

Office of Science Priority Research Areas for SCGSR Program

Priority Research Areas for SCGSR 2017 Solicitation 2

The applicants to the SCGSR Program must be pursuing graduate research in an area that is aligned with one or more of the Priority Research Areas for the SCGSR 2017 Solicitation 2. 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 below.

Applicants will need to identify in the online application system which Office of Science priority research area their proposed SCGSR research project is aligned with. Applications with a proposed research project that does not address an Office of Science research priority area and does not make specific reference to the stated aims of one the listed areas will not be considered.

It is recommended that applicant's become familiar with the Office of Science research program(s) most closely aligned with their graduate thesis research and the priority research area(s) below that are most closely aligned with their research objectives as they begin to formulate ideas for a SCGSR research proposal. A short overview of the Office of Science is available here [link to SCGSR SC overview]. Program descriptions for the Office of Science's six research program offices are summarized below to provide the context for the scientific and technical areas of priority interest to the Office of Science. Specific areas excluded in their research portfolios, and thus excluded in the SCGSR program, are also noted.

I. Advanced Scientific Computing Research (ASCR)

- (a) Applied Mathematics
- (b) Computer Science
- (c) Next Generation Networking for Science
- (d) Research and Evaluation Prototypes

II. Basic Energy Sciences (BES)

- (a) Accelerator and Detector R&D
- (b) Nuclear Chemistry and Radiochemical Separations
- (c) Neutron Scattering Research and Instrumentation
- (d) Predictive Materials Science and Chemistry
- (e) Fundamental Electrochemistry related to Energy Transduction, Storage, Chemical Conversion, and Corrosion
- (f) Crystal Growth
- (g) Ultrafast Materials and Chemical Sciences
- (h) Electron and Scanning Probe Microscopy Research and Instrumentation
- (i) Basic Geosciences
- (j) Gas Phase Chemical Physics
- (k) Radiation Effects in Materials

- (l) Catalysis Science with NMR Spectroscopy and Neutron Scattering
- (m) Highly Ionizing Radiation in Chemistry

III. Biological and Environmental Research (BER)

- (a) Computational Biology and Bioinformatics
- (b) Novel in Situ Imaging and Measurement Technologies for Biological Systems Science
- (c) Plant Science for Sustainable Bioenergy
- (d) Soil Microbiology
- (e) Environmental Systems Science
- (f) Atmospheric System Research
- (g) Earth System Modeling

IV. Fusion Energy Sciences (FES)

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

V. High Energy Physics (HEP)

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

VI. Nuclear Physics (NP)

- (a) Medium Energy Nuclear Physics
- (b) Heavy Ion Nuclear Physics
- (c) Low Energy Nuclear Physics
- (d) Nuclear Theory
- (e) Nuclear Data and Nuclear Theory Computing
- (f) Isotope Development and Production for Research and Applications
- (g) Accelerator Research and Development for Current and Future Nuclear Physics Facilities

I. 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.energy.gov/ascr/>

ASCR mission areas:

- To develop mathematical descriptions, models, methods, and algorithms to accurately describe and understand the behavior of complex systems involving processes that span vastly different time and/or length scales.
- To develop the underlying understanding and software to make effective use of computers at extreme scales.
- To transform extreme scale data from experiments and simulations into scientific insight.
- To advance key areas of computational science and discovery that further advance the missions of the Office of Science through mutually beneficial partnerships.
- To deliver the forefront computational and networking capabilities to extend the frontiers of science.
- To develop networking and collaboration tools and facilities that enable scientists worldwide to work together.

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 algorithms, software tools, the software libraries 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 two Leadership Computing Facilities, a high-performance production computing center, and a high-speed network and implements 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 well beyond the multi-petascale within a few years.

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

(a) Applied Mathematics

This program supports basic research leading to fundamental mathematical advances and computational breakthroughs across DOE and Office of Science missions. Applied Mathematics efforts span a range of research in scalable high-performance solvers, adaptive multiscale mathematical models, and coupled scientific data analysis and algorithms. These research developments are the foundation for enabling predictive models, simulations, and analysis of DOE-relevant science and engineering applications. The specific topic areas of interest are:

1. Adaptive Algorithms, Solvers, and Optimization for Extreme-Scale Computing
Basic research in the design, synthesis, analysis, and demonstration of algorithms that provide numerical solutions to mathematical models of physical systems with relevance to the DOE missions. Solver research opportunities include new classes of algorithms with one or more of the follow characteristics: low-communication, asynchronous, mixed-precision, fault-tolerant, resilient, energy-efficient, stochastic, and reproducible. A key research characteristic is that the results will also be useful for extreme-scale

simulations.

2. **Multiscale Mathematics for Coupled Extreme-Scale Scientific Simulations**
Innovative mathematics research to improve the fidelity and predictability of continuous and/or distributed complex systems that accurately capture the physics and/or subcomponent interactions across vastly different time and length scales.
3. **Research Foundations for Scalable Scientific Data Analysis and Algorithms**
Rigorous mathematical and computationally efficient approaches for analyzing and extracting information and insight from large-scale datasets relevant to the DOE missions. Of particular interest are computational approaches addressing the integration of observational data, experimental data, simulations and/or models.

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 program 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.

Topics of interest for this solicitation are focused on the following key research challenges for exascale and post-exascale platforms, namely:

1. **Extreme Scale**
Innovative programming models for developing applications on exascale platforms, exploiting unprecedented parallelism, heterogeneity of memory systems (e.g. Non-Uniform Memory Access (NUMA), non-coherent shared memory, hybrid memory cube, scratchpads), and heterogeneity of processing (e.g., Graphics Processing Units (GPUs), accelerators, big-small cores, processing in memory and near memory); algorithms and methods that support automated and semi-automated refinements from high-level specification of an application to low-level code, optimized at runtime to different HPC platforms. The focus is on enabling performance portability of applications developed for exascale computing and beyond.
2. **Resiliency**
Understanding the causes, frequency, and impact of various types of hard and soft faults and the detection and categorization thereof and methods to ensure the correctness of

applications in the presence of faults, including but not limited to machine learning, self-healing and reconfiguration, and heterogeneous paths of computation.

3. Data Analysis and Visualization

Visual analytic methods and environments for petabyte to exabyte multi-scale, multi-physics scientific data sets from simulations and/or experimental platforms; visual analytic environments to support understanding of HPC system and/or application behavior at extreme scale; and/or software visualization of highly parallel codes.

4. Data Management

Management of in-situ and complex distributed scientific workflows for high-end data-centric science applications; solutions to storage system and input/output bottlenecks for HPC applications; and alternatives to the file metaphor for science applications at scale.

5. Novel Methods

Novel methods, and abstract machines to analyze and understand common memory access patterns to improve data locality, minimize excessive data movement, which minimizes power. Machine abstractions should provide a theoretical framework to reason about extreme-scale architectures and their idealized software boundary.

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 networking, computer-supported collaboration, mathematics, mathematical formulations, social computing, natural language processing/understanding/generation and/or analysis, generalized research in human-computer interaction, discipline-specific data analytics and informatics, research focused on the World Wide Web and/or Internet, or research that is only applicable to hand-held, portable, desktop, embedded or cloud computing.

(c) Next Generation Networking for Science

This program supports research that advances the development, operation, and management of High Performance Networks and Distributed Computing environments. These environments include traditional compute, storage, and visualization resources, but extend deep into numerous scientific communities that operate unique scientific instruments. These globally distributed resources are interconnected via high-performance networks that operate at or above 100 Gbps. For this solicitation topics of interest are:

1. Distributed Resource Management

Development of software and middleware that will significantly enhance the ability of large collaborative science communities to dynamically assemble and use all the resources required to collect, process, and interpret an experiments data.

2. Intelligent Network Infrastructure

Development of a new generation of intelligent terabit optical network capabilities that leverage the emerging technologies such as Software Defined Networks (SDN), Network Function Virtualization (NFV), and Network Service Chaining (NSC), as well as recent advances in related fields such as machine learning and parallel computing.

3. Workflow Modeling

Advanced analytical models that significantly enhance our ability to predict how scientific workflows perform and to explain workflow behavior on distributed extreme-scale infrastructures built from computers, storage, instruments and multi-gigabit networks.

4. End-to-End Network Services

Data-aware network technologies that can deliver 100 Gbps end-to-end throughputs to distributed data-intensive science applications.

EXCLUSIONS: Topics that are NOT within the scope for this program area include: Proposals with a primary goal of developing hardware components, Intelligent Network Interface Cards, or network acceleration hardware; technologies that optimize wireless or other low-speed network infrastructures; proposals with a primary focus on development or deployment activities; and proposals that suggest incremental upgrades to existing network architectures, protocols, tools, or services.

(d) Research and Evaluation Prototypes

This program supports research to advance the evaluation, development, and operation of emerging systems for Leadership Class and production high performance computing facilities and advanced scientific networks at DOE National Labs. Grant applications are solicited in the following technical areas:

1. Machine Learning

Scalable software, methods, and techniques that ensure algorithm scalability to extreme scales and applications that are generalizable to scientific computing applications and operation of HPC systems.

2. Neuromorphic Computing

Specific to HPC-enabled modeling and simulation of computing architecture at extreme scales for generalizable applications of the proposed approach.

3. HPC Cybersecurity

Investigate methods and techniques to achieve scientific integrity through repeatable computing results whose process, origin, and data provenance is understood, whose correctness is understood, and for which uncertainty estimates are provided with associated metrics analytics and with specific emphasis to low system overhead approaches.

EXCLUSIONS: Topics that are NOT within the scope for this program area include research not addressing any of the challenges described above, and research primarily focusing on networking, computer-supported collaboration, mathematics, mathematical formulations, social computing, natural language processing/understanding/generation and/or analysis, generalized research in human-computer interaction, discipline-specific data analytics and informatics, research focused on the World Wide Web and/or Internet, or research that is only applicable to hand-held, portable, desktop, embedded or cloud computing.

II. 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 physical 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.energy.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) 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 materials. Applications encouraged under this topic should address the fundamental science underpinning the extraction and separation of fission products and actinides explored using experiment and theory, 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.

(c) 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 to accelerate the discovery of advanced materials to address the future energy challenges. This program offers opportunities for graduate students to work with neutron scattering scientists at these facilities in utilizing the cutting edge techniques for neutron scattering research, interacting with the scientific user community, and planning for the next-generation neutron scattering facilities for U.S. leadership.

(d) Predictive Materials Science and Chemistry

There is a growing need for materials and chemical scientists with expertise and experience in predictive theory and modeling, driven by the goal to reduce the time to develop and deploy new materials and chemical systems as well as by remarkable advances in computer power, algorithms, data repositories, and data science. The BES activities in this area include the development of new, experimentally validated, software tools and associated data that contribute to a fully integrated approach from material discovery to applications, with an emphasis on research that will provide the foundations for new energy technologies. BES supports research that advances ab-initio and multiscale methods for materials and chemical processes and underpins the development of user friendly software that captures the essential physics and chemistry of relevant systems.

Applications should focus on opportunities for graduate students in advanced theory and multiscale computational techniques in chemistry and materials science including first principles methods, implementation of new mathematics and algorithms, time dependent response, Monte Carlo and molecular dynamics, data mining, artificial intelligence, and code generation or optimization on next generation computer systems.

EXCLUSIONS: Based on programmatic priorities, activities that seek collaboration/training in experimental techniques will NOT be considered.

(e) Fundamental Electrochemistry related to Energy Transduction, Storage, Chemical Conversion, and Corrosion

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 enhance chemical synthesis and separations, 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 semiconductor surfaces under reaction conditions; and electrochemistry of separations processes and in catalytic and biocatalytic systems.

Specific issues for electrochemistry in energy transduction, energy storage, 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), and Materials under Extreme Environments (2007).

EXCLUSIONS: Research that is focused on identifying or producing new or optimized materials for battery systems or corrosion resistance, instead of focusing on electrochemical mechanisms, will NOT be considered.

(f) 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 three-dimensional single crystal growth; applications that target biomedical applications or systems (e.g., animal/human health) will NOT be considered.

(g) 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 should 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 should 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 should advance understanding of attosecond-to-femtosecond dynamics and electron-electron or electron-nuclear correlations in molecules.

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.

(h) 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 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, <http://science.energy.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 chemical sciences.

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

(i) 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 <http://science.energy.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.

(j) Gas Phase Chemical Physics

This priority research area includes research on gas-phase chemical processes important in energy applications. The overall goal is to understand energy flow and reaction mechanisms in complex, non-equilibrium, gas-phase environments, especially those in which the coupling of chemical and transport processes is poorly understood.

Several challenges for the gas phase chemical physics community voiced at research meetings,

workshops, and strategic planning sessions are described below. Applications should focus on these areas:

- Understanding the kinetics and dynamics of gas - particle/droplet interactions.
- Developing a better understanding of gas phase processes in heterogeneous catalysis.
- Developing a more detailed understanding of growth, formation, and reactions of new particles formed from gas precursors.
- Developing a conceptual framework and computational methodologies for thermochemistry and kinetics at high temperatures and/or high pressures.
- Developing new experimental techniques to probe high pressure reactions.
- Understanding the role of non-thermal kinetics, i.e., the effect of reactions occurring during the thermalization process.
- Understanding kinetics at high pressures where collisions do not occur as isolated binary events.
- Gaining insight into intramolecular dynamics, molecular photophysics, and new particle formation via high energy coherent light sources, e.g. VUV and x-ray radiation.
- Developing artificial intelligence methodologies to automate gas phase chemical physics modeling, calculations, and analysis of experimental data.
- Developing experimental and computational methods that can handle more complex molecules, multi-species, and multi-reaction systems.

EXCLUSIONS: Topics of research that will NOT be considered are: non-reacting fluid dynamics and spray dynamics, data-sharing software development, end-use combustion device development, and characterization or optimization of end-use combustion devices.

(k) 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 Basic Energy Sciences reports Basic Research Needs for Advanced Nuclear Energy Systems (2006) and Basic Research Needs for Materials under Extreme Environments (2007).

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 or flux pinning for superconductivity will NOT be considered.

(l) Catalysis Science with NMR Spectroscopy and Neutron Scattering

There have been a number of significant recent advances in nuclear magnetic resonance (NMR) spectroscopy and neutron scattering 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, a pulsed source with the world’s highest pulsed neutron flux, and the High Flux Isotope Reactor, a continuous source with an integrated flux rivaling the world’s highest intensity neutron scattering facilities. These neutron scattering facilities 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).

Applications should focus on advancing catalysis science research by utilizing the cutting edge NMR and neutron scattering techniques at the above-described facilities.

EXCLUSIONS: Technique development or 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.

(m) 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.

III. 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 transformation of materials such as nutrients and contaminants 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.energy.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 understand the relationships between climate change and Earth's ecosystems, develop and assess options for carbon sequestration, and provide science to underpin a fully predictive understanding of the complex Earth system and the potential impacts of climate change on ecosystems.
- To understand the behavior of DOE-relevant contaminants in subsurface environments, enabling prediction of their fate and transport in support of long term environmental stewardship and development of new, science-based remediation strategies.
- 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 Climate and Environmental Sciences Division (CESD).

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 facilities through the development of instrumentation at DOE's national user facilities.

The CESD supports fundamental science and research capabilities that enable major scientific developments in climate-relevant atmospheric-process and ecosystem research and modeling, in support of DOE's mission goals for basic science, energy, and national security. This includes research on clouds, aerosols, and the terrestrial carbon cycle; large-scale climate change and earth system modeling; the effects of climate change on ecosystems; and integrated analysis of climate change impacts on 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 energy byproducts. CESD also supports two national scientific user facilities: the Atmospheric Radiation Measurements Climate Research Facility (ARM) and the Environmental Molecular Sciences Laboratory (EMSL). ARM provides unique, multi-instrumented capabilities for continuous, long-term observations needed to develop and test understanding of the central role of clouds and aerosols on the earth's climate. EMSL provides integrated experimental and computational resources needed to understand the physical, chemical, and biological processes that underlie 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. Future research efforts across BER's Biological Systems Science Division will require basic life science researchers trained in interdisciplinary fields of computational biology and bioinformatics to advance a predictive understanding and design of biological processes in order to remain competitive in the global drive to develop renewable resources. *Candidates for this topic should focus on new innovative computational strategies, 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) Novel in situ Imaging and Measurement Technologies for Biological Systems Science

BER's current focus on developing a scientific basis for plant biomass-based biofuel production requires trained scientific work-force for detailed understanding of cellular metabolism in order to optimize beneficial properties into bioenergy relevant plants and microbes. Aligned with that goal, BER encourages development of new imaging instrumentation and technologies for in situ, dynamic, and nondestructive imaging of biological systems to visualize and measure the spatial/temporal relationships, physical connections, and chemical exchanges that facilitate the flow of information and materials across membranes and between intracellular partitions.

Candidates for this topic are expected to draw upon imaging techniques/capabilities from other disciplines that could be adapted to biological research, and to have a systems biology perspective to understand how the novel technological developments would advance the understanding of the biology of diverse plant and microbial species of relevance to BER.

Candidates are expected to seek research collaboration with imaging 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.

(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 life style are beneficial traits for bioenergy feed stocks. Current DOE Genomic Science Program research efforts in renewable feed stocks for bioenergy focus on the manipulation of metabolic pathways and carbon allocation in plant tissues to produce plant strains with enhanced biofuel production characteristics. *Candidates for this topic should focus on systems biology research and genome engineering approaches seeking to improve bioenergy crop characteristics such as biomass yields, cell wall recalcitrance, and optimized growth and development in marginal lands. Research is also encouraged to further understanding of plant-microbe interactions and/or molecular mechanisms underlying traits that increase sustainable production of such crops, such as nitrogen/water use efficiency and drought tolerance.* Future DOE bioenergy research will require plant scientists trained in genetics and breeding to translate such studies to the field.

(d) Soil Microbiology

Basic knowledge of how soil microbial communities (e.g. bacteria, viruses, fungi) operate and interact with broader environmental processes, including nutrient cycling and role in maintaining "healthy" soils, remains limited in many ways. These experimental challenges are mainly due to soil's compositional heterogeneity and the complex microbial consortia found in

terrestrial ecosystems and sedimentary environments. With the use of sophisticated approaches in “metaomics” coupled with high-resolution analytical technologies, researchers are at the precipice of being able to more fully investigate the functional properties of the interrelationships between and among soil microbes. *Candidates for this topic should focus on adapting genome-enabled techniques (e.g., metagenomics, metatranscriptomics, metaproteomics, and community- scale metabolomics) to interrogate relevant functional processes of microbes in terrestrial environments. Systems biology studies on regulatory and metabolic networks of microbes and microbial consortia involved in major biogeochemical cycling (e.g., carbon, nitrogen, sulfur, and phosphorus) are also encouraged.* Future research in this area requires an understanding of the reaction of soils and their microbial communities to environmental perturbations to maintain and/or manage healthy terrestrial ecosystems.

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

Current land process, watershed, ecosystem, and climate models inadequately represent the structure and function of key environmental and ecological processes that span the continuum from the bedrock, through the soil and vegetation, and to the atmospheric interface. These processes (e.g., soil biogeochemical reactions, plant-rhizosphere interactions, reactive transport, microbe-mineral interactions, vegetative, etc.), have interfaces and interactions between the various components of the continuum and land surface, riverine environments, coastal zones and the subsurface environment. The inadequate representation of these terrestrial ecosystem, subsurface structures, biogeochemical processes and hydrologic interactions represents a major roadblock in our ability to predictively understand the Earth and environmental systems. Improving our representation of the complex Earth system requires a better understanding of terrestrial ecosystem and/or subsurface processes that can affect the cycling and transport of water, elements (including carbon), nutrients, and other constituents from process-level observational, ecosystem and hydrobiogeochemical research. *Candidates for this topic are required to delineate an integrative, hypothesis-driven approach and clearly describe the existing needs in state-of-the-art models through terrestrial ecosystem and subsurface biogeochemical process research projects that will inform land process, watershed, and ecosystem models, and aligns with the scope and focus of the DOE Terrestrial Ecosystem Science and/or Subsurface Biogeochemical Research programs.* Developing a workforce with experience in innovative, experimental approaches efforts in subsurface/belowground process research will enable DOE to make significant advances in the high resolution predictive understanding of the Earth and environmental system and to foster innovative research.

(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 climate

change and its impacts on energy and related infrastructure. Applications should target one or more of these processes that need to be better represented in climate models to improve climate 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, convective initiation, cold pools, and organization on a range of scales. High priority research efforts in atmospheric sciences within DOE's Climate and Environmental Sciences Division (CESD) require new expertise in coupling observational data from the Atmospheric Radiation Measurement (ARM) Climate Research Facility with high resolution numerical models to advance predictive understanding of aerosol and cloud processes. *Of particular interest are applications for this topic that 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 Modeling: 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 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.*

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;
- 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 and 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;
- Medically related research; plant pests, biomass process engineering optimization, molecular dynamics simulations towards enzyme engineering; or DNA sequencing technology.

IV. 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.energy.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).

V. 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.energy.gov/hep>

The HEP experimental research program focuses on three scientific frontiers:

- *The Energy Frontier*, where powerful accelerators are used to create new particles, reveal their interactions, and investigate fundamental forces;
- *The Intensity Frontier*, where intense particle beams and highly sensitive detectors are used to pursue alternate pathways to investigate fundamental forces and particle interactions by studying events that occur rarely in nature, and to provide precision measurements of these phenomena; and
- *The Cosmic Frontier*, where non-accelerator-based experiments observe the cosmos and detect cosmic particles, making measurements of natural phenomena that can provide information about the nature of dark matter, dark energy, and other fundamental properties of the Universe that impact our understanding of matter and energy.

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 four 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; and
- *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.

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:

http://science.energy.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 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; 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 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 which 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.

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 man-made and 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 as well as neutrinos from nuclear reactors; sensitive measurements of rarely occurring phenomena that can indicate new physics beyond the Standard Model; measurements of dark energy; 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 and large-scale computing for HEP. Programmatic priority in this topic will be given to those applications that most effectively address this issue.

VI. Nuclear Physics (NP)

One of the enduring mysteries of the universe is the nature of matter—what are its basic constituents and how do they interact to form the properties we observe? The largest contribution by far to the mass of the matter we are familiar with comes from the nuclei of atoms. The mission of the Nuclear Physics (NP) program is to discover, explore, and understand all forms of nuclear matter. 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.

Program Website: <https://science.energy.gov/np/>

The priority areas for NP include the following:

- Understand how nucleons—protons and neutrons—combine to form atomic nuclei and how these nuclei have emerged since the origin of the cosmos.

- Using particle accelerators illuminate the structure of the nucleon—the core building block of matter; understand how quarks and gluons assemble to form matter’s core; and study the properties of the quark gluon plasma.
- Penetrate mysteries surrounding the fundamental properties of the neutron and the neutrino.
- Conceive, construct, and operate national scientific user facilities.
- Steward Isotope development, production, and technologies for research and applications.

To carry out its mission and address these priorities, the NP program focuses on three frontiers, Quantum Chromodynamics; Nuclei and Nuclear Astrophysics; and Fundamental Symmetries and Neutrinos. NP supports basic research in five subprograms: Medium Energy, Heavy Ion, Low Energy, Nuclear Theory, and Nuclear Data and Nuclear Theory Computing. The program is the steward of the DOE Isotope Program for the nation and supports the development of the tools and capabilities that make fundamental research possible.

The NP’s priority research areas for SCGSR program include:

(a) Medium Energy Nuclear Physics

The Medium Energy Nuclear Physics subprogram focuses primarily on experimental tests of the mathematical description of how quarks and gluons in nuclear matter interact, referred to as Quantum Chromodynamics (QCD) and in particular, the behavior of quarks inside protons and neutrons. Specific questions addressed include: *What is the internal landscape of the protons and neutrons (collectively known as nucleons)? What does QCD predict for the properties of strongly interacting matter? 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?* Various experimental approaches are pursued to determine the distribution of up, down, and strange quarks (and implicitly their antiquarks) in nucleons, as well as the roles of the gluons that bind the quarks; the effects of the quark and gluon spins within the nucleon; and the effect of the nuclear environment on the quarks and gluons. The subprogram also produces and studies higher-mass “excited states” of hadrons (composite particles, including nucleons, made of quarks, antiquarks, and gluons) predicted by QCD in order to determine how the theory leads to the observed properties of these strongly interacting particles. In pursuing these goals, the Medium Energy subprogram supports experimental research primarily at the Thomas Jefferson National Accelerator Facility (TJNAF) and the Relativistic Heavy Ion Collider (RHIC).

(b) Heavy Ion Nuclear Physics

The Heavy Ion Nuclear Physics subprogram focuses on studies of nuclear matter at extremely high densities and temperatures that are directed primarily at answering the overarching questions defining one of the three nuclear physics frontiers—Quantum Chromodynamics (QCD). The fundamental questions addressed include: *What are the phases of strongly interacting matter, and what roles do they play in the cosmos? What*

governs the transition of quarks and gluons into pions and nucleons? What determines the key features of QCD, and what is their relation to the nature of gravity and space-time? With careful measurements, scientists are accumulating data which offers insights into the processes early in the creation of the universe, and how protons, neutrons, and other bits of normal matter developed from the quark-gluon plasma predicted to exist about 1 microsecond after the Big Bang. Important avenues of investigation are directed at learning more about the physical characteristics of the quark-gluon plasma created in relativistic collisions of nuclei including exploring the energy loss mechanism for quarks and gluons traversing the plasma, determining the speed of sound in the plasma and locating the critical point for the transition between the plasma and normal matter. Experimental research is carried out primarily using the U.S. Relativistic Heavy Ion Collider (RHIC) facility and the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN).

(c) Low Energy Nuclear Physics

The Low Energy Nuclear Physics subprogram is the most diverse within the NP portfolio, supporting research activities aligned with scientific thrusts focusing primarily on answering the overarching questions associated with two science frontiers: Nuclei and Nuclear Astrophysics, and Fundamental Symmetries and Neutrinos. Questions associated with the Nuclei and Nuclear Astrophysics frontier include: *What is the nature of the nuclear force that binds protons and neutrons into stable nuclei and rare isotopes? 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?* One major goal of this subprogram is to develop a comprehensive description of nuclei using beams of stable and rare isotopes to yield new insights and reveal new nuclear phenomena. A second is to measure the cross sections of nuclear reactions powering stars and resulting in spectacular stellar explosions responsible for the synthesis of the elements. Questions addressed in the Fundamental Symmetries and Neutrinos frontier, which uses neutrinos and neutrons as primary probes, include: *What experimental approach for a next generation, ton-scale neutrino-less double beta decay detector is capable of achieving the sensitivity necessary to determine if the neutrino is its own anti-particle? Is there evidence from the electric-dipole moments of atomic nuclei and the neutron that demonstrate our current understanding of the fundamental laws governing nuclear physics is incomplete? Does evidence for parity violation in electron scattering and possible lepton number violation in the decay of nuclei indicate forces present at the dawn of the universe that disappeared from view as the universe evolved?* This subprogram also seeks to measure or set a limit on the neutrino mass and to determine if the neutrino is its own anti-particle (a Majorana particle). Neutrino properties are believed to play an important role in the evolution of the cosmos. Beams of cold and ultra-cold neutrons are used to study fundamental properties of neutrons. Precision studies to observe or set a limit on violation of time-reversal invariance in nucleonic, nuclear, and atomic systems investigate the origin of dominance of matter over antimatter in the universe, addressing fundamental questions in nuclear and particle physics, astrophysics, and cosmology.

(d) Nuclear Theory

The Nuclear Theory subprogram provides the theoretical support needed to interpret the wide range of data obtained from the experimental nuclear science subprograms, and to advance new ideas and hypotheses that identify potential areas for future experimental investigations. Nuclear Theory addresses all three of NP's scientific frontiers. One major theme of theoretical research is the development of an understanding of the mechanisms and effects of quark confinement and deconfinement. A quantitative description of these phenomena, QCD, is one of this subprogram's greatest intellectual challenges. New theoretical and computational tools are also being developed to describe nuclear many-body phenomena; these approaches will likely also see important applications in condensed matter physics and in other areas of the physical sciences. Another major research area is nuclear astrophysics, which includes efforts to understand the origins of the elements and the consequences that neutrino masses have for nuclear astrophysics and for the current Standard Model of elementary particles and forces.

(e) Nuclear Data and Nuclear Theory Computing

The mission of the United States Nuclear Data Program (USNDP) is to provide current, accurate, authoritative data for workers in pure and applied areas of nuclear science and engineering. The USNDP also addresses gaps in the data, through targeted experimental studies, and the use of theoretical models. The USNDP involves the efforts of ~50 nuclear physicists at ~15 national labs, research centers, institutes and universities, and is an important resource for workers in a wide range of pure and applied topics in nuclear physics.

Nuclear Theory Computing supports research in nuclear physics with "extreme" computational requirements, which has been enabled by the advent of high performance computing (HPC). Funding for NP research involving HPC is currently provided primarily through the Scientific Discovery through Advanced Computation (SciDAC) program, through major joint projects with the Office of Advanced Scientific Computing Research (ASCR) and the National Nuclear Security Agency (NNSA). The three current NP SciDAC projects use HPC techniques and facilities to investigate the properties of quark and gluon bound states and the QCD phase diagram using lattice QCD, and the properties of nuclei, calculated using various approximate techniques. Resources for NP HPC activities are also provided by the National Energy Research Scientific Computing (NERSC) center.

Theoretical NP research involving HPC, and both theoretical and experimental work of relevance to Nuclear Data, could be considered under this subprogram.

(f) Isotope Development and Production for Research and Applications

The Isotope Development and Production for Research and Applications subprogram supports the production, distribution, and development of production techniques for radioactive and enriched isotopes in short supply and critical to the Nation. Isotopes are commodities of

strategic importance for the Nation that are essential for energy exploration and innovation, medical applications, national security, and basic research. An important goal of the program is to make key isotopes more readily available to meet U.S. needs. To achieve this goal, the program provides facilities and capabilities for the production of research and commercial stable and radioactive isotopes, scientific and technical staff associated with general isotope research and production, and a supply of critical isotopes. Isotopes are made available by using the Department's unique facilities, the Brookhaven Linear Isotope Producer (BLIP) at BNL and the Isotope Production Facility (IPF) at LANL, of which the subprogram has stewardship responsibilities. The Program also coordinates and supports isotope production at a suite of university, national laboratory, and commercial accelerator and reactor facilities throughout the Nation to promote a reliable supply of domestic isotopes. Topics of interest include research to develop new or improved production or separation techniques for high priority isotopes in short supply. Examples for planned research include the need for positron-emitting radionuclides to support the rapidly growing area of medical imaging using positron emission tomography (PET), development of isotopes that support medical research used to diagnose and treat diseases, development of production methods for alpha-emitting radionuclides that exhibit great potential in disease treatment, development and use of research isotopes for various biomedical applications, development of stable isotope enrichment technologies, and the need for alternative isotope supplies for national security applications and advanced power sources. One of the high priorities is to conduct R&D aimed at re-establishing a domestic capability for stable isotope enrichment in the U.S. All R&D activities are peer reviewed. Another high priority is to provide opportunities for workforce development in the areas of nuclear chemistry and radiochemistry. These disciplines are essential to the long-term health of the fields of radioisotope production and applications.

(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 beam; the development of a future Nuclear Physics accelerator facility such as an electron-ion collider (EIC); 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 Facility for Rare Isotope Beams (FRIB).

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