

Office of Science Priority Research Areas for SCGSR Program

Priority Research Areas for SCGSR 2021 Solicitation 1

It is an **Eligibility** Requirement [link to Eligibility page] 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 2021 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 six SC program offices are: Advanced Scientific Computing Research (**ASCR**), Basic Energy Sciences (**BES**), Biological and Environmental Research (**BER**), Fusion Energy Sciences (**FES**), High Energy Physics (**HEP**), and Nuclear Physics (**NP**), which in this solicitation, temporarily includes the DOE Isotope Program (**DOE IP**) (Office of Isotope R&D and Production). A short overview of the Office of Science is available here [link to SCGSR SC overview], 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 2020 Solicitation 2. 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 read carefully the full descriptions of priority areas of consideration and, consult with the SCGSR program [link to Contact] 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

- (a) Microelectronics (ASCR, BES, HEP, and NP)
- (b) Data Science (ASCR, BES, BER, FES, HEP, and NP)
- (c) Conservation Laws and Symmetries (BES, HEP, and NP)
- (d) Accelerator Science (ASCR, BES, BER, FES, HEP, and NP)

II. Advanced Scientific Computing Research (ASCR)

- (a) Applied Mathematics
- (b) Computer Science

III. Basic Energy Sciences (BES)

- (a) Accelerator and Detector R&D
- (b) Basic Geosciences
- (c) Catalysis Science with NMR Spectroscopy, Neutron Scattering, and X-Ray Absorption Spectroscopy Techniques
- (d) Condensed Phase and Interfacial Molecular Science (CPIMS)
- (e) Crystal Growth
- (f) Data Science for AI Applications to Chemical, Geological, Biochemical, and Materials Sciences
- (g) Electron and Scanning Probe Microscopy Research and Instrumentation
- (h) Energy Transfers in Large Proteins and Protein Complexes
- (i) Fundamental Electrochemistry for Chemical and Materials Sciences
- (j) Gas Phase Chemical Physics
- (k) Highly Ionizing Radiation in Chemistry
- (l) Materials Science and Chemistry for Microelectronics
- (m) Neutron Scattering Research and Instrumentation
- (n) Nuclear Chemistry and Radiochemical Separations
- (o) Quantum Information Science for Experimental Condensed Matter Physics
- (p) Quantum Information Science for Theoretical Condensed Matter Physics
- (q) Radiation Effects in Materials
- (r) Separation Science
- (s) Ultrafast Materials and Chemical Sciences

IV. Biological and Environmental Research (BER)

- (a) Computational Biology and Bioinformatics
- (b) Biomolecular Characterization and Imaging Science
- (c) Plant Science for Sustainable Bioenergy
- (d) Environmental Microbiology
- (e) Environmental Systems Science
- (f) Atmospheric System Research
- (g) Earth System Model Development
- (h) Regional and Global Model and Analysis

V. Fusion Energy Sciences (FES)

- (a) Burning Plasma Science & Enabling Technologies
- (b) Discovery Plasma Science

VI. High Energy Physics (HEP)

- (a) Theoretical and Computational Research in High Energy Physics
- (b) Advanced Accelerator and Advanced Detector Technology Research and Development in High Energy Physics
- (c) Experimental Research in High Energy Physics

VII. Nuclear Physics (NP)

- (a) Medium Energy Nuclear Physics
- (b) Heavy Ion Nuclear Physics
- (c) Fundamental Symmetries
- (d) Nuclear Structure and Nuclear Astrophysics
- (e) Nuclear Theory
- (f) Nuclear Data and Nuclear Theory Computing
- (g) Accelerator Research and Development for Current and Future Nuclear Physics Facilities
- (h) Quantum Information Science for Experimental and Computational Nuclear Physics
- (i) Artificial Intelligence and Machine Learning for Nuclear Physics
- (j) Advanced Detector Technology Research and Development in Nuclear Physics
- (k) DOE Isotope Program (**DOE IP**) (Office of Isotope R&D and Production)
 - (i) Isotope Production Research
 - (ii) Isotope Processing and Purification
 - (iii) Nuclear Chemistry and Radiochemical Separations
 - (iv) Biological Tracers and Imaging
 - (v) Isotope Enrichment Technology

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 collaborating DOE laboratory scientist at the DOE host laboratory. Due to the convergence 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 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 course of 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 (<https://www.whitehouse.gov/wp-content/uploads/2018/12/STEM-Education-Strategic-Plan-2018.pdf>). Since its inception in 2014, the SCGSR program has demonstrated strength in preparing graduate students for science, technology, engineering, or mathematics (STEM) careers critically important 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 team science culture and world-class scientific facilities at national laboratories nurtures a workforce development eco-system readily addressing 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 them for careers in cutting edge transdisciplinary research fields and community environment.

The Department of Energy's Office of Science (<https://science.osti.gov/>) supports basic research endeavors in a broad spectrum from fundamental studies within a single academic discipline to collaborations involving efforts from 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 as shown, and are subject to evaluation by its 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 SC program office, it is recommended to submit it to the convergence area first.**

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

The Department of Energy's Office of Science programs have always been at the cutting edge of microelectronics, making major contributions to the scientific understanding, materials, and advanced instrumentation that enabled innovations to promote scaling. This has driven transformative advances in microelectronics for the challenging demands of DOE's high performance computing and science facilities. Now, strong evidence exists that scaling is approaching its physical and economic limits, and yet, the growth of data-centric computing and sensor networks is redefining computing workloads and microelectronics needs. 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 demand and power 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.

To enable continued advances in computing technologies, a fundamental rethinking is needed of the science behind the materials, physics, synthesis and placement technologies, architectures and algorithms. 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 materials discovery, device physics, architectures, and the software stack for developing information processing systems of the future.

Applications should take a multi-disciplinary approach to address future DOE needs in computing, power grid management, and science facility workloads. Potential areas of focus include discovery science that can lead to, for example, microelectronics for exascale computers and beyond with a small footprint and low power utilization. Such high performance computation will be necessary for analyzing and managing the vast amount of data that will be generated by future research facilities as well as pushing the boundaries of scientific computing. In addition, advances in new microelectronics materials, and their integration within a co-design framework, would transform power electronics and the electricity grid into a modern, agile, resilient, and energy-efficient system.

Relevant topics are outlined in the priority research directions from the Basic Research Needs for Microelectronics (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) 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, astronomy and particle physics. Many opportunities still remain for data science to accelerate the rate of fundamental discovery. Applications should focus on innovative applications of modern data science approaches (artificial intelligence, machine learning, graph theory, uncertainty quantification, etc.) and/or approaches to data management that would enable data science for cutting-edge research relevant to the Office of Science. A priority outcome

from this research should be novel, robust, data-driven, hypothesis-based models that lead to improved understanding; or the unleashing of high-value DOE research data in ways that are findable, accessible, interoperable, and reuseable by other researchers. Use of these 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. Identifying new physical descriptors may be important to manage the complexity of multidimensional datasets and enable inverse or statistically driven design concepts.

EXCLUSIONS: Quantum computing or quantum systems for quantum information science; energy storage; ‘omics’ data and systems biology approaches; applied research, such as design or optimization of instruments, devices, tools or processes; an exclusive focus on database development and management; areas covered already in the topics for ASCR, BES, BER, FES, HEP, and NP.

(c) Conservation Laws and Symmetries (Participating Programs: BES, 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, and NP)

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, and NP), 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, and 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, and NP). 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 the convergence area or a non-convergence area under a single program office, it is recommended to submit it 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 mission of the Advanced Scientific Computing Research (ASCR) program is to advance applied mathematics and computer science; deliver the most advanced 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, in partnership with the research community, including U.S. industry. The strategy to accomplish this has two thrusts: developing and maintaining world-class computing and network facilities for science; and advancing research in applied mathematics, computer science and advanced networking.

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 the Office of Science 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 Office of Science 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 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 science, computational science and network research to solve complex problems on computational resources that are on a trajectory to reach exascale within a few years.

The ASCR's research priority areas for SCGSR program include:

(a) Applied Mathematics

This subprogram supports research and development of applied mathematical models, methods, and algorithms for understanding complex natural and engineered systems related to DOE's mission.

Important areas of supported research include:

- Novel 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, multi-physics 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; and
- Innovative approaches for analyzing and extracting insight from large-scale data sets.

Scientific Machine Learning and Artificial Intelligence are emerging trends with the potential to transform science and energy research. The topic area considers how computational technology can be developed and used to assist, augment, or automate human skills for scientific purposes. Foundational research themes correspond to the need for incorporating domain-awareness, interpretability, and robustness into the development of new approaches. The capability research themes correspond to the three major use cases of massive scientific data analysis, machine-learning enhanced modeling and simulation, and intelligent automation and decision-support for complex systems such as autonomous experiments.

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

This subprogram supports basic research in computer science needed to create computational capabilities that support DOE and Office of Science mission and goals. Computer science research includes high performance systems hardware and software architecture, languages, compilers, programming models and environments, execution models, runtime systems, operating systems, scientific data management, data analytics, and visualization of scientific applications running at scale.

In the context of ASCR-supported high performance computing environments, research topics of interest are:

- Data analysis and visualization: visual analytic techniques for comparative and/or integrated analysis of two or more data sets; visual analytic approaches to understanding the state and behavior of a supercomputing system at scale; visual analysis of uncertainty and the sources thereof;
- Techniques for in situ data analysis and workflow management in high performance computing environments;
- Techniques and tools for advancing fundamental practices of management, archiving, curation, and/or reuse, of data generated by experimental, observational, and simulation data relevant to SC mission areas.
- Knowledge representation and machine learning for analysis of extreme scale scientific data from simulations and/or experiments;
- Storage system software and/or scientific databases for extreme scale data that support scientists' models of their data and the use thereof;

- Programming models, environments and tools that increase code portability, increase levels of abstraction, increase developer productivity, and/or make programming for HPC more accessible for newcomers to the field.
- Operating and runtime systems, including intelligent resource management, and workflow management systems, that support use of heterogeneous computing technologies, including diverse processors, accelerators, and memory and storage systems.
- Execution models and metrics to guide development and evaluation of software systems and applications for heterogeneous hardware environments.
- Neuromorphic Computing and/or Quantum Computing: research focused on information processing and computation systems beyond von Neumann/Turing architectures and Moore's Law Limits, including hardware architectures, development of programming environments, languages, libraries, compilers, simulators, and research and development of algorithms for physical simulation;
- Machine learning in the narrow context of high performance computing, relevant to SC user facilities including those supported by ASCR, and extreme scale applications for the acceleration of scientific discovery and its applications.
- 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 to deliver means that assure trustworthiness within open high-end networking and data centers.
- Autonomic computing and communication systems that integrate advances in applied artificial intelligence, Software Defined Networks (SDN), Science Internet of Things (S-IoT), and network analytics to support a new generation smart science facilities.

EXCLUSIONS: Topics that are NOT within the scope for this program area include research not addressing ~~the~~ any of the challenges described above and research primarily focusing on:

- Proposals with primary emphasis on hardware design (except as noted above), resilient solvers, and/or new development of machine probabilistic methods and their mathematical formalisms;
- All aspects of computer-supported collaboration, social computing, natural language processing / understanding / generation and/or analysis, and generalized research in human-computer interaction; Discipline-specific data analytics and informatics;
- Research focused on the World Wide Web, the dark web, and/or data about it; and
- Research that is primarily to advance cloud computing, and/or hand-held, portable, desktop, and/or embedded computing.

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.

Program Website: <https://science.osti.gov/bes/>

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.

The 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 opportunities 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.

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) Catalysis Science with NMR Spectroscopy, Neutron Scattering, and X-ray Absorption Spectroscopy Techniques

There have been a number of significant recent advances in nuclear magnetic resonance (NMR) spectroscopy, neutron scattering, and in-situ/operando x-ray techniques that hold great promise for advancing catalysis science. DOE has made considerable investments in ultra-high magnetic field and new generation dynamic nuclear polarization NMR spectrometers at Ames Laboratory and Pacific Northwest National Laboratory. In particular, ultra-high field instruments now provide enhanced sensitivity for rare and low-sensitivity NMR nuclei thereby enabling spectroscopic studies of important catalytic species that previously could not be observed. DOE also currently operates two world-leading neutron scattering facilities at Oak Ridge National Laboratory (the Spallation Neutron Source and the High Flux Isotope Reactor) that provide unique capabilities to probe catalyst structure and dynamics; in particular, unique scattering cross-sections enable visualization of light and heavy atoms in complex materials (e.g., zeolites and metal-organic frameworks). In addition, dedicated x-ray absorption spectroscopy beamlines at SLAC National Accelerator Laboratory, Brookhaven National Laboratory, and Argonne National Laboratory synchrotron facilities are uniquely equipped with in-situ/operando tools to enable the understanding of the relationship between the electronic and geometric structures of working catalysts and their performance.

Applications should focus on advancing catalysis science research by utilizing the cutting-edge NMR, neutron scattering, and x-ray absorption techniques at the above-described facilities. Graduate students interested in advancing ultrafast dynamics and spectroscopy in catalysis at the LCLS at SLAC National Accelerator Laboratory are encouraged to apply under topic (g) Ultrafast Materials and Chemistry.

EXCLUSIONS: Non-catalysis-driven research will not be considered. Topics in catalysis that pertain to health or medical sciences, biology, environmental, or geological sciences (atmospheric or subsurface) will not be considered.

(d) Condensed Phase and Interfacial Molecular Science (CPIMS)

Chemical physics and physical chemistry in liquids and at solid interfaces is important to a wide variety of energy technologies, providing a molecular-level understanding of chemical and physical processes. Experimental, theoretical, and computational investigations in the condensed phase and at interfaces aim at elucidating the molecular-scale chemical and physical properties and interactions that govern chemical reactivity, solute/solvent structure, and transport. Studies of reaction dynamics at well-characterized surfaces and clusters lead to the development of theories on the molecular origins of surface-mediated catalysis and heterogeneous chemistry. Studies of model condensed-phase systems target first-principles understanding of molecular reactivity and dynamical processes in solution and at surfaces, including complex interfaces. The transition from molecular-scale chemistry to collective phenomena in complex systems is also of interest, allowing knowledge gained at the molecular level to be exploited through the dynamics and kinetics of collective interactions.

EXCLUSIONS: Applications should focus on transformative research opportunities for graduate students to work with national laboratory scientists in advancing experimental and computational approaches at DOE National Laboratories. The CPIMS program supports reductionist science, with electronic, atomic, and molecular-level detail. Therefore, projects aimed at the bulk scale, including fluid dynamics, will not be considered. In addition, projects focused on technological applications, device development or medical science will not be considered.

(e) Crystal Growth

The importance of large, high quality crystals for fundamental research spans many scientific disciplines including chemistry, materials science, physics, biochemistry, and geochemistry. This program will provide opportunities for graduate students to focus on the growth of large single crystals and assess their properties with national laboratory instrumentation. This program emphasis is in keeping recommendations of 2009 NRC study report (<http://www.nap.edu/catalog/12640/frontiers-in-crystalline-matter-from-discovery-to-technology>) which calls for programs specifically designed to strengthen and sustain education and training in the field of the discovery and growth of crystalline materials. DOE laboratories provide a unique venue for both the growth and characterization of materials, with the availability of specialized state-of-the-art crystal growth equipment and furnaces that are generally not available in academic research laboratories. For inorganic materials, growth of single crystals can require processing at high temperatures in vacuum, high pressures of reactive gases, or hydrothermal conditions. Large single crystal growth under extreme and geochemical-relevant conditions can serve as important models of natural systems, in particular to determine molecular-level mechanisms, growth in heterogeneous environments, non-

equilibrium crystallization, and elemental or isotopic distribution under different dynamic conditions. For characterization, the DOE labs have extensive capabilities for x-ray, electron and neutron scattering, for measurement of properties including low temperatures (mK) and high magnetic fields (up to 100 T), and for handling radioactive materials.

Applications should focus on expanding and enriching graduate student's experience and proficiency in single crystal growth, characterization, and crystalline materials discovery.

EXCLUSIONS: Applications will only be considered if they expand the student's experience in experimental three-dimensional single crystal growth; applications that target biomedical applications or systems (e.g., animal/human health) will NOT be considered. Projects aimed at the synthesis of nanosized crystals with any dimensions being in the nanosize (including two-dimensional films), hierarchical assemblies including liquid crystals, or porous materials will NOT be considered. Applications focused on theory or computation will NOT be considered.

(f) Data Science for AI Applications to Chemical, Geological, Biochemical, and Materials Sciences

Artificial intelligence (AI) approaches include, for example, machine learning, deep learning, neural networks, and natural language processing. AI promises to be disruptive and to accelerate the scientific discovery progress for complex chemical, geological, biochemical, and materials systems. New chemical and physical property databases, comprised of experimental measurements and theoretical calculations from multiple research groups, are quickly evolving in size, complexity, and diversity. However, this heterogeneous data is often not structured for immediate application of AI methods, motivating the immersion of graduate students specializing in data science within these groups.

The proposed research must fit within the scope of basic research programs funded by the Chemical Sciences, Geosciences, and Biosciences (CSGB) Division (<https://science.osti.gov/bes/csgb/research-areas/chemical-transformations/>) and Materials Sciences and Engineering (MSE) Division (<https://science.osti.gov/bes/mse/Research-Areas>) in BES. Applicants must propose innovative approaches to incorporate data science and AI methods to advance the understanding of fundamental mechanisms.

EXCLUSIONS: Applied research, such as design or optimization of instruments, devices, tools or processes, or an exclusive focus on database development and management, are NOT considered.

(g) Electron and Scanning Probe Microscopy Research and Instrumentation

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 use or development of advanced electron and scanning probe microscopy instrumentation and techniques to image and characterize functional matter to answer fundamental questions in materials or chemical sciences.

EXCLUSIONS: Applications that target biomedical applications or systems (e.g., animal/human health) will NOT be considered.

(h) Energy Transfers in Large Proteins and Protein Complexes

Biological energy conversions frequently involve multiple transfers of electrons or excitation energy between molecular cofactors embedded in complex protein matrices. Examples of this include the transfers of electrons or excitation energy that occur in photosystems, respiratory complexes, and large enzymes like nitrogenases or hydrogenases. These transfers are often specific, directed, and highly efficient. They provide biochemical models that can inform the design of man-made energy conversion systems having comparable specificity and efficiency at the molecular scale. Research projects focused on electron and excitation transfers through proteins are supported by the Office of Basic Energy Sciences (BES) at several national laboratories. These projects address atomic-scale structures of the proteins, their dynamics, and how they promote efficiency and specificity of the transfers. This SCGSR research area invites graduate student participation in these projects to promote research interactions between national laboratories and university-based scientists and to provide training and experience that will empower the next generation of U.S. scientists and engineers to employ knowledge from biochemical systems in the design of advanced energy technologies.

EXCLUSIONS: Based on programmatic priorities, topics of research that will NOT be considered include: studies of animals, medically-oriented studies, development or optimization of

microbes or plants for biofuel or biomass production, phenotype analyses that do not test specific hypotheses, and intensive data collection that does not test specific hypotheses.

(i) 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 for Energy (2007), Solar Energy Utilization (2005), Next Generation Electrical Energy Storage (2017), Advanced Nuclear Energy Systems (2006), Future Nuclear Energy (2017), and Materials under Extreme Environments (2007) 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.

(j) Gas Phase Chemical Physics

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.

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.

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.

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.

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.

EXCLUSIONS: Topics of research that will NOT be considered are: non-reacting fluid dynamics (transport phenomena including computational fluid dynamics (CFD), 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.

(k) Highly Ionizing Radiation in Chemistry

There is a strong need for fundamental research to enhance the knowledge, understanding and utilization of the effects of ionizing radiation on chemical systems, for instance for the management of existing nuclear reactors and the development of next-generation reactors, waste streams and safe storage techniques. This priority research area addresses research in the chemistry of highly ionizing radiation related to these needs. Though in demand, there are few existing programs for graduate study in the U.S. in this field. National laboratories have capabilities and expertise in this field as well as unique facilities for research on this topic. This program will provide opportunities for graduate students to work with scientists with expertise

in the molecular basis of the chemistry of radiation effects, and to access advanced irradiation, analytical and computational capabilities at the national laboratories.

Typical topics in this area include 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 of particular interest. Basic research on how radiation chemistry of aqueous systems modifies, or is modified by a nearby interfaces can provide a fundamental foundation to address challenges in reactor chemistry, waste separation, and waste storage related to nuclear power generation.

EXCLUSIONS: Based on programmatic priorities, applications involving studies of human/animal health, using animal systems, or focusing on medical research will NOT be considered.

(l) Materials Science 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 the opportunity to reshape computing as we know it, seeking to make it orders of magnitude more energy efficient and powerful than it is today. 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 discover new 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 the manner in which 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 that focus primarily on Quantum Information Science or Quantum Computing will NOT be considered.

(m) Neutron Scattering Research and Instrumentation

There is a critical need for scientific and technical staff with expertise in developing and operating advanced neutron scattering instruments for materials research at the DOE's neutron scattering facilities. Based on the importance of neutron scattering, DOE currently operates two world-leading neutron scattering facilities at Oak Ridge National Laboratory (ORNL) – the Spallation Neutron Source (SNS), a pulsed source with the world's highest pulsed neutron flux, and the High Flux Isotope Reactor (HFIR), a continuous source with an integrated flux rivaling the world's highest intensity neutron scattering facilities. Both of these unique facilities have a number of highly optimized neutron scattering instruments for the study of structure and dynamics in materials by using a broad spectrum of techniques including diffraction, reflectometry, quasielastic and inelastic scattering, and imaging. In concert, BES supports several materials research projects, focused on neutron scattering, at the U.S. universities and national laboratories. Also supported is science-driven development of next-generation instrumentation concepts, novel tools, in-situ capabilities and software infrastructure for machine learning and data analytics to accelerate the discovery of advanced materials to address the future energy challenges.

Applications should focus on transformative materials research opportunities for graduate students to work with national laboratory neutron scattering scientists in advancing neutron scattering instrumentation, techniques and computational tools at the DOE neutron scattering facilities.

(n) Nuclear Chemistry and Radiochemical Separations

This priority research area involves basic research on nuclear chemistry and radiochemical separations, and in particular, the chemistry of transuranic elements and separation research involving radioactive isotopes. All aspects of transuranic chemistry are encouraged. 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. Of particular interest is research for resolving the f-electron challenge; the chemical and physical properties of these elements to determine solution, interfacial and solid-state bonding and reactivity; fundamental transactinide chemical properties; and bonding relationships among the actinides.

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.

(o) Quantum Information Science for Experimental Condensed Matter Physics

There is a growing need for experimental efforts to advance our understanding of quantum phenomena in systems that could be used for Quantum Information Science (QIS).

Next-Generation Quantum Systems: Proposals are requested for basic experimental research focused on phenomena that will enable the design and discovery of novel quantum information systems. Proposals should address Priority Research Opportunities 2, 3, and 4 identified in the report from the Basic Energy Sciences Roundtable on Opportunities for Basic Research for Next-Generation Quantum Systems (available at https://science.osti.gov/~media/bes/pdf/reports/2018/Quantum_systems.pdf). These targeted research areas include: enhance creation and control of coherence in quantum systems; discover novel approaches for quantum-to-quantum transduction; implement new quantum methods for advanced sensing and process control.

EXCLUSIONS: Based on programmatic priorities, applications solely involving fundamental research in quantum phenomena, quantum materials and materials discovery will not be considered. Further, proposals that solely focus on engineering design or systematic optimization of devices will not be considered.

(p) Quantum Information Science for Theoretical Condensed Matter Physics

There is a growing need for theoretical efforts to advance our understanding of quantum phenomena in systems that could be used for Quantum Information Science (QIS), and the use of quantum computing in materials sciences research.

Proposals are requested in support of the Roundtable reports “Quantum Computing in Materials Sciences” and “Next-Generation Quantum Systems” for basic research focused on using quantum computers to solve scientific problems in condensed matter physics or theories that will enable the design and discovery of improved qubits for QIS. Proposals should address the Priority Research Opportunities identified in these reports (https://science.osti.gov/~media/bes/pdf/reports/2018/Quantum_computing.pdf or https://science.osti.gov/~media/bes/pdf/reports/2018/Quantum_systems.pdf).

Targeted areas of theoretical research to advance future quantum systems include: (a) controlling quantum coherence and entanglement for improved qubits and quantum sensors, (b) quantum-classical hybrid computing approaches to quantum phenomena in condensed matter physics suitable for NISQ computing devices.

EXCLUSIONS: Based on programmatic priorities, applications that are focused on fundamental research in quantum phenomena, quantum materials, and materials discovery for systems unrelated to quantum information sciences will not be considered. Applications that focus solely on algorithmic advances, software tools, engineering and/or building quantum computers, or systematic optimization of devices will not be considered.

(q) Radiation Effects in Materials

Fundamental research into the effects of radiation on materials plays an important role in supporting a growing need for nuclear energy supply in the U.S. Radiation can be detrimental to properties, such as embrittlement, or beneficial to properties through doping or strengthening through structural modification. Fundamental research in this area allows a basic understanding of these processes such that structures and properties can be tuned for a given behavior such as radiation resistance or enhanced toughness. The 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>).

This research topic will provide opportunities for graduate students to work with scientists with expertise in radiation effects on materials, and to access advanced irradiation, analytical and computational capabilities at the national laboratories. 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. These processes and structures may be evaluated by a combination of experiment, theory, and modeling, with an emphasis on matching of time and length scales and in-situ observations.

EXCLUSIONS: Based on programmatic priorities, applications involving polymers research, fusion research, or flux pinning for superconductivity will NOT be considered.

(r) Separation Science

Research in chemical separations is critical for ensuring a sustainable chemical enterprise, securing essential elements needed for advanced energy technologies, and addressing contemporary issues of fuel, feedstock, and effluent processing in all phases of matter. Among the most acute chemical separation challenges are those wherein the targeted species are dilute or have very similar properties to other species that must be removed. For example, consider the capture of carbon dioxide from air (ca. 410 ppm CO₂), or the downstream separation of lanthanide species from each other to produce individual rare earth oxides or metals (>99.99% purity). Fundamental research in this area forms the basis for future technological development by providing an advanced understanding of underlying selective sorption and transport mechanisms, energy transfer processes, charge separation, and other elementary processes. The national laboratories have unique capabilities, expertise, and activities that address these most acute separation challenges. This program provides opportunities for graduate students to work with leading separation scientists at the national laboratories, and to gain relevant training and experience.

EXCLUSIONS: The topic does not support the synthesis or testing of separations materials as the principal or only goal; applied research; engineering design or scale-up; development of narrowly defined processes or devices; desalination; microfluidics; sensors; or research directed toward medical or pharmaceutical applications.

(s) Ultrafast Materials and Chemical Sciences

There is an identified need to advance ultrafast science based experimental and theoretical methods, capabilities, and facilities at the electronic, atomic, and molecular levels. This topic will provide opportunities for graduate students to develop and apply new ultrafast science capabilities utilizing x-rays, VUV, and other lower frequency sources using national laboratory instrumentation and facilities. Ultrafast science addresses key grand challenge areas in its ability to probe how quantum systems are organized and assembled; to reveal how materials are arranged and transformed at the atomic and electronic level; to uncover the fundamental rules of correlation and emergence; and to create and track non-equilibrium structures at relevant ultrafast time scales (a few picoseconds or less). By measuring and isolating fundamental excitations and using these as the lever for manipulating materials properties, the dynamics of order parameters may be probed and resolved, dominating fluctuations can be uncovered, and key length scales may be identified.

Applications must focus on the use of ultrafast probes to characterize and understand spin, charge, energy, and phase dynamics in materials and chemical processes for energy-relevant materials and chemical systems. For materials sciences, applications must focus on studying excitations in quantum systems to gain a fundamental mechanistic understanding of how the various quantum particles or quasi-particles interact and flow through an excited system. Applications in chemical sciences must advance understanding of attosecond-to-femtosecond dynamics and electron-electron or electron-nuclear correlations in molecules and electronic states involved in chemical conversions.

EXCLUSIONS: Applications that target biomedical applications or systems (e.g., animal/human health) and applications that focus on benchmarking materials performance and/or rank ordering of sample systems based on a chemical composition or nano-structural arrangement will NOT be considered. For materials sciences, applications that do not focus on studying excitations in quantum systems to gain a fundamental mechanistic understanding of how the various quantum particles or quasi-particles interact and flow through an excited system will be excluded.

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 BSSD 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. BSSD 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.

The BER's priority research areas for SCGSR program include:

(a) Computational Biology and Bioinformatics

The Biological Systems Science Division supports the genomic- and molecular- and 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 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, 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. *Candidates for this topic should focus on developing new innovative computational approaches, predictive models and analytics that enhance, scale and optimize the management and processing of large, complex and heterogeneous data generated from different scales for effective integration and interpretation of system-wide data, simulation of biological phenomena, processes and systems (including whole bacterial cells) relevant to BER science, and analysis of biological networks using computational systems biology approaches 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 www.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 Systems 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: Coupling Atmospheric Observational Data with Numerical Models

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 its 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 (EESDD) require new expertise in coupling observational data from the Atmospheric Radiation Measurement (ARM) Research Facility with high resolution numerical models to advance predictive understanding of aerosol and cloud processes. *Applications for this topic should enable observationally-focused graduate students to develop skills in numerical modeling or modeling-focused graduate students to develop skills in working with advanced observational data.*

(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 \(https://climatemodeling.science.energy.gov/\)](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, 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 by physical processes that are common to many subfields. Because of the wide range of plasma densities and temperatures encountered in fusion applications, it is valuable to support plasma science 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.

The 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.
- *Exploratory Magnetized Plasma* – Research on complex, magnetized plasma systems that spontaneously evolve toward a state of long-range order through dissipative processes (e.g., compact toroidal plasma).

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 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.

The 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.

While officially its own program office (Office of Isotope R&D and Production), for FY 2021, the DOE Isotope Program (DOE IP) will continue to be listed under the NP topics. The DOE IP produces isotopes in short supply and supports research on the improvement or development of production or process technology for isotopes. Radioisotopes are produced with reactors and accelerators at national laboratories and universities and enriched stable isotopes are produced with electromagnetic separation and centrifuge technologies.

- (i) Isotope Production Research
- (ii) Isotope Processing and Purification
- (iii) Nuclear Chemistry and Radiochemical Separations
- (iv) Biological Tracers and Imaging
- (v) Isotope Enrichment Technology

The 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 the National “Nuclear Data” effort, as well as several activities that facilitate the application of high performance computing to Nuclear Physics. The U.S. Nuclear Data Program (USNDP) collects, evaluates, and disseminates nuclear physics data for basic and applied nuclear research, maintains open databases of scientific information gathered over the past 100+ years of research in nuclear physics, and addresses gaps in the data through targeted experimental studies and the use of theoretical models. “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, 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). The current status of accelerator R&D, the present design concepts, and a list of R&D priorities for EIC are described in the February 2017 Report of the Community Review of EIC Accelerator R&D for the Office of Nuclear Physics. This report may be accessed at <https://science.osti.gov/np/community-resources/reports/>.

(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 Electron-Ion Collider (EIC), to be built at Brookhaven National Laboratory, will generate novel detector research and development efforts. 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.

(k) DOE Isotope Program (DOE IP) (Office of Isotope R&D and Production)

The mission of the DOE Isotope Program (DOE IP) is to support isotope production and research 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. The program lies at the intersection of many scientific communities including nuclear and radiochemistry, nuclear physics, accelerator and reactor science, materials science and engineering, separations science, and nuclear data to name just a few. The DOE IP provides facilities and capabilities for the production and/or distribution of research and commercial stable and radioactive isotopes. The scientific and technical staff associated with general isotope production and isotope production research are also supported. Radioactive isotopes and enriched stable isotopes are made available by using unique facilities stewarded by the Isotope Program at Brookhaven National Laboratory, Los Alamos National Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory. The Program 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 principle topics of interest to the Program are listed 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 enriching stable isotopes.

Topics of interest:

- Isotope Production Research
- Isotope Processing and Purification
- Nuclear Chemistry and Radiochemical Separations
- Biological Tracers and Imaging
- Isotope Enrichment Technology

Excluded from this call are applications related to the production of Mo-99, as this isotope is under the purview of the National Nuclear Security Agency Office of Materials Management and Minimization. A primary document currently guiding Isotope Program 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. Additional information about the Isotope Program may be found at <https://science.osti.gov/np/research/idpra/>.

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