

Office of Science Priority Research Areas for SCGSR Program

Priority Research Areas for SCGSR 2018 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 2018 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

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

- (n) Energy Transfers in Large Proteins and Protein Complexes
- (o) Quantum Information Science for Experimental Condensed Matter Physics
- (p) Quantum Information Science for Theoretical Condensed Matter Physics

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/>

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.

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.

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 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.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 methods for first-principles electronic structure, quantum Monte Carlo, and molecular dynamics. Other priorities include the implementation of new mathematics and algorithms (e.g., construction of rigorously complete quasi-analytical density-informed basis sets), techniques for ultrafast and driven quantum systems, machine learning, 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. Projects aimed at the synthesis of nanosized crystals with any dimensions being in the nanosize (including two-dimensional films) or hierarchical assemblies including liquid crystals 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 or 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 report Basic Research Needs for Future Nuclear Energy (2017).

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.

(n) 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.

(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.energy.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.

Quantum Computing in Materials Sciences and Next-Generation Quantum Systems: Proposals are requested for basic theoretical research focused on using quantum computers to solve scientific problems in materials sciences or quantum phenomena that will enable the design

and discovery of novel quantum information systems. Proposals should address the Priority Research Opportunities identified in the reports from the Basic Energy Sciences Roundtable on Opportunities for Quantum Computing in Chemical and Materials Sciences (https://science.energy.gov/~media/bes/pdf/reports/2018/Quantum_computing.pdf) or Basic Energy Sciences Roundtable on Opportunities for Basic Research for Next-Generation Quantum Systems (https://science.energy.gov/~media/bes/pdf/reports/2018/Quantum_systems.pdf). Areas of research for quantum computing include: controlling the quantum dynamics of nonequilibrium materials systems; unraveling the physics of strongly correlated electron systems; embedding quantum hardware in classical frameworks; and bridging the classical–quantum computing divide. Proposals must focus on fundamental research that will target computation for realistic problems relevant to Basic Energy Sciences using quantum computers that are available today. For example, quantum sensors based on solid materials could be greatly improved with insight from quantum computation, as could superconductors, complex magnetic materials, and materials for information technologies.

Targeted areas of theoretical research to advance future quantum systems include: advancement of artificial quantum-coherent systems with unprecedented functionality, enhanced creation and control of coherence in quantum systems; discovery of novel approaches for quantum-to-quantum transduction; and implementation of new quantum methods for advanced sensing and process control.

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.

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 enable major scientific developments in Earth system-relevant atmospheric, hydrological, 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 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 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 integrated analysis of Earth system variability and change 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 DOE-relevant energy byproducts. CESD 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) 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 terrestrial 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 Watershed Systems Research to Inform Models of the Earth and Environmental System

Current land process, watershed, ecosystem, and regional to global earth system 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 flow and transport, microbe-mineral interactions, vegetative change, etc.), are due to the many types of interfaces and interactions between the various physical, chemical and biological components of the land and vegetative surface, watershed

systems, coastal zones, and the subsurface environment. The inadequate representation of the functioning of ecosystems, from the terrestrial surface through the subsurface environment, and especially the biogeochemical processes and hydrologic interactions that occur within them, 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, DOE-relevant contaminants, 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, reactive transport, 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 in ecological process science and watershed systems science 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 changes to the Earth system and its impacts on energy and related infrastructure. Applications should target one or more of these 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, 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) 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 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/Earth/atmospheric 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 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.

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 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 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 for High Energy Physics*, where novel capabilities for modeling, optimization, event classification, and improved measurements are developed by taking advantage of superposition, entanglement, and squeezed states.

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 (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 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 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 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.

VI. 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.energy.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.energy.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.

The NP Program also includes the DOE Isotope Program which 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 technology.

Quantum Information Science (QIS) has been identified as an important cross-cutting topic, with potential impact across all SC mission areas (see https://science.energy.gov/~media/sc-2/pdf/presentations/2017/DOE-Office_of_Science_Dear_Colleague_Letter_on_QIS.pdf). NP encourages submission of innovative research ideas to address QIS in any of its priority areas.

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. In the aftermath of collisions at RHIC and at the LHC, researchers have seen signs of the same

quark-gluon plasma that is believed to have existed shortly after the Big Bang. 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 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 Structure and Nuclear Astrophysics subprogram 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.

The Low Energy Fundamental Symmetries subprogram 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 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.

(e) 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.

(f) Isotope Development and Production for Research and Applications

The mission of the Isotope Development and Production for Research and Applications subprogram (DOE Isotope Program) 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 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. Topics of interest are focused on the development of advanced, cost-effective and efficient technologies for producing, processing, 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. 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.energy.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.energy.gov/np/research/idpra/>.

(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.energy.gov/np/community-resources/reports/>.

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