PROGRAM ANNOUNCEMENT
TO DOE NATIONAL LABORATORIES

U. S. Department of Energy
Office of Science

Early Career Research Program

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Encourage/Discourage Date:	**02/27/2018 at 5 PM Eastern Time**
Proposal Due Date:	**04/04/2018 at 5 PM Eastern Time**

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UPDATES AND REMINDERS

DATA MANAGEMENT PLAN

The Office of Science has published a new Statement on Digital Data Management, published at http://science.energy.gov/funding-opportunities/digital-data-management/, which governs applications submitted under this DOE National Laboratory Announcement, and is detailed in Part IV of this DOE National Laboratory Announcement.

ACKNOWLEDGMENT OF FEDERAL SUPPORT

The Office of Science published guidance about how its support should be acknowledged at http://science.energy.gov/funding-opportunities/acknowledgements/.

RECOMMENDATION

The Office of Science encourages you to register in all systems as soon as possible. You are also encouraged to submit letters of intent, pre-applications, and applications well before the deadline.

Section I – DOE NATIONAL LABORATORY OPPORTUNITY DESCRIPTION

GENERAL INQUIRIES ABOUT THIS ANNOUNCEMENT SHOULD BE DIRECTED TO:

Technical/Scientific Program Contact:
Questions regarding the specific program areas/technical requirements can be directed to the program managers / technical contacts listed for each program within the DOE National Laboratory Announcement.

Administrative Contact (questions about program rules):
Questions about program rules should be sent to early.career@science.doe.gov

SUMMARY

The Office of Science of the Department of Energy hereby invites grant applications for support under the Early Career Research Program in the following program areas: Advanced Scientific Computing Research (ASCR); Biological and Environmental Research (BER); Basic Energy Sciences (BES), Fusion Energy Sciences (FES); High Energy Physics (HEP), and Nuclear Physics (NP). The purpose of this program is to support the development of individual research programs of outstanding scientists early in their careers and to stimulate research careers in the areas supported by the DOE Office of Science.

SUPPLEMENTARY INFORMATION

The mission of the DOE Office of Science is to deliver the scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy, economic, and national security of the United States. The Office of Science is the Nation's largest Federal sponsor of basic research in the physical sciences and the lead Federal agency supporting fundamental scientific research for our Nation's energy future.

The Office of Science accomplishes its mission and advances national goals by supporting:

- The frontiers of science—exploring nature's mysteries from the study of fundamental subatomic particles, atoms, and molecules that are the building blocks of the materials of our universe and everything in it to the DNA, proteins, and cells that are the building blocks of life. Each of the programs in SC supports research probing the most fundamental disciplinary questions.

- The 21st Century tools of science—providing the nation's researchers with 27 state-of-the-art national scientific user facilities - the most advanced tools of modern science - propelling the U.S. to the forefront of science, technology development and deployment through innovation.

- Science for energy and the environment—paving the knowledge foundation to spur discoveries and innovations for advancing the Department's mission in energy and

environment. SC supports a wide range of funding modalities from single principal investigators to large team-based activities to engage in fundamental research on energy production, conversion, storage, transmission, and use, and on our understanding of the earth systems.

Early Career Research Program opportunities exist in the following Office of Science research programs. Additional details about each program, websites, and technical points of contacts are provided in the materials that follow.

I. Advanced Scientific Computing Research (ASCR)

(a) Applied Mathematics: Adaptive Algorithms, Solvers, and Optimization for Extreme-Scale Computing
(b) Applied Mathematics: Multiscale Mathematics for Coupled Extreme-Scale Scientific Simulations
(c) Applied Mathematics: Research Foundations for Scalable Scientific Data Analysis and Algorithms
(d) Computer Science: Systems
(e) Computer Science: Data Management, Visualization, and Analytics
(f) Computer Science: Artificial Intelligence and Cybersecurity
(g) Computer Science: Advanced Network Architectures
(h) Computer Science: Workflow Science

II. Biological and Environmental Research (BER)

(a) Systems-Level Design and Engineering of Microbial or Plant Systems for the Production of Biofuels and Bioproducts
(b) Atmospheric Processes

III. Basic Energy Sciences (BES)

(a) Materials Chemistry
(b) Biomolecular Materials
(c) Synthesis and Processing Science
(d) Experimental Condensed Matter Physics
(e) Theoretical Condensed Matter Physics
(f) Physical Behavior of Materials
(g) Mechanical Behavior and Radiation Effects
(h) X-ray Scattering
(i) Neutron Scattering
(j) Electron and Scanning Probe Microscopies
(k) Atomic, Molecular, and Optical Sciences (AMOS)
(l) Gas Phase Chemical Physics (GPCP)
(m) Computational and Theoretical Chemistry
(n) Condensed Phase and Interfacial Molecular Science (CPIMS)
(o) Catalysis Science
(p) Separation Science
(q) Heavy Element Chemistry (HEC)
(r) Geosciences Research

(s) Solar Photochemistry
(t) Photosynthetic Systems
(u) Physical Biosciences
(v) Nanoscale Science Research Centers
(w) Accelerator and Detector Research
(x) X-ray Instrumentation and Technique Development
(y) Neutron Scattering Instrumentation and Technique Development

IV. Fusion Energy Sciences (FES)
(a) Magnetic Fusion Energy Science Experimental Research
(b) Magnetic Fusion Energy Science Theory and Simulation
(c) High-Energy-Density Plasma Science
(d) General Plasma Science Experiment and Theory
(e) Fusion Nuclear Science, Materials Research and Enabling R&D Programs for Fusion

V. High Energy Physics (HEP)
(a) Experimental Research at the Energy Frontier in High Energy Physics
(b) Experimental Research at the Intensity Frontier in High Energy Physics
(c) Experimental Research at the Cosmic Frontier in High Energy Physics
(d) Theoretical Research in High Energy Physics
(e) Accelerator Science and Technology Research & Development in High Energy Physics
(f) Detector Research and Development in High Energy Physics

VI. Nuclear Physics (NP)
(a) Medium Energy Nuclear Physics
(b) Heavy Ion Nuclear Physics
(c) Low Energy Nuclear Physics - Nuclear Structure and Nuclear Astrophysics
(d) Low Energy Nuclear Physics - Fundamental Symmetries
(e) Nuclear Theory
(f) Nuclear Data and Nuclear Theory Computing
(g) Accelerator Research and Development for Current and Future Nuclear Physics Facilities
(h) Isotope Development and Production for Research and Applications

I. Advanced Scientific Computing Research (ASCR)

Program Website: http://science.energy.gov/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 ASCR program gives the science and technology community, including U.S. industry, access to world-class supercomputers and the tools to use them for science and engineering. ASCR accomplishes this by developing and maintaining world-class computing and network facilities for science; and advancing research in applied mathematics, computer science, and advanced networking.

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 Leadership Computing facilities, a high-performance production computing center, and a high-speed network, and implements a broad base research portfolio to solve complex problems on computational resources that are on a trajectory to reach well beyond hundreds of petaflops within a few years.

For the purposes of the Early Career Research Program, proposed research must be responsive to one of the specific topic areas below:

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, statistical methodologies, 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:

(a) Applied Mathematics: Adaptive Algorithms, Solvers, and Optimization for Extreme-Scale Computing
Technical Contact: Steven Lee, 301-903-5710, Steven.Lee@science.doe.gov

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

References
Applied Mathematics Research for Exascale Computing
http://science.energy.gov/~/media/ascr/pdf/research/am/docs/EMWGreport.pdf

Report on the Extreme Scale Solvers Workshop
http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/reportExtremeScaleSolvers2012.pdf

(b) Applied Mathematics: Multiscale Mathematics for Coupled Extreme-Scale Scientific Simulations
Technical Contact: Steven Lee, 301-903-5710, Steven.Lee@science.doe.gov

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. Novel discretizations, scale bridging, and uncertainty analysis in such systems are of particular interest.

References
DOE Workshop Report on Multiphysics Simulations
http://science.energy.gov/~/media/ascr/pdf/programdocuments/docs/MultiPhysics-Simulations-Report.pdf

A Multifaceted Mathematical Approach for Complex Systems
http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Multifaceted_Mathematical_Approach_for_Complex_Systems.pdf

(c) Applied Mathematics: Research Foundations for Scalable Scientific Data Analysis and Algorithms
Technical Contact: Steven Lee, 301-903-5710, Steven.Lee@science.doe.gov

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 using new statistical methodology for large-scale datasets.

For Research Areas (a), (b), and (c) above, topics and approaches that are out of scope include:
- Research where the mathematical challenges are not clearly articulated in the pre-application;
- Approaches for specific scientific or engineering problems that are not applicable to a broader class of problems;
- Approaches with primary emphasis on tailoring or implementation of existing numerical methods for specific scientific problems; or
- High-performance computing (HPC) implementation or "framework" for scientific or engineering calculations that are primarily based on specific programming models or architectures.

Important note for encourage and discourage decisions: Pre-proposals must clearly articulate the main scientific motivations and barriers to progress, the technical basis for overcoming those barriers, and the key insights or novel approaches for addressing the scientific and technical challenges. The lack of such details is sufficient for discouragement of the proposed research.

Computer Science
This program supports research to advance the development, operation and systems management of Leadership Class and production high performance computing facilities and high performance

networks at DOE National Labs, application software development for scientific modeling and simulation for extreme-scale computing and beyond, high performance computing systems architecture and software, and scientific data management and analysis at scale.

Topics of interest for this solicitation are focused on the following key core computer science research areas:

(d) Computer Science: Systems
Technical Contact: Lucy Nowell, 301-903-3191, Lucy.Nowell@science.doe.gov

a. **Programming Models and Environments**: Innovative programming models for developing applications on next-generation platforms, exploiting unprecedented parallelism, heterogeneity of memory systems (e.g. Non-Uniform Memory Access (NUMA), non-coherent shared memory, hybrid memory cube, scratchpads), and heterogeneity of processing (e.g., Graphics Processing Units (GPUs), accelerators, big-small cores, processing in memory and near memory), with particular emphasis on making it easier to program at scale; and
b. **Performance Portability**: 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 extreme-scale computing and beyond.

(e) Computer Science: Data Management, Visualization, and Analytics
Technical Contact: Laura Biven, 301-903-9556, Laura.Biven@science.doe.gov

a. **Data management**, including compression and other approaches to data reduction, data indexing, data curation, provenance capture and use, and in-situ workflow management; and
b. **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.

(f) Computer Science: Artificial Intelligence and Cybersecurity
Technical Contact: Robinson Pino, 301-903-1263, Robinson.Pino@science.doe.gov

a. **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.
b. **Neuromorphic Computing:** Specific to HPC-enabled modeling and simulation of computing architecture at extreme scales for generalizable applications of the proposed approach.
c. **HPC Cybersecurity:** Investigate methods and techniques to achieve scientific integrity through repeatable computing results whose process, origin, and data provenance are 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.

(g) Computer Science: Advanced Network Architectures
Technical Contact: Thomas Ndousse-Fetter, 301-903-9960, Thomas.Ndousse-Fetter@science.doe.gov

a. **Network architectures and protocols** that effectively exploit 100 Gbps or greater networks or advanced information-centric science discovery services as opposed to today's data-centric services.

(h) Computer Science: Workflow Science
Technical Contact: Richard Carlson, 301-903-9486, Richard.Carlson@science.doe.gov

a. **Workflow Science**: Advanced analysis tools or services that enable scientists and engineers to determine why a distributed application or workflow achieves the observed performance with actionable suggestions when performance is below expectations.

Computer Science pre-applications and applications must explain their relevance to current and future high performance computing platforms as well as their relevance to the mission of the Office of Science and the Advanced Scientific Computing Research programs.

Topics that are out of scope include:

- Pre-applications and applications with primary emphasis on computer hardware design, fabrication, or integration; materials science; and computing devices and/or device/circuit design and/or manufacturing;
- All aspects of 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;
- Research that is only applicable to hand-held, tablets, laptops, portable, desktop, embedded or cloud computing;
- Research with a primary goal of developing hardware components, including Intelligent Network Interface Cards, or network acceleration hardware; and technologies that optimize wireless or other low-speed network infrastructures;
- Pre-proposals and proposals with a primary focus on development or deployment activities; or that suggest incremental upgrades to existing network architectures, protocols, tools, or services; and/or
- Research and applications not specific and justified in the context of current and future supercomputing facilities and networks supported by ASCR (i.e., Argonne Leadership Computing Facility (ALCF), National Energy Research Scientific Computing Center (NERSC), Oak Ridge Leadership Computing Facility (OLCF), and ESnet). http://science.energy.gov/ascr/facilities/

References

DOE Workshop report. "DOE Network 2025: Network Research Problems and Challenges for DOE Scientists Workshop,"

http://science.energy.gov/~/media/ascr/pdf/programdocuments/docs/2017/DOE_Network_2025.pdf

DOE Workshop report. "Software Defined Networking for Extreme-Scale Science: Data, Computer, and Instrument Facilities," https://www.orau.gov/ionInfrastructure2014/intelligent-network-infrastructure-workshop-report.pdf

DOE Workshop report. "STREAM2016: Streaming Requirements, Experience, Applications, and Middleware workshop," https://science.energy.gov/~/media/ascr/pdf/programdocuments/docs/2017/STREAM2016.pdf

II. Biological and Environmental Research (BER)

Program Website: http://science.energy.gov/ber/

The mission of the Biological and Environmental Research (BER) program is to support transformative science and scientific user facilities to achieve a predictive understanding of complex biological, earth, and environmental systems for energy and infrastructure security and resilience.

Biological Systems Science

The Biological Systems Science Division (BSSD) within DOE's Office of Biological and Environmental Research supports fundamental research to achieve a predictive systems-level understanding of microbes, plants, and biological communities to advance DOE missions in energy and the environment. By integrating genome-enabled science with advanced computation and experimental biology, BSSD seeks to uncover the foundational principles that drive complex biological systems, enabling the re-design of plants and microbes for beneficial purposes. Recent breakthroughs in genome editing and biological engineering continue to produce rapid advances in biotechnology. BSSD's goal is to develop and utilize these advances to provide the fundamental understanding needed to produce biofuels and related bioproducts from renewable biomass resources.

BER is seeking Biological Systems Science research in the following area:

(a) Systems-Level Design and Engineering of Microbial or Plant Systems for the Production of Biofuels and Bioproducts

Technical Contact: Pablo Rabinowicz, 301-903-0379, pablo.rabinowicz@science.doe.gov

Applications are requested for -omics driven plant or microbial systems biology research to develop genome-wide design and editing approaches, and *in vivo* or cell-free engineering technologies to produce high levels of biofuels and bioproducts. Applications that propose highly innovative genome-scale design and engineering approaches, supported by novel computational tools and coupled to high-throughput platforms for testing of the engineered organisms, are encouraged. Microbial systems may include eukaryote or prokaryote photosynthetic or fermentative microbes that can synthesize biofuels and bioproducts directly from light or by conversion of lignocellulosic biomass. Plant systems may include oil- or lignocellulosic biomass-

producing bioenergy crops that can be engineered for facilitated cell wall deconstruction and conversion into fuels and products, or for high productivity in marginal environments or under abiotic stress.

A focus on new or emerging model systems to expand the breadth of platform microorganisms and plants for engineering is encouraged. Research on traditional model systems should be kept to a minimum. Applications should consider biocontainment of engineered organisms and potential unintended outcomes of the proposed engineering approaches.

The following topics are **not** within the scope of the BSSD research area: food crops; starch-, waste-, natural gas-, petroleum-, or coal-derived biofuels and bioproducts; microbial fuel cells; wastewater treatment; bioremediation; production of ethanol, hydrogen, pharmaceuticals, nutraceuticals, cosmetics, or food products.

Applicants are encouraged to consider the use of resources provided by DOE Science User Facilities and Community Resources. These include the DOE Systems Biology Knowledgebase (KBase; www.kbase.us), DOE Joint Genome Institute (JGI; http://jgi.doe.gov/), DOE Environmental Molecular Sciences Laboratory (EMSL; http://www.emsl.pnl.gov/emslweb/), National Energy Research Scientific Computing Center (NERSC; http://www.nersc.gov), and DOE Structural Biology Infrastructure Facilities (http://science.energy.gov/ber/research/bssd/structural-biology/).

If an award is made, at least one project participant will be required to attend an annual investigator meeting each year of funding. Reasonable travel expenses may be included as part of the project budget.

Earth and Environmental Systems Sciences

The Earth and Environmental Systems Sciences subprogram supports fundamental science and research capabilities that enable major scientific developments in earth system-relevant atmospheric and ecosystem process and modeling research in support of DOE's mission goals for transformative science for energy and national security. There are five goals which frame the subprogram and investments: (a) synthesize new process knowledge and innovative computational methods that advance next generation, integrated models of the earth system; (b) develop, test and simulate process-level understanding of atmospheric systems and terrestrial ecosystems, extending from bedrock to the top of the canopy; (c) advance fundamental understanding of coupled biogeochemical processes in complex subsurface environments to enable systems-level environmental prediction and decision support; (d) enhance the unique capabilities and impacts of the ARM and EMSL scientific user facilities and other BER community resources to advance the frontiers of earth and environmental science; and (e) identify and address science gaps that limit translation of BER fundamental science into solutions for DOE's most pressing energy and environmental challenges.

BER is seeking Earth and Environmental Systems Sciences research in the following area:

(b) Atmospheric Processes
Technical Contact: Sally McFarlane, 301-903-0943, Sally.McFarlane@science.doe.gov

Atmospheric research within BER is focused on improving physical understanding of atmospheric processes that impact the Earth's energy budget (https://asr.science.energy.gov/). Applications are sought that will improve fundamental process-level understanding of the atmospheric system through analysis of BER observational data. Applications must focus on one or more of the following atmospheric processes: aerosol formation, growth, or removal; secondary organic aerosol processes; aerosol-cloud interactions; boundary layer processes that impact cloud formation, microphysical properties, or lifetime; convective cloud processes; ice or mixed phase microphysical processes; or radiative transfer processes. Applications must include discussion of error sources in observational data and how these uncertainties may impact the proposed analyses. The primary observational data used in the proposed research must be from one or more BER-supported user facilities, including the Atmospheric Radiation Measurement (ARM) Research Facility, Environmental Molecular Sciences Laboratory (EMSL), or from BER-supported field activities.

Complementary laboratory studies, instrument development, or additional small-scale field activities may be included as part of the proposed work, but must directly tie to existing BER-supported observations. Applications proposing field work at an ARM facility site must submit a separate pre-application to the ARM facility (https://www.arm.gov/research/campaign-proposal) by the same date as the Early Career application. Applications proposing field work at another BER-supported observational site must include a letter from the site manager or principal investigator indicating that the observational site can support the proposed activities, if selected.

Applicants may use data from other sources that complements the BER observations, but must clearly illustrate how the BER data is primary to the proposed work. Applicants may propose the use of process, regional, or global models, but must directly tie any modeling work to the observational analysis and to the improved understanding of atmospheric processes. The program will not consider applications that: focus primarily on model development, use BER observations only to drive a model simulation, or focus primarily on air quality or satellite validation.

Pre-applications for the Atmospheric Processes topic must clearly identify the atmospheric process being investigated and the BER-supported observational data to be used in the proposed research. If an award is made, at least one project participant will be required to attend an annual investigator meeting for each year of funding. Reasonable travel expenses may be included as part of the project budget.

More detailed information about BER Earth and Environmental Systems Sciences sponsored research can be found at: https://science.energy.gov/ber/research/cesd/.

III. Basic Energy Sciences (BES)
Program Website: http://science.energy.gov/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 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 biosciences. BES-supported scientific facilities provide specialized instrumentation and expertise that enable scientists to carry out experiments not possible at individual laboratories.

More detailed information about BES sponsored research can be found at the BES website listed above. There you will find BES-sponsored workshop reports that address the current status and possible future directions of some important research areas. Also, Principal Investigators' Meetings Reports contain abstracts of BES supported research in topical areas associated with Division-sponsored technical conferences. Finally, the websites of individual BES Divisions may also be helpful. The following web pages are listed for convenience:
BES overview information, including the latest BES Summary Report:
https://science.energy.gov/bes/community-resources/overview-brochures/
BES Workshop Reports:
http://science.energy.gov/bes/community-resources/reports/
Materials Sciences and Engineering Division Principal Investigators' Meetings:
http://science.energy.gov/bes/mse/principal-investigators-meetings/
Chemical Sciences, Geosciences, & Biosciences Division Principal Investigators' Meetings:
http://science.energy.gov/bes/csgb/principal-investigators-meetings/
Scientific User Facilities Division web page:
http://science.energy.gov/bes/suf/

This year, many of the core research areas are limiting early career applications to a subset of topics within their regular research programs. In those cases, the intention is to rotate topics on an annual basis. Proposed research must be responsive to a supported topic in one of the core research areas listed below:

(a) Materials Chemistry
Technical Contacts: Michael Sennett, 301-903-6051, Michael.Sennett@science.doe.gov (select Michael Sennett in PAMS) and Craig Henderson, 301-903-0805, Craig.Henderson@science.doe.gov

This program supports scientific research on materials with a focus on the *chemical synthesis, chemical control, and chemical dynamics* of material composition and structure across the range of length scales from atomic to mesoscopic, with a view to elucidating fundamental aspects of materials' structure-property relationships. The major programmatic focus is on the discovery, design and synthesis of novel, energy-relevant materials with an emphasis on the *chemistry* and *chemical* control of composition and structure across the range of length scales from atomic to mesoscopic, and consequent materials properties.

Recent BES Basic Research Needs (and other) workshops and reports have articulated those areas of the materials sciences that are most relevant to energy. All of the reports variously identify the overarching goal of fundamental materials chemistry research as providing the *knowledge* needed to *design and produce* new materials with *tailored properties from first principles.* This program will therefore emphasize research on the chemistry-based discovery, synthesis and transformations of materials and/or morphologies with the goal of providing fundamental knowledge with the potential to enable the development of next generation energy technologies.

For the early career program, the topic for applications in this year is strictly limited.

The program will accept hypothesis-driven applications ONLY in the following topical area:

- **Synthesis and characterization of hierarchically structured materials – chemical control of material morphologies in multiple dimensions and at multiple length scales**

Applicants should emphasize the impactful fundamental science aspects of their proposed project and the project should be focused on hypothesis-driven fundamental research that is transformative in nature.

The program will NOT consider applications this year on any other topic than the one listed above. Future Early Career Research Program competitions in Materials Chemistry will call for applications in a different limited topical area or areas, to be determined by programmatic needs and priorities at the time of the announcement.

The program will NOT accept applications describing the following categories of research activity: *Optimization* of material properties for any applications, *nanoparticle synthesis* as a primary goal, studies of *energetic materials* (i.e. propellants and explosives), *device fabrication and testing* as a primary goal, and *developing materials* for specific applications.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division-funded programs at the laboratory of the applicant.

(b) Biomolecular Materials
Technical Contact: Michael Markowitz, 301-903-6779, mike.markowitz@science.doe.gov

This activity supports basic research in the discovery, design and synthesis of functional materials and complex structures based on principles and concepts of biology. Since biology provides a blueprint for translating atomic and nanoscale phenomena into mesoscale materials that display complex yet well-coordinated collective behavior, the major programmatic focus is on the hypothesis-driven creation of energy-relevant versions of these materials optimized for harsher, non-biological environments.

Recent BES Basic Research Needs (and other) workshops and reports have clearly identified mastering the capabilities of living systems as a Grand Challenge that could provide the knowledge base to discover, design, and synthesize new materials with totally new properties for next-generation energy technologies. Biomolecular Materials research activity seeks to advance the ability for materials that can coherently manage collective chemical, optical, electronic, magnetic, mechanical, and thermal signals and processes; self-repair; regulate, clean, and sequester impurities; and tolerate abuse.

For the early career program, two separate topics (A and B shown below) are planned for alternate fiscal years. Based on programmatic priorities, science-driven research for assembly that incorporates error correcting and defect-managing mechanisms will be emphasized for both topics. **For this announcement, only applications focused on Topic B will be considered**.

> Topic A (Alternate years): The specific focus will be on research to design and create future next-generation materials for energy conversion and storage with programmable selectivity and transport based on biological gating and pumping functions.
>
> Topic B (This year): The focus should be creation of beyond-equilibrium multicomponent, resilient, self-regulating materials that can reconfigure function and energy transfer, transport, and communication pathways; repair and rebuild structure without external input; and self-replicate.

For both of these topics, science-driven coupling of theory and experiment to achieve synthesis of materials with predetermined functions, assembly management attributes noted above, and morphology will be emphasized. The program **will not** support projects that do not have a clear focus on materials science or are aimed at optimization of materials properties for any applications, device fabrication, sensor development, tissue engineering, and biological or biomedical research.

For DOE national laboratory applicants, the proposed research must fit within the BES MSE-funded programs at the laboratory of the applicant.

(c) Synthesis and Processing Science
Technical Contact: Bonnie Gersten, 301-903-0002, bonnie.gersten@science.doe.gov

This program supports basic scientific research on materials to understand the physical principles that underpin materials synthesis including diffusion, nucleation, and phase transitions, often using *in situ* diagnostics, and developing new techniques to synthesize materials. An important element of this activity is the development of real-time monitoring tools that probe the dynamic environment and the progression of structure and properties as a material is formed. This information is essential to the physical understanding of the underlying mechanisms in materials synthesis and processing that help gain atomic level control.

Recent BES Basic Research Needs (and other) workshops and reports (https://science.energy.gov/bes/community-resources/reports/) have identified the challenges in synthesis and processing that are most relevant to next-generation energy technologies. In

particular, the BES Advisory Committee's Grand Challenges report, *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science* and other BES workshop reports highlight the needs and challenges for the field.

This year's Early Career Research Program invites applicants to submit hypothesis driven proposals that present novel understanding and creative approaches elucidating the physical mechanisms underlying the synthesis and processing of three-dimensional bulk materials. Proposals that integrate a creative experimental methodology with a theoretical-based approach to accelerate progress in understanding unifying principles for synthesis and/or processing are of particular interest. The focus of this activity on materials discovery and design by physical means is complementary to the BES Materials Chemistry and Biomolecular Materials research activities, which emphasize chemical and biomimetic approaches.

The program **will not** support projects aimed at *optimization* of material properties for specific applications, device fabrication, or nanoparticle synthesis as a primary goal. In addition, projects that mainly focus on tribology, fluid dynamics, manufacturing or engineering scale-up and development will not be supported. Moreover, projects that involve biological materials or involve organic chemical synthesis as the primary focus will not be supported by this activity. For this year, projects involving the synthesis or processing of two-dimensional materials **will not** be supported.

For DOE national laboratory applicants, the proposed research must fit within the BES MSE-funded programs at the laboratory of the applicant.

(d) Experimental Condensed Matter Physics
Technical Contact: Michael Pechan, 301-903-0540, Michael.Pechan@science.doe.gov

The Experimental Condensed Matter Physics (ECMP) program supports research that will advance our fundamental understanding of the relationships between intrinsic electronic structure and the properties of complex materials.

This year the Early Career call in ECMP will focus on nanostructured and low dimensional quantum materials wherein electronic, structural, charge and magnetic states are controlled to produce novel functionality. Next year's call is anticipated to focus on bulk quantum materials. The ECMP Program does not support applications on electrochemistry, thermoelectric materials or photovoltaic materials; nor does it support projects aimed at materials optimization. In addition, the ECMP Early Career Program will not accept proposals on topics in the following areas: conventional semiconductors, heavy fermion superconductivity, quantum Hall physics in compound semiconductor materials, cuprate superconductivity, cold atom physics.

For DOE national laboratory applicants, the proposed research must fit within the BES MSE-funded programs at the laboratory of the applicant.

(e) Theoretical Condensed Matter Physics
Technical Contact: James Davenport, 301-903-0035, james.davenport@science.doe.gov (select James Davenport in PAMS) or Matthias Graf, 301-903-0874, matthias.graf@science.doe.gov

This program supports research in theoretical condensed matter physics with an emphasis on quantum materials, materials discovery, systems out of equilibrium (including transport and ultrafast response), and fundamental research in materials related to energy technologies. Examples of current research include strongly correlated electron systems, quantum phase transitions, magnetism, superconductivity, wide bandgap semiconductor physics, computational and data driven materials design, thermoelectric materials, optical response, and neutron and photon scattering. Novel, physics-based computational techniques are supported for quantum many-body problems. This year, applications are only sought in the areas of quantum materials and systems out of equilibrium, including transport and ultrafast response. Next year, the plan is to invite applications in targeted areas of high-throughput computations, data-driven materials discovery, and materials theory/modeling solely related to energy technologies**.**

For DOE national laboratory applicants, the proposed research must fit within the BES MSE-funded programs at the laboratory of the applicant.

(f) Physical Behavior of Materials
Technical Contact: Refik Kortan, 301-903-3308, refik.kortan@science.doe.gov

This program supports research to understand the physical behavior of materials. This year, the program invites early career proposals on the BES grand challenge (https://science.energy.gov/~/media/bes/besac/pdf/Reports/Challenges_at_the_Frontiers_of_Matter_and_Energy_rpt.pdf) topic of Harnessing Coherence in Light and Matter that are relevant to physical behavior of materials. The applicants should heavily emphasize the impactful fundamental science aspects of their projects and these projects should be centered around hypothesis driven fundamental research that is transformative in nature. This program also supports theory, modeling, and simulation activities, especially in combination with experimental research.

The program **will not** support projects aimed at optimization of materials properties for any applications, device fabrication, or sensor development.

For DOE national laboratory applicants, the proposed research must fit within the BES MSE-funded programs at the laboratory of the applicant.

(g) Mechanical Behavior and Radiation Effects
Technical Contact: John Vetrano, 301-903-5976, john.vetrano@science.doe.gov

This activity supports hypothesis-driven basic research to understand defects in materials and their effects on the properties of strength, structure, deformation, and failure. Defect formation, growth, migration, and propagation are examined by coordinated experimental and modeling efforts over a wide range of spatial and temporal scales. Topics this year include fundamental

studies of radiation resistance in structural materials, radiation effects on mechanical properties, and radiation in conjunction with additional environments such as stress and a corrosive medium; in all cases the radiation aspect needs to be the key topic to be studied. The long-term goals of this program are to develop the scientific underpinning that will allow the development of predictive models for the design of materials having superior radiation resistance, and to understand how materials can be manipulated by radiation. This year the emphasis is on radiation effects on materials, with the plan to alternate this topic with an emphasis on mechanical behavior annually. Applicants are encouraged to look at the priority research directions in the brochure for the recent workshop Basic Research Needs for Future Nuclear Energy (available on the BES web site); while not exclusive to this program they do outline priorities for BES in general.

Radiation is increasingly being used as a tool and a probe to gain a greater understanding of fundamental atomistic behavior of materials. Incoming fluxes can be uniquely tuned to generate a materials response that can be detected *in situ* over moderate length and time scales. Materials also sustain damage after long times in high-radiation environments typical of current and projected nuclear energy reactors and in geological waste storage. As nuclear energy is projected to play a larger role in U.S. energy production, these are issues that need to be addressed at a fundamental level. High-dose studies **will not** be explored in this program at this time, nor will radiation effects on concrete/cement, superconductivity, or magnetism.

For DOE national laboratory applicants, the proposed research must fit within the BES MSE-funded programs at the laboratory of the applicant.

(h) X-ray Scattering
Technical Contact: Lane Wilson, 301-903-5877, lane.wilson@science.doe.gov

This activity supports basic research on the fundamental interactions of photons with matter to achieve an understanding of atomic, electronic, and magnetic structures and excitations and their relationships to materials properties. The main emphasis is on x-ray scattering, spectroscopy, and imaging research, primarily at major BES-supported user facilities. Instrumentation development and experimental research directed at the study of ultrafast physical phenomena in materials is an integral part of the portfolio. Based on programmatic priorities, this activity **will not** support ultra-fast source development, but will focus on the application of ultra-fast probe interactions with materials and the resulting connection to materials dynamics.

Advances in x-ray scattering and ultrafast sciences will continue to be driven by scientific opportunities presented by improved source performance and optimized instrumentation. The x-ray scattering activity will continue to fully develop the capabilities at the DOE facilities by providing support for instrumentation, technique development and research. A continuing theme in the scattering program will be the integration and support of materials preparation (especially when coupled to *in situ* investigation of materials processing) as this is a core competency that is vital to careful structural measurements related to materials properties. New investments in ultrafast science will focus on research that uses radiation sources associated with BES facilities and beam lines but also includes materials research employing ultra-short pulse x-ray, electron beam and terahertz (THz) radiation probes created by tabletop laser sources.

For DOE national laboratory applicants, the proposed research must fit within the BES MSE-funded programs at the laboratory of the applicant.

(i) Neutron Scattering
Technical Contact: P. Thiyagarajan (Thiyaga), 301-903-9706, p.thiyagarajan@science.doe.gov

This activity supports basic research on the fundamental interactions of neutrons with matter to achieve an understanding of the atomic, electronic, and magnetic structures and excitations of materials and their relationship to macroscopic properties. Main emphasis is on innovative science of materials and phenomena using neutron scattering, coupled with advancement of neutron scattering techniques, primarily at BES-supported user facilities. A continuing theme of this program is the integration of material synthesis, neutron scattering experiments, and computational modeling. Integration of careful neutron scattering measurements on high quality model systems with modeling is vital for an in-depth understanding of the relationship between structure and dynamics and macroscopic properties.

The focus for this year's Early Career Research Program is on fundamental science on quantum materials based on the priority research directions in "Basic Research Needs Workshop on Quantum Materials for Energy Relevant Technology" (https://science.energy.gov/~/media/bes/pdf/reports/2016/BRNQM_rpt_Final_12-09-2016.pdf). Characterizing and controlling the emergent behavior are keys to optimizing and exploiting a wide range of quantum materials' performance and functionality. *In situ* studies can measure structure and dynamics of materials in the appropriate environment and operational conditions, yielding direct data for comparison to predictions. The program will develop novel approaches that will exploit the unique aspects of neutron scattering and *in situ* capabilities to investigate quantum materials with hierarchical structures and excitations in a wide range of length and time scales.

Based on programmatic priorities, applications focused on superconductivity (both conventional and unconventional) **will not** be considered.

For DOE national laboratory applicants, the proposed research must fit within the BES MSE-funded programs at the laboratory of the applicant.

(j) Electron and Scanning Probe Microscopies
Technical Contact: Jane Zhu, 301-903-3811, jane.zhu@science.doe.gov

This activity supports basic research in materials sciences using microscopy and spectroscopy techniques. The research includes experiments and theory to understand the atomic, electronic, and magnetic structures and properties of materials. This activity also supports the development of new instrumentation and techniques, including ultrafast diffraction and imaging techniques, to advance basic science and materials characterizations for energy applications. The goal is to develop a fundamental understanding of materials through advanced microscopy and spectroscopy.

The focus for this year's Early Career Research Program is on basic science based on the priority research directions in "Basic Research Needs Workshop on Quantum Materials for Energy Relevant Technology" (https://science.energy.gov/~/media/bes/pdf/reports/2016/BRNQM_rpt_Final_12-09-2016.pdf). New methods and approaches could provide an array of opportunities for groundbreaking science. These include understanding and controlling nano- or meso-scale inhomogeneity as well as the interplay between charge, orbital, spin and lattice degrees of freedom. Other areas of emphasis are imaging the functionality of materials; investigation of the electronic structure, spin dynamics, magnetism, phase transitions and transport properties from atomistic to mesoscopic scales; and development of advanced *in situ* analysis capabilities or combination of multiple probes for study of quantum materials.

This year applications are limited to the scanning probe microscopy and spectroscopy area. Based on programmatic priorities, projects aimed at technique development without science goals **will not be** considered.

For DOE national laboratory applicants, the proposed research must fit within the BES MSE-funded programs at the laboratory of the applicant.

(k) Atomic, Molecular, and Optical Sciences (AMOS)
Technical Contact: Tom Settersten, 301-903-8428, thomas.settersten@science.doe.gov

This program supports basic experimental and theoretical research aimed at understanding the structural and dynamical properties of atomic and molecular systems. The research emphasizes fundamental interactions of photons and electrons with atomic and molecular systems to characterize and control their behavior. The goal is to develop accurate quantum-mechanical descriptions of dynamical processes such as chemical bond breaking and forming, interactions in strong fields, and electron correlation. Topics of interest include the development and application of novel, ultrafast optical probes of matter; the interactions of atoms and molecules with intense electromagnetic fields; and quantum control of atomic and molecular systems. Projects involving technical development of sources or instrumentation must include a well-integrated scientific research focus.

The AMOS activity will continue to support science that advances DOE and BES mission priorities. Closely related experimental and theoretical efforts will be encouraged. AMOS will continue to have a prominent role at BES facilities in understanding and controlling the interaction of intense, ultrafast x-ray pulses with matter. Key targets for greater investment include attosecond science, ultrafast x-ray science, and ultrafast electron diffraction from molecular systems.

The program emphasizes ultrafast, strong-field, short-wavelength science, and correlated dynamics in atoms and molecules. Examples include the use of high-harmonic generation or its variants as soft x-ray sources; intense, ultrafast x-ray science at the Linac Coherent Light Source (LCLS); and development and characterization of femtosecond and attosecond pulses of x-rays at accelerator-based and table-top sources. Applications of these light sources include ultrafast

imaging of chemical reactions, diffraction and harmonic generation from aligned molecules, and inner-shell photoionization of atoms and molecules. Coherent control of nonlinear optical processes and tailoring of quantum-mechanical wave functions with lasers will continue to be of interest, particularly in molecular systems.

The AMOS program **is not** accepting applications in the areas of nanoscience, bioscience, and ultracold science.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) -funded programs at the laboratory of the applicant.

(l) Gas Phase Chemical Physics (GPCP)
Technical Contact: Wade Sisk, 301-903-5692, wade.sisk@science.doe.gov

The Gas Phase Chemical Physics (GPCP) Program supports research on gas-phase chemical processes important in energy applications. The overall goal of this program is to understand energy flow and reaction mechanisms in complex, non-equilibrium, gas-phase environments in which the coupling of chemical and transport processes is poorly understood.

The program may be divided into four basic science research thrusts described below.

1. *Light-Matter Interactions*. This thrust consists of research in molecular spectroscopy and diagnostics development to probe molecular structure, dynamics and interactions in complex gas-phase systems. This research is expected to provide approaches for chemical and physical analysis of heterogeneous and dynamic gas-phase environments. (OPEN)
2. *Chemical Reactivity*. This thrust includes chemical kinetics and mechanisms, chemical dynamics, collisional energy transfer, and construction of, and calculations on, molecular potential energy surfaces. This research is expected to develop fundamental understanding of energy flows and chemical reactions, which is the basis for determining accurate rate constants and predictive chemical mechanisms, and to develop and validate new theoretical methods to improve accuracy of theoretical chemical kinetics. (OPEN)
3. *Chemistry-Transport Interactions.* Research in this area focuses on gaining a better understanding of how non-equilibrium, non-uniform environments impact kinetics and mechanisms. Efforts include both experimental and theoretical studies probing mechanistic processes and how they change in complex environments. This research can lead to development of multiplexed diagnostics that measure many variables simultaneously to overcome irreproducibility associated with non-uniform and dynamic environments such as those in turbulent reacting flows. (CLOSED)
4. *Gas-Particle Interconversions*. This thrust consists of research on the formation, growth and evaporation of small particulates and aerosols and the transition to supercritical fluids at high pressures. This research is expected to lead to the development of mechanistic models of particle formation and growth, as well as a better understanding of particle evaporation. (CLOSED)

Research proposal applications will be accepted from only two of the selected four research thrusts each year, with the remaining thrusts offered in alternate years. For this announcement, only applications focused on thrusts **1** and **2** will be considered. Research applications for thrusts 3 and 4 will not be considered this year, but considered in alternate years.

The GPCP program **does *not*** support research in the following areas: 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.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

(m) Computational and Theoretical Chemistry
Technical Contact: Mark Pederson, 301-903-9956, mark.pederson@science.doe.gov

Computational and Theoretical Chemistry emphasizes sustained development and integration of new and existing theoretical and massively parallel computational approaches for the deterministic, accurate and efficient prediction of processes and mechanisms relevant to the BES mission, especially in relation to providing groundwork for computational design of molecular- to meso-scale materials and processes. Part of the focus is on next-generation simulation of processes that are so complex that efficient computational implementation must be accomplished in concert with development of theories and algorithms. Efforts should be tightly integrated with the research and goals of BES, especially the chemical physics programs, and should provide fundamental solutions that enhance or enable conversion to clean, sustainable, renewable, novel or highly efficient energy use. Efforts should include application to real molecular- and nano-scale systems. This may include the development or improvement of reusable computational tools that enhance analysis of measurements at the DOE facilities or efforts aimed at enhancing accuracy, precision, and applicability or scalability of all variants of quantum-mechanical simulation methods. This includes the development of spatial and temporal multi-scale/multistage methodologies that allow for time-dependent simulations of resonant, non-resonant and dissipative processes as well as rare events. Development of capabilities for simulation of light-matter interactions, conversion of light to chemical energy or electricity, and the ability to model and control externally driven electronic and spin-dependent processes in real environments are encouraged. These phenomena may be modeled using a variety of time-independent and time-dependent simulation approaches. Examples include:

- Practical predictive methods for excited-state phenomena in complex molecular systems.
- Nontraditional or novel basis sets, meshes and approaches for quantum simulation.
- Simulation and coupling of all interactions/scales in a system including: electronic, vibrational and atomistic structure, dissipative interactions, interactions between matter, radiation, fields and environment, spin-dependent and magnetic effects and the role of polarization, solvation and weak interactions.

Current interest includes applications to (i) energy storage, (ii) solar light harvesting including sunlight-to-fuel, (iii) interfacial phenomena, (iv) selective carbon-dioxide/gas separation, storage

and capture (v) next-generation combustion modeling, (vi) reactivity and catalysis (vii) molecular and nano-scale electronic-, spin- and energy transport, (viii) quantum simulation of biologically inspired mechanisms for energy management and (ix) alternative fuel.

Methods and/or investigations that do not require consideration of electronic rearrangements or coupling of electronic and vibrational degrees of freedom to external stimuli are not supported by this program.

For this year, the Computation and Theoretical Chemistry program will support efforts that focus upon improving the fundamental underpinnings of computational and theoretical methods for description of particle-particle, including many-body, interactions. Methods that do so by decreasing the number of empirical parameters in an existing capability, (2) increasing the computational/algorithmic efficiency of a specific existing capability, or (3) removing known fundamental issues from existing capabilities are of special interest. Methods that seek improvements of existing empirical parameterizations through introduction of additional empirical parameters, even if based upon results from other theoretical methods or experiment, will be discouraged.

For DOE national laboratory applicants, the proposed research must fit within the BES CSGB-funded programs at the laboratory of the applicant.

(n) Condensed Phase and Interfacial Molecular Science (CPIMS)
Technical Contact: Gregory Fiechtner, 301-903-5809, gregory.fiechtner@science.doe.gov

The CPIMS program emphasizes basic research at the boundary of chemistry and physics, pursuing a molecular-level understanding of chemical, physical, and electron- and photon-driven processes in liquids and at interfaces. With its foundation in chemical physics, the impact of this crosscutting program on DOE missions is far reaching, including energy utilization, catalytic and separation processes, energy storage, chemical synthesis, and subsurface chemical and transport processes. Experimental and theoretical investigations in the gas phase, condensed phase, and at interfaces aim at elucidating the molecular-scale chemical and physical properties and interactions that govern chemical reactivity, solute/solvent structure and transport. Studies of reaction dynamics at well-characterized surfaces and clusters lead to the development of theories on the molecular origins of surface-mediated catalysis and heterogeneous chemistry. Studies of model condensed-phase systems target first-principles understanding of molecular reactivity and dynamical processes in solution and at interfaces, including complex interfaces. Fundamental studies of reactive processes driven by radiolysis in condensed phases and at interfaces provide improved understanding of radiation-driven chemistry in nuclear fuel and waste environments.

Basic research is also supported to develop new experimental and theoretical tools that push the horizon of spatial and temporal resolution needed to probe chemical behavior selectively at interfaces and in solution, enabling studies of composition, structure, bonding and reactivity at the molecular level. The transition from molecular-scale chemistry to collective phenomena in complex systems is also of interest, allowing knowledge gained at the molecular level to be exploited through the dynamics and kinetics of collective interactions. In this manner, the desired evolution is toward predictive capabilities that span the microscopic to mesoscale domains,

enabling the computation of individual molecular interactions as well as their role in complex, collective behavior at continuum scales.

Recent Early Career Research Program awards managed in the CPIMS portfolio include (1) studies of ion solvation and charge transfer at electrochemical interfaces using nonlinear soft x-ray spectroscopy; (2) research that pushes accurate quantum simulations toward large mesoscale systems; (3) explorations of multidimensional infrared microscopy for visualizing chemical dynamics in heterogeneous environments; and (4) investigations of photochemical reactions of relevance to chemical synthesis in charged micro-droplets. Descriptions of earlier awards are found in CPIMS Meeting Reports at the link http://science.energy.gov/bes/csgb/principal-investigators-meetings/, under "Condensed-Phase and Interfacial Molecular Science". A more extensive description of program evolution can be found at the following link: https://science.energy.gov/~/media/bes/pdf/brochures/bes-cras/2017/cra_17_CPIMS.pdf.

The CPIMS program **does not** fund research in bulk fluid mechanics or fluid dynamics, applications such as the development of micro-scale devices, and research that is of principle importance to medical sciences and applications.

For DOE national laboratory applicants, the proposed research must fit within the BES CSGB-funded programs at the laboratory of the applicant.

(o) Catalysis Science
Technical Contact: Viviane Schwartz, 301-903-0448, viviane.schwartz@science.doe.gov (select Viviane Schwartz in PAMS) and Chris Bradley, 301-903-2047, chris.bradley@science.doe.gov

This activity develops the fundamental scientific principles enabling catalyst design and chemical transformation control for energy-related catalytic processes. Research includes: identification of the elementary steps of catalytic reaction mechanisms and their kinetics; the synthesis of catalytic sites and their environment at the atomic and molecular level; the study of structure-reactivity relationships of catalytic species in solution or on solids; the dynamics of catalyst structure relevant to catalyst reactivity, selectivity and stability; the experimental determination of potential energy landscapes for catalytic reactions; the development of novel spectroscopic, structural and multimodal techniques for *in situ* and *operando* characterization of catalytic processes; and the development and application of theory, modeling, and simulation for determining catalyst structure/function and catalytic pathways.

The primary goal for all submissions must be to understand and control reaction mechanisms of full catalytic cycles relevant to energy applications. For phenomenological catalysis to evolve into predictive catalysis, the principles connecting catalytic structure, activity, selectivity, and reaction mechanisms must be clearly and thoroughly identified. This activity **encourages hypothesis-driven** applications in all classical areas of catalysis but this year in particular in the following areas:

- Selective and low-temperature activation of lower or higher alkanes or multifunctional molecules using non-precious or non-metallic catalysts;

- Catalytic reaction mechanisms influenced by weak forces, confinement effects or secondary coordination effects;
- Catalytic mechanisms in electrochemical conversions of complex molecules into chemicals and fuels. However, some electrocatalytic processes involving carbon dioxide (CO_2), oxygen (O_2), hydrogen (H_2), water (H_2O) or nitrogen (N_2) are excluded this year (see details below);
- Fast and ultrafast characterization of reaction intermediates and transition states with the intent of unraveling catalytic mechanisms.

New strategies for design of selective catalysts for fuel and chemical production from both fossil and renewable biomass feedstocks are of interest. Additionally, applications and pre-applications MUST clearly identify the reaction system to be studied indicating the scientific rationale for selecting the chemical reactions and their relevance to the development of structure-reactivity relationships. The program **will not consider** applications on the following topics:

- Process or reactor design and optimization, including fabrication or optimization of batteries, sensors, or catalytic devices;
- Stoichiometric organometallic reactions that are not part of a full catalytic cycle;
- Applications where the focus resides on environmental and engineering aspects of chemical processes;
- Applications to study primarily the synthesis of catalytic materials;
- Applications where developing theoretical, computational, or characterization methods is the main objective, while understanding catalytic reaction mechanisms is secondary;
- High-throughput methods with the purpose of synthesizing, characterizing, or screening catalysts;
- Research focused on catalytic synthesis of pharmaceuticals or, more generally, fine chemicals unrelated to energy applications.

Additionally, **this year,** the program will NOT support the following categories of research:

- Photochemically activated processes;
- Electrocatalytic processes where the main objective is the reduction of CO_2, O_2 or N_2; the oxidation of H_2 or H_2O; or the evolution of H_2 or O_2.

Examples of research funded in catalysis can be found in Catalysis Science Program Meeting Reports at the link 'Chemical Sciences, Geosciences, & Biosciences Division Principal Investigators' Meetings', http://www.science.energy.gov/bes/csgb/principal-investigators-meetings/ (search for "catalysis" in the book title), and in the BES Research Summaries (http://science.energy.gov/bes/community-resources/program-summaries/). Basic Energy Sciences Advisory Committee (BESAC) -sponsored workshops, Basic Research Needs: Catalysis for Energy (2007), and Basic Research Needs for Catalysis Science (2017), outlining the current challenges and needs in this field, can also be found on Community Resources - Reports' web page link (https://science.energy.gov/bes/community-resources/reports/).

For DOE national laboratory applicants, the proposed research must fit within the BES CSGB-funded programs at the laboratory of the applicant.

(p) Separation Science
Technical Contact: Philip Wilk, 301-903-4537, philip.wilk@science.doe.gov

This activity supports fundamental research to predict and control the atomic and molecular interactions and energy exchanges determining the efficiency of chemical separations. This basic research is motivated by a desire to advance discovery and predictive design of future chemical separations utilizing novel, multifunctional, and/or energy- and atom-efficient methods; as well as the development and investigation of novel structures with the desired nano-, meso-, and macroscopic functionalities and dynamic and transport properties. Research topics include, but are not limited to: the structural and molecular dynamics of elementary separation steps at complex solid-fluid interfaces utilizing fast and ultrafast spectroscopy; the influence of nanoscale environments, such as ligands, electrolytes, confining structures, hybrid membranes, solvation or ionic spheres, etc., on separation mechanisms and kinetics at the molecular level; the role of amorphous, disordered, and non-equilibrium heterogeneous structures in separation mechanisms and efficiency; ultraselective separations in diverse aqueous environments (acid/base, saline, high T); reactive and non-reactive separations involving charge transport, complex mixtures and complex interfaces, and non-traditional solvents such as ionic liquids and deep eutectic solvents; the influence of electromagnetic or other fields affecting transport and bonding of charged or neutral species; and the mechanisms of energy absorption and dissipation in separating systems. A range of multidisciplinary experimental, theoretical and computational basic research approaches are employed, inspired by the multidimensional and time-dependent complexity of chemical separation problems.

Hypothesis-based separations research that is responsive to the reports on Basic Research Needs for Environmental Management, Energy and Water and Future Nuclear Energy, is well-aligned with the goals of this activity (https://science.energy.gov/bes/community-resources/reports/). However, research focused on understanding the chemistry and physical properties of actinides is better covered under (q) Heavy Element Chemistry.

This activity does not support applied research, engineering or scale up of processes, mineral or materials processing, devices or sensors, microfluidics, or research directed toward medical or analytical applications. The activity does not support the synthesis or testing of separations materials as the main goal, as such is covered under other activities.

To obtain more information about this research area, please see the proceedings of the Principal Investigators' Meetings at: http://science.energy.gov/bes/csgb/principal-investigators-meetings.

For DOE national laboratory applicants, the proposed research must fit within the BES CSGB-funded programs at the laboratory of the applicant.

(q) Heavy Element Chemistry (HEC)
Technical Contact: Philip Wilk, 301-903-4537, philip.wilk@science.doe.gov

This activity supports basic research on the fundamental chemistry of the actinide and transactinide elements with the goal to understand the underlying chemical and physical

principles that determine their behavior. The unique molecular bonding of the heavy elements is explored using theory and experiment to elucidate electronic and molecular structure as well as reaction thermodynamics. Emphasis is placed on: the chemical and physical properties of these elements to determine their bonding and reactivity in solution, at the interface, and in the solid-state; on the fundamental transactinide chemical properties; and on the overarching goal of resolving the *f*-electron challenge. The *f*-electron challenge refers to the inadequacy of current electronic structure methods to accurately describe the behavior of *f*-electrons, in particular: strong correlation, spin-orbit coupling, multiplet complexity, and associated relativistic effects. While the majority of the research supported by this activity is experimental, theoretical proposals are considered that integrate closely with existing experimental research. Synthetic and spectroscopic research is pursued within this activity on molecules that contain heavy elements and on how ligands interact with these elements.

The role of 5*f* electrons in bond formation remains the fundamental topic in actinide chemistry and is an overarching emphasis for this program. Resolving the role of the *f*-electrons is one of the three grand challenges identified in the *Basic Research Needs for Advanced Nuclear Energy Systems* report of the Basic Energy Sciences Workshop (2006) (https://science.energy.gov/~/media/bes/pdf/reports/files/Basic_Research_Needs_for_Advanced_Nuclear_Energy_Systems_rpt.pdf) and echoed in the report from the Basic Energy Sciences Advisory Committee: *Science for Energy Technology: Strengthening the Link between Basic Research and Industry* (August 2010) (https://science.energy.gov/~/media/bes/pdf/reports/files/Science_for_Energy_Technology_rpt.pdf). The 5*f* orbitals participate in the band structure of metallic and ceramic materials that contain the actinides and the nature of this participation down the actinide series is an area of active research. Theory and experiment show that 5*f* orbitals participate significantly in molecular actinide compounds, for example, compounds required for advanced nuclear energy systems. The majority of this activity is pursued at the national laboratories or coordinated directly with them because of the infrastructure needed to handle these materials safely. Research in heavy element chemistry at universities through single-investigator grants is supported, encouraging collaborations between university and laboratory projects. Sophisticated quantum-mechanical calculations that treat spin-orbit interactions accurately need further development so that they can predict the properties of molecules that contain actinides and predict the migration of radioactive species. Experimental validation of the theoretical properties of models will be the key to understanding the role of the 5*f* electrons.

Based on programmatic priorities, the HEC program does not fund research on: the processes affecting the transport of subsurface contaminants, the form and mobility of contaminants including wasteforms, projects focused on the use of heavy-element surrogates, projects aimed at optimization of materials properties including radiation damage, device fabrication, or biological systems; which are all more appropriately supported through other DOE programs. Research that is focused primarily on separations and does not address the unique properties of the heavy elements would be better aligned with the BES Separation Science program, which is described in section (p).

Applications should be hypothesis-based. Research funded in this category in the recent past can be found in Heavy Element Chemistry and Separation Science Principal Investigators' Meetings

Reports at http://science.energy.gov/bes/csgb/principal-investigators-meetings.

For DOE national laboratory applicants, the proposed research must fit within the BES CSGB-funded programs at the laboratory of the applicant.

(r) Geosciences Research
Technical Contact: James Rustad, 301-903-1717, james.rustad@science.doe.gov

This activity covers fundamental geochemical and geophysical sciences driven by novel measurements ideally coupled with theoretical/simulation methods directed at revolutionary understanding with broad implications. This year's focus is restricted to research addressing the micromechanics of time-dependent brittle processes in rocks under shallow crustal conditions. This activity is particularly concerned with (i) the collective processes behind crack network coalescence and localization at multiple scales and (ii) chemical-mechanical stress corrosion processes giving rise to subcritical crack growth in earth and related materials. Proposals may concentrate on theory, and modeling, or experiment. Experimental studies dealing with seismic signatures of crack coalescence at multiple length scales would be particularly germane to this activity.
The Geosciences program will not consider:

- Studies that are irrelevant to this year's focus—described above.
- Studies targeting particular single applications such as exploitation of a single resource, or remediation of a particular waste/contaminant type. Applicants in those cases should consult the appropriate DOE technology program;
- Studies that primarily develop technological applications of earth materials;
- Combined modeling-experimental studies that do not utilize measurement techniques that are appropriate for the model scale;
- Studies focused on molecular structure determination unless they are convincingly related to underlying energetics and/or reaction rates;
- Studies focusing on hydrological modeling and/or upscaling methods.

BES Geosciences project abstracts for the most recent principal investigators' meeting can be found through the following link:
http://science.energy.gov/~/media/bes/csgb/pdf/docs/Geosciences/2014_Geoscience_Models_Where_are_the_Rocks_Program.pdf. Note, however, this year's Early Career program is restricted to a subset of the research sponsored by the BES Geosciences Program.

For DOE national laboratory applicants, the proposed research must fit within the BES CSGB-funded programs at the laboratory of the applicant.

(s) Solar Photochemistry
Technical Contacts: Mark Spitler, 301-903-4568, mark.spitler@science.doe.gov **and Chris Fecko, 301-903-1303,** christopher.fecko@science.doe.gov **(select Chris Fecko in PAMS)**

This activity supports fundamental, molecular-level research on solar energy capture and conversion in the condensed phase and at interfaces. These investigations of solar photochemical energy conversion focus on the elementary steps of light absorption, charge separation, and

charge transport within a number of chemical systems, including those with significant nanostructured composition. Although the long-term mission of this Program is an understanding of the science behind solar-driven production of fuels and electricity, it is recognized that fundamental research in the interaction of light, matter and electrons in these systems is essential to the achievement of Program goals.

Supported research areas include organic and inorganic photochemistry, catalysis and photocatalysis, and photoinduced electron and energy transfer in the condensed phase and across interfaces, photoelectrochemistry, and artificial assemblies for charge separation and transport that mimic natural photosynthetic systems. An enhanced theory and modeling effort is needed for rational design of these artificial solar conversion systems.

Among the challenges for catalytic fuels production, knowledge gained in charge separation and electron transfer needs to be applied in a meaningful way to activation of small molecules including, among others, CO_2 in its reduction to fuels and H_2O in its oxidation or reduction via transformative catalytic cycles. This spans the range from dark catalytic reactions to those driven by the energy of an absorbed photon and in both homogeneous and heterogeneous environments. The major scientific challenge for photoelectrochemical energy conversion for fuel generation is that small band gap semiconductors capable of absorbing solar photons are susceptible to oxidative degradation, whereas wide band gap semiconductors, which are resistant to oxidative degradation in aqueous media, absorb too little of the solar spectrum. Also of emphasis is research on the principles of new hybrid systems that feature molecular catalysis at solid surfaces and of new nanoscale structures for the photochemical generation of fuels.

Research areas concerned with separation of charge that might result in electricity include multibandgap, multilayer cascade-type semiconductors, photosensitized nanoparticulate solids, and the study of the mechanism of multiple exciton generation within nanoparticles. There are also challenges in fundamental understanding of photoconversion processes – energy transfer and the generation, separation, and recombination of charge carriers – in organic-based molecular semiconductors, which could lead to a new type of inexpensive and flexible solar cell.

Another regime of chemistry initiated through creation of high energy excited states is highly ionizing radiation, as can be produced through electron pulse radiolysis, to investigate reaction dynamics, structure, and energetics of short-lived transient intermediates in the condensed phase. Among many topics, fundamental research is of interest in areas which have a long term impact upon the understanding of radiolytic degradation of nuclear tank waste, the reactivity of solid surfaces in reactor coolant systems, and the chemistry of reagents used in separations processes in nuclear cycles.

Solar Photochemistry does not fund research on device development or optimization.

For DOE national laboratory applicants, the proposed research must fit within the BES CSGB-funded programs at the laboratory of the applicant.

(t) Photosynthetic Systems
Technical Contact: Stephen Herbert, 301-903-0383, stephen.herbert@science.doe.gov

This activity supports basic research on the capture and conversion of solar energy to chemically stored forms of energy in plants, algae, and photosynthetic microbes. Topics of study include, but are not limited to, photosynthetic light harvesting, photosynthetic proton and electron transport, photosynthetic reduction of carbon dioxide into organic compounds, and the self-assembly, dynamics, and self-repair of photosynthetic proteins, complexes and membranes. The goal of the program is to foster greater knowledge of the structure and function of the diverse photosynthetic systems found in nature. Projects funded by the program combine biochemistry, biophysics, molecular biology, computational chemistry, and other approaches to understand the biological capture of sunlight and its conversion to and storage as chemical energy at a fundamental level.

All submitted applications must clearly state the energy relevance of the proposed basic research. Photosynthetic Systems does not fund: 1) development or optimization of devices or processes; 2) development or optimization of microbial strains or plant varieties for biofuel or biomass production. 3) phenotype analyses that do not test specific hypotheses relevant to the program; 4) genomic or other "omic" data acquisition that does not test specific hypotheses relevant to the program; and 5) projects that are primarily computational in nature.

For DOE national laboratory applicants, the proposed research must fit within the BES CSGB-funded programs at the laboratory of the applicant.

(u) Physical Biosciences
Technical Contact: Robert Stack, 301-903-5652, robert.stack@science.doe.gov

This activity supports basic research that combines physical science techniques with biochemical, chemical, and molecular biological approaches to discover the underlying physical and chemical principles that govern how plants and non-medical microbes capture, convert, and store energy. Fundamental research supported by the program includes studies that will provide a better understanding of the structure/function, mechanistic and electrochemical properties of enzymes that catalyze complex multielectron redox reactions (especially those involved in the interconversion of CO_2/CH_4, N_2/NH_3, and H^+/H_2), determine how the complex metallocofactors at the active sites of these enzymes are synthesized, and understand how the potential of these cofactors can be "tuned" using ligand coordination to reduce overpotential and better enable catalysis using earth-abundant metals. The program also funds mechanistic studies on electron bifurcation and catalytic bias in enzyme systems, and identifies the factors that direct and regulate the flow of electrons through energy-relevant metabolic pathways on larger spatial and temporal scales.

Physical Biosciences **does not** fund research in: 1) animal systems; 2) prokaryotic systems related to human/animal health or disease; 3) development and/or optimization of devices and/or processes; 4) development and/or optimization of microbial strains or plant varieties for biofuel/biomass production; 5) cell wall breakdown or deconstruction; 6) transcriptional or translational regulatory mechanisms and/or processes; 7) environmental remediation and/or

identification of environmental hazards. Projects should ideally be hypothesis-driven; projects that develop or rely primarily on high-throughput screening approaches **will not** be supported nor will projects that are primarily computational in nature.

All submitted applications must clearly state the energy relevance of the proposed research: How will the knowledge gained from the proposed project better our understanding of the structure, function, and/or mechanistic aspects of energy-relevant biological redox reactions at the molecular level?

For DOE national laboratory applicants, the proposed research must fit within the BES CSGB-funded programs at the laboratory of the applicant.

(v) Nanoscale Science Research Centers
Technical Contact: George Maracas, 301-903-1264, george.maracas@science.doe.gov

This research area supports work that advances the instruments, techniques, and capabilities of the existing BES Scientific User Facilities and/or contributes to capabilities of future facilities in this area. Research topics that develop and exploit the unique potential of co-located facilities within and across the BES scientific user facilities are encouraged. We do not intend to support applications to establish new, unrelated types of facilities or to develop techniques that do not relate to the missions of the Nanoscale Science Research Centers (NSRCs) (https://science.energy.gov/bes/suf/user-facilities/nanoscale-science-research-centers/).

Five NSRCs support the synthesis, fabrication, characterization, and analysis of materials and structures at the nanoscale (https://science.energy.gov/bes/suf/user-facilities/nanoscale-science-research-centers/). These centers are DOE's premier user facilities for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools for synthesis, fabrication, characterization, and new computing approaches and capabilities. As such, research is supported across the spectrum of scientific and engineering disciplines to understand and exploit phenomena exhibited by materials and structures at the nanoscale. Areas include energy conversion and storage, structured materials derived from or inspired by nature, directed assembly of nanostructures, hard and crystalline materials (including the structure of macromolecules), magnetic and soft materials (including polymers and ordered structures in fluids), quantum structures for future computers and integration from nano to meso scales. Tools for probing nanomaterials and phenomena are increasingly multi-modal, to enable synthesis and characterization of electrical, optical, and/or magnetic properties simultaneously in real time with high resolution over a range of length scales. The ability to characterize functional nanoscale materials in-situ, under operating conditions (operando), is also increasingly important, from, for example, battery electrode charging/discharging, to catalysts at high pressures and temperatures, to biologically-inspired, soft, and/or hybrid materials behavior in liquid environments.

New approaches to probe at the nanoscale, notably leveraging complementary modalities at the co-located x-ray, neutron and other facilities are of particular interest. Closely coupling theory and modeling with experiment to accelerate understanding nanoscale phenomena and their resulting innovations is encouraged.

The electron-beam micro-characterization area focuses on developing next generation electron-beam instrumentation and on conducting corresponding research. Electron scattering techniques have key attributes making them complementary to x-ray and neutron beam techniques. They have unsurpassed spatial resolution and can simultaneously obtain structural, chemical, and other types of information from sub-nanometer regions. This enables the study of the fundamental mechanisms of catalysis, energy conversion, corrosion, charge transfer, magnetic behavior, and many other processes dynamically and at short time scales. Key is acquiring fundamental understanding to develop new and to improve existing materials and structures for energy and security applications.

Allowed topics for instrumentation and technique development efforts are limited to scanning, transmission, and scanning transmission electron microscopes, atom probes and related field ion instruments, related surface characterization apparatus and scanning probe microscopes. Instrumentation that advances multi-modal, in situ and operando studies of materials and chemical processes is preferred.

See the Relevant BES Reports (https://science.energy.gov/bes/community-resources/reports/)

- Challenges at the Frontier of Matter and Energy report: Transformative Opportunities for Discovery Science
- Future of Electron Scattering and Diffraction
- Quantum Materials for Energy Relevant Technology
- From Quanta to the Continuum: Opportunities for Mesoscale Science

For DOE national laboratory applicants, the proposed research must fit within the BES Scientific User Facilities (SUF) -funded programs at the laboratory of the applicant.

(w) Accelerator and Detector Research
Technical Contact: Eliane Lessner, 301-903-9365, eliane.lessner@science.doe.gov

This program supports work that advances the instruments, techniques, and capabilities of the existing and/or future BES Scientific User Facilities. We do not intend to support applications to establish new, unrelated types of facilities or to develop techniques that do not relate to the missions of the light sources and neutron scattering centers.
In the accelerator and detector research program, the objective is to improve the output and capabilities of light sources and neutron scattering facilities that are the most advanced of their kind in the world. Two major components are required for the advancement of light sources: the production of photon beams with increased average flux and brightness, and the detection tools capable of responding to the high photon-beam intensity. The first component requires higher repetition-rate photocathode guns and radiofrequency (RF) systems, and photon beams of enhanced temporal coherence, such as produced by improved seeding techniques or x-ray oscillators in the case of free electron lasers. Secondly, detectors require higher computational capabilities per pixel, improved readout rates, radiation hardness, and better energy and temporal resolutions. Additionally, R&D is required to produce ultrafast beam instrumentation capable of measuring accurately femto- and atto-second bunch lengths. Higher neutron-flux capabilities at the Spallation Neutron Source will demand high-intensity H^- currents, possibly provided by the development of high-power and high-frequency lasers, and detectors designed

for advanced neutron imaging with very high throughput.

An excellent reference for accelerator physics needs for light sources can be found in *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Volume 618, Issues 1-3*. A detailed discussion of opportunities and needs for future electron sources and neutron and photon detector development at the existing and future BES facilities can be found in the Future Electron Sources Workshop report and in the Neutron and Photon Detector Workshop report available at https://science.energy.gov/bes/community-resources/reports/

This program strongly interacts with BES programmatic research that uses synchrotron radiation and neutron sources.

For DOE national laboratory applicants, the proposed research must fit within the BES SUF-funded programs at the laboratory of the applicant.

(x) X-ray Instrumentation and Technique Development
Technical Contact: Peter Lee, 301-903-8484, Peter.Lee@science.doe.gov

This program supports work that advances the instruments, techniques, and capabilities of the existing and/or contributes to capabilities of future BES supported light source facilities. This program **will not** support applications to establish new, unrelated types of facilities or to develop techniques not applicable to BES x-ray light source facilities.

The unique properties of the light source facilities include, for storage-ring based synchrotron sources, a continuous spectrum, high flux, and brightness and, for the Linac Coherent Light Source (LCLS), ultra-short pulses, high peak power, and high coherence, making them indispensable tools for the exploration of matter. The wide range of emitted photon wavelengths provide incisive probes for advanced research. The three broad categories of experimental measurement techniques performed at the light sources - spectroscopy, scattering, and imaging - probe the fundamental parameters by which we perceive the physical world (energy, momentum, position, and time). By exploiting the short pulse lengths of these light sources, especially the LCLS, each technique can also be performed in a timing fashion.

In order to fully exploit the wide range of capabilities of these x-ray light source facilities, this program will encourage the development of imaginative concepts for new types of x-ray instruments as well as innovative uses of existing instruments, especially in the area of novel instrumentation for new experimental capabilities, development of advanced x-ray optics[1] and novel approaches to data visualization and analysis.

For DOE national laboratory applicants, the proposed research must fit within the BES SUF-funded programs at the laboratory of the applicant.

[1] Report for the X-ray Optics for BES Light Source Facilities Workshop, http://science.energy.gov/~/media/bes/pdf/reports/files/X-ray_Optics_for_BES_Light_Source_Facilities_rpt.pdf.

(y) Neutron Scattering Instrumentation and Technique Development
Technical Contact: James J. Rhyne, 301-903-6827, James.Rhyne@science.doe.gov

This program supports work that advances instrumentation and technique capabilities of the existing and/or future BES supported neutron scattering facilities.

Thermal neutron scattering is a unique and effective tool for probing many aspects of the atomic structure and dynamics of materials. It is particularly well-suited for determining the atomic positions of both light and heavy atoms in solid or soft matter systems. In addition, the neutron scatters from magnetic moments in the material thus providing information on the magnetic structure. The neutron energy is well-matched to that of elementary atomic and magnetic excitations (spin waves and phonons) in a material and, via inelastic scattering, can provide data crucial for understanding dynamics in a variety of systems including superconductors, magnetic, and multi-ferroic materials.

In order to fully exploit the wide range of capabilities of the BES neutron scattering facilities, this program will encourage the development of imaginative concepts for new types of scattering instruments as well as innovative uses of existing instruments, advanced optics, sample environments, and novel approaches to data visualization and analysis.

Note: This program **will not** support applications to establish new, unrelated types of facilities or to develop techniques not applicable to BES neutron scattering facilities.

For DOE national laboratory applicants, the proposed research must fit within the BES SUF-funded programs at the laboratory of the applicant.

IV. Fusion Energy Sciences (FES)

Program Website: http://science.energy.gov/fes/

The mission of the Fusion Energy Sciences (FES) program is to expand the fundamental understanding of matter at very high temperatures and densities and to build the scientific foundation needed to develop a fusion energy source. This is accomplished through the study of plasma, the fourth state of matter, and how it interacts with its surroundings.

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. Accordingly, the FES program has four strategic goals:

- Advance the fundamental science of magnetically confined plasmas to develop the predictive capability needed for a sustainable fusion energy source;
- Support the development of the scientific understanding required to design and deploy the materials needed to support a burning plasma environment;

- Pursue scientific opportunities and grand challenges in high-energy-density plasma science to better understand our universe, and to enhance national security and economic competitiveness, and;
- Increase the fundamental understanding of basic plasma science, including both burning plasma and low temperature plasma science and engineering, to enhance economic competiveness and to create opportunities for a broader range of science-based applications.

Research is guided by the FES strategic plan, **Fusion Energy Sciences, a Ten-Year Perspective (2015-2025)** (http://science.energy.gov/~/media/fes/pdf/program-documents/FES_A_Ten-Year_Perspective_2015-2025.pdf), and a series of community research needs workshops held in 2015. The final reports from these workshops can be found here: http://science.energy.gov/fes/community-resources/workshop-reports/

Excluded from this call are low-energy nuclear reactions and "cold fusion" research.

To address the strategic goals and the high-priority plasma science issues identified by the workshops, FES program supports research on the specific topics below:

(a) Magnetic Fusion Energy Science Experimental Research
Technical Contact: Mark Foster, 858-455-3360, mark.foster@science.doe.gov

This Experimental Research program seeks to utilize existing unique magnetic fusion research facilities to develop the physics knowledge needed to advance the FES energy mission. The effort requires operation of a set of diversified experimental facilities, ranging from smaller-scale university experiments to large national facilities that involve extensive collaborations. The extensive plasma diagnostic systems operating on these facilities provide the experimental data required to study fusion science, basic plasma physics, and fusion energy production and to validate theoretical understanding and computer models, leading ultimately to a predictive understanding of plasma properties, including their dynamics and interactions with surrounding materials. Operation of major fusion facilities will be focused on science issues relevant to the design and operation of International Thermonuclear Experimental Reactor (ITER) and other high-performance tokamaks, burning plasma physics, magnetic confinement, and other high priority plasma physics issues identified by the community research needs workshops.

Research in this area also involves stellarators and small-scale facilities that explore emerging concepts for plasma confinement and stability, address critical issues that may affect the tokamak concept (e.g. plasma disruptions, impulsive heat loads, and operational maintenance and complexity), and investigate topics common to all fusion power plant concepts (e.g. interactions between plasma and material surfaces, and material science issues associated with the high fluxes of heat, charged-particles, and neutrons in a fusion power plant).

The program also supports development of diagnostic systems relevant to ITER and other high-performance tokamaks, advanced diagnostic capabilities to enable close coupling of experiments and theory/computations, and sensors or actuators required for active control of plasma properties to optimize device operation and plasma performance.

Scientists from the U.S. also participate in leading experiments on fusion facilities abroad and conduct comparative studies to supplement the scientific understanding they can obtain from domestic facilities.

(b) Magnetic Fusion Energy Science Theory and Simulation
Technical Contact: John Mandrekas, 301-903-0552, john.mandrekas@science.doe.gov

The Magnetic Fusion Theory and Simulation program focuses on advancing the scientific understanding of the fundamental physical processes governing the behavior of magnetically confined plasmas and contributes to the FES goal of developing the predictive capability needed for a sustainable fusion energy source. Specific areas of interest include:

- Macroscopic stability and dynamics of fusion plasmas, with a strong focus on the prediction, avoidance, control, and mitigation of deleterious or performance-limiting instabilities, such as plasma disruptions and other transient or off-normal events;
- Understanding and control of the multiscale, collisional and turbulent physical mechanisms responsible for the loss of heat, momentum, and particles from the confining region;
- Interaction of externally launched radiofrequency waves designed to heat the plasma and drive current, with the background plasma and surrounding structures;
- Nonlinear interaction between background plasma, various instabilities, and energetic particle populations, including the alpha particles generated by the fusion reactions, and its impact on the confinement of these particles and the overall plasma performance; and,
- The effect of multiscale and multiphysics processes at the plasma boundary, including the pedestal and scrape-off layer regions, on the plasma performance and on the interaction and interface of the hot plasma boundary with the material walls.

The efforts supported by this program provide the foundations for integrated whole-device modeling simulations of fusion systems and range from analytical work to the development and application of advanced simulation codes capable of exploiting the potential of current and next-generation high performance computers.

(c) High-Energy-Density Plasma Science
Technical Contact: Kramer Akli, 301-903-2943, kramer.akli@science.doe.gov

High-energy-density laboratory plasma (HEDLP) physics is the study of ionized matter at extremely high density and temperature, specifically when matter is heated and compressed to a point that the stored energy in the matter reaches approximately 100 billion Joules per cubic meter (the energy density of a hydrogen molecule). This corresponds to a pressure of approximately 1 million atmospheres or 1 millibar (Mbar). Systems in which free electrons play a significant role in the dynamics and for which the underlying assumptions and methods of traditional ideal-plasma theory and standard condensed matter theory do not apply (e.g., Warm Dense Matter at temperatures of a few electronvolt (eV)) can have pressures as low as 0.1 Mbar and are also considered high-energy-density (HED) plasmas. Discovery-driven scientific explorations of HED states of matter are being supported in this program. Topical examples being emphasized include (1) high-energy-density hydrodynamics, (2) radiation-dominated

dynamics and material properties, (3) magnetized HED plasmas, (4) nonlinear optics of plasmas and laser-plasma interactions, (5) relativistic HED plasmas and intense beam physics, and (6) warm dense matter.

(d) General Plasma Science Experiment and Theory
Technical Contact: Nirmol Podder, 301-903-9536, nirmol.podder@science.doe.gov

The General Plasma Science (GPS) activity supports research in frontier areas of fundamental plasma science and engineering. The program is focused on advancing the understanding of 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, thermal, radiative and particle transport, waves, structures, flows and their interactions. Areas of research responsive to this subprogram may include:

- Understanding electric self-organization and the physics of coherent structures in plasmas (e.g., How are coherent structures or patterns formed, controlled, or manipulated?);
- Understanding magnetic self-organization and the energetics of the plasma universe (e.g., Understanding the formation of coherent structures in magnetized plasmas and the processes for plasma dynamo, magnetic reconnection, particle acceleration, and turbulent cascade); and
- Low-temperature plasma at the interface of chemistry and biology (e.g., How is the interaction of plasma with solids, liquids, and gases are controlled for societal benefit? What novel diagnostics are needed to be developed for high-pressure or atmospheric-pressure plasmas?).

For more information, please see the 2015 Frontiers of Plasma Science Workshops report (https://science.energy.gov/~/media/fes/pdf/program-news/Draft_Frontiers_of_Plasma_Science_Report_2016-05-01.pdf).

(e) Fusion Nuclear Science, Materials Research and Enabling R&D Programs for Fusion
Technical Contact: Daniel Clark, 301-903-3883, daniel.clark@science.doe.gov

The Fusion Nuclear Science, Materials Research and Enabling R&D programs support the advancement of fusion science for both the near and long-term by carrying out research on technological topics that: (1) enable domestic experiments to achieve their full performance potential and scientific research goals; (2) permit scientific exploitation of the performance gains being sought from physics concept improvements; (3) allow the U.S. to enter into international collaborations, thus gaining access to experimental conditions not available domestically; (4) develop the technology and materials required for future fusion facilities, and (5) explore the science underlying these technological advances. Due to the harshness of the fusion environment and the significant challenge to overcome it, one of the four major goals of the FES program is to support the development of the scientific understanding required to design and deploy the materials and technology needed to support a sustained burning plasma environment. Given this goal, these programs are interested in fundamental research focused on advancing the following topics:

- Development of plasma-facing materials and components (including both solids and liquid metals)
- Development of advance structural and functional materials
- Development of breeder blanket concepts
- Development of tritium fuel cycle technologies
- Development of plasma enabling technologies (superconducting magnets, plasma heating, and fueling)

For more information, please see the 2012 Fusion Energy Sciences Advisory Committee (FESAC) report titled *Opportunities for Fusion Materials Science and Technology Research Now and During the ITER Era* (http://science.energy.gov/~/media/fes/pdf/workshop-reports/20120309/FESAC-Materials-Science-final-report.pdf) and the 2015 workshop Report on Science Challenges and Research Opportunities in Plasma Materials Interactions (https://science.energy.gov/~/media/fes/pdf/workshop-reports/2016/PMI_fullreport_21Aug2015.pdf).

V. High Energy Physics (HEP)
Program Website: http://science.energy.gov/hep/

The mission of the High Energy Physics (HEP) program is to understand how the universe works at its most fundamental level by discovering the elementary constituents of matter and energy, probing the interactions between them, and exploring the basic nature of space and time.

The scientific objectives and priorities for the field recommended by the High Energy Physics Advisory Panel (HEPAP) are detailed in its recent long-range strategic Particle Physics Project Prioritization Plan (P5), available at: http://science.energy.gov/~/media/hep/hepap/pdf/May-2014/FINAL_P5_Report_Interactive_060214.pdf

The HEP program focuses on three experimental 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 three 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;

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

Detector Research and Development, where the basic science and technologies needed to design and build the High Energy Physics detectors essential for making new discoveries are developed.

The three frontiers and the three cross-cutting research areas are collectively the six research subprograms supported by HEP. Proposed research should address specific research goals in one or more of the six research subprograms, and explain how the research or technology development supports the broad scientific objectives and mission of the HEP program. Principal investigators should submit their application to the HEP subprogram that they consider to be the best "fit" to the preponderance of their research effort. Applications for support of generic detector R&D efforts should be directed to the Detector Research and Development research area described below. However, applicants proposing physics studies and pre-conceptual R&D efforts directed towards a specific experiment within an experimental frontier should submit their application to the relevant HEP scientific frontier research area. Experimental HEP applications that include an R&D component within the overall research scope are specifically encouraged.

Applications should not attempt to bolster the case for facilities not currently approved for funding or not expected to be available during the course of the work.

(a) Experimental Research at the Energy Frontier in High Energy Physics
Technical Contact: Abid Patwa, 301-903-0408, Abid.Patwa@science.doe.gov

This research area seeks to support studies of fundamental particles and their interactions using proton-proton collisions at the highest possible energies. This is accomplished through direct detection of new phenomena or through sensitive measurements that probe the Standard Model and new physics beyond it. In particular, applications are sought for physics research utilizing data being collected at the Large Hadron Collider (LHC) by the ATLAS (A Toroidal LHC Apparatus) and Compact Muon Solenoid (CMS) experiments. This research area also provides graduate and postdoctoral research training for the next generation of scientists, and equipment and computational support for physics research activities. Applications addressing physics studies and pre-conceptual R&D directed towards specific future Energy Frontier experiments are also accepted. Support for Heavy Ion Physics research is not provided under this research area.

(b) Experimental Research at the Intensity Frontier in High Energy Physics
Technical Contact: Glen Crawford, 301-903-4829, Glen.Crawford@science.doe.gov

This research area seeks to support precision studies that are sensitive to new physical processes at very high energy scales, beyond what can be directly probed with energy frontier colliders, and that typically require intense particle beams. This research area includes studies of the fundamental properties of neutrinos produced by a variety of sources, including accelerators and nuclear reactors; studies of rare processes or precision measurements probing new physics processes as described above with either high intensity stored beams or beams incident on fixed targets; and studies of high intensity electron-positron collisions. In addition, this research area includes searches for proton decay. Graduate and postdoctoral research training for the next generation of scientists, and equipment and computational support for physics research activities are also provided. Applications addressing physics studies and pre-conceptual R&D directed towards specific future Intensity Frontier experiments are also accepted. Support for Large Hadron Collider beauty experiment (LHCb) research or studies of neutrinoless double beta decay is not provided under this research area.

(c) Experimental Research at the Cosmic Frontier in High Energy Physics
Technical Contact: Kathy Turner, 301-903-1759, Kathy.Turner@science.doe.gov

This research area seeks to support precision studies using observations of the cosmos and naturally occurring cosmic particles to understand the properties of fundamental particles and fields. Priorities include studies of the nature of dark energy, direct-detection searches for dark matter particles and research efforts towards planning the next generation of ground-based cosmic microwave background experiments to explore the inflationary epoch, the nature of dark energy and place constraints on neutrino masses. Measurements using high-energy cosmic rays, gamma rays and other phenomena are included, but at a lower priority. Applications are sought for physics research efforts in support of current experiments in the Cosmic Frontier, as well as physics studies and pre-conceptual planning directed towards specific future experiments being considered for the program. This research area also provides graduate and postdoctoral research training for the next generation of scientists, and equipment and computational support for physics research activities.

Research efforts aimed at developing techniques or understanding experimental data within the context of theoretical models that are expressly for or as part of an experimental research collaboration are included in this area. General theoretical or computational research applications not specifically carried out as part of a particular Cosmic Frontier experimental collaboration should be directed to the Theoretical Research subprogram. Studies of gravitational physics (other than for cosmic acceleration), classical astrophysics phenomena, fundamental symmetries, or planning for future cosmic ray or gamma ray experiments are not included in this research area.

(d) Theoretical Research in High Energy Physics
Technical Contact: William Kilgore, 301-903-3711, William.Kilgore@science.doe.gov

This research area seeks to support theoretical activities that provide the vision and the

mathematical framework for understanding and extending our knowledge of particles, forces, space-time, and the universe. Theoretical research is essential to support current experiments at the Energy, Intensity and Cosmic Frontiers, to identify new directions for High Energy Physics and to provide a deeper understanding of nature. Topics studied in theoretical high energy physics research include but are not limited to: phenomenological studies that seek to interpret experimental data, suggest searches for new physics at existing facilities and develop a research program for future facilities; precision calculations of experimental observables to test our current theories at the level of quantum corrections; the development of new models of physical interactions to describe unexplained phenomena or to unify seemingly distinct concepts; progress in quantum field theory, quantum gravity and other possible frameworks to develop a deeper understanding of nature; and the development of analytical and numerical computational techniques to facilitate studies in these areas. This research area also provides graduate and postdoctoral research training for the next generation of scientists and the computational resources needed for theoretical calculations. Activities that rely on experimental data, performed expressly for or with an experimental research collaboration, are not included in this research area.

(e) Accelerator Science and Technology Research & Development in High Energy Physics
Technical Contact: L.K. Len, 301-903-3233, Lk.Len@science.doe.gov

The accelerator technology R&D subprogram develops the next generation of particle accelerators and related technologies that are essential for discoveries in HEP. This research area supports world-leading research in the physics of particle beams and long-range, exploratory research aimed at developing new concepts. This research area also provides graduate and postdoctoral research training, equipment for experiments and related computational efforts.

Topics studied in the accelerator science and technology R&D subprogram 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 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. R&D applications, which are focused on accelerator applications outside of high-energy physics, are now coordinated through the Accelerator Stewardship program and are outside the scope of this particular FOA.

(f) Detector Research and Development in High Energy Physics
Technical Contact: Helmut Marsiske, 301-903-6989, Helmut.Marsiske@science.doe.gov

The detector R&D subprogram develops the next generation of instrumentation for HEP. It supports research leading to fundamental advances in the science of particle and radiation detection, and the development of new experimental techniques. This is typically long-term, "generic" R&D that may be high-risk, but has the potential for wide applicability and/or high-impact.

Topics studied in the detector R&D research 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; detectors for photons from ultraviolet to infrared wavelengths; detectors for cosmic microwave background radiation; detectors and experimental techniques for ultralow-background experiments; and advanced electronics and data acquisition systems. Support for graduate and postdoctoral research training, engineering and other technical efforts, and equipment and computational efforts required for experimental detector R&D and fabrication is included in this research area.

VI. Nuclear Physics (NP)
Program Website: http://science.energy.gov/np/

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. 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* http://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. Specific questions within these areas are addressed by the research activities of subprograms supported by NP as described below. In addition, the NP isotope subprogram produces and/or distributes stable and radioactive isotopes that are critical for the Nation and supports research into production techniques for such isotopes.

The NP program supports the development of the tools and capabilities that make fundamental research possible, including accelerator research and development for current and future nuclear physics facilities. It also supports applications of nuclear science and technology to help bridge the gap between basic nuclear physics research and applied science, and an initiative on advanced detector technology research and development. Research, development and fabrication of equipment directed toward research in any NP subprogram may be proposed, but applications including extensive projects requiring detailed review of scope, budget and schedule beyond the procedures for this announcement will not be considered. Applications should not attempt to bolster the case for facilities or major items of equipment not currently approved for funding or not expected to be available during the course of the work. Under this FOA, NP does not support investigations into the development of nuclear reactors for purposes outside the scope of the NP subprograms described below.

Applications are solicited for research in any of the NP subprograms and areas described below.

(a) Medium Energy Nuclear Physics
Technical Contact: Gulshan Rai, 301-903-4702, gulshan.rai@science.doe.gov

The Medium Energy subprogram of NP 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
Technical Contact: James Sowinski, 301-903-7587, james.sowinski@science.doe.gov

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. RHIC facility and the LHC at the European Organization for Nuclear Research (CERN).

(c) Low Energy Nuclear Physics - Nuclear Structure and Nuclear Astrophysics
Technical Contact: Chris Gould, 301-903-1963, christopher.gould@science.doe.gov

The Low Energy Nuclear Structure and Nuclear Astrophysics subprogram aims primarily at answering the overarching questions associated with the second frontier identified by Nuclei and Nuclear Astrophysics (NSAC). These 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.

(d) Low Energy Nuclear Physics – Fundamental Symmetries
Technical Contact: Paul Sorensen, 301-903-1952, paul.sorensen@science.doe.gov

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.

(e) Nuclear Theory
Technical Contact: George Fai, 301-903-8954, george.fai@science.doe.gov

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

(f) Nuclear Data and Nuclear Theory Computing
Technical Contact: Frank E (Ted) Barnes, 301-903-3212, ted.barnes@science.doe.gov

This subarea includes the National "Nuclear Data" effort, as well as several activities that facilitate the application of high performance computing to Nuclear Physics. The US 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, including nuclear astrophysics, and the development of theoretical techniques for incorporating LQCD results in traditional many-body nuclear physics calculations. Early Career applications in this subarea might include for example highly computational research programs in nuclear theory, or experimental studies of relevance to the national nuclear data program.

(g) Accelerator Research and Development for Current and Future Nuclear Physics Facilities
Technical Contact: Manouchehr Farkhondeh, 301-903-4398, manouchehr.farkhondeh@science.doe.gov

This NP 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 (BNL) RHIC, with heavy ion and polarized proton beams; linear accelerators such as the Continuous Electron Beam Accelerator Facility (CEBAF) at 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/ .

(h) Isotope Development and Production for Research and Applications
Technical Contact: Michelle Shinn, 301-903-8363, michelle.shinn@science.doe.gov

The mission of the Isotope Development and Production for Research and Applications subprogram (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. Isotopes are made available by using unique facilities stewarded by the Isotope Program at BNL, Los Alamos National Laboratory (LANL), and Oak Ridge National Laboratory (ORNL). 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 molybdenum-99 (Mo-99), as this isotope is under the purview of the National Nuclear Security Administration (NNSA) 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 http://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 http://science.energy.gov/np/research/idpra/.

Section II – AWARD INFORMATION

A. TYPE OF AWARD INSTRUMENT

DOE anticipates awarding laboratory work authorizations under this DOE National Laboratory Announcement.

B. ESTIMATED FUNDING

It is anticipated that up to $10,000,000 per year will be available under this DOE National Laboratory Announcement, contingent on satisfactory peer review and the availability of appropriated funds. Between 15 and 25 awards are anticipated, and applicants should request project support for five years, with out-year support contingent on the availability of appropriated funds, progress of the research, and programmatic needs. Awards are expected to begin in **FY 2018**.

DOE reserves the right to fund, in whole or in part, any, all, or none of the proposals submitted in response to this DOE National Laboratory Announcement.

C. MAXIMUM AND MINIMUM AWARD SIZE

The award size will depend on the number of meritorious proposals and the availability of appropriated funds.

Ceiling
The largest award made under the previous seven versions of this DOE National Laboratory Announcement received no more than $2,588,000 over five years. However, the median award size is $2,500,000, with more than 90% of awards made for exactly $2,500,000 over five years.

Floor
$2,500,000 over five years

D. EXPECTED NUMBER OF AWARDS

DOE anticipates making 15-25 awards under this DOE National Laboratory Announcement. The exact number of awards will depend on the number of meritorious applications and the availability of appropriated funds.

E. ANTICIPATED AWARD SIZE

While the minimum award size is $2,500,000, DOE expects the typical award size will be $2,500,000 over five years. Applicants are encouraged to propose research expenditures as close to the funding minimum as possible. Typical budgets will be $500,000 per year for five years. The size of a national laboratory award is commensurate with the requirement to charge twelve-month annual salaries (compared with professors, who are partially paid by academic institutions). Thus, a minimum of 50% and up to 100% of the Principal Investigator's salary

should be proposed.

F. PERIOD OF PERFORMANCE

DOE anticipates making awards with a project period of five years.

G. TYPE OF PROPOSAL

DOE will accept new DOE National Laboratory Proposals under this DOE National Laboratory Announcement. Please only submit a PAMS lab technical proposal in response to this announcement; do not submit a DOE Field Work Proposal (FWP) at this time. The Office of Science will request FWPs later from those selected for funding consideration under this announcement.

Section III – ELIGIBILITY INFORMATION

A. ELIGIBLE APPLICANTS AND TOPICS

Only DOE National Laboratories are eligible to apply.

The Principal Investigator must be a full-time, permanent, non-postdoctoral national laboratory employee as of the deadline for the proposal. No more than ten (10) years can have passed between the year the Principal Investigator's Ph.D. was awarded and the year that this funding announcement was posted. For the present competition, those who received doctorates no earlier than 2007 are eligible.

There can be no co-Principal Investigators.

Principal investigator means the scientist or other individual designated by the recipient to direct the project.

Each Principal Investigator may only submit one Office of Science Early Career Research Program proposal per annual competition. Additionally, a Principal Investigator may not participate in more than three Office of Science Early Career Research Program competitions.

Participation in the competition is defined as submission of a full proposal. In rare cases, it is necessary to withdraw a proposal early in the process; a proposal withdrawn prior to being sent for merit review by the DOE Office of Science will not count as a submission. Likewise, a proposal declined without merit review by the DOE Office of Science will not count as a submission.

The act of submitting a proposal implies that the submitting institution has checked, confirmed, and certifies that the Principal Investigator is eligible. No additional certifying documentation is required.

Proposals must be submitted through a DOE national laboratory. A companion Funding Opportunity Announcement (DE-FOA-0001761) describes the Early Career Research Program opportunity for tenure-track untenured assistant professors and tenure-track untenured associate professors at U.S. academic institutions. An employee with a joint appointment between a university and a DOE national laboratory must apply through the institution that pays his or her salary and provides his or her benefits; the eligibility criteria above must also be met.

Eligibility exemptions **will not** be granted.

Each proposal must be accompanied by a letter from the national laboratory director to the technical point of contact confirming that the proposed research idea fits within the scope of Office-of-Science-funded programs at the national laboratory. Proposing research that falls within this category ensures that investigators have the opportunity to belong to or join, at the laboratory's discretion, funded research groups. Investigators funded under this program are allowed to charge as little as 50 % of their time to the award, freeing up time to develop or

maintain funded collaborations within the lab over the course of the award. Making sure that investigators have potential connections with Office-of-Science funded programs encourages the laboratory to actively plan to address funding transition issues that may arise when an award ends.

Proposals from DOE National Laboratories should not (a) attempt to revive previously terminated research areas within the laboratory or (b) topically isolate investigators.

While there is no limit on the number of preproposals from a DOE national laboratory in a given year, each laboratory is responsible for ensuring that the research ideas submitted in its preproposals fit within the scope of Office-of-Science-funded programs at the national laboratory.

B. COST SHARING

Cost sharing is not required.

C. ELIGIBLE INDIVIDUALS

There is NOT a U.S. citizenship requirement for the Principal Investigator or any project participants.

Principal Investigators of early career awards funded by other agencies or entities are eligible, but the proposed research must have a scope different from that already funded by the other organization.

Principal Investigators who have received awards previously under the Office of Science Early Career Research Program are not eligible.

If a Principal Investigator has multiple doctorates, the discipline of the one they have earned within the ten-year eligibility window should be relevant to the proposed research.

Letters of recommendation are not allowed. Proposals that include recommendation letters will be subject to elimination from consideration during DOE's initial review.

The Principal Investigator must be employed in the eligible position as of the closing date for this announcement.

Eligible individuals with the skills, knowledge, and resources necessary to carry out the proposed research as a Principal Investigator are invited to work with their organizations to develop a proposal. Individuals from underrepresented groups as well as individuals with disabilities are always encouraged to apply.

Section IV – PROPOSAL AND SUBMISSION INFORMATION

A. ADDRESS TO REQUEST PROPOSAL PACKAGE

Proposal submission instructions are available in this announcement on the DOE Office of Science Portfolio Analysis and Management System (PAMS). Screenshots showing the steps in DOE National Laboratory proposal submission are available in the PAMS External User Guide, accessible by navigating to https://pamspublic.science.energy.gov and clicking on the "PAMS External User Guide" link.

Proposals submitted outside of PAMS will not be accepted.

B. LETTER OF INTENT AND PRE-PROPOSAL

1. Letter of Intent

A Letter of Intent is not required.

2. Pre-proposal

PRE-PROPOSAL DUE DATE
01/25/2018, 5 PM Eastern Time

ENCOURAGE/DISCOURAGE DATE
02/27/2018, 5 PM Eastern Time

A preproposal is required and must be submitted by 01/25/2018 at 5 PM Eastern Time. The preproposal must be submitted electronically through the DOE Office of Science Portfolio Analysis and Management System (PAMS) website https://pamspublic.science.energy.gov/.

Note: Make sure you choose "View / Respond to DOE National Laboratory Announcements." Do not choose "View / Respond to Funding Opportunity Announcements." If you choose the latter, you will respond to the wrong solicitation, and your preproposal might not be considered.

While there is no limit on the number of preproposals from a DOE national laboratory in a given year, each laboratory is responsible for ensuring that the research ideas submitted in its preproposals fit within the scope of Office-of-Science-funded programs at the national laboratory.

Preproposals will be reviewed for responsiveness of the proposed work to the research topics identified in this DOE National Laboratory Announcement. DOE will send a response by email to each applicant encouraging or discouraging the submission of a full proposal by 02/27/2018. Applicants who have not received a response regarding the status of their preproposal by this date are responsible for contacting the program to confirm this status. **Only those applicants that receive notification from DOE encouraging a full proposal may submit full proposals.** No other full proposals will be considered.

The pre-proposal attachment must include, at the top of the first page, the following information:

Title of Preproposal
Principal Investigator Name, Job Title
Institution
PI Phone Number, PI Email Address
Year Doctorate Awarded: XXXX
Number of Times Previously Applied†:
Topic Area*:
DOE National Laboratory Announcement Number: **LAB 17-1761**

† Indicate how many times the PI has previously submitted a full proposal in the Office of Science Early Career Research Program. The program has been offered in eight previous years, FY 2010 – FY 2017. Participation in the competition is defined as submission of a full, formal proposal. A PI who has participated in three past Office of Science Early Career Research Program competitions is not eligible.

* The topic area can be found in Part I, Supplementary Information, of this DOE National Laboratory Announcement. For example, the topic area might be Synthesis and Processing Science or Magnetic Fusion Energy Science Theory and Simulation. Please select from the list in Part I.

This information must be followed by a clear and concise description of the objectives and technical approach of the proposed research. The preproposal may not exceed two pages, with a minimum text font size of 11 point and margins no smaller than one inch on all sides. Figures and references, if included, must fit within the two-page limit.

Only one preproposal per Principal Investigator is allowed.

To help the Office of Science avoid conflicts of interest in identifying potential reviewers, a one-page list of the Principal Investigator's collaborators, co-editors, and graduate/postdoctoral advisors and advisees must be submitted with the preproposal. The one-page list must be the last page in the preproposal file and will not count against the two-page limit for the pre proposal. Further guidance on how to prepare this list is included in the next two paragraphs:

Collaborators and Co-editors: List, in alphabetical order, all persons, including their current organizational affiliations, who are, or who have been, collaborators or co-authors with the Principal Investigator on a research project, book or book article, report, abstract, or paper during the 48 months preceding the closing date of this announcement. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the Principal Investigator interacted on a regular basis while the research was being done. Also, list any individuals who are currently or have been in the past co-editors with the Principal Investigator on a special issue of a journal, compendium, or conference proceedings during the 24 months the closing date of this announcement. If there are no collaborators or co-editors to report, state "None."

Graduate and Postdoctoral Advisors and Advisees: List the names of the Principal Investigator's own graduate advisor(s) and principal postdoctoral sponsor(s) and their current organizational affiliations. Also list the names of the Principal Investigator's graduate students and postdoctoral associates during the past five years and their current organizational affiliations.

Since the Office of Science will never use individuals from your institution as reviewers, you may omit them from the preproposal list to save space. Listing collaborators on your preproposal is to help us identify reviewers and does not affect the decision to encourage or discourage submission of a full proposal.

Those preproposals that are encouraged are used to help the Office of Science begin planning for the full proposal peer review process. The intent of the Office of Science in discouraging submission of certain full proposals is to save the time and effort of applicants in preparing and submitting full proposals not responsive to this DOE National Laboratory Announcement.

The Principal Investigator will be automatically notified when the preproposal is encouraged or discouraged. The DOE Office of Science Portfolio Analysis and Management System (PAMS) will send an email to the Principal Investigator from PAMS.Autoreply@science.doe.gov, and the status of the preproposal will be updated at the PAMS website https://pamspublic.science.energy.gov/. Notifications are sent as soon as the decisions to encourage or discourage are finalized.

It is important that the preproposal be a single file with extension .pdf, .docx, or .doc. The filename should not exceed 50 characters. The preproposal must be submitted electronically through the DOE Office of Science Portfolio Analysis and Management System (PAMS) website https://pamspublic.science.energy.gov/. The Principal Investigator and anyone submitting on behalf of the Principal Investigator must register for an account in PAMS before it will be possible to submit a preproposal. All PIs and those submitting preproposals on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to avoid submission delays.

To access PAMS, you may use the Internet Explorer, Firefox, Google Chrome, or Safari browsers. For best results, we recommend the use of Internet Explorer 11.

Registering to PAMS is a two-step process; once you create an individual account, you must associate yourself with ("register to") your institution. Detailed steps are listed below.

Create PAMS Account:

- To register, click the "Create New PAMS Account" link on the website https://pamspublic.science.energy.gov/.
- Click the "No, I have never had an account" link and then the "Create Account" button.
- You will be prompted to enter your name and email address, create a username and password, and select a security question and answer. Once you have done this, click the "Save and Continue" button.
- On the next page, enter the required information (at least one phone number and your mailing address) and any optional information you wish to provide (e.g., FAX number, website,

mailstop code, additional email addresses or phone numbers, Division/Department). Click the "Create Account" button.

- Read the user agreement and click the "Accept" button to indicate that you understand your responsibilities and agree to comply with the rules of behavior for PAMS.
- PAMS will take you the "Having Trouble Logging In?" page. (Note: If you reviewed for or were listed as PI on a prior submission to the Office of Science but have not previously created an account, you may already be linked to an institution in PAMS. If this is the case, PAMS will take you to the PAMS home page.)

Register to Your Institution:

- Click the link labeled "Option 2: I know my institution and I am here to register to the institution." (Note: If you previously created a PAMS account but did not register to an institution at that time, you must click the Institutions tab and click the "Register to Institution" link.)
- PAMS will take you to the "Register to Institution" page.
- Type a word or phrase from your institution name in the field labeled, "Institution Name like," choose the radio button next to the item that best describes your role in the system, and click the "Search" button. A "like" search in PAMS returns results that contain the word or phrase you enter; you need not enter the exact name of the institution, but you should enter a word or phrase contained within the institution name. (Hint: If your institution has an acronym, such as ANL for Argonne National Laboratory or UCLA for the Regents of the University of California, Los Angeles, you may search for the acronym under "Institution Name like." Many institutions with acronyms are listed in PAMS with their acronyms in parentheses after their names.)
- Find your institution in the list that is returned by the search and click the "Actions" link in the Options column next to the institution name to obtain a dropdown list. Select "Add me to this institution" from the dropdown. PAMS will take you to the "Institutions – List" page.
- If you do not see your institution in the initial search results, you can search again by clicking the "Cancel" button, clicking the Option 2 link, and repeating the search.
- All DOE National Laboratories have established profiles in PAMS, so please keep searching until you find your laboratory.

Submit Your Pre-Proposal:

- Create your pre-proposal (called a preproposal in PAMS) outside the system and save it as a file with extension .docx, .doc, or .pdf. Make a note of the location of the file on your computer so you can browse for it later from within PAMS.
- Log into PAMS and click the Proposals tab. Click the "View / Respond to DOE National Laboratory Announcements" link and find the current announcement in the list. Click the "Actions/Views" link in the Options column next to this announcement to obtain a dropdown menu. Select "Submit Preproposal" from the dropdown. Note: Make sure you choose "View / Respond to DOE National Laboratory Announcements." Do not choose "View / Respond to Funding Opportunity Announcements." If you choose the latter, you will respond to the wrong solicitation, and your preproposal might not be considered.

- On the Submit Preproposal page, select the institution from which you are submitting this preproposal from the Institution dropdown. If you are associated with only one institution in the system, there will only be one institution in the dropdown.
- Note that you must select one and only one Principal Investigator (PI) per preproposal; to do so, click the "Select PI" button on the far right side of the screen. Find the appropriate PI from the list of all registered users from your institution returned by PAMS. (Hint: You may have to sort, filter, or search through the list if it has multiple pages.) Click the "Actions" link in the Options column next to the appropriate PI to obtain a dropdown menu. From the dropdown, choose "Select PI."
- If the PI for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, click the "Invite PI" link at the top left of the "Select PI" screen. You can enter an optional personal message to the PI in the "Comments" box, and it will be included in the email sent by PAMS to the PI. You must wait until the PI registers before you can submit the preproposal. Save the preproposal for later work by clicking the "Save" button at the bottom of the screen. It will be stored in "My Preproposals" for later editing.
- Enter a title for your preproposal.
- Select the appropriate technical contact from the Program Manager dropdown.
- To upload the preproposal file into PAMS, click the "Attach File" button at the far right side of the screen. Click the "Browse" (or "Choose File" depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the "Upload" button to upload the file.
- At the bottom of the screen, click the "Submit to DOE" button to save and submit the preproposal to DOE.
- Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the preproposal.

You are encouraged to register for an account in PAMS at least a week in advance of the preproposal submission deadline so that there will be no delays with your submission.

Collection of demographic data such as gender, race, and ethnicity allows the DOE Office of Science to gauge whether its programs and opportunities are fairly reaching and benefiting everyone regardless of demographic category. Knowledge of the demographic distributions within a portfolio, particularly those collected over many years, allows assessments of trends and demonstrates responses to actions taken on the part of agencies. To gather the information needed, we ask that registrants provide the demographic information requested in their PAMS user profiles. Submission of the requested information is voluntary and is not a precondition of award.

For help with PAMS, click the "External User Guide" link on the PAMS website, https://pamspublic.science.energy.gov/. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this DOE National Laboratory Announcement should reference **LAB 17-1761.**

Preproposals submitted outside PAMS will not be considered.

C. CONTENT AND PROPOSAL FORMS

PROPOSAL DUE DATE
04/04/2018, 5 PM Eastern Time

Note: PDF files attached in PAMS must be plain files consisting of text, numbers, and images without editable fields, signatures, passwords, redactions, or other advanced features available in some PDF-compatible software. Do not attach PDF portfolios.

Concurrent submission of a proposal to other organizations for simultaneous consideration will not prejudice its review. However, you can only be funded once by the federal government for a given scope of work. Thus, if both proposals are selected for funding, you will only be able to accept one award. To avoid this situation, you can submit proposals for completely different scopes of work to the two agencies.

LETTERS

Letters of recommendation are not allowed. Proposals that include recommendation letters will be subject to elimination from consideration during DOE's initial review.

Each proposal must be accompanied by a letter from the national laboratory director to the technical point of contact confirming that the proposed research idea fits within the scope of Office-of-Science-funded programs at the national laboratory.

Optional letters of collaboration for unfunded or funded collaborations may be placed in Appendix 7 (Other Attachments). Letters of collaboration should state the intention to participate, but they should not be written as recommendation or endorsement letters, which are not allowed.

Each optional letter of collaboration may contain <u>two and only two</u> sentences and must use the following format:

Dear <Principal Investigator Name>:

If your proposal entitled, "<Proposal Name>," is selected for funding under the DOE Office of Science Early Career Research Program, it is my intent to collaborate in this research by <Complete Sentence With a Very Short Description of What the Collaborator Offers to Do or Provide>. Thank you for the opportunity to participate.

Sincerely,

<Collaborator's Name and Signature Block>

1. Summary of Proposal Contents and Information about PAMS

Each DOE National Laboratory proposal will contain the following sections:

- Budget, entered into PAMS as structured data using the PAMS budget form
- Abstract (one page), entered into PAMS as a separate pdf
- Budget justification, entered into PAMS as a separate pdf
- Proposal, combined into a single pdf containing the following information:
    - Proposal Cover Page
    - Project Narrative (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel – 15 page limit)
    - Appendix 1: Biographical Sketch(es)
    - Appendix 2: Current and Pending Support
    - Appendix 3: Bibliography and References Cited
    - Appendix 4: Facilities and Other Resources
    - Appendix 5: Equipment
    - Appendix 6: Data Management Plan

Appendix 7: Other Attachments (optional)

SUBMISSION INSTRUCTIONS

Full proposals must be submitted into the DOE Office of Science Portfolio Analysis and Management System (PAMS). For help with PAMS, click the "External User Guide" link on the PAMS website, https://pamspublic.science.energy.gov/. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free number) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submissions and inquiries about this Program Announcement should reference **LAB 17-1761.** Full proposals submitted in response to this Program Announcement must be submitted to PAMS no later than 4/4/2018 at 5 PM Eastern Time.

All PIs and those submitting on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to ensure timely submissions**.** To register, click "Create New PAMS Account" on the website https://pamspublic.science.energy.gov/ and follow the instructions for creating an account.

The following information is provided to help with proposal submission. Detailed instructions and screen shots can be found in the user guide. To find the user guide, click the "External User Guide" link on the PAMS home page. Onscreen instructions are available within PAMS.

- Log into PAMS. From the proposals tab, click the "View DOE National Laboratory Announcements" link and find the current announcement in the list. Click the "Actions/Views" link in the Options column next to this announcement to obtain a dropdown menu. Select "Submit Proposal" from the dropdown.
- Note that you must select one and only one Principal Investigator (PI) per proposal; to do so, click the "Select PI" button on the far right side of the screen. Find the appropriate PI from

the list of all registered users from your institution returned by PAMS. (Hint: You may have to sort, filter, or search through the list if it has multiple pages.) Click the "Actions" link in the Options column next to the appropriate PI to obtain a dropdown menu. From the dropdown, choose "Select PI."

- If the PI for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, click the "Invite PI" link at the top left of the "Select PI" screen. You can enter an optional personal message to the PI in the "Comments" box, and it will be included in the email sent by PAMS to the PI. You must wait until the PI registers before you can submit the proposal.
- New This Year: You must select one and only one Sponsored Research Official/Business Official/Administrative Official (SRO/BO/AO) per proposal; to do so, click the "Select SRO/BO/AO" button on the far right side of the screen. Find the appropriate SRO/BO/AO from the list of all registered users from your institution returned by PAMS. (Hint: You may have to sort, filter, or search through the list if it has multiple pages.) Click the "Actions" link in the Options column next to the appropriate SRO/BO/AO to obtain a dropdown menu. From the dropdown, choose "Select SRO/BO/AO."
- If the SRO/BO/AO for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the SRO/BO/AO to register in PAMS. To do so, click the "Invite SRO/BO/AO" link at the top left of the "Select SRO/BO/AO" screen. You can enter an optional personal message to the SRO/BO/AO in the "Comments" box, and it will be included in the email sent by PAMS to the SRO/BO/AO. You must wait until the SRO/BO/AO registers before you can submit the proposal.
- Save the proposal for later work by selecting "Save" from the dropdown at the bottom of the screen and then clicking the "Go" button. It will be stored in "My Proposals" for later editing. As a minimum, you must complete all the required fields on the PAMS cover page before you can save the proposal for the first time.
- The cover page, budget, and attachments sections of the lab proposal are required by PAMS before it can be submitted to DOE.
- Complete the sections in PAMS one at a time, starting with the cover page and following the instructions for each section.
- Click the "+View More" link at the top of each section to expand the onscreen instructions. On the budget section, click the "Budget Tab Instructions" link to obtain detailed guidance on completing the budget form.
- Save each section by selecting either "Save" (to stay in the same section) or "Save… and Continue to the Next Section" (to move to the next section) from the dropdown menu at the bottom of the screen, followed by clicking the "Go" button.
- If you save the proposal and navigate away from it, you may return later to edit the proposal by clicking the "View My Existing Proposals" or "My Proposals" links within PAMS.
- You must enter a budget for each annual budget period.
- You must also enter a budget for each proposed sub-award. The sub-award section can be completed using the same steps used for the budget section.
- In the attachments section of the lab proposal, the abstract, the budget justification, and the proposal narrative are required and must be submitted as separate files.

- You must bundle everything other than the budget, abstract, and budget justification into one single PDF file to be attached under "Proposal Attachment."
- Do not attach anything under "Other Attachments."
- To upload a file into PAMS, click the "Attach File" button at the far right side of the screen. Click the "Browse" (or "Choose File" depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the "Upload" button to upload the file.
- Once you have saved all of the sections, the "Submit to DOE" option will appear in the dropdown menu at the bottom of the screen.
- To submit the proposal, select "Submit to DOE" from the dropdown menu and then click the "Go" button.
- Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the proposal.
- The proposal will also appear under My Proposals with a Proposal Status of "Submitted to DOE."

Please only submit a PAMS lab technical proposal in response to this announcement; do not submit a DOE Field Work Proposal (FWP) at this time. The Office of Science will request FWPs later from those selected for funding consideration under this announcement.

For help with PAMS, click the "External User Guide" link on the PAMS website, https://pamspublic.science.energy.gov/. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free number) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submissions and inquiries about this Program Announcement should reference **LAB 17-1761.**

2. Detailed Contents of the Proposal

BUDGET AND BUDGET EXPLANATION

The budget must be submitted into PAMS using the PAMS budget form. Research proposed under this announcement should have five annual budget periods. Please enter the following budget period start and end dates into PAMS for proposals submitted to this announcement:

- Budget Period 1: 09/01/2018 – 08/31/2019
- Budget Period 2: 09/01/2019 – 08/31/2020
- Budget Period 3: 09/01/2020 – 08/31/2021
- Budget Period 4: 09/01/2021 – 08/31/2022
- Budget Period 5: 09/01/2022 – 08/31/2023

PAMS will calculate the cumulative budget totals for you.

A written justification of each budget item is to follow the budget pages. The budget justification must be placed in a separate, single pdf document and attached on the appropriate screen in PAMS. Further instructions regarding the budget and justification are given below and in the

PAMS software.

PROJECT SUMMARY/ABSTRACT (NO MORE THAN ONE PAGE)

The project summary/abstract must contain a summary of the proposed activity suitable for dissemination to the public. It must be a self-contained document that identifies the name of the applicant, the Principal Investigator (PI), the project title, the objectives of the project, a description of the project, including methods to be employed, the potential impact of the project (i.e., benefits, outcomes). This document must not include any proprietary or sensitive business information as the Department may make it available to the public. The project summary must not exceed 1 page when printed using standard 8.5" by 11" paper with 1" margins (top, bottom, left and right) with font not smaller than 11 point. The one-page project summary/abstract must be placed in a separate, single pdf document and attached on the appropriate screen in PAMS.

The abstract may be used to prepare publicly accessible reports about DOE-supported research.

DOE COVER PAGE
(PART OF PROJECT NARRATIVE PDF)

The following proposal cover page information may be placed on a plain page. No form is required. This cover page will not count in the project narrative page limitation.

- **Institution:**
- **Street Address/City/State/Zip:**
- **Principal Investigator (PI):**
- **Position Title of PI:**
- **Business Mailing Address of PI:**
- **Telephone Number of PI:**
- **Email of PI:**
- **DOE National Laboratory Announcement Number: LAB 17-1761**
- **DOE/Office of Science Program Office (ASCR, BER, BES, FES, HEP, or NP):**
- **Topic Area*:**
- **Topic Area Program Manager:**
- **Year Doctorate Awarded:**
- **Number of Times Previously Applied[†]:**
- **PAMS Preproposal Number:**
- **PECASE Eligible**: (Yes or No)?**
- **Proposal Contains Biosketch in Appendix 1 (Yes or No)?**
- **Proposal Contains Data Management Plan in Appendix 6[§]: (Yes or No)?**

* The topic area can be found in Part I, Supplementary Information, of this DOE National Laboratory Announcement. For example, the topic area might be Synthesis and Processing Science or Magnetic Fusion Energy Science Theory and Simulation. Please select from the list in Part I.

† Indicate how many times the PI has previously submitted a full proposal in the Office of Science Early Career Research Program. The program has been offered in eight previous years, FY 2010 – FY 2017. Participation in the competition is defined as submission of a full, formal proposal. A PI who has participated in three past Office of Science Early Career Research Program competitions is not eligible.

** The White House Office of Science and Technology Policy may ask federal agencies each year to nominate candidates for the Presidential Early Career Awards for Scientists and Engineers (PECASE). Investigators from the top proposals in the Office of Science Early Career Research Award competition may be nominated for PECASE if they are eligible. A PI is PECASE-eligible if he or she is, as of the closing date of this DOE National Laboratory Announcement, a U.S. citizen, U.S. national or permanent resident and if she or he has not received a PECASE previously through any agency. PECASE eligibility is not required for an award under the current DOE National Laboratory Announcement.

§ The Office of Science will decline without review any proposal without a data management plan.

PROJECT NARRATIVE (NO MORE THAN 15 PAGES LONG)

The project narrative **must not exceed 15 pages** of technical information, including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right). The font must not be smaller than 11 point. Merit reviewers will only consider the number of pages specified in the first sentence of this paragraph.

The Project Narrative comprises the research plan for the project. It should contain enough background material in the Introduction, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. The narrative should provide a clear, concise statement of the specific objectives/aims of the proposed project. The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the methods to be used. It should also include a timeline for the major activities of the proposed project.

Do not include any Internet addresses (URLs) that provide supplementary or additional information that constitutes a part of the proposal. Using Internet sites in an attempt to avoid page limits will fail: The content of those sites will not be reviewed. See Section VIII Part D for instructions on how to mark proprietary proposal information.

APPENDIX 1: BIOGRAPHICAL SKETCH

Provide a biographical sketch for the Principal Investigator (PI) as an appendix to your technical narrative. As part of the sketch, provide information that can be used by reviewers to evaluate the PI's potential for leadership within the scientific community. Examples of information of interest are invited and/or public lectures, awards received, scientific program committees, conference or workshop organization, professional society activities, special international or

industrial partnerships, reviewing or editorship activities, or other scientific leadership experiences. The biographical information (curriculum vitae) must not exceed 3 pages when printed on 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 11 point and must include the following:

Education and Training: Undergraduate, graduate and postdoctoral training, provide institution, major/area, degree and year.

Research and Professional Experience: Beginning with the current position list, in chronological order, professional/academic positions with a brief description.

Publications: Provide a list of up to 10 publications most closely related to the proposed project. For each publication, identify the names of all authors (in the same sequence in which they appear in the publication), the article title, book or journal title, volume number, page numbers, year of publication, and website address if available electronically. Patents, copyrights and software systems developed may be provided in addition to or substituted for publications. An abbreviated style such as the Physical Review Letters (PRL) convention for citations (list only the first author) may be used for publications with more than 10 authors.

Synergistic Activities: List professional and scholarly activities related to the effort proposed. Some examples might be invited and/or public lectures, awards received, scientific program committees, conference or workshop organization, professional society membership and/or activities, special international or industrial partnerships, reviewing or editorship activities, or other scientific leadership experiences.

Collaborators and Co-editors: List in alphabetical order all persons, including their current organizational affiliation, who are, or who have been, collaborators or co-authors with you on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of this proposal. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the Principal Investigator interacted on a regular basis while the research was being done. Also, list any individuals who are currently, or have been, co-editors with you on a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of this proposal. If there are no collaborators or co-editors to report, state "None."

Graduate and Postdoctoral Advisors and Advisees: List the names and current organizational affiliations of your graduate advisor(s) and principal postdoctoral sponsor(s). Also, list the names and current organizational affiliations of your graduate students and postdoctoral associates during the past 5 years.

Personally Identifiable Information: Do not include sensitive personally identifiable information such as social security number, birth date, citizenship, marital status, or home address. Do not include information that a merit reviewer should not make use of.

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

- The biographical information (curriculum vitae) must not exceed 3 pages when printed on 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 11 point.

APPENDIX 2: CURRENT AND PENDING SUPPORT

Provide a list of all current and pending support (both Federal and non-Federal) for the Principal Investigator (PI) for ongoing projects and pending proposals.

List all sponsored activities or awards requiring a measurable commitment of effort, whether paid or unpaid.
For every activity, list the following items:

- The sponsor of the activity or the source of funding
- The award or other identifying number
- The title of the award or activity
- The total cost or value of the award or activity, including direct and indirect costs. For pending proposals, provide the total amount of requested funding.
- The person-months of effort per year being dedicated to the award or activity
- A description of the similarities, differences, and synergies of the award or activity with the research described in the current proposal.

Do not list start-up funds provided to the PI by the employing academic institution. If the PI has submitted a similar research proposal to an early career program at another agency or foundation, she or he should provide a few sentences explaining the similarities and/or differences with the current Early Career Research Program proposal. Provide the Current and Pending Support as an appendix to your project narrative. Concurrent submission of a proposal to other organizations for simultaneous consideration will not prejudice its review.

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

APPENDIX 3: BIBLIOGRAPHY & REFERENCES CITED

Provide a bibliography of any references cited in the Project Narrative. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. For research areas where there are routinely more than ten coauthors of archival publications, you may use an abbreviated style such as the Physical Review Letters (PRL) convention for citations (listing only the first author). Include only bibliographic citations. Applicants should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the proposal. Provide the Bibliography and References Cited information as an appendix to your project narrative.

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

APPENDIX 4: FACILITIES & OTHER RESOURCES

This information is used to assess the capability of the organizational resources, including subawardee resources, available to perform the effort proposed. Identify the facilities to be used (Laboratory, Animal, Computer, Office, Clinical and Other). If appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Describe only those resources that are directly applicable to the proposed work. Describe other resources available to the project (e.g., machine shop, electronic shop) and the extent to which they would be available to the project. Please provide the Facility and Other Resource information as an appendix to your project narrative.

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

APPENDIX 5: EQUIPMENT

List equipment already available for this project and, if appropriate, identify location and pertinent capabilities. Provide the Equipment information as an appendix to your project narrative.

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

APPENDIX 6: DATA MANAGEMENT PLAN

Provide a Data Management Plan (DMP) that addresses the following requirements:

1. DMPs should describe whether and how data generated in the course of the proposed research will be shared and preserved. If the plan is not to share and/or preserve certain data, then the plan must explain the basis of the decision (for example, cost/benefit considerations, other parameters of feasibility, scientific appropriateness, or limitations discussed in #4). At a minimum, DMPs must describe how data sharing and preservation will enable validation of results, or how results could be validated if data are not shared or preserved.
2. DMPs should provide a plan for making all research data displayed in publications resulting from the proposed research open, machine-readable, and digitally accessible to the public at the time of publication. This includes data that are displayed in charts, figures, images, etc. In addition, the underlying digital research data used to generate the displayed data should be made as accessible as possible to the public in accordance with the principles stated in the Office of Science Statement on Digital Data Management (http://science.energy.gov/funding-opportunities/digital-data-management/). This requirement could be met by including the data as supplementary information to the published article, or through other means. The published article should indicate how these data can be accessed.
3. DMPs should consult and reference available information about data management resources to be used in the course of the proposed research. In particular, DMPs that explicitly or implicitly commit data management resources at a facility beyond what is conventionally made available to approved users should be accompanied by written approval from that

facility. In determining the resources available for data management at Office of Science User Facilities, researchers should consult the published description of data management resources and practices at that facility and reference it in the DMP. Information about other Office of Science facilities can be found in the additional guidance from the sponsoring program.

4. DMPs must protect confidentiality, personal privacy, Personally Identifiable Information, and U.S. national, homeland, and economic security; recognize proprietary interests, business confidential information, and intellectual property rights; avoid significant negative impact on innovation, and U.S. competitiveness; and otherwise be consistent with all applicable laws, and regulations. There is no requirement to share proprietary data.
5. Applications must meet the published additional requirements of the program office to which the application is submitted, as identified on the DOE Cover Page of the application. Program office requirements will be considered during merit review and award selection. Advanced Scientific Computing Research (ASCR) and Biological and Environmental Research (BER) have published additional requirements, available through http://science.energy.gov/funding-opportunities/digital-data-management/. Applications will not be transferred between program offices.

DMPs will be reviewed as part of the overall Office of Science research proposal merit review process. Applicants are encouraged to consult the Office of Science website for further information and suggestions for how to structure a DMP: http://science.energy.gov/funding-opportunities/digital-data-management/

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

APPENDIX 7: OTHER ATTACHMENTS

Information not easily accessible to a reviewer may be included in this appendix, but do not use this appendix to circumvent the page limitations of the proposal. Reviewers are not required to consider information in this appendix, and reviewers may not have time to read extensive appendix materials with the same care they would use with the proposal proper. Do not include scientific publications. Although the preference of this program is to support PI-led efforts without paid collaborators, if a funded or unfunded collaboration is proposed, an optional letter of collaboration may be included in this appendix. Letters of collaboration should state the intent to participate and nothing else. They should not be written as recommendation or endorsement letters, which are not allowed. Each optional letter of collaboration may contain two and only two sentences and must use the following format:

Dear <Principal Investigator Name>:

If your proposal entitled, "<Proposal Name>," is selected for funding under the DOE Office of Science Early Career Research Program, it is my intent to collaborate in this research by <Complete Sentence With a Very Short Description of What the Collaborator Offers to Do or Provide>. Thank you for the opportunity to participate.

Sincerely,

<Collaborator's Name and Signature Block>

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

3. Detailed Instructions for the Budget

Budgets are required for the entire project period. A budget form must be completed for each budget period of the award, and a cumulative budget form for the entire project period will be populated by PAMS. A detailed budget justification narrative must be included after the budget pages. The justification should cover labor, domestic travel, equipment, materials and supplies, and anything else that will be covered with project funds.

To edit a section on the budget, click the edit icon ( ) for each section on the page. Remember to save all budget periods before moving on to the next section. You can save the budget periods by selecting "Save All Budget Periods" from the dropdown on the lower right corner of the PAMS budget entry screen and then clicking the "Go" button. You can also save any data entry page in PAMS using the blue diskette icon ( ) in the floating toolbar on the bottom of the screen.

Section A. Senior/Key Person (Required)
For each Senior/Key Person, enter the appropriate information. List personnel, salary funds, and the number of months that person will be allocated to the project. Also include a written narrative in the budget justification that fully justifies the need for requested personnel.

Section B. Other Personnel
List personnel, salary funds, and the number of months that person will be allocated to the project. Also include a written narrative in the budget justification that fully justifies the need for requested personnel.

Section C. Equipment Description
For the purpose of this budget, equipment is designated as an item of property that has an acquisition cost of $5,000 or more and an expected service life of more than one year. (Note that this designation applies for proposal budgeting only and differs from the DOE definition of capital equipment.) List each item of equipment separately and justify each in the budget justification section. Allowable items ordinarily will be limited to research equipment and apparatus not already available for the conduct of the work. General-purpose office equipment, such as a personal computer, is not eligible for support unless primarily or exclusively used in the actual conduct of scientific research.

Section D. Travel
In the budget justification, list each trip's destination, dates, estimated costs including transportation and subsistence, number of staff traveling, the purpose of the travel, and how it

relates to the project. Indicate whether travel cost estimates are based upon quotes from travel agencies; upon past experience of similar number of trips to similar travel destinations; or something else (describe). To qualify for support, attendance at meetings or conferences must enhance the investigator's capability to perform the research, plan extensions of it, or disseminate its results.

Section E. Participant/Trainee Support Costs:
If applicable, submit training support costs. Educational projects that intend to support trainees (precollege, college, graduate and post graduate) must list each trainee cost that includes stipend levels and amounts, cost of tuition for each trainee, cost of any travel (provide the same information as needed under the regular travel category), and costs for any related training expenses. Participant costs are those costs associated with conferences, workshops, symposia or institutes and breakout items should indicate the number of participants, cost for each participant, purpose of the conference, dates and places of meetings and any related administrative expenses. In the budget justification, indicate whether trainee cost estimates are based upon past experience of support of similar number of trainees on similar projects; past experience of support of similar number of participants attending similar conferences/workshops/symposia; or something else (describe).

Section F. Other Direct Costs:
Enter Other Direct Costs information for each item listed.

- **Materials and Supplies:** Enter total funds requested for materials and supplies in the appropriate fields. In the budget justification, indicate general categories such as glassware, and chemicals, including an amount for each category (items not identified under “Equipment”). Categories less than $1,000 are not required to be itemized. In the budget justification, indicate whether cost estimates are based upon past experience of purchase of similar or like items; quotes/catalog prices of similar or like items; or something else (describe).
- **Publication Costs:** Enter the total publication funds requested. The proposal budget may request funds for the costs of documenting, preparing, publishing or otherwise making available to others the findings and products of the work conducted under the award. In the budget justification, include supporting information. In the budget justification, indicate whether cost estimates are based upon past experience of purchase of similar or like items; vendor quotes of similar publication services; or something else (describe).
- **Consultant Services:** Enter total funds requested for all consultant services. In the budget justification, identify each consultant, the services he/she will perform, total number of days, travel costs, and total estimated costs. In the budget justification, indicate whether consultant cost estimate is based upon previous experience/quotes for similar or like services; or something else (describe).
- **ADP/Computer Services:** Enter total funds requested for ADP/Computer Services. The cost of computer services, including computer-based retrieval of scientific, technical and education information may be requested. In the budget justification, include the established computer service rates at the proposing organization if applicable. In the budget justification, indicate whether cost estimates are based upon quotes/past experience of purchase of similar computer services; established computer service rates at the proposing institution; or something else (describe).

- **Subawards/Consortium/Contractual Costs:** Enter total costs for all subawards/consortium organizations and other contractual costs proposed for the project. In the budget justification, justify the details.
- **Equipment or Facility Rental/User Fees:** Enter total funds requested for Equipment or Facility Rental/User Fees. In the budget justification, identify each rental/user fee and justify. In the budget justification, indicate whether cost estimates are based upon past experience with similar or like items; vendor quotes of similar items; or something else (describe).
- **Alterations and Renovations:** Enter total funds requested for Alterations and Renovations.
- **In the budget justification**, itemize by category and justify the costs of alterations and renovations, including repairs, painting, removal or installation of partitions, shielding, or air conditioning. Where applicable, provide the square footage and costs.
- **Other:** Add text to describe any other Direct Costs not requested above. Enter costs associated with "Other" item(s). Use the budget justification to further itemize and justify.

Section G. Direct Costs
This represents Total Direct Costs (Sections A thru F) and will be calculated by PAMS.

Section H. Other Indirect Costs
Enter the Indirect Cost information for each field. Only four general categories of indirect costs are allowed/requested on this form, so please consolidate if needed.

Section I. Total Direct and Indirect Costs
This amount will be calculated by PAMS (Sections G + H)

D. SUBMISSIONS FROM SUCCESSFUL APPLICANTS

If selected for award, DOE reserves the right to request additional or clarifying information.

E. SUBMISSION DATES AND TIMES

1. Letter of Intent Due Date

A letter of intent is not required.

2. Pre-proposal Due Date

01/25/2018, 5 PM Eastern Time

You are encouraged to submit your preproposal well before the deadline.

3. Proposal Due Date

04/04/2018, 5 PM Eastern Time

You are encouraged to transmit your proposal well before the deadline.

Modifications to the proposal are not allowed after the proposal due date.

4. Late Submissions

Delays in submitting letters of intent, preproposals, and proposals may be unavoidable. DOE has accepted late submissions when applicants have been unable to make timely submissions because of technological disruptions, significant natural disasters, and severely incapacitating or life-threatening illnesses. Other circumstances may or may not justify late submissions. Unacceptable justifications include but are not limited to the following:

- Failure to begin submission process early enough.
- Failure to provide sufficient time to complete the process.
- Failure to understand the submission process.
- Failure to understand the deadlines for submissions.
- Failure to satisfy prerequisite registrations.
- Unavailability of administrative personnel.

The applicant is responsible for beginning the submission process in sufficient time to accommodate reasonably foreseeable incidents, contingencies, and disruptions.

An applicant that waits to receive feedback from letters of intent or preproposals incurs the risk of having insufficient time to finish writing the proposal: Applicants should not delay drafting their proposals.

Scheduled medical events that are known at the time this FOA is published do not justify late submissions: Applicants should draft their submissions in sufficient time to meet the deadlines.

Applicants must email early.career@science.doe.gov
to discuss the option of a late submission in the case of unavoidable circumstances.

DOE notes that not all requests for late submission will be approved.

Changes to preproposals or proposals after the deadline are not allowed.

F. FUNDING RESTRICTIONS

Funding for all awards and future budget periods are contingent upon the availability of funds appropriated by Congress and the availability of future-year budget authority.

Support for paid collaborators of the Principal Investigator will be considered only in rare cases where a collaborator (either early career or senior) brings something unique to the project. However, preference will be given to Principal-Investigator-led efforts without paid collaborators for which the budget covers research support staff (e.g., students and postdoctoral fellows), travel, supplies, equipment, and other expenses necessary for the Principal-Investigator-led project.

Preference will be given to proposals without subawards with the exception of those that propose small subawards for essential supporting work such as sample analysis. Subawards that pay salary for scientific collaborators outside the proposing institution are discouraged.

Execution of the annual funding is solely at the discretion of the principal investigator in accordance with the DOE-approved budget.

G. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS

1. Where to Submit

Proposals must be submitted through PAMS to be considered for award.

Please only submit a PAMS lab technical proposal in response to this announcement; do not submit a DOE Field Work Proposal (FWP) at this time. The Office of Science will request FWPs via the Searchable FWP system later from those selected for funding consideration under this announcement.

2. Registration Process

ONE-TIME REGISTRATION PROCESS

DOE Office of Science Portfolio Analysis and Management System (PAMS)

The DOE Office of Science performs many functions for DOE national laboratory proposals in the Portfolio Analysis and Management System (PAMS), which is available at https://pamspublic.science.energy.gov.

There are many activities that you can perform in PAMS, and more functionality will be added throughout the near future. DOE national laboratories will submit preproposals, letters of intent, and proposals directly into PAMS.

You must register in PAMS to submit a preproposal, letter of intent, or DOE national laboratory proposal.

To access PAMS, you may use the Internet Explorer, Firefox, Google Chrome, or Safari browsers. For best results, we recommend using Internet Explorer 11.

Notifications sent from the PAMS system will come from the PAMS email address <PAMS.Autoreply@science.doe.gov>. Please make sure your email server/software allows delivery of emails from the PAMS email address to yours.

Registering to PAMS is a two-step process; once you create an individual account, you must associate yourself with ("register to") your institution. Detailed steps are listed below.

1. CREATE PAMS ACCOUNT:

To register, click the "Create New PAMS Account" link on the website https://pamspublic.science.energy.gov/.

- Click the "No, I have never had an account" link and then the "Create Account" button.
- You will be prompted to enter your name and email address, create a username and password, and select a security question and answer. Once you have done this, click the "Save and Continue" button.
- On the next page, enter the required information (at least one phone number and your mailing address) and any optional information you wish to provide (e.g., FAX number, website, mailstop code, additional email addresses or phone numbers, Division/Department). Click the "Create Account" button.
- Read the user agreement and click the "Accept" button to indicate that you understand your responsibilities and agree to comply with the rules of behavior for PAMS.
- PAMS will take you the "Having Trouble Logging In?" page. (Note: If you reviewed for or were listed as PI on a prior submission to the Office of Science but have not previously created an account, you may already be linked to an institution in PAMS. If this is the case, PAMS will take you to the PAMS home page.)

2. REGISTER TO YOUR INSTITUTION:

- Click the link labeled "Option 2: I know my institution and I am here to register to the institution." (Note: If you previously created a PAMS account but did not register to an institution at that time, you must click the Institutions tab and click the "Register to Institution" link.)
- PAMS will take you to the "Register to Institution" page.
- Type a word or phrase from your institution name in the field labeled, "Institution Name like," choose the radio button next to the item that best describes your role in the system, and click the "Search" button. A "like" search in PAMS returns results that contain the word or phrase you enter; you need not enter the exact name of the institution, but you should enter a word or phrase contained within the institution name. (Hint: If your institution has an acronym, such as ANL for Argonne National Laboratory or UCLA for the Regents of the University of California, Los Angeles, you may search for the acronym under "Institution Name like." Many institutions with acronyms are listed in PAMS with their acronyms in parentheses after their names.)
- Find your institution in the list that is returned by the search and click the "Actions" link in the Options column next to the institution name to obtain a dropdown list. Select "Add me to this institution" from the dropdown. PAMS will take you to the "Institutions – List" page.
- If you do not see your institution in the initial search results, you can search again by clicking the "Cancel" button, clicking the Option 2 link, and repeating the search.
- All DOE National Laboratories have established profiles in PAMS, so please keep searching until you find your laboratory.

3. Proposal Receipt Notices

Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the proposal.

4. Viewing Submitted Proposals

Upon submission, the proposal will appear under My Proposals for the PI and the Submitter with a Proposal Status of "Submitted to DOE."

Section V - PROPOSAL REVIEW INFORMATION

A. CRITERIA

1. Initial Review Criteria

Prior to a comprehensive merit evaluation, DOE will perform an initial review to determine that (1) the applicant is eligible for the award; (2) the information required by the DOE National Laboratory Announcement has been submitted; (3) all mandatory requirements are satisfied, , including attachment of a biosketch and a data management plan; (4) the proposed project is responsive to the objectives of the DOE National Laboratory Announcement, and (5) the proposed project is not duplicative of programmatic work. Proposals that fail to pass the initial review will not be forwarded for merit review and will be eliminated from further consideration.

A proposal declined without merit review by the DOE Office of Science will not count as one of the three allowed submissions to the Early Career Research Program. Likewise, a proposal withdrawn prior to being sent for merit review by the DOE Office of Science will not count as one of the three allowed submissions.

2. Merit Review Criteria

Proposals will be subjected to scientific merit review (peer review) and will be evaluated against the following criteria, listed in descending order of importance.

1. Scientific and/or Technical Merit of the Project;
2. Appropriateness of the Proposed Method or Approach;
3. Competency of Applicant's Personnel and Adequacy of Proposed Resources; and
4. Reasonableness and Appropriateness of the Proposed Budget.

The following announcement-specific evaluation criteria will also be used during the scientific merit review (peer review):

5. Relevance to the mission of the specific program (e.g., ASCR, BER, BES, FES, HEP, or NP) to which the proposal is submitted.
6. Potential for leadership within the scientific community.

The evaluation process will include the following program policy factors:

- Relevance of the proposed activity to Office of Science priorities
- Ensuring an appropriate balance of activities within the Office of Science programs
- Fostering the development of a diverse cadre of supported Principal Investigators
- The availability of funds

Note that external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Both Federal and non-Federal reviewers may be used,

and submission of a proposal constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

The following questions will be posed to reviewers for each of the review criteria listed above:

1. Scientific and/or Technical Merit of the Project
What is the scientific innovation of proposed research? How does the proposed research compare with other research in its field, both in terms of scientific and/or technical merit and originality? How might the results of the proposed research impact the direction, progress, and thinking in relevant scientific fields of research? What is the likelihood of achieving influential results? Is the Data Management Plan suitable for the proposed research and to what extent does it support the validation of research results?

2. Appropriateness of the Proposed Method or Approach
Does the proposed research employ innovative concepts or methods? How logical and feasible are the research approaches? Are the conceptual framework, methods, and analyses well justified, adequately developed, and likely to lead to scientifically valid conclusions? Does the applicant recognize significant potential problems and consider alternative strategies?

3. Competency of Applicant's Personnel and Adequacy of Proposed Resources
Does the proposed work take advantage of unique facilities and capabilities? What are the past performance and potential of the Principal Investigator (PI)? How well qualified is the research team to carry out the proposed research? Are the research environment and facilities adequate for performing the research?

4. Reasonableness and Appropriateness of the Proposed Budget
Are the proposed budget and staffing levels adequate to carry out the proposed research? Is the budget reasonable and appropriate for the scope?

5. Relevance to the mission of the specific program (e.g., ASCR, BER, BES, FES, HEP, or NP) to which the proposal is submitted
How does the proposed research contribute to the mission of the program in which the proposal is being evaluated?

6. Potential for leadership within the scientific community
Scientific leadership can be defined very broadly and can include direct research contributions. How has the PI demonstrated the potential for scientific leadership and creative vision? How has the PI been recognized as a leader?

For criterion 5, the missions of the program areas are:

Advanced Scientific Computing Research (ASCR): 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.

Biological and Environmental Research (BER): To support transformative science and scientific user facilities to achieve a predictive understanding of complex biological, earth, and environmental systems for energy and infrastructure security and resilience.

Basic Energy Sciences (BES): To support fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security.

Fusion Energy Sciences (FES): To expand the fundamental understanding of matter at very high temperatures and densities and to build the scientific foundation needed to develop a fusion energy source. This is accomplished through the study of plasma, the fourth state of matter, and how it interacts with its surroundings.

High Energy Physics (HEP): To understand how the universe works at its most fundamental level by discovering the elementary constituents of matter and energy, probing the interactions between them, and exploring the basic nature of space and time.

Nuclear Physics (NP): 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.

In addition to providing narrative comments associated with each of the six merit review criteria, each reviewer will be asked to provide an overall integer numerical rating between 1 and 6 for each proposal, where the scale follows:
Strongly Encourage Funding (5 or 6);
Encourage Funding (3 or 4); or
Discourage Funding (1 or 2).

B. REVIEW AND SELECTION PROCESS

1. Merit Review

Proposals that pass the initial review will be subjected to a formal merit review and will be evaluated based on the criteria above.

2. Program Policy Factors

The following Program Policy Factors will be considered:
- Relevance of the proposed activity to Office of Science priorities
- Ensuring an appropriate balance of activities within the Office of Science programs
- Fostering the development of a diverse cadre of supported Principal Investigators
- The availability of funds

3. Selection

The Selection Officials will consider the results of the merit review along with program policy factors.

4. Discussions and Award

The Government may enter into discussions with a selected applicant for any reason deemed necessary. Failure to resolve satisfactorily the issues identified by the Government will preclude award to the applicant.

C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES

DOE is striving to make **selections under this program within 6 months**. The time interval begins on the date proposals are due. **Awards are expected to be made in Fiscal Year 2018**.

Section VI - AWARD ADMINISTRATION INFORMATION

Office of Science Early Career Research Program investigators intending to transfer to a new institution must submit a request for transfer along with a new proposal. If the scope of work has not changed, the award may be transferred. If the scope of work has changed, the new proposal will be subject to merit review as described below. Transfer awards will be for the remaining award period only, and the requested budget cannot exceed the remaining budget for the original award. If a laboratory employee transfers to a university, the requested budget should be as close to $150,000 per year as possible for each remaining year. While a transfer proposal can be submitted any time of the year, it should be submitted at least six months before the transfer to allow time for execution of merit review.

To transfer an award to an academic institution, the investigator must move into a tenure-track or tenured position at the academic institution.

To transfer an award to a DOE National Laboratory, the investigator must move into a full-time, permanent, non-postdoctoral national laboratory position. The transfer proposal must be accompanied by a letter from the national laboratory director to the technical point of contact confirming that the proposed research idea fits within the scope of Office-of-Science-funded programs at the national laboratory. Transferring research that falls within this category ensures that investigators have the opportunity to belong to or join, at the laboratory's discretion, funded research groups. Making sure that DOE National Laboratory investigators have potential connections with Office-of-Science funded programs encourages the laboratory to actively plan to address funding transition issues that may arise when an award ends.

To retain an award at a DOE National Laboratory, the investigator must remain in a full-time, permanent, non-postdoctoral national laboratory position.

Execution of the annual funding is solely at the discretion of the principal investigator in accordance with the DOE-approved budget.

The award period is five years, conditional on adequate annual progress and appropriation of funds. At the end of this period, the DOE national laboratory employing the principal investigator has the primary responsibility to address funding transition issues that arise when the award ends.

A minimum of 50% and up to 100% of the Principal Investigator's salary must be charged to the award annually.

A. AWARD NOTICES

1. Notice of Selection

Selected Applicants Notification: DOE will notify applicants selected for award. This notice of selection is not an authorization to begin performance.

Non-selected Notification: Organizations whose proposals have not been selected will be advised as promptly as possible. This notice will explain why the proposal was not selected.

2. Notice of Award

A work authorization/contract modification issued by the contracting officer is the authorizing award document.

B. REPORTING

Annual progress reports and a final technical report from the award investigator will be required.

Annual progress reports will be due 90 days before the end of each budget year.

A final technical report will be required 90 days after the award ends.

Section VII - QUESTIONS/AGENCY CONTACTS

A. QUESTIONS

For help with PAMS, click the "External User Guide" link on the PAMS website, https://pamspublic.science.energy.gov/. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this DOE National Laboratory Announcement should reference **LAB 17-1761.**

Please contact the PAMS help desk for technological issues with the PAMS system.

Questions regarding the specific program areas and technical requirements may be directed to the technical contacts listed for each program within the DOE National Laboratory Announcement or below.

Please contact the program staff with all questions not directly related to the PAMS system.

B. AGENCY CONTACTS

PAMS Customer Support	855-818-1846 (toll-free) 301-903-9610 sc.pams-helpdesk@science.doe.gov
Administrative Contact	Questions about program rules should be sent to early.career@science.doe.gov.
Program Manager Scientific Contact	Questions regarding the specific program areas/technical requirements can be directed to the program managers / technical contacts listed for each program within the DOE National Laboratory Announcement.

Section VIII - OTHER INFORMATION

A. MODIFICATIONS

Notices of any modifications to this DOE National Laboratory Announcement will be posted on the Grants and Contracts website (http://science.doe.gov/grants/).

B. GOVERNMENT RIGHT TO REJECT OR NEGOTIATE

DOE reserves the right, without qualification, to reject any or all proposals received in response to this DOE National Laboratory Announcement and to select any proposal, in whole or in part, as a basis for negotiation and/or award.

C. COMMITMENT OF PUBLIC FUNDS

The Contracting Officer is the only individual who can make awards or commit the Government to the expenditure of public funds. A commitment by other than the Contracting Officer, either explicit or implied, is invalid.

D. PROPRIETARY PROPOSAL INFORMATION

Patentable ideas, trade secrets, proprietary or confidential commercial or financial information, disclosure of which may harm the applicant, should be included in a proposal only when such information is necessary to convey an understanding of the proposed project. The use and disclosure of such data may be restricted, provided the applicant includes the following legend on the first page of the project narrative and specifies the pages of the proposal which are to be restricted:

"The data contained in pages _____ of this proposal have been submitted in confidence and contain trade secrets or proprietary information, and such data shall be used or disclosed only for evaluation purposes."

To protect such data, each line or paragraph on the pages containing such data must be specifically identified and marked with a legend similar to the following:

"The following contains proprietary information that (name of applicant) requests not be released to persons outside the Government, except for purposes of review and evaluation."

E. EVALUATION AND ADMINISTRATION BY NON-FEDERAL PERSONNEL

In conducting the merit review evaluation, the Government may seek the advice of qualified non-Federal personnel as reviewers. The Government may also use non-Federal personnel to conduct routine, nondiscretionary administrative activities. The applicant, by submitting its application, consents to the use of non-Federal reviewers/administrators. All non-Federal and Federal reviewers must sign conflict of interest and confidentiality statements prior to reviewing a proposal. Non-Federal personnel conducting administrative activities must sign a non-

disclosure agreement.

F. AVAILABILITY OF FUNDS

Funds are not presently available for this award. The Government's obligation under this award is contingent upon the availability of appropriated funds from which payment for award purposes can be made. No legal liability on the part of the Government for any payment may arise until funds are made available to the Contracting Officer for this award and until the awardee receives notice of such availability, to be confirmed in writing by the Contracting Officer.