of simulation and analysis of systems that account for the uncertainties of the systems, or are inherently stochastic or uncertain;
- innovative approaches for analyzing, extracting insight from, or reducing large-scale data sets; and
- foundational research in Scientific Machine Learning (Scientific ML) and Artificial Intelligence (AI) as a cross-cutting area of interest for enabling greater adaptivity, automation, and predictive capabilities in scientific computing.

EXCLUSIONS: Development and/or implementation of existing numerical methods to a specific application is NOT within the scope of this program, no matter how challenging the application.

(b) Computer Science

The Computer Science research program supports research that enables computing and networking at extreme scales and the understanding of extreme scale, or complex data from both simulations and experiments. It aims to make high performance scientific computers and networks highly productive and efficient to solve scientific challenges while attempting to reduce domain science application complexity as much as possible. The computer science program does this in the context of sharp increases in the heterogeneity and complexity of computing systems; the need to seamlessly and intelligently integrate simulation, data analysis, and other tasks into coherent and usable workflows; and the challenges posed by highly novel computing platforms such as neuromorphic systems. Priority interests for the program include the following:

- Data management, analysis, and visualization: SC-supported researchers and facilities are generating large, complex, multi-modal data at unprecedented rates. There is a need for advanced visualizations and visual analytics tools for making sense of these data and making operational decisions. This program solicits research to develop techniques for deriving and visualizing insights from large scale and/or complex simulation, experimental, or observational data or combinations of these as relevant to SC and DOE priority applications: Visual analysis of high-dimensional data at scale, data from multiple sources and of varying types, attributes such as uncertainty, and data in the context of domain-specific knowledge; and Visual analytic approaches to understanding artificial intelligence/machine learning outcomes or the state and behavior of a supercomputing system at scale. This program also solicits techniques and tools for advancing findable, accessible, interoperable reusable (FAIR) data practices of management, archiving, curation, and/or reuse, of data generated by experimental, observational, and simulation relevant to SC mission areas. Additional areas of interest include combining of data streaming and cloud storage uses for SC infrastructure as well as visualization needs at the edge for SC experimental facilities.
- In Situ Data Management (ISDM): Scientific computing will increasingly incorporate a number of different tasks that need to be managed along with the main simulation or experimental tasks—for example, ensemble analysis, data-driven science, artificial intelligence, machine learning, surrogate modeling, and graph analytics. Many of these tasks will need to execute concurrently, that is, in situ, with simulations and experiments sharing the same computing resources. ISDM capabilities can enable scientific discovery from a broad range of data sources—i.e. HPC simulations, experiments, scientific instruments, and sensor networks—over a wide scale of computing platforms: leadership-class HPC, clusters, clouds, workstations, and embedded devices at the edge. ISDM capabilities can also manage large data volumes from computations and experiments to minimize data movement, save storage space, and boost resource efficiency—often while simultaneously increasing scientific precision. This program solicits research to advance ISDM capabilities to run on computing platforms at a variety of scales; to be automated and controllable; to be more interoperable and composable; and to use provenance and metadata for transparent results. This program also solicits co-designed research activities for ISDM as well as new in situ algorithms.
- Storage Systems and I/O: The success of the DOE computational, experimental, and observational sciences is inextricably tied to the usability, performance, and reliability of emerging storage systems and input/output (SSIO) technologies. SSIO technologies involve the organization, movement, placement, and efficient retrieval of data to enhance computation and discovery. This program solicits research to improve SSIO capabilities that enable science understandability and reproducibility; accelerate scientific discovery; enhance SSIO usability,

performance, and resilience; and improve efficiency and integrity of data movement and storage. One particular focus of this program is to improve pipelines for analysis-centric, data intensive workflows on high performance computing (HPC) systems, and that use large-scale storage.

- Programming Models, Environments, and Portability: Innovative programming models for developing applications on next-generation platforms, exploiting unprecedented parallelism, heterogeneity of memory systems (e.g. Non-Uniform Memory Access [NUMA], non-coherent shared memory, high-bandwidth memory [HBM], scratchpads, and heterogeneity of processing (e.g., Graphics Processing Units [GPUs], Field Programmable Gate Arrays [FPGAs], Coarse-Grained Reconfigurable Architectures [CGRAs], other types of accelerators, big-small cores, processing in memory, and near memory, etc.), with particular emphasis on making it easier to program at scale. Basic research on programming tools for all phases of the software-development cycle are relevant, including but not limited to, design, implementation, verification, optimization, and integration. Particularly welcome are methods that infuse artificial intelligence/machine learning into the programming environment.
- Operating and Runtime Systems: System software that provides intelligent, adaptive resource management and support for highly-parallel software and workflow-management systems, and that facilitates effective and efficient use of heterogeneous computing technologies, including diverse execution models, processors, accelerators, memory, and storage systems. Target workloads include modeling and simulation, data analysis, and the processing of large-scale, streaming data from experiments.
- Performance Portability and Co-design: Methods that support performance portability, which provides the ability to efficiently use diverse kinds of hardware platforms with minimal changes to the application source code, and/or hardware/software co-design, which is a method for designing and/or adapting both hardware and software design as part of a holistic process. These methods include automated and semi-automated refinements from high-level specification of an application and/or hardware design to low-level code, optimized when compiled and/or, for software, at runtime, to different HPC platforms. The focus is on enabling performance portability of, and/or the design of future hardware for, applications developed for extreme-scale computing and beyond.
- Distributed Scheduling and Resource Management: As scientific-computing resources are being called upon to support a wide variety of workloads, including those that tightly integrate large-scale and ensemble simulation and data-analysis workflows with experimental data collection and control, the algorithms and implementations matching computational requirements to resources need to scale to handle more tasks, more resources, and more-widely-distributed resources. Specifically sought are methods for decentralized, resilient, secure resource management, scheduling, and coupled data transfer across widely-distributed computing facilities; and modeling of such distributed systems.

EXCLUSIONS: Topics that are out of scope for Computer Science include:

- Applications that address topics not covered in the list of Computer Science Priority Interests above;

- Applications with primary emphasis on resilient solvers, and/or new development of machine probabilistic methods and their mathematical formalisms;
- Applications aimed at advancing computer-supported collaboration, social computing, and generalized research in human-computer interaction;
- Discipline-specific data analytics and informatics without a clear articulation of how the research will generalize to other disciplines and/or advance computer science capabilities;
- Research focused on the World Wide Web, the dark web, and/or data about it;
- Research that is primarily to advance cloud computing, hand-held, portable, desktop, and/or embedded computing that is not applicable to ASCR-supported computational and data science environments; and Research and applications not motivated and justified in the context of current and future SC user facilities, especially those supported by ASCR (i.e., Argonne Leadership Computing Facility or ALCF, Oak Ridge Leadership Computing Facility or OLCF, and National Energy Research Scientific Computing Center or NERSC): https://science.osti.gov/ascr/Facilities.

(c) Computational Partnerships

This subprogram supports computational research that will advance partnerships with SC, National Nuclear Security Administration (NNSA), other DOE programs, and the National Cancer Institute (NCI). This includes research in pioneering science applications for the next generation of high-performance computing and research that incorporates and integrates applied mathematics, computer science, and computational sciences, to enable scientists to exploit effectively extreme scale computers in their pursuit of transformational scientific discovery through simulation and modeling. For examples of SciDAC partnerships, refer to the website https://www.scidac.gov. For examples of extreme scale computing systems, refer to the website: https://science.osti.gov/ascr/Facilities/Accessing-ASCR-Facilities. Additionally, this subprogram supports basic research to enable scientists to easily find and interact with unique scientific facilities and data, and to work with peers or facilities staff involved in a scientific discovery process. Research topics of interest include:

- Theories, algorithms, tools, and services needed to create diverse computing environments where multiple resources can be combined in unique ways to suit the needs of an individual science community,
- Mechanisms and theories to enable scientists to interact with their peers and technical staff that operate a distributed scientific facility,
- Tools and services needed to support physical experiments in testbeds and production networks, and
- Advanced modeling and simulation methods and capabilities that can accurately predict and reliably validate the suitability and performance characteristics of large globally distributed infrastructures and workflows.

(d) Advanced Computing Technologies (ACT)

This activity supports quantum computing and networking efforts and Research and Evaluation Prototypes (REP). The Research and Evaluation Prototypes (REP) activity addresses the 11 challenges of next generation computing systems. By actively partnering with the research community, including industry and Federal agencies, on the development of technologies that enable next-generation machines, ASCR ensures that commercially available architectures serve the needs of the scientific community. The REP activity also prepares researchers to effectively use future generation of scientific computers, including novel technologies, and seeks to reduce risk for future major procurements. Research topics currently of interest for ACT include:

- Research focused on information processing and computation systems for emerging computing technologies including hardware architectures, accelerators, development of programming environments, languages, libraries, compilers, simulators, and research and development on their algorithms for physical simulation;
- Cybersecurity for scientific computing integrity: research on security techniques appropriate for open scientific environments, with a focus on ensuring scientific integrity in the context of extreme scale high performance computing and other SC Scientific User facilities to deliver means that assure trustworthiness within open high-end networking and data centers;
- Machine Learning: Scalable software, methods, and techniques that ensure algorithm scalability to extreme scales and applications that are generalizable to scientific computing applications and operation of HPC systems.
- Neuromorphic Computing: Specific to HPC-enabled modeling and simulation of computing architecture at extreme scales for generalizable applications of the proposed approach.
- Advanced Wireless for Science focusing is on communications that cover higher frequencies, THz, of 5G+ or WiFi6+ and software defined capabilities. The expanding national rollout of advanced wireless networks is creating opportunities for scientific applications;
- Microelectronics for Scientific Computing: For continued advances in computing technologies, a fundamental rethinking is needed of the science behind computing processor synthesis, placement, architectures, and algorithms. No longer can the approach be modular and linear, as it has been in the past. Rather, these advances must be developed collectively, in a spirit of co-design, where each scientific discipline informs and engages the other to achieve orders of magnitude improvements in system-level performance.
- Research to evaluate the suitability of specific quantum computing hardware architectures for science applications, including resource estimates for quantum computing applications of interest to SC;
- Theoretical methods and software tools to:
    - Assess the performance of real-world quantum processors
    - Facilitate device-specific optimization of individual operations ranging from state preparation and measurement through gate implementation and compilation

- Suppress noise, mitigate crosstalk, control errors, and maintain optimally high-fidelity operations in the absence of formal error correction; and
- Adaptation of promising new quantum computing technologies for testbed use.

Proposed research in quantum computing should focus on applications of quantum computing relevant to the SC and on devices that are already available or that become available during the term of the award rather than large-scale, high-fidelity, fault-tolerant machines.

EXCLUSIONS: Topics that are out of scope include:

- Research that does not address the specific ACT topics described above;
- Development of quantum algorithms;
- Development of new candidate qubit systems or improvements to physical qubits;
- Development of integrated circuits for quantum computing;
- Quantum transduction;
- Quantum communication, networking, and key distribution;
- Cryptography and cryptanalysis;
- Error correction codes and implementation of error correction codes;
- Research solely relevant to large-scale, high-fidelity, fault-tolerant machines; and
- Projects that are duplicative of or competitive with industry.

III. Basic Energy Sciences (BES)

The mission of the Basic Energy Sciences (BES) program is to support fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support other aspects of DOE missions in energy, environment, and national security. The portfolio supports work in the natural sciences by emphasizing fundamental research in materials sciences, chemistry, geosciences, and aspects of biosciences. BES-supported scientific facilities provide specialized instrumentation and expertise that enable scientists to carry out experiments not possible at individual laboratories.

Additional information can be found on the BES website. BES-sponsored workshop reports address the current status and possible future directions of some important research areas. PI Meetings Reports contain abstracts of BES supported research in topical areas associated with Division-sponsored technical conferences.

- BES Website: https://science.osti.gov/bes
- BES Workshop Reports: http://science.osti.gov/bes/community-resources/reports/

- Materials Sciences and Engineering Division PI Meetings: http://science.osti.gov/bes/mse/principal-investigators-meetings/
- Chemical Sciences, Geosciences, & Biosciences Division PI Meetings: http://science.osti.gov/bes/csgb/principal-investigators-meetings/

BES mission areas:

- To design, model, synthesize, characterize, analyze, assemble, and use a variety of new molecules, materials, and structures, including metals, alloys, ceramics, polymers, bioinspired and biomimetic materials and more for energy-related applications.
- To understand, model, and control chemical reactivity and energy transfer processes in the gas phase, in solutions, and at interfaces for energy-related applications, employing lessons from inorganic and biological systems.
- To develop new concepts and improve existing methods to assure a secure energy future utilizing any or all renewable and fossil energy sources.
- To conceive, design, fabricate, and use new scientific instruments to characterize and ultimately control materials, especially instruments for x-ray, neutron, and electron beam scattering and for use with high magnetic and electric fields.

BES' priority research areas for SCGSR program include:

(a) Accelerator and Detector R&D

Basic Energy Sciences (BES) supports accelerator and detector research and development in support of its current and future x-ray and neutron sources. These facilities give graduate students the opportunity to work side-by-side with accelerator and instrument scientists that are operating some of the world's cutting-edge facilities and also developing advanced technology for next-generation facilities. Accelerator physics has always relied on inventing, developing, and adapting advanced technologies to enable state-of-the-art research. With the adoption of particle accelerator and detector technologies by many scientific fields, the demand for skilled practitioners in these areas has grown significantly. As the scale of particle accelerators and their associated detectors has grown, very few universities have been able to maintain the infrastructure needed to provide such practical training, and students typically have to rely on short residencies at accelerator laboratories to receive such experience. BES is particularly interested in the training of graduate students in radio frequency (rf) engineering, new electron source technologies for x-ray free electron lasers including photocathodes, beam diagnostics instrumentation, nonlinear beam dynamics analysis, beam optics design, and detector technology. Also of interest are Artificial Intelligence and Machine Learning tools applied to optimization and control of accelerators and data analytics.

EXCLUSIONS: Based on programmatic priorities, topics of research that will NOT be considered are: the development of materials for detectors or x-ray optics, or the development of mathematical algorithms for detector data management, which are supported through other DOE programs.

(b) Basic Geosciences

Basic research in geosciences underpins knowledge of the terrestrial impacts and limitations of energy technologies and informs the nation's strategy for mitigating these impacts in a safe and cost-effective manner. This priority research area involves basic research on imaging strain fields, inferring stress through constitutive relations, and measuring and predicting the evolution of permeability and porosity and fracture networks in response to changes in stress in the earth's subsurface and in response to precipitation/dissolution reactions. Example topics include induced seismicity, rock physics and integrity, poro-elastic deformation, slow fracture nucleation and growth, and large-scale strain measurements with GPS and InSAR techniques. Research focused on permeability and porosity evolution and dynamics is particularly well aligned with this priority area and is one of the key focus areas identified in the Basic Energy Sciences Roundtable Report, Controlling Subsurface Fractures and Fluid Flow: A Basic Research Agenda (May 2015), available at https://science.osti.gov/bes/community-resources/reports/.

EXCLUSIONS: Topics of research that will NOT be considered are: wellbore integrity, advanced drilling methods, hydraulic fracturing technologies, remediation tools, stimulation methods, and specific CO2 sequestration or nuclear waste repository performance assessment, all of which are covered under other DOE programs.

(c) Basic Science for Advanced Manufacturing

This research area addresses the need to lay the scientific foundation to create new, transformative technologies for manufacturing that are energy efficient, environmentally clean, and sustainable. This requires fundamental advances in synthesis, processing, mechanistic investigation, computation and validation, and operando characterization. Science that advances precise, scalable synthesis and processing of atomic-scale building blocks will enable manufacture of materials and chemical systems with unparalleled structures and functions. New approaches for combining multiscale modeling with in-situ diagnostics and data science techniques are needed to enable real time adaptive manufacturing processes. Innovative science-based methodologies are needed to achieve atom and energy efficiency for sustainable manufacturing and to enable adaptive and resilient manufacturing across scales that exploits renewable or recycled feedstocks. New co-design approaches to control matter in the presence of impurities, defects, and/or nonequilibrium states across multiple length scales during manufacture are needed to simultaneously achieve multiple complex performance objectives. Next-generation materials and manufacturing processes need to be intrinsically more circular to enable remanufacturing to be less wasteful and require less energy. The national laboratory system has expertise and experimental and computational capabilities in the design and synthesis of materials, investigation of chemical mechanisms, in situ and in operando characterization, and development of data science AI and ML techniques to achieve these objectives. This program will provide opportunities for graduate students to work with scientists with expertise in these areas and to access advanced synthesis, analytical, and computational capabilities at the national laboratories. The 2020 Basic Research Needs Workshop for Transformative Manufacturing report identifies basic science priority research directions that could accelerate innovation to transform manufacturing in the future. Fundamental research areas of interest include but are not limited to:

- Research in the discovery of new crystal growth methods and thin-film deposition techniques are needed to create large, high quality crystals and complex materials under non-equilibrium conditions and through multiscale and external interactions.

- Studies to seamlessly integrate self-assembly mechanisms, for coherent management and self-regulation of multiple complex and simultaneous functions, from one size domain across multiple length scales during the construction of materials or chemical systems for clean energy.
- Research focused on understanding the chemical and catalytic dynamics and transformations of functional materials in operational environments, including development of new in situ or operando tools and techniques that provide knowledge needed to tailor and control materials and processes across multiple length scales relevant to manufacturing-related environments so that they perform as designed with minimum energy consumption and maximum efficiency.
- Research for development of predictive models, including AI/ML for data-driven science, that accelerate discovery of innovative methods and support fundamental science to precisely direct multiscale synthesis and assembly, and chemical system performance, with real-time adaptive control.
- Research for designing and integrating conversion and separations to produce, refine, recover, or recycle important chemical and materials chemical processing feedstocks by coupling highly active catalysts with membranes and solvation and by replacing thermally controlled separations.
- Convergent theoretical and experimental approaches for understanding and controlling multiphase reactions under the influence of chemical and electrochemical potential within complex reactive manufacturing-related environments.

EXCLUSIONS: The topic does not support projects primarily aimed at optimization of properties of materials for applications, device fabrication and testing; engineering design or scale-up; applied research; microfluidics; sensors; research directed toward medical or pharmaceutical applications; biofuel production; development or optimization of microbes or plants for biofuel, bioproduct, or biomass production; and intensive data collection that does not test specific hypotheses.

(d) Basic Science for Clean Energy and Decarbonization

This research area addresses the foundational science needed for future clean energy systems including the investigation and design of materials and chemical processes for decarbonization. Development of clean energy technologies will depend on the fundamental understanding, and ultimately control, of material properties and chemical mechanisms. Materials will need to be more functional and durable than today's energy materials, and chemical mechanisms will require increased control at the level of electronic structure and dynamics. Such advances will build on principles revealed by basic science, allowing materials and chemical processes to be designed to exacting standards. The national laboratory system has expertise and experimental and computational capabilities in the design and synthesis of materials and in the mechanistic understanding and control of complex chemical processes for energy capture, conversion, and storage. This program will provide opportunities for graduate students to work with scientists with expertise in these areas and to access advanced analytical and computational capabilities at the national laboratories. Fundamental research areas of interest include:

- Research in chemical separations and reactive separations critical for ensuring a sustainable chemical, clean energy enterprise, addressing contemporary issues of fuel, feedstock, and effluent processing in all phases of matter.

- Studies of energy transfers in proteins, protein complexes, and biohybrid constructs that are relevant to the design of new technologies benefitting from highly specific and efficient flows of energy at the molecular scale.
- Research is requested to address the materials and chemical challenges of carbon dioxide removal (CDR) approaches and that can accelerate the science-based synthesis and assembly of transformative materials and the discovery of chemical mechanisms for this purpose. Proposals should focus on fundamental understanding of important CDR processes such as direct air capture, and catalytic or photo-, electro-, or bio-catalytic conversion, and mineralization. Direct air capture may consider a plurality of dilute source phases including but not limited to ambient air, ocean, and surface waters.
- Materials and chemical studies to discover and understand mechanisms for highly selective energy delivery to natural or synthetic chemical separations systems containing captured carbon dioxide or its immediate derivative species and reaction intermediates.
- Materials and chemical research to develop lower-carbon or no-carbon containing fuels (such as light alkanes, hydrogen, ammonia, alcohols, and other oxygenated compounds) that can substitute for carbon-rich fossil fuels. Of particular interest are efforts that couple approaches for production of low-carbon or no-carbon containing fuels with approaches for carbon capture such as subsurface mineralization, ocean capture, and direct air capture.
- Studies of materials and chemical mechanisms (including photo-, electro-, thermal-, and/or catalysis or bio-catalysis) for carbon dioxide conversion to high value products such as fuels and chemicals.
- Detailed investigations of the fundamental dynamics and mechanisms of clean energy conversion systems and their active material components, and of materials that exhibit novel emergent phenomena or unique properties that could impact clean energy technologies, utilizing innovative approaches.
- Fundamental understanding of the relationships between intrinsic electronic structure and properties of complex materials, light-matter interactions, and/or new, unique deformation and failure mechanisms of materials such as polymers, membranes, coating materials, and electrodes used in clean energy systems.
- Research that integrates new chemical, physical, or bioinspired experimental, theory, and data science approaches for control of dynamic synthesis and assembly pathways to create resilient multiscale systems that exhibit well-coordinated functionality and manipulation of energy and information for a broad range of clean energy technologies.

EXCLUSIONS: The topic does not support projects focused on the synthesis or testing of separations materials as the principal or only goal; applied research; synthesis of small molecules or nanoparticles; engineering design or non-science-based scale-up; device fabrication and testing; development of narrowly defined processes or devices; desalination; microfluidics; sensors; research directed toward medical or pharmaceutical applications; studies of animals; biofuel production; development or optimization of microbes or plants for biofuel, bioproduct, or biomass production; phenotype analyses that do not test specific hypotheses; intensive data collection that does not test specific hypotheses; and engineering, device optimization, or designing/building carbon capture systems.

(e) Chemical and Materials Sciences for Quantum Information Science (QIS)

This topic provides opportunities for graduate students to engage in fundamental theoretical and experimental QIS research with DOE National Laboratory scientists. Applications are sought in two topical areas: 1) Quantum Computing in Chemical and Materials Sciences; and 2) Next-Generation Quantum Systems.

Quantum Computing in Chemical and Materials Sciences: Applications are requested for theoretical research using quantum computers, emulators and/or annealers to solve scientific problems in chemical and materials sciences. Applications must describe how the proposed research addresses one or more of the Priority Research Opportunities identified in the report Basic Energy Sciences Roundtable on Opportunities for Quantum Computing in Chemical and Materials Sciences:

1. Controlling the quantum dynamics of non-equilibrium chemical and materials systems
2. Unraveling the physics and chemistry of strongly correlated electron systems
3. Developing algorithms for embedding quantum hardware in classical frameworks
4. Bridging the classical-quantum computing divide.

Next-Generation Quantum Systems: Applications are requested for basic experimental or theoretical research focused on the discovery and characterization of quantum phenomena to enable the design and discovery of novel quantum information systems. Applications must describe how the proposed research addresses one or more of the Priority Research Opportunities identified in the report Basic Energy Sciences Roundtable on Opportunities for Basic Research for Next-Generation Quantum Systems:

1. Advance artificial quantum-coherent systems with unprecedented functionality for QIS
2. Enhance creation and control of coherence in quantum systems
3. Discover novel approaches for quantum-to-quantum transduction
4. Implement new quantum methods for advanced sensing and process control

EXCLUSIONS: Applications that emphasize engineering, device optimization, or designing/building quantum computers and devices will not be considered. Applications that are focused on fundamental chemical and materials science research of quantum phenomena in systems unrelated to QIS will not be considered. Applications that focus solely on algorithmic advances or software tools without a connection to BES-relevant science will not be considered.

(f) Data and Computational Sciences for Materials and Chemical Sciences

This topic will provide opportunities for graduate students to engage in design and development of the tools required for fundamental data and computational sciences research to understand, design, and predictively control matter and energy at the electronic, atomic, and molecular levels.

Applications must develop novel data and/or computational science tools and techniques to address one or more of the following three topics:

- **Predictive control of reactions and nonequilibrium processes** for efficient chemical and energy transduction in complex nonequilibrium and/or field-driven environments.
- **Harnessing quantum phenomena in many-particle systems driven far from equilibrium** by manipulating quantum effects such as coherence, entanglement, and novel states of matter.
- **Uncovering hidden correlations, emergent behavior, and functional relationships** to develop novel, robust, data-driven or hybrid models that lead to improved understanding and advancement of fundamental energy science research that is unlikely to be achievable otherwise.

Applicants must propose to advance computational and/or data science research that can appropriately capture or accurately describe the essential physics and chemistry of relevant materials and chemical systems and processes. Efforts aimed at extending currently attainable length and time scales or increasing complexity are sought. Computational science research that makes use of, integrates with, or improves upon the open-source codes and data developed under the BES Computational Chemical Sciences (CCS) and Computational Materials Science (CMS) programs is encouraged. Data science research that facilitates the integration of highly heterogeneous chemical and materials data of diverse provenance to promote findable, accessible, interoperable, and reusable (FAIR) data sharing for model generalization and extrapolation to data-poor regions, creation of unique reference datasets, and the extension of fundamental theories to complex many-parameter systems, is encouraged.

EXCLUSIONS: Applied research, such as design or optimization of user facility instruments, devices, tools, or processes will not be considered. Applications that focus on research without a connection to BES-relevant science will not be considered.

(g) Fundamental Electrochemistry for Chemical and Materials Sciences

Electrochemistry is central to energy conversion and storage as well as chemical processes and systems. There is a strong need for fundamental research on electrochemistry to solve longstanding scientific challenges related to next generation batteries for transportation and grid-level storage, to significantly improve chemical energy and solar energy conversion, to enable the discovery of novel chemical synthesis and separations processes, and to mitigate or prevent corrosion in energy production systems (particularly nuclear and fossil energy plants). The national laboratory system has expertise in this field and has developed advanced experimental and computational capabilities to better understand electrochemical mechanisms at a fundamental level to address needs in energy research. This program will provide opportunities for graduate students to work with scientists with expertise in electrochemistry and to access advanced analytical and computational capabilities at the national laboratories. Areas of particular interest include: high resolution, in-situ studies of electrochemical processes in materials; electrochemistry of non-equilibrium or metastable materials; electrochemistry at the nanoscale (effect of nanoscale morphology); electrochemistry in extreme conditions (at high temperature and/or stress, and in radiation environments); dynamic behavior of electrode-electrolyte interphases, catalyst-electrolyte interfaces, or catalytic systems under in-situ/operando conditions; and electrochemical mechanisms of electroorganic synthesis, separations processes and in catalytic and biocatalytic systems.

Specific issues for electrochemistry in energy transduction, energy storage, chemical conversion, and corrosion have been identified in the Basic Energy Sciences report Basic Research Needs for Catalysis Science (2017), Next Generation Electrical Energy Storage (2017), Future Nuclear Energy (2017), and Materials under Extreme Environments (2007). Important issues have also been identified in reports from the Roundtable on Foundational Science for Carbon-Neutral Hydrogen Technologies (2021) and on Liquid Solar Fuels (2019). The reports are available at https://science.osti.gov/bes/Community-Resources/Reports, along with the consensus study report, "A Research Agenda for Transforming Separation Science" (https://doi.org/10.17226/25421).

EXCLUSIONS: Research that is focused on identifying or producing new or optimized materials or on structure-property relationships, instead of focusing on electrochemical mechanisms, will NOT be considered.

(h) Gas Phase Chemical Physics

This program supports research on fundamental gas-phase chemical processes that provide understanding and scientific foundations for clean energy. Research in this program explores chemical reactivity, kinetics, and dynamics in the gas phase at the level of electrons, atoms, molecules, and nanoparticles. A continuing goal of this program is to understand energy flow and reaction mechanisms in complex, nonequilibrium, gas-phase environments. A new goal for this program is to understand how these gas-phase processes can influence and be influenced by surface phenomena.

The program currently supports the following five research thrusts:

1. *Light-Matter Interactions* includes research in the development and application of novel tools, such as molecular spectroscopy, for probing the nuclear and electronic structure of gas-phase molecules to enable chemical and physical analysis of heterogeneous and dynamic gas-phase environments and to understand the dynamic behavior of isolated molecules, such as energy flow (e.g., relaxation of excited states), nuclear rearrangements, and loss of coherence and entanglement. Applications are encouraged that develop automated methods based on artificial intelligence and machine learning (AI/ML) methods to facilitate the analysis of complex molecular spectra, or seek to improve the understanding of quantum phenomena in systems that could be used for quantum information science.

2. *Chemical Reactivity* comprises research in chemical kinetics and mechanisms, chemical dynamics, collisional energy transfer, and construction of, and calculations on, molecular potential energy surfaces to develop fundamental insight into energy flow and chemical reactions important in clean energy and transformative manufacturing processes. Applications are encouraged that develop AI/ML methods for the construction of potential energy surfaces and optimization of chemical kinetic mechanisms.

3. *Gas-Particle Interconversions* comprises research on the chemistry of small gas-phase particles, including their interactions with gas-phase molecules and dynamic evolution to understand the molecular mechanisms of formation, growth and transformation (such as evaporation, phase transition, and reactive processing) of small particles.

4. *Gas-Surface Chemical Physics* retains a strong emphasis on molecular-scale investigations of gas-phase chemical processes with the goal of gaining a better understanding of the cooperative effects of coupling gas phase chemistry with surface chemistry. Applications are encouraged that explore the cooperative effects of gas-surface coupling for systems relevant to clean energy or transformative manufacturing.

5. *Ultrafast Imaging/Spectroscopy*includes studies of the short timescale phenomena underlying photochemical and photophysical processes, such as photodissociation, isomerization, and nonadiabatic dynamics in the gas phase. Applications are encouraged that develop AI/ML methods for analyzing ultrafast images/spectra or to provide insight into chemical systems associated with clean energy or transformative manufacturing.

EXCLUSIONS: Topics of research that will NOT be considered are: non-reacting fluid dynamics (transport phenomena including computational fluid dynamics (CFD), reacting and non-reacting turbulent flow, and the impact of transport of chemical reactions), spray dynamics, data-sharing software development, end-use combustion device development, and characterization or optimization of end-use combustion devices.

(i) Instruments R&D for Neutron and X-ray Facilities

There is a critical need to train scientific and technical staff to develop, upgrade, and operate a large suite of scattering and imaging instruments at the high brilliance light and high flux neutron sources to enable state-of-the-art research in science and technology. BES operates five light sources (ALS, APS, NSLS-II, SSRL and LCLS) and two neutron sources (SNS and HFIR) with about 200 instruments of different classes operating day and night and over 11,000 annual scientific users. In addition, BES is upgrading NSLS-II with new instruments, ALS-U and APS-U, with new accelerator technologies and is constructing new facilities such as LCLS-II and STS to sustain US leadership in this important area. These facilities provide graduate students the opportunities to work side-by-side with the teams of instrument scientists who conduct research, operate some of the world's cutting-edge instruments, and develop advanced instruments for next-generation facilities. The different classes of instruments (e.g. diffraction, reflectometry, quasielastic and inelastic scattering, and imaging) are highly optimized for the study of structure and dynamics in a wide range of length and time scales at unprecedented speed (from ultrafast) and spatial and energy resolution. Also supported is science-driven development of next-generation instrumentation concepts, novel tools, time resolved, in-situ and operando and multimodal measurement capabilities, and software infrastructure for machine learning, data analytics, and remote access to accelerate the discovery of solutions for clean energy and forefront scientific challenges.

Applications should focus on transformative opportunities for graduate students to carry out research in collaboration with instrument scientists at the facilities to develop instrumentation, novel techniques, and computational tools for enhancing the impact of the world leading BES neutron and light sources.

EXCLUSIONS: Applications will only be considered if they emphasize the development of instrumentation, technique, or software for the instruments at the facilities. Those focused solely on using the facilities for science will NOT be considered as that scope is being covered by other topics.

(j) Instruments and Techniques R&D for Electron and Scanning Probe Microscopy

BES supports research and development in electron and scanning probe microscopy for fundamental understanding of matter at the national laboratories. These facilities provide opportunities for graduate students to work side-by-side with scientists with expertise in operation of some of the world's cutting-edge facilities and in the development of advanced techniques and instrumentation for next-generation microscopy. Recent advances in imaging capabilities at the laboratories provide an opportunity to observe and study matter from the 3D spatial perspectives to true "4D" time-resolved maps that allow quantitative predictions of material properties. New capabilities are emerging to image functionalities that are critical for enabling significant progress in measuring and understanding functional materials and grand challenges in materials, chemical, and nano sciences. Imaging capabilities across multiple scales were recently identified as a transformative opportunity for materials research (see the report Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science, https://science.osti.gov/bes/community-resources/reports/). These impacts include accelerating the discovery of new materials and new functionalities, the understanding of materials properties, and progress in materials synthesis, as well as solving longstanding challenges in the relationship between the structure of inhomogeneous matter and its behavior. The ability to correlate the atomic and nanoscale structure of matter with physical properties (e.g., mechanical, electrical, magnetic, catalytic, and optical) and functionality forms the core of many disciplines.

Applications should focus on the advancement of electron and scanning probe microscopy instrumentation and techniques to image and characterize functional matter to answer fundamental questions in nanoscience, materials, or chemical sciences. Also of interest are Artificial Intelligence and Machine Learning tools applied to data analytics, visualization and optimization and control of electron and scanning probes.

EXCLUSIONS: Applications that target biomedical applications or systems (e.g., animal/human health) will NOT be considered. Applications that focus solely on using the instruments for science will NOT be considered as that scope is being covered by other topics.

(k) Materials Sciences and Chemistry for Microelectronics

As the semiconductor industry faces mounting challenges to continue the decades-long success of Moore's Law scaling it is becoming increasingly clear that there is a pressing need and an opportunity to reshape computing as we know it, seeking to make it orders of magnitude more energy efficient and powerful. We need a deeper understanding of the physics underlying information transfer, processing, and storage to identify new ways of using electrical, optical, magnetic, and thermal excitations at nanometer scales to design the efficient computing hardware of the future. And we need to identify new materials and improved ways of synthesizing, processing, characterizing, and configuring them at atomic length scales. In parallel with the need to develop a new energy-efficient computing paradigm, a pressing need exists to revolutionize how electrical power is generated, transmitted, and consumed, which brings similar materials science and chemistry challenges. This priority research area emphasizes basic research to discover, design, and characterize next-generation electronic, magnetic, and optical materials, including research to understand and control interfacial chemical reactions to enable the synthesis of new materials. Of particular interest are materials and systems that could leverage unexploited physical phenomena to revolutionize the computation, control, communication, and storage of information. Additional details are described in the priority research directions from the Basic

Research Needs for Microelectronics Workshop Report: https://science.osti.gov/-/media/bes/pdf/reports/2019/BRN_Microelectronics_rpt.pdf

EXCLUSIONS: Research related to system architecture, network design, algorithms, and software is outside the scope of the BES mission and therefore will NOT be considered. Activities with a primary focus on Quantum Information Science or Quantum Computing will NOT be considered.

(l) Nuclear Chemistry and Radiochemical Separations

This priority research area encourages actinide and transactinide fundamental chemical research that underpins the DOE missions in energy, environment, and national security. Research performed in this program is essential to a clean-energy future, such as but not limited to, the fundamental research supporting carbon-free nuclear energy. Emphasis is placed on the chemical and physical properties of the transuranic elements to determine their bonding and reactivity as well as determining fundamental transactinide chemical properties. Separation science applications encouraged under this topic should address the fundamental science underpinning the extraction and separation of fission products and actinides, emphasizing separation research that is directly responsive to the research needs described in the report from the Office of Science workshop on Basic Research Needs for Environmental Management (July 8-11, 2015) to elucidate electronic and molecular structure as well as reaction thermodynamics.

EXCLUSIONS: Based on programmatic priorities, topics of research that will NOT be considered are: the processes affecting the transport of subsurface contaminants, isotope development, microfluidics, medical research, and projects aimed at optimization of materials properties including radiation damage, device fabrication, or biological systems.

(m) Radiation Effects in Materials and Chemistry

There is a strong need for fundamental research to enhance the knowledge, understanding, and utilization of the effects of radiation on chemical systems and materials that ultimately may improve the management of existing nuclear reactors, the development of next-generation reactors, and spent-fuel disposition.

Though in demand and highly relevant to the mission of the Department of Energy, there are few existing programs for graduate study in the U.S. focused on this research area. National laboratories have expertise as well as unique facilities for research in this area that will provide new dimensions to graduate research.

Topics of interest include radiation in the form of electrons, ions, or neutrons, and its effects on the production, migration, and growth of defects as well as the effects of irradiation on the behavior of materials and molecules including the study of energy deposition and the transport following the absorption of ionizing radiation in media ranging from low-temperature ices, through aromatic liquids to supercritical fluids. Track structure effects and the structure, properties, and reactions of the radicals formed in these tracks are also of particular interest. Understanding chemical and materials processes initiated by ionization radiation at interfaces of aqueous solutions with solids can provide a fundamental foundation to address challenges in reactor chemistry, waste separation, and waste storage related to nuclear power generation. Particularly relevant topics are outlined in the priority research directions from the 2017 Basic Energy Sciences report Basic Research Needs for Future Nuclear Energy (https://science.osti.gov/bes/Community-Resources/Reports#BRNFNE).

EXCLUSIONS: Based on programmatic priorities, topics of research that will NOT be considered are: isotope development, polymers research, fusion research, flux pinning for superconductivity, medical research, animal systems, or anything focused on human or animal health.

IV. Biological and Environmental Research (BER)

The mission of the Biological and Environmental Research (BER) program is to support fundamental research and scientific user facilities to achieve a predictive understanding of complex biological, climatic, and environmental systems for a secure and sustainable energy future. The program seeks to understand how genomic information is translated to functional capabilities, enabling more confident redesign of microbes and plants for sustainable biofuels production, improved carbon storage, and understanding the biological and biogeochemical processes that drive elemental and nutrient cycling in the environment. BER research also advances understanding of the roles of the earth's biogeochemical systems (the atmosphere, land, oceans, sea ice, and subsurface) in determining climate in order to predict climate decades or centuries into the future to provide information that will inform plans for future energy and resource needs.

Program Website: https://science.osti.gov/ber

BER mission areas:

- To obtain new molecular-level insight into the functioning and regulation of plants, microbes, and biological communities to provide the science base for cost-effective production of next generation biofuels as a major secure national energy resource.
- To enable major scientific developments in Earth system-relevant atmospheric, hydrological, biogeochemical, ecosystem, and cryospheric process and modeling research in support of DOE's mission goals.
- To understand the relationships between Earth system (including climate) change and terrestrial ecosystems, and provide science to underpin a fully predictive understanding of the complex Earth system, including the potential impacts of Earth system change on DOE mission-relevant infrastructures.
- To understand processes and controls needed to describe elemental and nutrient cycling in the environment, based on laboratory and field experiments and system modeling.
- To make fundamental discoveries at the interface of biology and physics by developing and using new, enabling technologies and resources for DOE's needs in climate, bioenergy, and subsurface science.

The BER program is organized into two divisions, the Biological Systems Science Division (BSSD), and Earth and Environmental Systems Sciences Division (EESSD).

The EESSD supports research that integrates discovery- and hypothesis-driven science with technology development on plant and microbial systems relevant to DOE bioenergy mission needs. Systems biology is the multidisciplinary study of complex interactions specifying the function of entire biological systems—from single cells to multicellular organisms—rather than the study of individual components. EESSD focuses on utilizing systems biology approaches to define the functional principles that drive living systems, from microbes and microbial communities to plants and other whole organisms. The division also supports operation of a scientific user facility, the DOE Joint Genome Institute (JGI), and use of structural biology capabilities through the development of instrumentation at DOE's national user facilities.

The EESSD supports fundamental science and research capabilities that enable major scientific developments in Earth system (including climate) relevant atmospheric, hydrological, biogeochemical, ecosystem, and cryospheric research and modeling, in support of DOE's mission goals for basic science, energy, and national security. This includes research on clouds, aerosols, hydrology, biogeochemistry, and cryospheric processes; scale-aware modeling of process interactions extending from local to global; and model development and analysis of the Earth system including interactions between the natural Earth system and energy and related infrastructures. It also supports subsurface biogeochemical research that advances fundamental understanding of coupled physical, chemical, and biological processes controlling the environmental fate and transport of DOE-relevant energy byproducts. EESSD also supports two national scientific user facilities: the Atmospheric Radiation Measurements (ARM) User Facility and the Environmental Molecular Sciences Laboratory (EMSL). ARM provides unique, multi-instrumented capabilities for continuous, long-term observations needed to develop and test improved understanding of the central role of clouds and aerosols as part of the atmospheric component of Earth system models. EMSL provides premier experimental and high-end computational resources needed to understand molecular- to meso-scale physical, chemical, and biological processes for addressing DOE's energy and environmental mission.

BER's priority research areas for SCGSR program include:

(a) Computational Biology and Bioinformatics

The Biological Systems Science Division supports genomic-, molecular imaging-based investigations to elucidate biological systems critical to DOE's fundamental science programs in bioenergy and the environment. Systems biology approaches allow integration of omics- (genomics, proteomics, metabolomics) and quantitative data across spatial, temporal, and functional scales to develop predictive multiscale models that can be used to derive testable hypotheses about emergent properties, functions, and dynamics of organismal systems. An enduring challenge is to develop the tools necessary to capture, annotate, integrate, analyze, and archive large, complex systems biology datasets such as those generated by BER programs. Currently, the ability to generate complex multi-"omic" and associated meta-datasets greatly exceeds the ability to interpret these data. Priority research areas for this topic include *development of new innovative computational approaches and AI based methods to identify relationships among different parts of the genomes , analysis of biological networks and integrated models; advanced algorithms and data-handling methods to process and integrate imaging and structural biology data with simulations and other biological measurements; analytical methods that enhance, scale and optimize the management and processing of large, complex and heterogeneous data* *generated from different scales for integration and interpretation of system-wide data, simulation of biological phenomena, processes and systems relevant to BER science.*

(b) Biomolecular Characterization and Imaging Science

The Biological Systems Science Division's focus on developing a scientific basis for biomass-based biofuel production requires a trained scientific workforce to develop a detailed understanding of cellular metabolism in order to optimize beneficial properties of bioenergy- relevant plants and microbes. Aligned with that goal, BER encourages development of new imaging and 3D structural characterization instrumentation and technologies for the study of cellular and molecular systems and networks critical to the functioning of those organisms. Of particular interest are technologies for probing biological systems in situ to characterize the dynamic spatial and temporal relationships, physical connections, and chemical exchanges that facilitate the flow of information and materials across membranes and between intracellular partitions. Also of interest are technologies for characterizing the structures of critical molecular and cellular components that inform understanding of the system and its essential dynamic processes. Candidates for this topic are encouraged to draw upon imaging techniques/capabilities from other disciplines that could be adapted to advance the understanding of the biological systems of diverse plant and microbial species of relevance to BER. Candidates are expected to seek research collaboration with imaging or structural biology scientists and engineers at the DOE National Laboratories in conceptualizing interdisciplinary approaches and leveraging tools and resources available to advance an imaging concept from proof of principle to use in common research practice.
See https://BERStructuralBioPORTAL.org/ for BER-supported beamline capabilities and contacts at the DOE synchrotron and neutron facilities and BER Bioimaging 2019 for DOE Lab-led Bioimaging projects.

(c) Plant Science for Sustainable Bioenergy

Crops grown for bioenergy purposes will possess characteristics quite different from those required of plants grown for food. Decreased or altered lignin composition, a longer juvenile period for increased biomass, and in some cases a perennial lifestyle are among traits considered favorable for bioenergy feed stocks. Current DOE Genomic Science Program research efforts in renewable feed stocks for bioenergy and bioproducts focus on the manipulation of metabolic pathways and carbon allocation in plant tissues to produce plant varieties with enhanced productivity, compositional quality and sustainability. *Candidates for this topic should focus on systems biology and genome engineering approaches seeking to improve terrestrial bioenergy crop characteristics such as biomass yields, optimized growth and development in marginal lands, and research to further understanding of plant-microbe interactions and/or molecular mechanisms underlying traits that increase sustainable production of such crops under various abiotic stresses.* Future DOE bioenergy research will require plant scientists trained in multiple scientific disciplines that enable translation of research to the field.

(d) Environmental Microbiology

Microbial activities are fundamental drivers of environmental processes across all scales. Despite notable advances over the past decade, significant gaps remain in our understanding of the way in which microbes contribute to and modulate global elemental cycles of carbon and nutrients. Given the compositional heterogeneity of terrestrial ecosystems, highly integrated research, drawing on '-omics', high-resolution analytical technologies, and sophisticated computational approaches, is needed to fully describe the functional properties and interrelationships among microbial populations. Research needs include studies of fundamental processes, as well as the metabolic interactions among microbial populations (bacteria, archaea, viruses, fungi, and protists) and with their environment. Also of interest are microbial responses to stress such as (but not limited to) warming, elevated CO2, or changes in water or nutrient availability over varying time scales. *Candidates for this topic should adopt a genome-enabled approach (e.g., meta-genomics, -transcriptomics, -proteomics, and metabolomics) to interrogate relevant functional microbial processes in terrestrial environments. Systems biology studies on regulatory and metabolic networks of microbes and microbial consortia involved in relevant biogeochemical processes (for example, but not limited to, carbon/nitrogen/sulfur/methane cycling or redox processes) are encouraged.*

(e) Environmental System Science: Process-Level Terrestrial Ecosystem and Watershed Systems Research to Inform Models of the Earth and Environmental System

Current models inadequately represent the structure and function of key ecological and hydro-biogeochemical processes of the terrestrial environment. These processes (e.g., nutrient/elemental reactions and cycling, plant-rhizosphere interactions, reactive flow and transport, microbe-mineral interactions, vegetative change, etc.) occur within ecosystems, watersheds, and subsurface systems, spanning a continuum from the bedrock, through the soil and vegetation, and to the atmosphere, and are the product of interactions among the various physical, chemical, and biological components of the Earth system. The inadequate representation of the functioning of ecosystems, watersheds, and subsurface systems, and especially the biogeochemical processes and hydrologic interactions that occur both within them and at their interfaces, represents a major roadblock to predictively understand Earth and environmental systems. Improving the representation of the complex Earth system requires advancing and integrating better understanding of ecological and hydro-biogeochemical processes that can affect the cycling and transport of water, elements, nutrients, and other constituents within the terrestrial system. *Proposals to this topic are required to delineate integrative, hypothesis-driven research that clearly identifies and advances existing needs in state-of-the-art models to better inform representation of the terrestrial system, including landscape and vegetation dynamics, ecosystem processes, watershed hydro-biogeochemistry, nutrient/elemental cycling, reactive transport, rhizosphere processes, and microbial processes in soils, sediments and groundwater. Proposed research must align with the scope and focus of the DOE Environmental System Science program (https://ess.science.energy.gov).* Developing a workforce with experience in innovative approaches in ecological, watershed, and subsurface process and systems science research and modeling will enable DOE to foster innovative research and make significant advances in the high-resolution predictive understanding of Earth and environmental systems.

(f) Atmospheric System Research: Aerosol and Cloud Processes

Cloud and aerosol feedbacks remain a large source of uncertainty in model projections of future climate change. Inadequate representation of the detailed processes controlling aerosol and cloud life cycles at the appropriate spatial scales inhibits our ability to predict changes to the Earth system and their impacts on energy and related infrastructure. Applications should target one or more of these climate-relevant processes that need to be better represented in Earth system models to improve the ability of models to confidently make projections: aerosol particle formation, growth, absorption, and aging; cloud microphysical processes such as ice nucleation, drizzle and precipitation formation, and phase partitioning; land-atmosphere interactions that impact aerosol and cloud formation; and interactions between clouds and the environment such as entrainment of air into clouds, convective initiation, cold pools, and organization of convective clouds on a range of scales. High priority research efforts in atmospheric sciences within DOE's Earth and Environmental Systems Sciences Division (EESSD) require new expertise in using observational data from the Atmospheric Radiation Measurement (ARM) Research Facility as well as high resolution numerical models to advance predictive understanding of aerosol and cloud processes. *Applications for this topic should use observations and/or modeling tools supported by Biological and Environmental Research (BER) to study the aerosol and cloud processes outlined above. Examples of BER-supported observations and models include observations from ARM, the Weather Research and Forecasting model (WRF), the WRF model coupled to Chemistry (WRF-Chem), the Community Atmosphere Model (CAM), the Large Eddy Simulation (LES) ARM Symbiotic Simulation and Observation (LASSO), and the Energy Exascale Earth System Model (E3SM). Applications that couple atmospheric observations with numerical models are encouraged. Applications that use artificial intelligence or machine learning (AI/ML) or advanced statistical techniques are also encouraged if doing so provides better understanding of atmospheric processes.*

(g) Earth System Model Development: Computational Climate Modeling

In order to advance the fidelity of Earth system models, there is ongoing need to improve physical process representation (complexity) as well as model resolution. At the same time, computing capabilities continue to advance and computer architectures are becoming increasingly complex. These computational advances present both a challenge and opportunity for Earth system modeling research, and there is need for the combined skill-set of computational and climate/Earth system sciences, in order to design and optimize model codes with methods that can effectively utilize the evolution and advances of computer systems. *Candidates for this topic should be developing new algorithms or computational methods for Earth system model codes that will both advance Earth system science and be designed to effectively and efficiently utilize emerging generations of Leadership class computers.*

Background in one area of earth system sciences as well as in either software engineering or mathematics, is desired but not required. Please refer to climate modeling site (https://climatemodeling.science.energy.gov/) for more information on the program and funded projects.

(h) Regional and Global Model and Analysis: Diagnostics for Water and Biogeochemical Cycles

The development of Earth system modeling systems requires process-oriented diagnostics to evaluate the deficiencies in model parameterizations. Current generation of Earth system models use parameterizations for cloud process, and biogeochemical processes among others. Clouds significantly influence precipitation, which is the major link between the water and biogeochemical cycles of the Earth system. The coupling between the atmosphere and the land surface provides the physical drivers of the linkage. As the Earth system models' resolution increases, the interactions between different components of the Earth system present new challenges for diagnosing relationships that connect precipitation with large-scale variables involved in parameterization of sub-grid scale processes. *Candidates for this topic should focus on water cycle and biogeochemical research seeking to develop new analysis frameworks that combine process-oriented diagnostics and other exploratory metrics with methods of improving parameter choice for existing parameterizations in Earth System Models. Use of Artificial Intelligence techniques is encouraged but not compulsory.*

Please refer to [climate modeling site](https://climatemodeling.science.energy.gov/) (https://climatemodeling.science.energy.gov/) for more information on the program and funded projects.

EXCLUSIONS: The following areas are NOT within the scope of the BER program of this solicitation:

- Bioenergy from sewage processing, bioremediation of organics, phytoremediation, marine biology, and oceanography;
- Design, modeling, or technology development related to renewable energy systems including wind farms, solar arrays, and hydropower;
- Existing or newly proposed processes for commercial, industrial, residential, and municipal solid and liquid waste management, even if those processes hold potential to positively impact the carbon cycle, nitrogen cycle, etc.;
- Experimentation in support of industrial processes, including feedstock substitutions, emissions scrubbing, and other processes designed for greenhouse gas emissions;
- Policy analysis and/or policy implementation studies related to climate change;
- General human behavioral research, even as it applies to such areas as biofuels acceptance and climate change; however, economic and risk research is very much on point and encouraged;
- Marine experimentation in support of climate research, including understanding of marine organisms and marine ecology even when it may impact carbon, nutrient, and other cycles and/or hold potential for marine carbon sequestration;
- Observations and experimentation on ocean currents, ocean heat transfer, and other physical ocean properties;
- Engineering of systems or instrumentation or deployment of innovative combinations of existing probes where basic research is not the main thrust;
- Technology development and testing for climate change mitigation or adaptation technology development;
- Air pollution measurements, control technology development or evaluation;
- Site-specific scientific studies of climate change where research may be focused on a particular community, localized resource, or region, but where more generalized extensions and interpretations of the research are not a central component;
- Applied contaminant remediation, including phytoremediation approaches.
- Medically related research; plant pests, biomass process engineering optimization, molecular dynamics simulations towards enzyme engineering; or DNA sequencing technology.

V. Fusion Energy Sciences (FES)

The mission of the Fusion Energy Sciences (FES) program is to expand the fundamental understanding of matter at very high temperature and density and to build the scientific foundation needed to develop a fusion energy source. This is accomplished by studying plasma and its interaction with its surroundings across wide ranges of temperature and density, developing advanced diagnostics to make detailed measurements of its properties and dynamics, and creating theoretical and computational models to resolve the essential physics principles. The National Research Council report *Plasma Science: Advancing Knowledge in the National Interest* has recognized that plasma science has a coherent intellectual framework unified byphysical processes that are common to many subfields. Because of the wide range of plasmadensities and temperatures encountered in fusion applications, it is valuable to support plasmascience across many of its subfields in order to advance the fusion energy mission.

Program Website: https://science.osti.gov/fes/

The size and complexity of world-leading experiments in the field of plasma physics are rapidly expanding beyond the scale of the single university investigator. Prime examples of this are research in burning plasma science and high-energy-density plasmas. It is essential that the U.S. develop a workforce with the necessary skills and experience in *burning plasma science* to maintain U.S. leadership in fusion and to fully capitalize on the U.S. investment in ITER and its operation in the coming decade. This means enabling students to pursue grand-challenge problems in burning plasma science by providing them access to parameter regimes only available at the highest pressures (thermal and magnetic) as well as state-of-the-art diagnostics, both of which are only available at FES's major magnetic confinement fusion science facilities. Student accessibility to these premier facilities is important for developing a workforce with the critical scientific and team-building skills necessary to achieve our mission and secure U.S. leadership in this emergent field of science in the coming decades.

FES's priority research areas for SCGSR program include:

(a) Burning Plasma Science & Enabling Technologies

Research supported in this area will advance the predictive understanding of plasma confinement, dynamics, and interactions with surrounding materials, through the use of major magnetic confinement fusion research facilities or leadership-class computing resources. Among the topics addressed by this program are the macroscopic stability and dynamics of fusion plasmas; the understanding and control of turbulent transport processes; radiofrequency (RF) and neutral beam heating and current drive; energetic particle dynamics; multi-scale and multi-physics processes at the plasma edge; and the interaction and interface of the hot plasma boundary with the material walls.

Additionally, FES actively encourages applications that utilize and advance technology needed to enhance the capabilities for existing and next-generation fusion research facilities, enabling these facilities to achieve higher levels of performance and flexibility needed to explore new science regimes. This includes but is not limited to RF and neutral beam physics and engineering.

This priority area also supports the development of advanced diagnostic capabilities to enable close coupling of experiments and theory/computations for existing facilities; diagnostic systems relevant for the extreme conditions to be encountered in ITER; and sensors and actuators required for active control of plasma properties to optimize device operation and plasma performance.

(b) Discovery Plasma Science

The ability to create and manipulate plasmas with densities and temperatures spanning many orders of magnitude has led to the establishment of plasma science as a multi-disciplinary field, necessary for understanding the flow of energy and momentum in astrophysical plasmas, as well as enabling the development of breakthrough technologies. Research supported in this priority area must be directed toward addressing problems at the frontiers of plasma science. Specifically in the areas of:

- *General Plasma Science* – Understanding the behavior of non-neutral and single-component plasmas, ultra-cold neutral plasmas, dusty plasmas, and micro-plasmas, as well as the study of dynamical processes in classical plasmas including turbulence and turbulent transport, plasma waves, structures, and flows.
- *High Energy Density Laboratory Plasmas* – Structural and dynamical studies of ionized matter at extreme densities and temperatures.

VI. High Energy Physics (HEP)

The mission of the High Energy Physics (HEP) program is to understand how our universe works at its most fundamental level. We do this by discovering the elementary constituents of matter and energy, probing the interactions between them, and exploring the basic nature of space and time. This effort is part of a global enterprise of discovery, with students and scientists world-wide working side-by-side to unlock the secrets of the universe.

Program Website: https://science.osti.gov/hep

The HEP experimental research program focuses on three scientific frontiers:

- *The Energy Frontier,* where powerful accelerators are used to create new particles, reveal their interactions, and investigate fundamental forces;
- *The Intensity Frontier,* where intense particle beams and highly sensitive detectors are used to pursue alternate pathways to investigate fundamental forces and particle interactions by studying events that occur rarely in nature, and to provide precision measurements of these phenomena; and
- *The Cosmic Frontier,* where precision measurements of naturally occurring cosmic particles and phenomena are used to reveal the nature of dark matter, understand the cosmic acceleration caused by dark energy and inflation, infer certain neutrino properties, and explore the unknown.

Together, these three interrelated and complementary discovery frontiers offer the opportunity to answer some of the most basic questions about the world around us. Also integral to the mission of HEP are five cross-cutting research areas that enable new scientific opportunities by developing the necessary tools and methods for discoveries:

- *Theoretical High Energy Physics,* where the vision and mathematical framework for understanding and extending the knowledge of particles, forces, space-time, and the universe are developed;

- *Computational High Energy Physics,* where the framework of simulation and computational techniques are developed for advancing the HEP mission;
- *Accelerator Science and Technology Research and Development,* where the technologies and basic science needed to design, build, and operate the accelerator facilities essential for making new discoveries are developed;
- *Particle Detector Research and Development,* where the technologies and basic science needed to design, build, and operate the detector facilities essential for making new discoveries are developed; and
- *Quantum Information Science (QIS*), where novel capabilities for advancing HEP research using QIS techniques are supported along with the development of QIS, aligned to the SC initiative in QIS.

The scientific objectives and priorities for the field recommended by the High Energy Physics Advisory Panel are detailed in the long-range plan available at: https://science.osti.gov/~/media/hep/pdf/files/pdfs/p5_report_06022008.pdf.

A thriving program in HEP theory and computation is essential for identifying new directions and opportunities for the field; moreover, the fields of experimental HEP and accelerator physics have always relied on inventing, developing, and adapting advanced technologies in order to enable new discoveries. In particular, HEP supports graduate training in priority areas that emphasize connections to current and future particle physics research facilities. These facilities give students the opportunities to work side-by-side with leading scientists on the latest research topics. With the adoption of many of the techniques and technologies used in HEP research by a wide range of scientific fields, the demand for skilled practitioners in many of these areas has grown significantly, while few universities have been able to maintain the infrastructure needed to provide practical, hands-on training. The SCGSR program supports students for extended residencies at HEP laboratories to receive this critical experience.

HEP's priority research areas for SCGSR program include:

(a) Theoretical and Computational Research in High Energy Physics

This priority area supports activities that range from detailed calculations of the predictions of the Standard Model to the extrapolation of current knowledge to a new level of understanding, and the identification of the means to experimentally verify such predictions. It also supports computational, simulation, and data tools that are important for HEP research – in particular those that exploit near-term advanced architectures (ranging from supercomputers to dedicated hardware that selects events of interest in under a microsecond) and computational solutions that can be applied across the HEP science drivers. Topics studied in this priority area include, but are not limited to: phenomenological and theoretical studies that support experimental HEP research at the Energy, Intensity and Cosmic Frontiers, both in understanding the data and in finding new directions for experimental exploration; development of analytical and numerical computational techniques for these studies including incorporation of concepts from big data and analytics, machine learning, and efficient parallel computing in distributed environments; computational science and simulations that advance theoretical high energy physics or scientific discovery aligned with the HEP mission; and construction and exploration of theoretical frameworks for understanding fundamental particles and forces at the deepest level possible.

(b) Advanced Accelerator and Advanced Detector Technology Research & Development in High Energy Physics

The advanced technology R&D priority area develops the next generation of particle accelerators and detectors and related technologies for discovery science; and also for possible applications in industry, medicine and other fields. This priority area supports world-leading research in the physics of particle beams and particle detection, particularly exploratory research aimed at developing new concepts. Proposals that address advanced training in critical supporting engineering disciplines or topical areas will also be considered (see below).

Topics studied in the advanced accelerator technology R&D priority area include, but are not limited to: accelerator and beam physics, including analytic and computational techniques for modeling particle beams and simulation of accelerator systems; novel acceleration concepts; the science of high gradients in accelerating cavities and structures; high-power radio frequency (RF) sources; high-brightness beam sources; and beam instrumentation. Also of interest are superconducting materials and conductor development; innovative magnet design and development of high-field superconducting magnets; as well as associated testing and cryogenic systems. Proposals which address advanced training in RF engineering, cryogenic engineering or superconducting magnet engineering as applied to accelerator technologies will also be considered.

Four areas in accelerator science and engineering have been identified as having critical mission need for the DOE, and are the focus of DOE Traineeship programs. Applications in these areas of critical need are strongly encouraged:

1. Physics of large accelerator and systems engineering,
2. Superconducting radiofrequency accelerator physics and engineering,
3. Radiofrequency power system engineering,
4. Cryogenic systems engineering (especially liquid helium systems).

Topics studied in the advanced particle detector R&D priority area include, but are not limited to: low-mass, high channel density charged particle tracking detectors; high resolution, fast-readout calorimeters and particle identification detectors; techniques for improving the radiation tolerance of particle detectors; and advanced electronics and data acquisition systems. Proposals which address advanced training in cryogenic engineering or low-radioactivity materials as applied to particle detector technologies will also be considered.

(c) Experimental Research in High Energy Physics

The experimental HEP research effort supports experiments utilizing human-made and/or naturally occurring particle sources to study fundamental particles and their interactions. Topics studied in the experimental research program include, but are not limited to: proton-proton collisions at the highest possible energies; studies of neutrino properties using accelerator-produced neutrino beams or cosmic data, neutrinos from nuclear reactors; sensitive measurements of rarely occurring phenomena that can indicate new physics beyond the Standard Model; measurements of cosmic acceleration caused by dark energy and inflation; and detection of the particles that make up cosmic dark matter.

Applications to this priority area should explicitly address how the proposed training will enhance the applicant's experience and abilities in the critical areas of particle detector instrumentation and/or computational science including incorporation of concepts from big data and analytics machine learning, efficient parallel computing in distributed environments, and large-scale computing for HEP. Programmatic priority in this topic will be given to those applications that most effectively address this issue.

VII. Nuclear Physics (NP)

The mission of the Office of Nuclear Physics (NP) program is to discover, explore, and understand all forms of nuclear matter.

Program Website: https://science.osti.gov/np

Although the fundamental particles that compose nuclear matter—quarks and gluons—are themselves relatively well understood, exactly how they interact and combine to form the different types of matter observed in the universe today and during its evolution remains largely unknown. It is one of the enduring mysteries of the universe: What, really, is matter? What are the units that matter is made of, and how do they fit together to give matter the properties we observe? To solve this mystery, the NP program supports experimental and theoretical research—along with the development and operation of particle accelerators and advanced technologies—to create, detect, and describe the different forms and complexities of nuclear matter that can exist, including those that are no longer commonly found in our universe.

In executing this mission, nuclear physics focuses on three broad yet tightly interrelated areas of inquiry. These areas are described in Reaching for the Horizon https://science.osti.gov/np/nsac/, a long range plan for nuclear science released in 2015 by the Nuclear Science Advisory Committee (NSAC). The three areas are:

- Quantum Chromodynamics,
- Nuclei and Nuclear Astrophysics, and
- Fundamental Symmetries and Neutrinos.

NP's priority research areas for SCGSR program include:

(a) Medium Energy Nuclear Physics

The Medium Energy subprogram of Nuclear Physics focuses primarily on questions having to do with the first frontier of Nuclear Physics, Quantum Chromodynamics (QCD), especially regarding the spectrum of excited mesons and baryons, and the behavior of quarks inside the nucleons (neutrons and protons). Specific questions that are being addressed include: *What does QCD predict for the properties of excited mesons and baryons? What governs the transition of quarks and gluons into pions and nucleons? What is the role of gluons and gluon self-interactions in nucleons and nuclei*? *What is the internal landscape of the nucleons?*

Experimental research is primarily carried out at the Thomas Jefferson National Accelerator Facility (TJNAF), the Relativistic Heavy Ion Collider (RHIC), the High Intensity Gamma-Ray Source (HIGS), and on a smaller scale at other international facilities. Two major goals of the research program at TJNAF are the discovery of “exotic mesons” which carry gluonic excitations, and the experimental study of the substructure of the nucleons using high-energy electron beams. At RHIC, the goals are to elucidate how much the spin of gluons contributes to the proton's spin and study the spin-flavor structure of sea quarks in polarized proton-proton collisions. This subprogram also supports investigations of some aspects of the second and third frontiers, Nuclei and Nuclear Astrophysics, and Fundamental Symmetries and Neutrinos.

(b) Heavy Ion Nuclear Physics

The Heavy Ion Nuclear Physics subprogram focuses on studies of condensed quark-gluon matter at extremely high densities and temperatures characteristic of the infant Universe. Only two facilities in the world are capable of exploring the properties nuclear matter in these conditions, the U.S. Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory and the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN). The goal is to explore and understand unique manifestations of QCD in this many-body environment and their influence on the Universe’s evolution. Important avenues of investigation are directed at resolving properties of the quark gluon plasma at different length scales and learning more about its physical characteristics including its temperature, the energy loss mechanism for quarks and gluons traversing the plasma, determining the speed of sound in the plasma, measuring the effect of the chiral magnetic force, understanding how quarks fragment and recombine to form hadronic matter (hadronization), and locating a possible critical point for the transition between the plasma and normal matter.

(c) Fundamental Symmetries

The Fundamental Symmetries program investigates aspects of the third frontier identified by NSAC - Fundamental Symmetries and Neutrinos. Questions addressed in this frontier include: *What is the nature of the neutrinos, what are their masses, and how have they shaped the evolution of the universe? Why is there now more matter than antimatter in the universe? What are the unseen forces that were present at the dawn of the universe but disappeared from view as the universe evolved?* The subprogram supports measurements addressing these questions via techniques and experiments that rely on capabilities unique to nuclear science. Examples include experiments to measure, or set a limit on, the neutrino mass and to determine if the neutrino is its own antiparticle. Experiments with cold neutrons also investigate the dominance of matter over antimatter in the universe, as well as other aspects of Fundamental Symmetries and Interactions.

(d) Nuclear Structure and Nuclear Astrophysics

The Nuclear Structure and Nuclear Astrophysics program investigates aspects of the second frontier identified by NSAC— Nuclei and Nuclear Astrophysics. Questions include: *What is the nature of the nucleonic matter? What is the origin of simple patterns in complex nuclei? What is the nature of neutron stars and dense nuclear matter? What is the origin of the elements in the cosmos? What are the nuclear reactions that drive stars and stellar explosions?* Major goals of this subprogram are to develop a comprehensive description of nuclei across the entire nuclear chart, to utilize rare isotope beams to reveal new nuclear phenomena and structures unlike those that are derived from studies using stable ion beams, and to measure the cross sections of nuclear reactions that power stars and spectacular stellar explosions and are responsible for the synthesis of the elements.

(e) Nuclear Theory

The Nuclear Theory subprogram supports theoretical research at universities and DOE national laboratories with the goal of improving our fundamental understanding of nuclear physics, interpreting the results of experiments, and identifying and exploring important new areas of research. This subprogram addresses all of the field’s scientific thrusts described in NSAC’s long range plan, as well as the specific questions listed for the experimental subprograms above. Theoretical research on QCD (the fundamental theory of quarks and gluons) addresses the questions of how the properties of the nuclei, hadrons, and nuclear matter observed experimentally arise from this theory, how the phenomenon of quark confinement arises, and what phases of nuclear matter occur at high densities and temperatures. In Nuclei and Nuclear Astrophysics, theorists investigate a broad range of topics, including calculations of the properties of stable and unstable nuclear species, the limits of nuclear stability, the various types of nuclear transitions and decays, how nuclei arise from the forces between nucleons, and how nuclei are formed in cataclysmic astronomical events such as supernovae and neutron star mergers. In Fundamental Symmetries and Neutrinos, nucleons and nuclei are used to test the Standard Model, which describes the interactions of elementary particles at the most fundamental level. Theoretical research in this area is concerned with determining how various (beyond) Standard Model aspects can be explored through nuclear physics experiments, including the interactions of neutrinos, unusual nuclear transitions, rare decays, and high-precision studies of cold neutrons.

(f) Nuclear Data and Nuclear Theory Computing

This area includes research related to the U.S. Nuclear Data Program (USNDP), as well as several activities that facilitate the application of high performance computing to nuclear physics. The USNDP collects, evaluates, and disseminates nuclear physics data for basic and applied nuclear research with its support of the National Nuclear Data Center (NNDC). The NNDC maintains open databases of scientific information gathered over the past 50+ years of research in nuclear physics. The USNDP also addresses gaps in the data through targeted experimental studies, modeling and simulation, and the use of theory. “Nuclear Theory Computing” includes the NP component of the ASCR program Scientific Discovery through Advanced Computing (SciDAC), which promotes the use of supercomputers to solve computationally challenging problems of great current interest. Recent topics in computational nuclear physics investigated under SciDAC include the theory of quarks and gluons on a lattice (LQCD), studies of a wide range of applications of models of nuclei and nuclear matter, internal structure of nucleons and nuclei in terms of quarks and gluons and their dynamics, and problems in nuclear astrophysics such as nucleosynthesis and gravity-wave generation in supernovae and neutron star mergers, and the development of theoretical techniques for incorporating LQCD results in traditional many-body nuclear physics calculations. SCGSR applications in this area might include for example highly computational research programs in nuclear theory, or experimental studies of relevance to the national nuclear data program.

(g) Accelerator Research and Development for Current and Future Nuclear Physics Facilities

The Nuclear Physics program supports a broad range of activities aimed at research and development related to the science, engineering, and technology of heavy-ion, electron, and proton accelerators and associated systems. Areas of interest include the R&D technologies of the Brookhaven National Laboratory's Relativistic Heavy Ion Collider (RHIC), with heavy ion and polarized proton beams; linear accelerators such as the Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF); and development of devices and/or methods that would be useful in the generation of intense rare isotope beams for the next generation rare isotope beam accelerator facility, the Facility for Rare Isotope Beams (FRIB) currently under construction at Michigan State University. Also of interest is R&D in accelerator science and technology in support of next generation Nuclear Physics accelerator facilities such as an electron-ion collider (EIC) under development to be built at BNL.

(h) Quantum Information Science for Experimental and Computational Nuclear Physics

The nuclear physics community seeks to fully develop the capabilities of Quantum Information Systems (QIS) and quantum computing for nuclear physics research with special emphasis on areas in quantum chromodynamics, fundamental symmetries, nuclear structure, and nuclear astrophysics. Proposals should address the Priority Research Opportunities as identified in the October 2019 report from the Nuclear Scientific Advisory Committee "Nuclear Physics and Quantum Information Science" https://science.osti.gov/-/media/np/pdf/Reports/NSAC_QIS_Report.pdf. Key areas include quantum computing and quantum simulation related to progress in quantum field theory and many-body physics and quantum sensor development applicable to nuclear physics research efforts. Further information can be found at https://science.osti.gov/np/Research/Quantum-Information-Science.

(i) Artificial Intelligence and Machine Learning for Nuclear Physics

Artificial Intelligence (AI) and Machine Learning (ML) have tremendous potential within NP Research. Advancements in the nuclear physics research infrastructure generate both experimental and computation data, and all top priorities in the NSAC Long Range Plan benefit from researching and applying AI and ML methods with well-understood uncertainty quantification, both systematic and statistical, to accelerator science, NP experimentation, and NP theory. Applicants should refer to Section 2 "Priority Research Directions" in the 2020 AI for Nuclear Physics Report, https://arxiv.org/abs/2006.05422, for detailed NP priority areas in AI and ML.

(j) Advanced Detector Technology Research and Development in Nuclear Physics

The advanced detector technology R&D is forward looking to innovative concepts and emerging technologies that provides new pathways to discovery science. This priority area supports detector R&D that is substantially beyond the current state-of-the-art. Proposals that are incremental improvements or test and characterize available detectors or systems are of less importance. Proposals that address advanced training in novel on-the-horizon disruptive technologies will also be considered.

The Electron-Ion Collider (EIC), to be built at Brookhaven National Laboratory, will generate novel detector research and development effort. The physics goals of the EIC requires advancements in detector technology to optimize the physics outcome of the experiments. Relevant details can be found in the "Electron-Ion Collider Detector Requirements and R&D Handbook," http://www.eicug.org/web/sites/default/files/EIC_HANDBOOK_v1.2.pdf. This resource identifies specific targeted technologies for research and development as well as the machine parameters, kinematics of the basic physics processes, and detector performance requirements specific to the EIC.

EXCLUSIONS: NP does NOT support investigations into the development of nuclear reactors for purposes outside the scope of the NP priority areas described above.

VIII. Isotope R&D and Production (DOE IP)

The mission of the Isotope R&D and Production Program, commonly referred to as the DOE Isotope Program (DOE IP), is to support isotope production research and development (R&D) into novel technologies for production of isotopes to assure availability of critical isotopes that are in short supply to address the needs of the Nation.

Program Website: https://science.osti.gov/Isotope-Research-Development-and-Production

The DOE IP relies on expertise across numerous technical disciplines to accomplish its mission, including nuclear and radiochemistry, nuclear physics, accelerator and reactor science, materials science and engineering, separations science, nuclear data, and others. The DOE IP utilizes facilities and capabilities for the production and distribution of stable and radioactive isotopes in short supply. Radioactive isotopes and enriched stable isotopes are made available by using unique facilities stewarded by DOE IP at Brookhaven National Laboratory, Los Alamos National Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory. DOE IP also coordinates and supports isotope production at a suite of university, national laboratory, and other federal accelerator and reactor facilities throughout the Nation to promote a reliable supply of isotopes domestically. The five principal topics of interest to DOE IP are described below and are focused on the development of advanced, cost-effective and efficient technologies for producing, processing (including isotopic separations, and the development of tracers), recycling, and distributing isotopes in short supply. This includes technologies for production of radioisotopes using reactor and accelerator facilities and new technologies for isotope enrichment.

A primary document currently guiding DOE IP priorities is entitled "Meeting Isotope Needs and Capturing Opportunities for the Future: The 2015 Long Range Plan for the DOE-NP Isotope Program." This document may be accessed at https://science.osti.gov/~/media/np/nsac/pdf/docs/2015/2015_NSACI_Report_to_NSAC_Final.pdf.

The DOE IP's priority research areas for SCGSR program include:

(a) Isotope Production Research

Proposals to this topic should be focused on novel or improved capabilities for inducing transmutation of atoms in targets to create radioisotopes. This includes aspects of targetry and target fabrication. The development of innovative approaches to isotope production are of interest, including integration of Artificial Intelligence and Machine Learning techniques to model and predict the behavior of targets undergoing irradiation to optimize one or more parameters. Both accelerator- and reactor-based isotope production modalities are understood to require different considerations. Proposals to this topic can address either or both production modalities. Robotics and advanced manufacturing techniques, as they apply to isotope production and processing, may also be proposed to this topic.

(b) Isotope Processing, Purification, Separations and Radiochemical Synthesis

Work in this topic might be directed toward the improvement and/or development of novel chemical and physical processes to recover and purify radioisotopes from activated targets. Applications proposing scopes of work dealing with isotopes not necessarily resulting from direct transmutation of target material (e.g., the recovery and purification of radioisotopes from legacy materials, facility components, used nuclear fuel, or waste streams/effluents of other processing efforts) would also be considered responsive.

Additionally, the development or synthesis of chemical constructs with physical or chemical properties that make them particularly useful in the isotope science landscape (e.g., the synthesis and development of novel chelating agents or other ligands) are programmatically very relevant. Development of automated production and processing techniques to enhance the efficiency and safety of radioisotope production and processing (including uses of AI or ML and advanced manufacturing) are also encouraged. It is important to note that the development of purification and separation techniques may but do not have to include the handling of radioactive materials or irradiation of targets (e.g., experiments based on surrogate material are acceptable).

(c) Biological Tracers and Imaging

Work in this topic should be focused on the development of isotopes and/or chemical constructs which have physical or chemical properties that make them particularly useful as biological tracers and/or imaging agents. Included in this topic are the synthesis and development of novel chelating agents or other ligands. Please note that the DOE IP funds only basic science R&D. Studies investigating the applications of isotopes will not be considered for funding.

(d) Isotope Enrichment Technology

DOE IP is presently making significant investments in the establishment of a broad-scope stable isotope enrichment capability using gas centrifuge and electromagnetic ion separation (EMIS) technologies, as well as modest investments in radioisotope EMIS and Atomic Vapor Laser Isotope Separation (AVLIS) technologies. Therefore, new proposals aimed at stable and radioisotope enrichment should focus on the improvement of throughput, design and yield of gas centrifuge, EMIS, and AVLIS technologies. Proposals involving energy and feedstock efficient enrichment technologies are also acceptable. R&D efforts that support analytical methods for synthesizing and purifying silane gas as well as those proposing technologies outside of the those listed may also be considered responsive. The development of enrichment techniques and capabilities to produce enriched stable isotopes relevant to advanced energy fuel cycles and technologies may also be considered responsive.

EXCLUSIONS: Excluded from this call are applications related to the production of Mo-99 and Pu-238, as these isotopes are under the purview of the National Nuclear Security Administration Office of Materials Management and Minimization (https://www.energy.gov/nnsa/national-nuclear-security-administration) and the DOE Office of Nuclear Energy (https://www.energy.gov/ne/office-nuclear-energy) respectively. Furthermore, the DOE IP does NOT support investigations into the development of nuclear reactors for purposes outside the scope of the DOE IP priority areas described above.

IX. Accelerator R&D and Production (ARDAP)

The mission of the Office of Accelerator R&D and Production (ARDAP) program is to ensure a robust pipeline of particle accelerator expertise and technology to build the billion-dollar-class scientific facilities of the future. Research in next-generation accelerator science and technology, followed by its successful transition to industrial production, is critical to supporting the physical sciences research and the industrial strength needed to position the U.S. to lead the world for decades to come. A key aspect of this mission is to develop a workforce with expertise in effective technology transfer R&D and accelerator component engineering.

ARDAP is particularly interested in training graduate students who can bridge the gap between accelerator science research and industrial adoption and production of accelerator technology. In addition to strong accelerator science and engineering skills, closely-coupled expertise in design-for-manufacture practices, manufacturing risk reduction, supply chain analysis and risk reduction, application of advanced manufacturing techniques, and application of data science techniques to improve accelerator component production are each of interest.

Applicants seeking to work on a specific Office of Science program's accelerator R&D who also wish to develop a solid background in general aspects of technology transfer and engineering may consider applying under the Accelerator Science convergence area.

Program Website: https://science.osti.gov/ARDAP

ARDAP welcomes proposals with either a Research focus or a Development focus, with the latter being strongly encouraged.

ARDAP's priority research areas for the SCGSR program include:

(a) Accelerator Technology Research

ARDAP supports accelerator technology research through the Accelerator Stewardship program which invests in use-inspired R&D technology areas to enable new accelerator applications in industry, medical treatment, and national security. ARDAP is interested in developing a workforce that can broadly enhance the ability of the DOE Office of Science and other federal agencies to conduct their accelerator-based missions, provide the basic R&D foundation necessary for sustained innovation across a broad range of accelerator applications, drive specific accelerator applications to practical and testable prototypes, and serve as a bridge between those who develop accelerator technology and those who apply accelerator technology.

Proposals in the ARDAP Accelerator Research area should have a strong emphasis on early-stage basic research and should include one or more well-defined activities related to transferring the results into practice, and ultimately into commercial production. Such activities can include (1) market analysis to understand the market potential if the research is successful, (2) market analysis to identify possible commercialization partners, (3) collaborating with industry experts, or (4) pursuing a research topic identified by industry, and other industry-centered activities. Proposals in this area may focus on work suitable for academic publication and must include a component related to commercialization.

(b) Accelerator Technology Development

ARDAP is particularly interested in training graduate students who can bridge the gap between accelerator science research and industrial adoption and production of accelerator technology. In addition to strong accelerator science and engineering skills, ARDAP is interested in developing a workforce with closely coupled expertise in design for manufacture, manufacturing risk reduction, supply chain analysis and risk reduction, application of advanced manufacturing techniques, and application of data science techniques to improve accelerator component production.

Proposals in the ARDAP Accelerator Development area should have a strong emphasis on partnering with industry to transfer technology and develop the means to produce the technology efficiently. Proposals in this area may advance knowledge generally but should focus on advancing the technology's manufacturing readiness level.