# DEPARTMENT OF ENERGY OFFICE OF SCIENCE



# EARLY CAREER RESEARCH PROGRAM Funding Opportunity Announcement (FOA) Number: DE-FOA-0002019

# FOA TYPE: AMENDMENT 00001 CFDA Number: 81.049

FOA Issue Date:	January 7, 2019
Submission Deadline for Letters of Intent:	NA
Submission Deadline for Pre-Applications:	February 6, 2019 at 5:00 PM Eastern Time A Pre-Application is required
<b>Pre-Application Response Date:</b>	March 8, 2019
Submission Deadline for Applications:	April 29, 2019 at 5:00 PM Eastern Time

Amendment 00001: This amendment clarifies the eligibility requirements regarding years from PhD, language used in some topical program descriptions, and the relevant technical points of contact.

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# UPDATES AND REMINDERS

#### RECOMMENDATION

The Department of Energy (DOE) Office of Science (SC) 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.

#### PRE-APPLICATION REVIEW

Pre-applications may be comparatively reviewed by DOE SC program managers to determine which pre-applications may yield the most competitive applications. Potential applicants whose pre-applications that are determined to be noncompetitive will not be permitted to submit applications.

#### **AVOIDING ERRORS**

The following advice is compiled from actual experiences of applicants for SC financial assistance awards.

- Please ensure that the research narrative is comprised of one and only one Portable Document Format (PDF) file, including all appendices, when it is attached to the SF-424 (R&R) form.
- When using the PAMS website at <u>https://pamspublic.science.energy.gov</u>, please avoid using the back-arrow button in your web browser to navigate.
- Please ensure that the application contains no personally identifiable information (PII).
- Please ensure that the budget is calculated using the applicable negotiated indirect cost and fringe benefit rates.

#### GRANTS.GOV WORKSPACE

Applications submitted through Grants.gov at <u>https://www.Grants.gov</u> must be submitted through a "Workspace." Workspace permits members of a team to simultaneously work on their application in an online collaborative environment. Application forms may exist as both online webforms and downloadable forms. More information is available at <a href="https://www.grants.gov/web/grants/applicants/workspace-overview.html">https://www.grants.gov/web/grants/workspace</a>.

#### DATA MANAGEMENT PLAN

Applications submitted under this FOA are subject to the Office of Science Statement on Digital Data Management, published at <u>https://science.energy.gov/funding-opportunities/digital-data-management/</u>. Compliance with this statement is detailed in Part IV of this FOA.

#### ACKNOWLEDGMENT OF FEDERAL SUPPORT

SC published guidance about how its support should be acknowledged at <u>https://science.energy.gov/funding-opportunities/acknowledgements/</u>.

# Section I – FUNDING OPPORTUNITY DESCRIPTION

# GENERAL INQUIRIES ABOUT THIS FOA 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 FOA.

#### Administrative Contact (questions about program rules):

Questions about program rules should be sent to <u>SC.Early@science.doe.gov</u>

# STATUTORY AUTHORITY

Public Law 95-91, US Department of Energy Organization Act Public Law 109-58, Energy Policy Act of 2005

# **APPLICABLE REGULATIONS**

Uniform Administrative Requirements, Cost Principles, and Audit Requirements for Federal Awards, codified at 2 CFR 200
U.S. Department of Energy Financial Assistance Rules, codified at 2 CFR 910
U.S. Department of Energy, Office of Science Financial Assistance Program Rule, codified at 10 CFR 605

# SUMMARY

SC 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 SC.

# SUPPLEMENTARY INFORMATION

SC's mission 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. SC 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.

SC 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-ofthe-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 SC research programs. Additional details about each program, websites, and technical points of contacts are provided in the materials that follow.

- I. <u>Advanced Scientific Computing Research</u> (ASCR);
- II. <u>Biological and Environmental Research</u> (BER);
- III. <u>Basic Energy Sciences</u> (BES),
- IV. Fusion Energy Sciences (FES);
- V. <u>High Energy Physics</u> (HEP), and
- VI. <u>Nuclear Physics</u> (NP)

The topics for the FOA are indicated by letters under each Program Office name (ASCR, BER, BES, FES, HEP, or NP). For example, under ASCR, the first topic is "Adaptive Algorithms, Solvers, and Optimization for High Performance Computing."

Advanced Scientific Computing Research (ASCR) **Program Website:** <u>http://science.energy.gov/ascr/</u>

ASCR's mission 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 and engineering, 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 the scientific needs of the future 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 and thousands 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 SC 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) Adaptive Algorithms, Solvers, and Optimization for High Performance Computing Technical Contact: Steven Lee, 301-903-5710, <u>Steven.Lee@science.doe.gov</u>

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, randomized, or stochastic. A key research characteristic is that the results will also be useful for high-performance computing simulations.

#### (b) Multiscale Mathematics for Coupled High Performance Scientific Simulations Technical Contact: Steven Lee, 301-903-5710, <u>Steven Lee@science.doe.gov</u>

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, multiphysics coupling approaches, scale bridging, uncertainty quantification, and sensitive analysis in such systems are of particular interest.

#### (c) Research Foundations for Scalable Scientific Data Analysis and Algorithms Technical Contact: Steven Lee, 301-903-5710, <u>Steven.Lee@science.doe.gov</u>

Rigorous mathematical and computationally efficient approaches for analyzing and extracting information and insight from large-scale data 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 methodologies for large-scale data.

For Topics (a), (b), and (c) above, crosscutting research that enables greater adaptivity and automation in scientific computing capabilities is of particular interest. Such forward-looking and versatile capabilities can stem from research advances in artificial intelligence, machine learning, uncertainty quantification, sensitivity analysis, error estimation, and related areas.

For Applied Mathematics, 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.

<u>Important note for encourage and discourage decisions</u>: Pre-applications 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.

# **References:**

Report on 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/programdocuments/docs/reportExtremeScaleSolvers2012.pdf

DOE Workshop Report on Multiphysics Simulations

https://science.energy.gov/~/media/ascr/pdf/programdocuments/docs/MultiPhysics-Simulations-Report.pdf

Report on A Multifaceted Mathematical Approach for Complex Systems <u>http://science.energy.gov/~/media/ascr/pdf/program-</u> documents/docs/Multifaceted\_Mathematical\_Approach\_for\_Complex\_Systems.pdf

DOE Workshop on Scientific Machine Learning Website: https://www.orau.gov/ScientificML2018/ Pre-Workshop report: https://www.orau.gov/ScientificML2018/workshop-report.htm

# **Computer Science**

This program supports research that enables computing and networking at extreme scales and the understanding of extreme scale and complex data from both simulations and experiments. It aims to make high performance scientific computers and networks highly productive and efficient to solve scientific challenges while attempting to reduce domain science application complexity as much as possible.

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

#### (d) Systems

Technical Contact: Robinson Pino, 301-903-1263, <u>Robinson.Pino@science.doe.gov</u>

- 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], Field-Programmable Gate Arrays [FPGAs], other types of accelerators, big-small cores, processing in memory and near memory, etc.), with particular emphasis on making it easier to program at scale. Particularly welcome are applications that infuse artificial intelligence/machine learning into the programming environment.
- b. **Operating and Runtime Systems**: System software that provides intelligent, adaptive resource management and support for workflow management systems, and that facilitates effective and efficient use of heterogeneous computing technologies, including diverse execution models, processors, accelerators, and memory and storage systems.
- c. **Performance Portability**: Algorithms and methods that support automated and semiautomated 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.

Applications are not restricted to a single Systems topic above and may span all of them, provided the scope of work remains appropriate for the program.

#### (e) Data Management, Visualization, and Analytics Technical Contact: Laura Biven, 301-903-9556, <u>Laura.Biven@science.doe.gov</u>

- a. **Data management** approaches for managing and analyzing large data from scientific instruments and simulation including methods for reducing the size and/or complexity of the data for further analysis, particularly in real time; in situ workflow management and techniques for carrying out data management and analysis in situ to meet research needs; and data management for preservation and archiving, to support collaboration and sharing, and to facilitate re-use.
- b. Analytic Methods and Environments to improve visual exploration and understanding of petabyte to exabyte multi-scale, multi-physics scientific data sets from simulations and/or experimental platforms; to support efficient analysis of data across federated resources; to support interactivity with simulation and/or real-time steering of experiments, including remote interactions; and to help answer scientifically relevant questions from the data about, for example, uncertainty, sensitivity analysis, causality, and the debugging of codes and methods. As appropriate, applicants are encouraged to consider evaluation methods for new visualization tools and techniques resulting from the proposed research.

#### (f) Emerging Computing Technologies Technical Contact: Robinson Pino, 301-903-1263, <u>Robinson.Pino@science.doe.gov</u>

- 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) Applied Network Science for Complex Interconnected Engineered Systems Technical Contact: Thomas Ndousse-Fetter, 301-903-9960, <u>Thomas.Ndousse-Fetter@science.doe.gov</u>

The focus of this subtopic is on the application of network science for the characterization and understanding of the behavior of complex interconnected engineered systems such as wide area communication networks, large-scale supercomputing facilities, networked scientific instruments, regional unity grids, super-facilities, and hybrid systems. Potential topics of interest include but are not limited to the following: machine learning-based techniques, network interdependencies and cascading failures, networks of networks, network sampling and measurement, and cascading dynamics in quantum networks.

# Topics that are out of scope include:

- Pre-applications and applications that do not address the specific Computer Science topics described above.
- Pre-applications and applications that do not explain/describe their relevance to current and future high performance computing platforms and/or data-centric science as well as their relevance to the mission of SC and ASCR.
- 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;
- Research primarily focused on advancing discipline-specific data analytics and informatics without a clear articulation of how the proposed research could be generalized to other SC priority mission areas;
- Research primarily focused on advancing Virtual Reality and Augmented Reality technologies;
- 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 for networks, including Intelligent Network Interface Cards, biological complex networks, social networks, or network acceleration hardware; and technologies that optimize wireless or other low-speed network infrastructures;
- Pre-applications and applications with a primary focus on development or deployment activities; or that suggest incremental upgrades to existing network architectures, protocols, tools, or services.
- Development and optimization of quantum algorithms; development of new candidate qubit systems; schemes based on qubits that have not yet demonstrated high-fidelity gates; schemes to improve the performance and functionality of qubits; quantum transduction; quantum communication, networking, and key distribution; cryptography and cryptanalysis; research solely relevant to large-scale, high-fidelity, fault-tolerant machines; projects that are duplicative of or competitive with industry; software development other than what is required to maintain efficient operation of the laboratory.

#### References

NITRD LSN Workshop Report on Complex Engineered Networks, https://www.nitrd.gov/pubs/nitrd\_lsn\_workshop\_report\_2012.pdf

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," <u>https://www.orau.gov/ionInfrastructure2014/intelligent-network-infrastructure-workshop-report.pdf</u>

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

DOE Workshop report: "Management, Analysis and Visualization of Experimental and Observational Data: The Convergence of Data and Computing," <u>https://science.energy.gov/~/media/ascr/pdf/programdocuments/docs/ascr-eod-workshop-2015-report\_160524.pdf</u>

DOE Workshop report: "Crosscut Report: Exascale Requirements Reviews," <u>https://science.energy.gov/~/media/ascr/pdf/programdocuments/docs/2018/DOE-ExascaleReport-CrossCut.pdf</u>

DOE Workshop report: "Neuromorphic Computing – Architectures, Models, and Applications Workshop," <u>https://science.energy.gov/~/media/ascr/pdf/programdocuments/docs/Post-</u> <u>Workshop\_Report\_2016\_Neuromorphic\_Computing.pdf</u>

DOE Workshop report: "Neuromorphic Computing – From Materials Research to Systems

Architecture Roundtable,"

https://science.energy.gov/~/media/ascr/pdf/programdocuments/docs/Neuromorphic-Computing-Report\_FNLBLP.pdf

DOE Workshop report: "The 2015 Cybersecurity for Scientific Computing Integrity - Research Pathways and Ideas Workshop,"

https://science.energy.gov/~/media/ascr/pdf/programdocuments/docs/ASCR\_Cybersecurity\_20\_ Research\_Pathways\_and\_Ideas\_Workshop.pdf

DOE Workshop report: "The 2015 Cybersecurity For Scientific Computing Integrity Workshop,"

https://science.energy.gov/~/media/ascr/pdf/programdocuments/docs/ASCR\_Cybersecurity\_For\_ Scientific\_Computing\_Integrity\_Report\_2015.pdf

DOE Workshop report: "The 2015 Machine Learning and Understanding For Scientific Discovery Workshop," <u>https://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Machine Learning DOE Workshop Report.pdf</u>

#### **Research and Evaluation Prototypes**

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

#### (h) Quantum Computing Technical Contact: Claire Cramer, 301-903-5384, <u>Claire.Cramer@science.doe.gov</u>

Research to evaluate the suitability of specific quantum computing hardware architectures for science applications. Feedback and control systems for physical qubits in quantum processors. Compilation and optimization tools, including efficient mapping of algorithms to circuits in real-

world hardware and research to develop more effective gates. Techniques for minimizing or mitigating error in real-world quantum processors.

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

Topics that are out of scope include:

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

#### References

DOE Workshop report: "Quantum Computing for Science", February 2015. <u>http://science.energy.gov/~/media/ascr/pdf/programdocuments/docs/ASCRQuantumReportfinal.</u> <u>pdf</u>

DOE Workshop report: "Quantum Testbeds Stakeholder Workshop", February 2017. https://science.energy.gov/~/media/ascr/pdf/programdocuments/docs/2017/QTSWReport.pdf

#### Biological and Environmental Research (BER) Program Website: <u>http://science.energy.gov/ber/</u>

BER's mission 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 BER supports fundamental research to achieve a predictive systems-level understanding of relevant biological systems to advance DOE missions in sustainable bioenergy development. BSSD programs aim at identifying the foundational principles that drive biological systems and developing modern "omics" tools to address the challenges associated with microbial production of advanced biofuels and bioproducts.

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

# (a) Fundamental Systems Biology-Driven Research to Enable Advanced Biofuels and Bioproducts Production

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

Applications are requested for systems biology research to advance the development of emerging model microorganisms and/or microbial communities relevant for the production of biofuels and/or bioproducts directly from light or by conversion of lignocellulosic biomass. Applications that propose multi-omics approaches coupled with advanced predictive modeling and high-throughput screening to understand biological systems with novel functional capabilities and biosynthetic potential are encouraged. Proposed studies could include but are not limited to: elucidation of relevant regulatory and metabolic networks or environmental signal processing related to product synthesis by microbes or multispecies consortia; development of genetic tools to facilitate the study and manipulation of emerging microbial model systems; and understanding and modification of phenotypes involved in the synthesis of biofuel and bioproduct precursors, deconstruction of plant cell wall biomass, and/or tolerance to stresses induced by altered biosynthetic pathways or culture conditions.

The following topics are not within the scope of the BSSD research area: Starch-, waste-, natural gas-, petroleum-, or coal-derived biofuels and bioproducts; microbial fuel cells; electrosynthesis; wastewater treatment; municipal solid waste; bioremediation; production of ethanol, hydrogen, pharmaceuticals, nutraceuticals, cosmetics, or food products. Applications focused solely on eukaryotic algal systems or technology development will not be considered.

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; <u>www.kbase.us</u>), DOE Joint Genome Institute (JGI; <u>http://jgi.doe.gov/</u>), DOE Environmental Molecular Sciences Laboratory (EMSL; <u>http://www.emsl.pnl.gov/emslweb/</u>), National Energy Research Scientific Computing Center (NERSC; <u>http://www.nersc.gov</u>), 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 grand challenges that frame the subprogram and investments: (a) advancing the understanding of the integrated water cycle by studying relevant processes involving the atmospheric, terrestrial, oceanic, and human system components and their interactions and feedbacks across local, regional, and global scales, thereby improving the predictability of the water cycle and reducing associated uncertainties in

response to short- and long-term perturbations; (b) advancing a robust, predictive understanding of coupled biogeochemical processes and cycles across spatial and temporal scales by investigating natural and anthropogenic interactions and feedbacks and their associated uncertainties within Earth and environmental systems; (c) understanding and quantifying the drivers, interactions, and feedbacks both among the high-latitude components and between the high latitudes and the global system to reduce uncertainties and improve predictive understanding of high-latitude systems and their global impacts; (d) advancing next-generation understanding of Earth system drivers and their effects on the integrated Earth-energy-human system; and (e) developing a broad range of interconnected infrastructure capabilities and tools that support the integration and management of models, experiments, and observations across a hierarchy of scales and complexity to address CESD scientific grand challenges.

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

#### (b) Environmental System Science (ESS) Technical Contact: David Lesmes, 301-903-2977, <u>David.Lesmes@science.doe.gov</u>

The goal of the Environmental System Science (ESS) activity, which consists of the Subsurface Biogeochemical Research (SBR) and Terrestrial Ecosystem Science (TES) programs, is to advance a robust predictive understanding of terrestrial environments, extending from bedrock to the top of the vegetated canopy and from molecular to global scales in support of DOE's energy and environmental missions. Using an iterative approach to model-driven experimentation and observation, interdisciplinary teams of scientists work to unravel the coupled physical, chemical and biological processes that control the structure and functioning of terrestrial ecosystems across vast spatial and temporal scales. State-of-science understanding is captured in conceptual theories and models which can be translated into a hierarchy of computational components and used to predict the system response to perturbations caused, for example, by changes in climate, land use/cover, or contaminant loading. Basic understanding of the system structure and function is advanced through this iterative cycle of experimentation and observation by targeting key system components and processes that are suspected to most limit the predictive skill of the models.

Within the integrated Earth system, watersheds are the fundamental organizing unit within which physical, biological, and chemical processes interact and co-evolve to mediate the hydrobiogeochemical (HBGC) functioning of terrestrial environments. Understanding how watersheds function requires an integrative examination of how surface and subsurface water flow and constituents are transported over a broad range of spatiotemporal scales and how biogeochemical processes mediated by microorganisms enable mineral dissolution and precipitation, organic matter deposition and degradation, oxidation and reduction reactions, and plant-rhizosphere interactions. Mechanistic models of watershed systems—extending from bedrock through soils to the vegetative canopy—have reactive transport codes at their core. These codes incorporate metabolic models of microbial processes; molecular-scale understanding of geochemical stability, speciation, and biogeochemical reaction kinetics; and diagnostic signatures of the system response at varying spatial and temporal scales. These models are powerful, however, their predictive skill is limited by our ability to parameterize and capture the multiscale dynamics of coupled biological, physical, and chemical interactions in real environments over a broad

range of spatial and temporal scales and environments, and to determine and capture hot spots and hot moments of disproportionately high levels of HBGC interaction and activity relative to the bulk of the environment. In addition, there is an increasing emphasis and need to couple reactive transport codes with land surface, river routing, and atmospheric models to more holistically represent the integrative processes influencing watershed HBGC across scales.

The SBR (https://doesbr.org/) and TES (https://tes.science.energy.gov/) programs, which make up the ESS activity, support multidisciplinary research programs at the DOE National Laboratories as well as a diverse portfolio of research projects led by university PIs. This programmatic approach recognizes that the National Laboratories are structured for conducting coordinated, team-oriented research in a manner that is distinct from, but complementary to, research conducted by financial assistance (10 CFR Part 605). For this topic, ESS is interested in applications from individual early-career scientists at universities, DOE National Laboratories, and eligible research institutes that complement, but do not duplicate, the existing Science Focus Area (SFA) research programs or major research projects, and which are focused on watershed system science (https://doesbr.org/research/sfa/index.shtml;

<u>https://tes.science.energy.gov/research/labs.shtml; https://doesbr.org/research/ideas.shtml</u>). Such applications are expected to provide unique or innovative insights into the research challenges facing the SFAs. While all applicants to this topic must identify in the pre-application how the proposed project is unique yet complements ongoing work within SBR or TES SFAs or major research projects, applicants will be required in the application submission to explain in full detail how the proposed work complements, does not duplicate, and introduces a unique scientific challenge that is different from ongoing SBR and/or TES SFAs and other major projects supported by BER.

All applications are required to clearly delineate an integrative, hypothesis-driven approach and clearly describe the existing needs/gaps in state-of-the-art models. Field investigations do not have to be performed at DOE-funded field sites but they must be performed at research sites within the United States, and we encourage applicants to use existing resources such as Ameriflux sites and NSF-funded Critical Zone Observatory sites as well as DOE-funded field sites which are primarily managed by the SFAs. Proposed efforts are expected to represent new or unique avenues of research. For all field projects, a letter of support must be provided in the full application from the lead PI responsible for the field site where the project will be conducted.

Applicants are encouraged to address one or more of the following research challenges by utilizing existing watershed testbeds and research sites and complementing, but not duplicating, existing SFA research efforts:

- Quantify how biological behavior, abiotic-biotic interactions, and molecular transformations control the mobility of contaminants (e.g., U, Tc, Hg), nutrients (e.g., N, P, C), and other inorganic elements involved in mediating biogeochemical processes (e.g., S, Fe, Mn).
- 2. Quantify and predict how hydrology drives fine-scale biogeochemical processes, especially hot spots and hot moments of disproportionally high interaction and activity, in surface-subsurface systems.
- 3. Translate biogeochemical behavior across relevant molecular to watershed scales to

accurately and tractably predict flows of water, nutrients, and contaminants.

4. Identify, quantify, and predict watershed responses to natural and anthropogenic perturbations extreme events, and shifts to new states.

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. In addition, funded projects are expected to at least mirror any data obtained or derived from the research supported under this ESS topic within the ESS Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) data archive.

More detailed information about BER Earth and Environmental Systems Sciences sponsored research can be found at: <u>https://science.energy.gov/ber/research/cesd/</u>. Information on data archiving within ESS-DIVE can be found at: <u>https://ess-dive.lbl.gov/</u>.

# Basic Energy Sciences (BES) Program Website: <u>http://science.energy.gov/bes/</u>

BES's mission 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: <u>http://science.energy.gov/bes/mse/principal-investigators-meetings/</u>

Chemical Sciences, Geosciences, & Biosciences Division Principal Investigators' Meetings: http://science.energy.gov/bes/csgb/principal-investigators-meetings/ Scientific User Facilities Division web page: <u>http://science.energy.gov/bes/suf/</u>

Many of the core research areas limit 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, <u>Michael.Sennett@science.doe.gov</u> (select Michael Sennett in PAMS) and Craig Henderson, 301-903-0805, <u>Craig.Henderson@science.doe.gov</u>

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, structure, and function 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 this year is strictly limited. The program will accept hypothesis-driven applications ONLY in the following topical area:

• Chemical synthesis of new metastable materials with novel compositions, structures, phases, and/or functions via understanding and control of non-equilibrium reaction pathways and conditions

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* or synthesis of *small molecules* 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. Further, the proposed research must be technically delineated from other research.

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

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 A will be considered.

- Topic A (This year): 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 (Alternate years): The focus should be creation of beyond-equilibrium multicomponent, resilient, self-regulating materials that can reconfigure function and/or energy transfer, transport, and communication pathways; repair and rebuild structure without external input; or 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. Bio-centric research **will be de-emphasized**, including activities focused on understanding of underlying biological synthetic or assembly processes, biologically-driven synthesis of monodisperse polymers, or creation of bio-hybrid materials. 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 Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

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

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 that help gain atomic level control in materials synthesis and processing.

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 applications that present novel understanding and creative approaches elucidating the physical mechanisms underlying the synthesis and processing of two-dimensional bulk materials. Applications 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 will not be supported by this activity. For this year, projects involving the synthesis or processing of two-dimensional materials **will** be the only applications supported.

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.

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

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 bulk quantum materials wherein electronic, structural, charge and magnetic states are controlled to produce novel functionality. Next year's call is anticipated to focus on nanostructured and low dimensional 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 or device development. In addition, the ECMP Early Career Program will not accept applications on topics in the following areas: conventional semiconductors, heavy fermion superconductivity, quantum Hall physics in compound semiconductor materials, cuprate superconductivity, and cold atom physics.

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.

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

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 targeted areas of high-throughput computations, datadriven materials discovery, and materials theory/modeling solely related to energy technologies. Next year, the plan is to invite applications in the areas of quantum materials and systems out of equilibrium, including transport and ultrafast response.

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.

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

This program supports research to understand the physical behavior of materials. This year, the program invites early career applications in the areas of thermoelectric, magnetocaloric, and multiferroic materials, and in the area of light-matter interactions in the fields of excitonics, plasmonics and metamaterials. The program will also consider applications relevant to the field of Quantum Information Science for research on the creation and control of coherent phenomena for transduction of quantum coherent states between different physical systems with high fidelity. 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 Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

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

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 Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

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

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 conventional tabletop laser sources.

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.

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

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 at mesoscale where macroscopic properties of polymer-based materials manifested. The program will develop novel approaches that will exploit the unique aspects of neutron scattering to investigate polymer-based materials with hierarchical structures or excitations over a wide range of length and time scales.

Based on programmatic priorities, applications focused on organic photovoltaics **will not** be considered.

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.

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

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 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; investigating the electronic structure, spin dynamics, magnetism, phase transitions and transport properties from atomistic to mesoscopic scales; and developing advanced *in situ* analysis capabilities or combination of multiple probes for study of quantum materials.

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 Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

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

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) Division funded programs at the laboratory of the applicant.

#### (1) Gas Phase Chemical Physics (GPCP) Technical Contact: Wade Sisk, 301-903-5692, <u>wade.sisk@science.doe.gov</u>

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. (CLOSED)

- 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. (CLOSED)
- 3. *Chemistry-Transport Interactions*. Research in this area focuses on gaining a better understanding of how non-equilibrium and/or 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. (OPEN)
- 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. (OPEN)

Research 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 FOA, only applications focused on thrusts **3** and **4** will be considered. Research applications for thrusts **1** and **2** 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, <u>mark.pederson@science.doe.gov</u>

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 molecularto 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 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) quantitative description of chemical- or molecular- based quantum or classical logic emulators (vi) reactivity and catalysis (vii) molecular and nano-scale electronic-, spin- and energy transport, and (viii) quantum simulation of biologically inspired mechanisms for energy management.

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.

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 Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

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

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.

The CPIMS program has recently added research projects that (1) explore quantum entanglement to drive and sense reactions and reaction dynamics remotely in solution and at interfaces, (2) study kinetics and reaction dynamics above surfaces of potential importance to quantum information devices, (3) examine rare electrochemical events (such as nucleation and self assembly) using machine learning and advanced sampling techniques of large data sets, and (4) study hydrogen bonding and solvation of ions in liquid electrolytes (including in conventional dipolar solvents, ionic liquids and deep eutectic solvents). The program has also added projects such as (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; and (3) explorations of multidimensional infrared microscopy for visualizing chemical dynamics in heterogeneous environments. Descriptions of earlier awards are found in CPIMS Meeting Reports at the link <a href="http://science.energy.gov/bes/csgb/principal-investigators-meetings/">https://science.energy.gov/bes/csgb/principal-investigators-meetings/</a>, under "Condensed-Phase and Interfacial Molecular Science". A more extensive description of program evolution can be found at the following link: <a href="https://science.energy.gov/~/media/bes/pdf/brochures/bes-cras/2017/cra\_17\_CPIMS.pdf">https://science.energy.gov/~/media/bes/pdf/brochures/bes-cras/2017/cra\_17\_CPIMS.pdf</a>.

The CPIMS program **does not** fund research in continuum fluid mechanics or fluid dynamics, applications such as the development of 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 Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

#### (o) Catalysis Science

# Technical Contact: Viviane Schwartz, 301-903-0448, <u>viviane.schwartz@science.doe.gov</u> and Chris Bradley, 301-903-2047, <u>chris.bradley@science.doe.gov</u>

This program supports basic research pursuing novel catalyst design and quantum- and molecular-level control of chemical transformations relevant to the sustainable conversion of energy resources. Emphasis is on the understanding of reaction mechanisms, enabling precise identification and manipulation of catalytic active sites, their environments, and reaction conditions for optimized efficiency and selectivity. Elucidation of *catalytic reaction mechanisms in diverse chemical environments* and *the structure-reactivity relationships of solid and molecular catalysts* comprise the central component of the program, with specific focus areas involving:

- Advanced concepts concerning catalyst design, including topics related to multifunctionality, confinement within porous materials, site cooperativity, nano- and singleatom stabilized structures, and manipulation of weak interactions;
- Design of catalysts for efficient interconversion of electrical and chemical energy, including investigation of *charge transport dynamics and reactivity* relevant to electrocatalytic reactions as well as thermally excited redox conversions in solution or at interfaces;
- Development of novel time-resolved spectroscopic techniques and structural probes for in situ/operando characterization of catalytic processes, including *ultrafast* bond formation and transition state conversion, as well as slower ionic or atomic or molecular species rearrangements during reaction;
- Examination of the dynamics of catalyst and electronic structures occurring during catalytic cycles and deactivation;
- Investigation of emerging approaches to direct catalytic transformations in multicomponent mixtures, multiple reactions, and integrated processes, such as cascade and tandem processes;
- Advanced theory, modeling, and data-science approaches to mechanism identification, catalyst discovery and development, and efforts leading to benchmarks for catalytic properties

A long-term objective is to promote the convergence of heterogeneous, homogeneous, and biocatalysis as a means to discover novel inorganic, organic, and hybrid catalysts selective for fuel and chemical production from both fossil and renewable feedstocks, including synthetic or natural polymers. Another enduring goal is to maximize the atom and energy efficiency of chemical transformations. This activity is especially receptive to novel and emerging approaches to fundamentally understand and manage complexity at various levels: active site structure and superstructure, feedstock molecular diversity and variability, multiple sources of excitation (thermal, electrical, electromagnetic), transient and discontinuous operation, and kinetic behavior for complex reaction networks. It also encourages integrated theory-experiment and predictive theoretical catalysis supported by data-intensive strategies.

The FY19 Early Career Research Program in Catalysis Science will exclude activities that are not hypothesis-driven and:

1. Studies that focus primarily on the synthesis of catalytic materials; and

2. Studies where developing theoretical, computational, or characterization methods is the main objective, while understanding the catalytic reaction mechanisms is secondary.

This program does not support: (1) the study of transformations appropriate for pharmaceutical applications; (2) studies where the primary focus is the elementary steps of light adsorption; (3) non-catalytic stoichiometric reactions; (4) whole cell or organismal catalysis; (5) process or reactor design and optimization; or (6) device development or optimization.

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', <u>http://www.science.energy.gov/bes/csgb/principal-investigators-</u> <u>meetings/</u> (search for "catalysis" in the book title), and in the BES Research Summaries (<u>https://science.energy.gov/bes/community-resources/program-summaries/</u>). A 2017 BESACsponsored workshop, Basic Research Needs for Catalysis Science, outlining the current challenges and needs in this field, can also be found on the 'Basic Research Needs Reports' web page link

(https://science.energy.gov/~/media/bes/pdf/reports/2017/BRN\_CatalysisScience\_rpt.pdf).

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.

# (p) Separation Science (SEP) Technical Contact: Philip Wilk, 301-903-4537, <u>philip.wilk@science.doe.gov</u>

Thematically, this research area supports fundamental separation science, with topics on Chemistry at Complex Interfaces, Charge Transport and Reactivity, Reaction Pathways in Diverse Environments, Chemistry in Aqueous Environments and Ultrafast Chemistry, studies that predict and control the atomic and molecular interactions and energy exchanges that determine the efficiency of chemical separations.

The overall goal is to obtain a thorough understanding at the molecular-, nano-, and meso-scales of basic chemical and physical principles leading to novel separation processes that utilize new, multifunctional and/or energy- and atom-efficient methods. Investigations of novel structures is included, such as complex interfaces, functionalized surfaces and architectures, and systems designed at multiple size- and time-scales. More details about the Separation Science program can be found on the web: <u>https://science.energy.gov/bes/csgb/research-areas/separation/</u>. For the positioning of the research of the Separation Science program in broader context with the main research themes of the Chemical Sciences, Geosciences, and Biosciences (CSGB) Division see https://science.energy.gov/bes/csgb/.

Based on programmatic priorities, the Separation Science program does not support applied research, engineering or scale up of processes, mineral or materials processing, devices or sensors, microfluidics or medical applications. The program will not consider applications on chemical analysis, though applications that contain analytical aspects, which fit the objectives of specific research topics, may be considered.

Applications should be hypothesis-based. Research funded in this category in the recent past can be found in Principal Investigators' Meetings Reports at: <u>http://science.energy.gov/bes/csgb/principal-investigators-meetings</u>.

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.

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

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 chemical 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, the fundamental transactinide chemical properties, and 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 applications 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.p\_df).

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 Separations 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 Separations Science Principal Investigators' Meetings Reports at <u>http://science.energy.gov/bes/csgb/principal-investigators-meetings</u>.

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.

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

This research area supports fundamental geoscience research, with emphasis on the molecularlevel origins of geochemical and geophysical processes. This year's geosciences early career call is aimed at earth science problems involving topics on Chemistry at Complex Interfaces; Charge Transport and Reactivity; Reaction Pathways in Diverse Environments; Chemistry in Aqueous Environments; and Ultrafast Chemistry. To be considered for funding for the FY19 Early Career Program, application ideas must make strong connections to one or more of these topics. Particular priority will be given to applications that put together compelling strategies for understanding geochemical reaction mechanisms. Applications that do not convincingly connect with at least one of the thematic areas above will not be considered.

For information about the relationship of the Geosciences program to the main research themes of the Chemical Sciences, Geosciences, and Biosciences (CSGB) Division see <u>https://science.energy.gov/bes/csgb/</u>.

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.

#### (s) Solar Photochemistry Technical Contact: Chris Fecko, 301-903-1303, <u>christopher.fecko@science.doe.gov</u>

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, photoinduced electron and energy transfer in the condensed phase and across interfaces, photoelectrochemistry, photodriven generation or manipulation of quantum coherence in artificial molecular systems, and artificial assemblies for charge separation and transport that mimic natural photosynthetic systems. An enhanced theory and modeling effort is needed to improve current understanding of many photochemical phenomena.

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 interest is research on the principles of 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 molecular 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, including energy transfer and the generation, separation, and recombination of charge carriers.

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 that 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 Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

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

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 in natural photosynthesis include, but are not limited to, light harvesting, quantum coherent energy transfer, proton and electron transport, 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 Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

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

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; and 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 Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

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

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.

Five Nanoscale Science Research Centers (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 Department of Energy'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 electronbeam 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, 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) Division funded programs at the laboratory of the applicant.

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

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, research and development (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<sup>-</sup> currents, requiring tight control of beam losses, and detectors designed for advanced neutron imaging with very high throughput. Particle accelerators are complicated interconnected machines and ideal for applications of artificial intelligence and machine learning algorithms.

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 Scientific User Facilities (SUF) Division funded programs at the laboratory of the applicant.

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

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 encourages 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 techniques for new experimental capabilities, advanced x-ray optics<sup>1</sup> development, and novel approaches to data visualization and analysis.

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

<sup>1</sup> Report for the X-ray Optics for BES Light Source Facilities Workshop, <u>http://science.energy.gov/~/media/bes/pdf/reports/files/X-ray\_Optics\_for\_BES\_Light\_Source\_Facilities\_rpt.pdf.</u>

## (y) Neutron Scattering Instrumentation and Technique Development Technical Contact: Pappannan Thiyagarajan, 301-903-9706, <u>P.Thiyagarajan@science.doe.gov</u>

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 multiferroic materials.

In order to fully exploit the wide range of capabilities of the BES neutron scattering facilities, this program will encourage the development of innovative 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 Scientific User Facilities (SUF) Division funded programs at the laboratory of the applicant.

## Fusion Energy Sciences (FES) Program Website: <u>http://science.energy.gov/fes/</u>

FES's mission 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.

One of the next frontiers for the FES program is the study of the burning plasma state, in which the fusion process itself provides the dominant heat source for sustaining the plasma temperature (i.e., self-heating). Production of strongly self-heated fusion plasma will allow the discovery and study of a number of new scientific phenomena. To achieve these research goals, FES invests in flexible U.S. experimental facilities of various scales, international partnerships leveraging U.S. expertise, large-scale numerical simulations based on experimentally validated theoretical models, development of advanced fusion-relevant materials, and invention of new measurement techniques.

FES also supports discovery plasma science, which is focused on research at the frontiers of basic and low temperature plasma science and high-energy-density laboratory plasmas.

Research is guided by the FES strategic plan, **Fusion Energy Sciences, a Ten-Year Perspective** (2015-2025) (<u>http://science.energy.gov/~/media/fes/pdf/program-documents/FES\_A\_Ten-Year\_Perspective\_2015-2025.pdf</u>), a series of community research needs workshops held in 2015 (<u>http://science.energy.gov/fes/community-resources/workshop-reports/</u>), and reports from the Fusion Energy Sciences Advisory Committee (FESAC) such as the recent 2018 report on "Transformative Enabling Capabilities for Efficient Advance Toward Fusion Energy" (<u>https://science.energy.gov/~/media/fes/fesac/pdf/2018/TEC\_Report\_1Feb20181.pdf</u>).

## 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 and other community input, the Fusion Energy Sciences program supports research on the specific topics below:

## (a) Magnetic Fusion Energy Science Experimental Research Technical Contact: Matt Lanctot, 301-903-1972, <u>matthew.lanctot@science.doe.gov</u>

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 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.

Applications to this area must have a primary focus on experimental research, and address critical issues that may affect the tokamak concept (e.g. plasma disruptions, impulsive heat loads, confinement and transport, and operational maintenance and complexity), or investigate topics common to all fusion power plant concepts (e.g. interactions between plasma and material surfaces). Innovative applications of transformational approaches and technologies such as machine learning, advanced manufacturing, and engineered materials are also encouraged.

Scientists from the U.S. may 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) Stellarator Research in Magnetic Fusion Energy Sciences Technical Contact: Samuel Barish, 301-903-2917, <u>sam.barish@science.doe.gov</u>

This program supports stellarator research on small-, medium-, and large-scale facilities, thereby enhancing the understanding of magnetically-confined plasmas. The stellarator offers attractive solutions to critical challenges to achieve fusion energy by providing a steady-state, disruption-free fusion reactor concept with minimal power requirements for plasma sustainment. Key issues include, but are not limited to, understanding and (if possible) reducing the level of turbulent transport, and improving the understanding of 3-D shaping in an integrated manner in plasmas with higher levels of performance.

Also of interest is stellarator research aimed at resolving magnetic-confinement fusion plasma science issues that will be faced in the next generation of machines, including ITER, and addressing new and unique scientific regimes that can be achieved with long-pulse superconducting international stellarators.

## (c) Magnetic Fusion Energy Science Theory and Simulation Technical Contact: John Mandrekas, 301-903-0552, <u>john.mandrekas@science.doe.gov</u>

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. Applications focusing on computational applications of Quantum Information Science (QIS) that can have a transformative impact on FES mission areas are also encouraged.

## (d) Measurement Innovation Technical Contact: Curt Bolton, 301-903-4914, <u>curt.bolton@science.doe.gov</u>

This program element supports the development of innovative diagnostics to make detailed measurements of the behavior of plasmas. Advances are sought in diagnostic systems to achieve higher resolution or higher reliability, reduce complexity, and improve the ability to function in a burning plasma environment or provide access to previously unmeasured parameters. The proposed measurement innovations should seek to enable breakthroughs in scientific understanding, the linking of theory/computation with experiments, or active control of plasma properties to optimize device operation and plasma performance in a variety of device configurations.

## (e) High-Energy-Density Plasma Science Technical Contact: Kramer Akli, 301-903-2943, <u>kramer.akli@science.doe.gov</u>

High-energy-density laboratory plasmas (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 1Mbar. 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 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 and intense beam physics, and (6) warm dense matter. Applications focusing on developing high energy density materials relevant to QIS are also strongly encouraged.

## (f) General Plasma Science Experiment and Theory Technical Contact: Nirmol Podder, 301-903-9536, <u>nirmol.podder@science.doe.gov</u>

The General Plasma Science (GPS) program is focused on research at the frontiers of basic and low temperature plasma science. The basic plasma science research that is usually funded

through the Magnetic Fusion Energy Science program or the High Energy Density Laboratory Plasmas program will not be considered. Focus areas include: (1) dynamical processes in laboratory plasmas, magnetospheric, solar, and astrophysical plasmas, such as magnetic reconnection, particle energization, plasma dynamo, turbulence and transport, energetic particles, flows, collisional and collisionless shocks; (2) understanding the behavior of dusty plasmas, nonneutral, single-component matter and/or anti-matter plasmas, and ultra-cold neutral plasmas; and (3) understanding plasma processes and/or plasma chemistry in low temperature plasma, interfacial plasma, plasma-surface interaction, interaction of plasma with materials and/or biomaterials, microplasmas, and the synthesis of nanomaterials.

For more information, please see the 2015 report of the panel on frontiers of plasma science (<u>https://science.energy.gov/~/media/fes/pdf/program-news/Frontiers\_of\_Plasma\_Science\_Final\_Report.pdf</u>).

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

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 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 the following topical areas:

- Development of plasma-facing materials and components
- Development of advanced structural and functional materials
- Development of breeder blanket concepts
- Development of tritium fuel cycle technologies
- Development of superconducting magnet technologies

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* (<u>http://science.energy.gov/~/media/fes/pdf/workshop-</u>reports/20120309/FESAC-Materials-Science-final-report.pdf</u>), the 2015 workshop Report on Science Challenges and Research Opportunities in Plasma Materials Interactions (<u>https://science.energy.gov/~/media/fes/pdf/workshop-</u>

<u>reports/2016/PMI\_fullreport\_21Aug2015.pdf</u>), and most recently, the 2018 FESAC report on Transformative Enabling Capabilities for Efficient Advance Towards Fusion Energy (https://science.energy.gov/~/media/fes/fesac/pdf/2018/TEC\_Report\_15Feb2018.pdf).

# High Energy Physics (HEP)

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

HEP's mission 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: <u>http://science.energy.gov/~/media/hep/hepap/pdf/May-2014/FINAL\_P5\_Report\_Interactive\_060214.pdf.</u>

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 from accelerators and reactors are studied using highly sensitive detectors to investigate fundamental forces and particle interactions 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 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, <u>Abid.Patwa@science.doe.gov</u>

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 CMS (Compact Muon Solenoid) 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 <u>not</u> provided under this research area.

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

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 often 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, <u>Kathy.Turner@science.doe.gov</u>

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 <u>not</u> included in this research area.

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

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, <u>Lk.Len@science.doe.gov</u>

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, <u>Helmut.Marsiske@science.doe.gov</u>

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 is 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 and fast-timing capabilities 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.

## Nuclear Physics (NP) Program Website: <u>http://science.energy.gov/np/</u>

NP's mission 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. Additionally, Quantum Information Science (QIS) has been identified as an important cross-cutting topic, with potential impact across all SC mission areas (see <u>https://science.energy.gov/~/media/sc-2/pdf/presentations/2017/DOE-Office\_of\_Science\_Dear\_Colleague\_Letter\_on\_QIS.pdf</u>). NP encourages submission of innovative research ideas to address QIS in any of its subprograms:

- (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

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

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 quarkgluon 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: Paul Sorensen, 301-903-1952, <u>paul.sorensen@science.doe.gov</u>

The Low Energy Nuclear Structure and Nuclear Astrophysics subprogram aims primarily at answering the overarching questions associated with the second frontier identified by NSAC-Nuclei and Nuclear Astrophysics. 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, <u>george.fai@science.doe.gov</u>

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 highprecision studies of cold neutrons.

### (f) Nuclear Data and Nuclear Theory Computing Technical Contact: George Fai, 301-903-8954, <u>george.fai@science.doe.gov</u>

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 manybody 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 <a href="https://science.energy.gov/np/community-resources/reports/">https://science.energy.gov/np/community-resources/reports/</a>.

## (h) Isotope Development and Production for Research and Applications Technical Contact: Ethan Balkin, 301-903-1861, <u>ethan.balkin@science.doe.gov</u>

The mission of the Isotope Development and Production for Research and Applications subprogram (DOE Isotope Program) is to support isotope production and research into novel or improved technologies for production of isotopes to assure the 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 Brookhaven National Laboratory, Los Alamos National Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory. The Program also coordinates and supports isotope production at a suite of university, national laboratory, and other federal accelerator and reactor facilities throughout the Nation to promote a reliable domestic supply of isotopes. 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 existing 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

<u>.pdf</u>. Additional information about the Isotope Program may be found at <u>http://science.energy.gov/np/research/idpra/</u>.

## **Open Science**

SC is dedicated to promoting the values of openness in Federally-supported scientific research, including, but not limited to, ensuring that research may be reproduced and that the results of Federally-supported research are made available to other researchers. These objectives may be met through any number of mechanisms including, but not limited to, data access plans, data sharing agreements, the use of archives and repositories, and the use of various licensing schemes.

The use of the phrase "open-source" does not refer to any particular licensing arrangement, but is to be understood as encompassing any arrangement that furthers the objective of openness.

## Section II – AWARD INFORMATION

## A. TYPE OF AWARD INSTRUMENT

DOE anticipates awarding grants under this FOA.

## **B. ESTIMATED FUNDING**

It is anticipated that up to \$49,000,000 will be available under this FOA, contingent on satisfactory peer review and the availability of appropriated funds. Up to 65 awards are anticipated. Applicants should request project support for five years, with the release of out-year support contingent on adequate progress of the research. Awards are expected to begin in **FY 2019**.

DOE is under no obligation to pay for any costs associated with preparation or submission of applications. DOE reserves the right to fund, in whole or in part, any, all, or none of the applications submitted in response to this FOA.

# C. MAXIMUM AND MINIMUM AWARD SIZE

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

## Ceiling

Historically, the average DOE Early Career Research award has been \$750,000 for five years. Larger awards (historic maximum of \$960,000) are possible with sufficient justification. The ceiling for an application is \$1,000,000 over five years.

## Floor

Applicants are encouraged to request the amount needed for their proposed research program. For this FOA, additional flexibility is anticipated to reflect the variation in research costs by discipline and institution. The minimum request for an application is \$750,000 over five years.

## **D. EXPECTED NUMBER OF AWARDS**

DOE anticipates up to 65 awards under this FOA. The exact number of awards will depend on the number of meritorious applications and the availability of appropriated funds.

# E. ANTICIPATED AWARD SIZE

Applicants are encouraged to propose research expenditures that correspond to the funding needed for their proposed research program. DOE expects the typical award size will be in a narrow range around \$750,000 over five years.

# F. PERIOD OF PERFORMANCE

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

# G. TYPE OF APPLICATION

DOE will only accept new applications under this FOA.

# Section III – ELIGIBILITY INFORMATION

# A. ELIGIBLE APPLICANTS

In accordance with 2 CFR 910.126, Competition, eligibility for award is restricted to the following:

Only U.S. academic institutions are eligible to apply. Other Federal agencies, Federally Funded Research and Development Center (FFRDC) Contractors, and nonprofit organizations described in section 501(c)(4) of the Internal Revenue Code of 1986 that engaged in lobbying activities after December 31, 1995 are not eligible to apply.

The act of submitting an application implies that the submitting institution has checked, confirmed, and certifies that the Principal Investigator is eligible, as outlined in Section III C and D. No additional certifying documentation is required.

Applications must be submitted through a U.S. academic institution. A companion announcement (LAB 19-2019) describes the Early Career Research Program opportunity for full-time DOE national laboratory employees. 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.

# **B. COST SHARING**

Cost sharing is not required.

# C. ELIGIBLE INDIVIDUALS

The Principal Investigator must be an **untenured** Assistant Professor on the tenure track or an **untenured** Associate Professor on the tenure track at a U.S. academic institution as of the deadline for the application. Principal investigator (PI) means the scientist or other individual designated by the recipient institution to direct the project.

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

No more than ten (10) years can have passed between the year the Principal Investigator's Ph.D. was awarded and 2018. For the present competition, those who received doctorates no earlier than 2008 are eligible. If a Principal Investigator has multiple doctorates, the discipline of the one they have earned within the 10-year eligibility window should be relevant to the proposed research.

There can be no co-Principal Investigators.

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

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

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 an application for assistance. Individuals from underrepresented groups as well as individuals with disabilities are always encouraged to apply for assistance.

Eligibility exemptions will not be granted.

# **D. LIMITATIONS ON SUBMISSIONS**

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

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

Letters of recommendation and department chair letters are not allowed. Applications that include recommendation or department chair letters will be subject to elimination from consideration during DOE's initial review.

# Section IV – APPLICATION AND SUBMISSION INFORMATION

# A. ADDRESS TO REQUEST APPLICATION PACKAGE

Application forms and instructions are available at Grants.gov. To access these materials, go to <u>https://www.grants.gov</u>, select "Apply for Grants", and then select "Download Application Package." Enter the CFDA number (81.049) and/or the funding opportunity number (DE-FOA-0002019) shown on the cover of this FOA and then follow the prompts to download the application package.

Applications submitted through <u>www.FedConnect.net</u> will not be accepted.

# **B. LETTER OF INTENT AND PRE-APPLICATION**

## 1. Letter of Intent

Not applicable.

## 2. Pre-application

## February 6, 2019 at 5:00 PM Eastern Time

ENCOURAGE/DISCOURAGE DATE

## March 8, 2019

A pre-application is required and must be submitted by February 6, 2019, at 5:00 PM Eastern Time. The pre-application must be submitted electronically through the DOE SC Portfolio Analysis and Management System (PAMS) website <u>https://pamspublic.science.energy.gov/</u>.

Pre-applications will be reviewed as outlined below. DOE will send a response by email to each applicant encouraging or discouraging the submission of an application by March 8, 2019. Applicants who have not received a response regarding the status of their pre-application by this date are responsible for contacting the program to confirm this status. **Only those applicants that receive notification from DOE encouraging an application may submit applications.** No other applications will be considered.

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

Title of Pre-application PI Name, Job Title Institution PI Phone Number, PI Email Address Year Doctorate Awarded: XXXX Number of Times Previously Applied†: Topic Area\*:

### FOA Number: DE-FOA-0002019

<sup>†</sup> Indicate how many times the PI has previously submitted a full application in the SC Early Career Research Program. The program has been offered in nine previous years, FY 2010 – FY 2018. Participation in the competition is defined as submission of a full, formal application. A PI who has participated in three past SC Early Career Research Program competitions is not eligible.

\* The topic area descriptions can be found in Section I, Supplementary Information, of this FOA. 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 Section I.

This information must be followed by a clear and concise description of the objectives and technical approach of the proposed research. The pre-application may not exceed three 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 three-page limit. If the pre-application narrative exceeds three-pages, only the first three pages will be evaluated in the review of the document.

The information described below on collaborators, advisors and advisees is required and does not count towards the three page limit for the pre-application. Failure to include this information will result in the pre-application being discouraged from submitting a full application.

*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 preceding the closing date of this announcement. If there are no collaborators or co-editors to report, state "None."

Since SC will never use individuals from your institution as reviewers, you may omit them from the pre-application list to save space. Listing collaborators on your pre-application is to help us identify reviewers and does not affect the decision to encourage or discourage submission of a formal application.

*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.

#### PRE-APPLICATION REVIEW

All complete pre-applications will be reviewed to determine their responsiveness to the objectives of the FOA. In addition, if a scientific topic receives a large number of pre-applications, federal Program Managers may evaluate the pre-applications to determine their competitiveness within the scientific topic, based on the following criteria:

- 1. Responsiveness to the objectives of the FOA.
- 2. Scientific and technical merit.
- 3. Appropriateness of the proposed research approaches.
- 4. Likelihood of scientific impact.
- 5. Ensuring a diverse pool of applicants.

Pre-application comparative reviews will compare pre-applications within a topical field with priority given to scientifically innovative and forward-looking basic research with the highest likelihood of success as a full application. These reviews will be conducted by no less than three federal program managers chosen for their topical knowledge and diversity of perspective. The results of the review will be documented.

Applicants with the highest rated pre-applications will be encouraged to submit applications; others will be discouraged from submitting applications. Upon request, feedback from the comparative review will be provided after the deadline for the receipt of applications.

The ratio of encourage/discourage results will differ between topical subjects. DOE is committed to ensuring that a sufficient number of applicants will be encouraged to submit applications to foster a competitive merit review of full applications. The intent in discouraging submission of certain pre-applications is to benefit applicants who otherwise would have prepared and submitted applications with a negligible likelihood of success; noting that the failed application would also then "count" towards the PI's three allowed applications to the SC Early Career Research program.

The PI will be automatically notified when the pre-application is encouraged or discouraged. The DOE SC Portfolio Analysis and Management System (PAMS) will send an email to the PI from <u>PAMS.Autoreply@science.doe.gov</u>, and the status of the pre-application will be updated at the PAMS website <u>https://pamspublic.science.energy.gov/</u>. Notifications are sent as soon as the decisions to encourage or discourage are finalized.

#### **PRE-APPLICATION SUBMISSION**

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

You may use the Internet Explorer, Firefox, Google Chrome, or Safari browsers to access PAMS.

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.

# Please see Section IV, Part I, 4., DOE SC Portfolio Analysis and Management System (PAMS), below, for instructions about how to register in PAMS.

# **Submit Your Pre-Application:**

- Create your pre-application (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 Funding Opportunity 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.
- 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 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 <<u>PAMS.Autoreply@science.doe.gov</u>> 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.

**WARNING**: The PAMS website at <u>https://pampspublic.science.energy.gov</u> will permit you to edit a previously submitted pre-application in the time between your submission and the deadline. If you choose to edit, doing so will remove your previously submitted version from consideration. If you are still editing at the time of the deadline, you will not have a valid submission. Please pay attention to the deadline.

For help with PAMS, click the "External User Guide" link on the PAMS website, <u>https://pamspublic.science.energy.gov/</u>. 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: <u>sc.pams-helpdesk@science.doe.gov</u>. All submission and inquiries about this FOA should reference **DE-FOA-0002019**.

Pre-applications submitted outside PAMS will not be considered. Pre-applications may not be submitted through Grants.gov or www.FedConnect.net.

# C. GRANTS.GOV APPLICATION SUBMISSION AND RECEIPT PROCEDURES

This section provides the application submission and receipt instructions for applications to SC. Please read the following instructions carefully and completely.

## **1. Electronic Delivery**

SC is participating in the Grants.gov initiative to provide the grant community with a single site to find and apply for grant funding opportunities. SC requires applicants to submit their applications online through Grants.gov.

## 2. How to Register to Apply through Grants.gov

a. Instructions: Read the instructions below about registering to apply for SC funds. Applicants should read the registration instructions carefully and prepare the information requested before beginning the registration process. Reviewing and assembling the required information before beginning the registration process will alleviate last-minute searches for required information.

Organizations must have a Data Universal Numbering System (DUNS) Number, active System for Award Management (SAM) registration, and Grants.gov account to apply for grants. If individual applicants are eligible to apply for this funding opportunity, then you may begin with step 3, Create a Grants.gov Account, listed below.

Creating a Grants.gov account can be completed online in minutes, but DUNS and SAM registrations may take several weeks. Therefore, an organization's registration should be done in sufficient time to ensure it does not impact the entity's ability to meet required application submission deadlines.

Complete organization instructions can be found on Grants.gov here: <u>https://www.grants.gov/web/grants/applicants/organization-registration.html</u>

1) *Obtain a DUNS Number*: All entities applying for funding, including renewal funding, must have a DUNS Number from Dun & Bradstreet (D&B). Applicants must enter the DUNS Number in the data entry field labeled "Organizational DUNS" on the SF-424 form. For more detailed instructions for obtaining a DUNS Number, refer to:

https://www.grants.gov/web/grants/applicants/organization-registration/step-1-obtain-dunsnumber.html

2) *Register with SAM*: All organizations applying online through Grants.gov must register with SAM at <u>https://www.sam.gov</u>. Failure to register with SAM will prevent your organization from applying through Grants.gov. SAM registration must be renewed annually. For more detailed instructions for registering with SAM, refer to:

https://www.grants.gov/web/grants/applicants/organization-registration/step-2-register-withsam.html

3) *Create a Grants.gov Account*: The next step is to register an account with Grants.gov. Follow the on-screen instructions or refer to the detailed instructions here: <u>https://www.grants.gov/web/grants/applicants/registration.html</u>

4) *Add a Profile to a Grants.gov Account:* A profile in Grants.gov corresponds to a single applicant organization the user represents (i.e., an applicant) or an individual applicant. If you work for or consult with multiple organizations and have a profile for each, you may log in to one Grants.gov account to access all of your grant applications. To add an organizational profile to your Grants.gov account, enter the DUNS Number for the organization in the DUNS field while adding a profile. For more detailed instructions about creating a profile on Grants.gov, refer to: <u>https://www.grants.gov/web/grants/applicants/registration/add-profile.html</u>

5) *EBiz POC Authorized Profile Roles*: After you register with Grants.gov and create an Organization Applicant Profile, the organization applicant's request for Grants.gov roles and access is sent to the EBiz POC. The EBiz POC will then log in to Grants.gov and authorize the appropriate roles, which may include the AOR role, thereby giving you permission to complete and submit applications on behalf of the organization. You will be able to submit your application online any time after you have been assigned the AOR role. For more detailed instructions about creating a profile on Grants.gov, refer to: https://www.grants.gov/web/grants/applicants/registration/authorize-roles.html

6) *Track Role Status*: To track your role request, refer to: https://www.grants.gov/web/grants/applicants/registration/track-role-status.html

b. *Electronic Signature*: When applications are submitted through Grants.gov, the name of the organization applicant with the AOR role that submitted the application is inserted into the signature line of the application, serving as the electronic signature. The EBiz POC **must** authorize people who are able to make legally binding commitments on behalf of the

organization as a user with the AOR role; this step is often missed and it is crucial for valid and timely submissions.

3. How to Submit an Application to SC via Grants.gov

Grants.gov applicants can apply online using Workspace. Workspace is a shared, online environment where members of a grant team may simultaneously access and edit different webforms within an application. For each FOA, you can create individual instances of a workspace.

Below is an overview of applying on Grants.gov. For access to complete instructions on how to apply for opportunities, refer to: <u>https://www.grants.gov/web/grants/applicants/apply-for-grants.html</u>

1) Create a Workspace: Creating a workspace allows you to complete it online and route it through your organization for review before submitting.

2) Complete a Workspace: Add participants to the workspace, complete all the required forms, and check for errors before submission.

a. Adobe Reader: If you decide not to apply by filling out webforms you can download individual PDF forms in Workspace so that they will appear similar to other Standard forms. The individual PDF forms can be downloaded and saved to your local device storage, network drive(s), or external drives, then accessed through Adobe Reader.

NOTE: Visit the Adobe Software Compatibility page on Grants.gov to download the appropriate version of the software at: <u>https://www.grants.gov/web/grants/applicants/adobe-software-compatibility.html</u>

b. Mandatory Fields in Forms: In the forms, you will note fields marked with an asterisk and a different background color. These fields are mandatory fields that must be completed to successfully submit your application.

c. Complete SF-424 Fields First: The forms are designed to fill in common required fields across other forms, such as the applicant name, address, and DUNS number. To trigger this feature, an applicant must complete the SF-424 information first. Once it is completed, the information will transfer to the other forms.

3) Submit a Workspace: An application may be submitted through workspace by clicking the Sign and Submit button on the Manage Workspace page, under the Forms tab. Grants.gov recommends submitting your application package at least 24-48 hours prior to the close date to provide you with time to correct any potential technical issues that may disrupt the application submission.

4) Track a Workspace: After successfully submitting a workspace package, a Grants.gov Tracking Number (GRANTXXXXXXX) is automatically assigned to the package. The number will be listed on the Confirmation page that is generated after submission.

For additional training resources, including video tutorials, refer to: https://www.grants.gov/web/grants/applicants/applicant-training.html

Applicant Support: Grants.gov provides applicants 24/7 support via the toll-free number 1-800-518-4726 and email at support@grants.gov. For questions related to the specific grant opportunity, contact the number listed in the application package of the grant you are applying for.

If you are experiencing difficulties with your submission, it is best to call the Grants.gov Support Center and get a ticket number. The Support Center ticket number will assist SC with tracking your issue and understanding background information on the issue.

## 4. Timely Receipt Requirements and Proof of Timely Submission

Proof of timely submission is automatically recorded by Grants.gov. An electronic date/time stamp is generated within the system when the application is successfully received by Grants.gov. The applicant AOR will receive an acknowledgement of receipt and a tracking number (GRANTXXXXXXX) from Grants.gov with the successful transmission of their application. Applicant AORs will also receive the official date/time stamp and Grants.gov Tracking number in an email serving as proof of their timely submission.

When SC successfully retrieves the application from Grants.gov, and acknowledges the download of submissions, Grants.gov will provide an electronic acknowledgment of receipt of the application to the email address of the applicant with the AOR role. Again, proof of timely submission shall be the official date and time that Grants.gov receives your application. Applications received by Grants.gov after the established due date for the program will be considered late and will not be considered for funding by SC.

Applicants using slow internet, such as dial-up connections, should be aware that transmission can take some time before Grants.gov receives your application. Again, Grants.gov will provide either an error or a successfully received transmission in the form of an email sent to the applicant with the AOR role. The Grants.gov Support Center reports that some applicants end the transmission because they think that nothing is occurring during the transmission process. Please be patient and give the system time to process the application.

# **D. CONTENT AND APPLICATION FORMS**

## APPLICATION PREPARATION

You must submit the application through Grants.gov at <u>https://www.grants.gov/</u>, using either the online webforms or downloaded forms. (Additional instructions are provided in <u>Section IV, Part</u> <u>C</u> of this FOA.)

You are required to use the compatible version of Adobe Reader software to complete a <u>Grants.gov</u> Adobe application package. To ensure you have the <u>Grants.gov</u> compatible version of Adobe Reader, visit the software compatibility page at <u>https://www.grants.gov/web/grants/applicants/adobe-software-compatibility.html</u>.

You must complete the mandatory forms and any applicable optional forms (e.g., Disclosure of Lobbying Activities (SF-LLL)) in accordance with the instructions on the forms and the additional instructions below.

Files that are attached to the forms must be PDF files unless otherwise specified in this FOA. Attached PDF files must be plain files consisting of text, numbers, and images without editable fields, signatures, passwords, redactions, or other advanced features available in some PDFcompatible software. Do not use PDF portfolios or binders.

Please note the following restrictions that apply to the names of all files attached to your application:

- Please limit file names to 50 or fewer characters
- Do not attach any documents with the same name. All attachments should have a unique name.
- Please use only the following characters when naming your attachments: A-Z, a-z, 0-9, underscore, hyphen, space, period, parenthesis, curly braces, square brackets, ampersand, tilde, exclamation point, comma, semi colon, apostrophe, at sign, number sign, dollar sign, percent sign, plus sign, and equal sign. Attachments that do not follow this rule may cause the entire application to be rejected or cause issues during processing.

#### LETTERS

Letters of recommendation are not allowed. A department chair letter is not required and should not be included. Applications that include recommendation letters or department chair letters will be subject to elimination from consideration during DOE's initial review.

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 must 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 application entitled, "<Application Name>," is selected for funding under the DOE SC 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

## **RESUBMISSION OF APPLICATIONS**

Applications submitted under this FOA may be withdrawn from consideration by using the PAMS website at <u>https://pamspublic.science.energy.gov</u>. Applications may be withdrawn at any time between when the applicant submits the application and when DOE makes the application available to merit reviewers. **Such withdrawals take effect immediately and cannot be reversed**. Please exercise due caution.

After an application is withdrawn, it may be resubmitted only if this FOA is still open for the submission of applications. Such resubmissions will only count as one submission.

Note that there may be a delay between the application's submission in Grants.gov and when it is available to be withdrawn in PAMS. SC will usually consider the last submission, according to its Grants.gov timestamp, to be the intended version. Please consult with your program manager to resolve any confusion about which version of an application should be considered.

## IMPROPER CONTENTS OF APPLICATIONS

Applications submitted under this FOA will be stored in controlled-access systems, but they may be made publicly available if an award is made. As such, it is critical that applicants follow these guidelines:

- Do not include information subject to any legal restriction on its open distribution, whether classified, export control, or unclassified controlled nuclear information.
- Do not include sensitive and protected personally identifiable information, including social security numbers, birthdates, citizenship, marital status, or home addresses. Pay particular attention to the content of biographical sketches and curriculum vitae.
- Do not include letters of support from Federal officials.
- Do not include letters of support on Federal letterhead. Letters that are not letters of support (such as letters confirming access to sites, facilities, equipment, or data; or letters from cognizant contracting officers) may be on Federal letterhead.
- Clearly mark all proprietary or trade-secret information.

## CHANGE OF AWARDEE INSTITUTION

If an awardee chooses to relinquish an award made under this FOA to permit the transfer of the award to a new institution, the new institution must submit an application under the thenavailable SC "annual" or "open" FOA.

## 1. SF-424 (R&R)

Complete this form first to populate data in other forms. Complete all the required fields in accordance with the pop-up instructions on the form. The list of certifications and assurances referenced in Field 17 is available on the DOE Financial Assistance Forms Page at

<u>https://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms</u> under Certifications and Assurances.

DUNS AND EIN NUMBERS (FIELDS 5 AND 6)

The DUNS and Employer Identification Number (EIN) fields on the SF-424 (R&R) form are used in PAMS to confirm the identity of the individual or organization submitting an application.

- Enter each number as a nine-digit number.
- Do not use hyphens or dashes.
- SC does not use the twelve-digit EIN format required by some other agencies.
- SC does not use the DUNS+4 format.

TYPE OF APPLICATION (FIELD 8)

A **new** application is one in which DOE support for the proposed research is being requested for the first time.

Only new applications will be accepted under this FOA.

Please answer "yes" to the question "Is this application being submitted to other agencies?" if substantially similar, identical, or closely related research objectives are being submitted to another Federal agency. Indicate the agency or agencies to which the similar objectives have been submitted.

# 2. Research and Related Other Project Information

## Note concerning question 4.a. and 4.b.

If any environmental impact, positive or negative, is anticipated, indicate "yes" in response to question 4.a., "potential impact – positive or negative - on the environment." Disclosure of the impact should be provided in response to question 4.b. First indicate whether the impact is positive or negative and then identify the area of concern (e.g., air, water, exposure to radiation, etc.).

DOE understands the phrase in field 4.a., "potential impact ... *negative*" to apply if the work described in the application could potentially have any of the impacts listed in (1) through (5) of 10 CFR 1021, Appendix B, Conditions that Are Integral Elements of the Classes of Action. (<u>https://www.ecfr.gov</u>)

Additionally, for actions which could have any other adverse impacts to the environment or have any possibility for adverse impacts to human health (e.g., use of human subjects, Biosafety Level 3-4 laboratory construction/operation, manufacture or use of certain nanoscale materials which are known to impact human health, or any activities involving transuranic or high level radioactive waste, or use of or exposure to any radioactive materials beyond de minimis levels), applicants should indicate a "negative" impact on the environment.

Lastly, 1) if there would be extraordinary circumstances (i.e., scientific or public controversy) related to the significance of environmental effects (10 CFR 1021.410 (b)(2)), 2) if the work is connected to other actions with potentially significant impacts (10 CFR 1021.410 (b)(3), or 3) if the work is related to other nearby actions with the potential for cumulatively significant impacts (10 CFR 1021.410 (b)(3)), applicants should indicate a "negative" impact on the environment.

Complete questions in fields 1 through 6 of the SF-424(R&R) form and attach files. The files must comply with the following instructions:

PROJECT SUMMARY/ABSTRACT (FIELD 7 ON THE FORM)

The project summary/abstract is a summary of the proposed activity suitable for distribution to the public and sufficient to permit potential reviewers to identify conflicts of interest. It must be a self-contained document. Provide the name of the applicant, the project title, the PI and the PI's institutional affiliation, any coinvestigators and their institutional affiliations, the objectives of the project, a description of the project, including methods to be employed, and the potential impact of the project (i.e., benefits, outcomes. A sample is provided below:

A Really Great Idea

A. Smith, Lead Institution (Principal Investigator)A. Brown, Institution 2 (Co-Investigator)A. Jones, Institution 3 (Co-Investigator)

Text of abstract

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. To attach a Project Summary/Abstract, click "Add Attachment."

If an application is recommended for award, the project summary will be used in preparing a public abstract about the award. Award abstracts and titles form a Government document that describes the project and justifies the expenditure of Federal funds in light of the DOE and SC mission statements at <u>https://energy.gov/mission</u> and <u>https://science.energy.gov/about/</u>.

- Do not include any proprietary or sensitive business information.
- DOE may use the abstract may to prepare public reports about supported research.

## DOE COVER PAGE (PART OF PROJECT NARRATIVE ATTACHED TO FIELD 8 ON THE FORM)

The application narrative must begin with a cover page that will not count toward the project narrative page limitation. The cover page must include the following items:

- The project title:
- Applicant Institution:
- Street Address/City/State/Zip:
- Principal Investigator (PI) name:
- Position title for the PI:
- PI telephone number, email:
- Funding Opportunity Announcement Number: DE-FOA-0002019
- DOE/SC Program Office (ASCR, BER, BES, FES, HEP, or NP):
- Topic Area\*:
- Topic Area Program Manager:
- Year Doctorate Awarded:
- Is the PI in a Tenure-Track Appointment: (Yes or No)?
- Does the PI have tenure: (Yes or No)?
- Number of Times Previously Applied<sup>†</sup>:
- PAMS Preproposal (Pre-application)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 FOA. 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.

<sup>†</sup> Indicate how many times the PI has previously submitted a full application in the SC Early Career Research Program. The program has been offered in nine previous years, FY 2010 - FY 2018. Participation in the competition is defined as submission of a full, formal application. A PI who has participated in three past SC 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 applications in the SC 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 FOA, 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 FOA.

§ SC will decline without review any proposal without an encouraged pre-application or without a data management plan.

**Important Instructions to the Sponsored Research Office of Submitting Institutions**: SC requires that you create one single PDF file that contains the DOE Cover Page, project narrative, biographical sketch, current and pending support, bibliography and references cited, facilities and other resources, equipment, data management plan, and other attachments. This single PDF file must be attached in Field 8 on the Grants.gov form. Do not attach any of the items listed in this paragraph separately in any other field in Grants.gov. If you do, these additional attachments

will not become part of the application in PAMS. The application will then either be declined without merit review or reviewed in incomplete form.

## PROJECT NARRATIVE (FIELD 8 ON THE FORM)

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. This page limit does not apply to the Cover Page, Budget Page(s), Budget Justification, Table of Contents, biographical material, publications and references, and appendices, each of which may have its own page limit.

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 application. Merit reviewers are not required to access Internet sites; however, Internet publications in a list of references will be treated identically to print publications. See Section VIII, Part D for instructions on how to mark proprietary application information. To attach a Project Narrative, click "Add Attachment."

Do not attach any files, including requested appendices described below as files, for fields 9, 10, 11, and 12 in Grants.gov. Follow the below instructions to include the information as appendices in the single, bundled project narrative file. These appendices will not count toward the project narrative's page limitation.

APPENDIX 1: BIOGRAPHICAL SKETCH

- Provide the biographical sketch information as an appendix to your project narrative.
- Do not attach a separate file.
- The biographical sketch appendix will not count in the project narrative page limitation.
- The biographical information (curriculum vitae) must not exceed three 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:

A biographical sketch for the PI must be included as an appendix to the technical narrative. Failure to include this information will result in the application being declined without review. 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. The biographical information (curriculum vitae) must not exceed three 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:

- **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.

In addition, the biographical sketch must include information to permit DOE to identify individuals who are conflicted with or potentially biased (favorably or unfavorably) against the investigator. Include a section entitled "**Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers**" that will not count in a page limit. Provide the following information in this section:

- **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 application. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the PI 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 applications 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.

**Personally Identifiable Information**: Do not include sensitive and protected personally identifiable information including social security numbers, birthdates, citizenship, marital status, or home addresses. Do not include information that a merit reviewer should not make use of.

APPENDIX 2: CURRENT AND PENDING SUPPORT

Provide a list of all current and pending support (both Federal and non-Federal) for the PI for

ongoing projects and pending applications. List all sponsored activities or awards requiring a measurable commitment of effort, whether paid or unpaid. Do not list start-up funds provided to the PI by the employing academic institution. If the PI has submitted a similar research application to an early career program at another agency or foundation, this application must be included as a pending application, with the required explanation of the similarities and/or differences with the current Early Career Research Program application.

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 award period (start date end date).
- The person-months of effort per year being dedicated to the award or activity
- Briefly describe the research being performed (or planned for pending applications) and explicitly identify any similarities, differences, overlaps, or synergies with the proposed research.

Provide the Current and Pending Support as an appendix to your project narrative. Concurrent submission of an application 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 application. 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. For proposed investigations requiring access to experimental user facilities maintained by institutions other than the applicant, please provide a document from the facility manager confirming that the researchers will have access to the facility. 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 major items of 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 SC Statement on Digital Data Management (<u>https://science.energy.gov/funding-opportunities/digital-data-management</u>. 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 SC 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 SC 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 <u>http://science.energy.gov/funding-opportunities/digital-data-management/</u>. Applications will not be transferred between program offices.

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

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

#### APPENDIX 7: OTHER ATTACHMENT

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 application. 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 application 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 format shown in Section IV D. Content and Application Forms, under the Letters subheading. Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

#### Follow the above instructions to include the information as appendices to the project narrative file. These appendices will not count toward the project narrative's page limitation.

• Do not attach any files to fields 9, 10, 11, or 12.

#### 3. Research And Related Budget

Complete the Research and Related Budget form in accordance with the instructions on the form (Activate Help Mode to see instructions) and the following instructions. You must complete a separate budget for each year of support requested. The form will generate a cumulative budget

for the total project period. You must complete all the mandatory information on the form before the NEXT PERIOD button is activated. You may request funds under any of the categories listed as long as the item and amount are necessary to perform the proposed work, meet all the criteria for allowability under the applicable Federal cost principles, and are not prohibited by the funding restrictions in this FOA (See Section IV, Part G).

A reasonable start date for use in completing the budget is 09/01/2019. The following budget period start and end dates may be used for proposals submitted to this FOA:

- Budget Period 1: 09/01/2019 08/31/2020
- Budget Period 2: 09/01/2020 08/31/2021
- Budget Period 3: 09/01/2021 08/31/2022
- Budget Period 4: 09/01/2022 08/31/2023
- Budget Period 5: 09/01/2023 08/31/2024

The following advice will improve the accuracy of your budget request:

- Funds requested for personnel must be justified as the product of their effort on the project and their institutional base salary.
- Funds requested for fringe benefits must be calculated as the product of the requested salary and, if present, the negotiated fringe benefit rate contained in an institution's negotiated indirect cost rate agreement.
- Funds requested for indirect costs must be calculated using the correct indirect cost base and the negotiated indirect cost rate.
- You are encouraged to include the rate agreement used in preparing a budget as a part of the budget justification.

If you are proposing indirect costs and do not already have an Indirect Cost Rate Agreement with your Cognizant Federal Agency or documentation of rates accepted for estimating purposes by DOE or another Federal agency, it is recommended that you begin preparing an Indirect Cost Rate Proposal to be submitted, upon request, to the DOE contract specialist/grants management specialist who will evaluate your application if you are selected for award.

For your convenience in preparing an Indirect Cost Rate proposal, a link to applicant resources, including indirect rate model templates, has been provided below: https://science.energy.gov/sbir/applicant-resources/grant-application/.

Section A Senior/Key Person	For each Senior/Key Person, enter the requested information. List personnel, base salary, the number of months that person will be allocated to the project, requested salary, fringe benefits, and the total funds requested for each person. The requested salary must be the product of the base salary and the effort. Include a written narrative in the budget justification that justifies the need for requested personnel.	
Section B	List personnel, the number of months that person will be allocated to	
Other Personnel	the project, requested salary fringe benefits, and the total funds	

Budget Fields

	requested for each person
	requested for each person.
	Include a written narrative in the budget justification that fully justifies
	the need for requested personnel.
Section C Equipment	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 <b>each</b> item of equipment separately and justify each in the budget justification section. Do not aggregate items of equipment. Allowable items ordinarily will be limited to research equipment and apparatus not already available for the conduct of the work. General-purpose office equipment is not eligible for support unless primarily or exclusively used in the actual conduct of scientific research.
Section D	For purposes of this section only, travel to Canada or to Mexico is
Travel	considered domestic 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 the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). 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. Domestic travel is to be justified separately from foreign travel.
Section E	If applicable, submit training support costs. Educational projects that
Participant/Trainee Support Costs	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. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).
Section F	• Materials and Supplies: Enter total funds requested for
Other Direct Costs	<ul> <li>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. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).</li> <li>Publication Costs: Enter the total publication funds requested.</li> </ul>
	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. Indicate the basis for the cost estimate
	(quotes from vendors or suppliers, past experience of similar
	items, or some other basis).
	• <b>Consultant Services:</b> 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. Indicate the basis for the
	cost estimate (quotes from vendors or suppliers, past experience
	of similar items, or some other basis).
	<ul> <li>ADP/Computer Services: Enter total funds requested for</li> </ul>
	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. Indicate the basis for the
	cost estimate (quotes from vendors or suppliers, past experience
	of similar items, or some other basis).
	• 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. Indicate the
	basis for the cost estimate (quotes from vendors or suppliers, past
	experience of similar items, or some other basis).
	• 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	This represents Total Direct Costs (Sections A through F)
Direct Costs	This represents Total Direct Costs (Sections A unough 17)
Section H	Enter the Indirect Cost information for each field. Only four general
Other Indirect Costs	, e
Other multeet Costs	categories of indirect costs are allowed/requested on this form, so
	please consolidate if needed. Include the cognizant Federal agency and
Castian I	contact information if using a negotiated rate agreement.
Section I	This is the total of Sections G and H

Total Direct and	
Indirect Costs	

BUDGET JUSTIFICATION (FIELD L ON THE FORM)

Provide the required supporting information for the following costs (See R&R Budget instructions): equipment; domestic and foreign travel; participant/trainees; materials and supplies; publication; consultant services; ADP/computer services; subaward/consortium/contractual; equipment or facility rental/user fees; alterations and renovations; and indirect cost type. Provide any other information you wish to submit to justify your budget request. **Attach a single budget justification file for the entire project period in field L.** The file automatically carries over to each budget year.

You may wish to include the indirect cost rate agreement as a part of the budget justification.

#### 4. R&R Subaward Budget Attachment(s) Form

Under the Early Career Research Program, preference will be given to applications 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.

**Budgets for Subawardees**: You must provide a separate R&R budget for each subawardee. Download the R&R Budget Attachment from the R&R SUBAWARD BUDGET ATTACHMENT(S) FORM and either e-mail it to each subawardee that is required to submit a separate budget or use the collaborative features of Workspace. After the subawardee has either e-mailed its completed budget back to you or completed it within Workspace, attach it to one of the blocks provided on the form. Use up to 10 letters of the subawardee's name (plus.pdf) as the file name (e.g., ucla.pdf or energyres.pdf). Filenames should not exceed 50 characters.

If the project involves more subawardees than there are places in the SUBAWARD BUDGET ATTACHMENT(S) FORM, the additional subaward budgets may be saved as PDF files and appended to the Budget Justification attached to Field L.

Applicants should consult their local information technology ("IT") support resources for any necessary assistance in converting the forms downloaded from Grants.gov into plain PDF files that can be combined into one non-Portfolio PDF file (the Budget Justification).

Ensure that any files received from subawardees are the PDF files extracted from the SUBAWARD BUDGET ATTACHMENT(S) FORM. Errors will be created if a subawardee sends a prime applicant a budget form that was not extracted from the application package.

Note: If an application proposes subawards to a DOE National Laboratory, a Federal agency, or another Federal agency's FFRDC, the value of such proposed subawards will be deducted from any resulting award: Those classes of organizations must be paid directly by SC. However, the details of such proposed budgets are an essential for understanding and analyzing the proposed research.

#### **5. Project/Performance Site Location(s)**

Indicate the primary site where the work will be performed. If a portion of the project will be performed at any other site(s), identify the site location(s) in the blocks provided.

Note that the Project/Performance Site Congressional District is entered in the format of the 2 digit state code followed by a dash and a 3 digit Congressional district code, for example VA-001. Hover over this field for additional instructions.

Use the Next Site button to expand the form to add additional Project/Performance Site Locations.

#### 6. Summary of Required Forms/Files

Name of Document	Format	Attach to
SF 424 (R&R)	Form	N/A
<b>RESEARCH AND RELATED Other</b> <b>Project Information</b>	Form	N/A
Project Summary/Abstract	PDF	Field 7
Project Narrative, including required appendices	PDF	Field 8
<b>RESEARCH &amp; RELATED BUDGET</b>	Form	N/A
Budget Justification	PDF	Field L
PROJECT/PERFORMANCE SITE LOCATION(S)	Form	N/A
SF-LLL Disclosure of Lobbying Activities, if applicable	Form	N/A

#### E. SUBMISSIONS FROM SUCCESSFUL APPLICANTS

If selected for award, DOE reserves the right to request additional or clarifying information for any reason deemed necessary, including, but not limited to:

- Indirect cost information
- Other budget information
- Name and phone number of the Designated Responsible Employee for complying with national policies prohibiting discrimination (See 10 CFR 1040.5)
- Representation of Limited Rights Data and Restricted Software, if applicable
- Commitment Letter from Third Parties Contributing to Cost Sharing, if applicable
- Environmental Information

Applicants that are not institutions of higher education, that request indirect costs, and that do not already have an Indirect Cost Rate Agreement with their Cognizant Federal Agency or documentation of rates accepted for estimating purposes by DOE or another Federal agency, are

advised to begin preparing an Indirect Cost Rate Proposal for submission, upon request, to the DOE contract specialist/grants management specialist who will evaluate your application if you are selected for award.

# F. SUBMISSION DATES AND TIMES

## **1. Letter of Intent Due Date**

A letter of intent is not required.

## 2. Pre-application Due Date

February 6, 2019 at 5:00 PM Eastern Time

A Pre-Application is required.

You are encouraged to submit your pre-application well before the deadline.

#### **3.** Application Due Date

April 29, 2019 at 5:00 PM Eastern Time

You are encouraged to transmit your application well before the deadline. Modifications to the application are not allowed after the application due date.

## 4. Late Submissions

Delays in submitting letters of intent, pre-applications, and applications may be unavoidable. DOE has accepted late submissions when applicants have been unable to make timely submissions because of widespread technological disruptions or significant natural disasters. DOE has made accommodations for incapacitating or life-threatening illnesses and for deaths of immediate family members. Other circumstances may or may not justify late submissions. Unacceptable justifications include 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.

You are responsible for beginning the submission process in sufficient time to accommodate reasonably foreseeable incidents, contingencies, and disruptions.

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 <u>SC.Early@science.doe.gov</u> 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.

## G. INTERGOVERNMENTAL REVIEW

This program is not subject to Executive Order 12372 Intergovernmental Review of Federal Programs.

## **H. FUNDING RESTRICTIONS**

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

Support for paid collaborators of the PI 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 PI-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 applications 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.

**Cost Principles**: Costs must be allowable, allocable and reasonable in accordance with the applicable Federal cost principles referenced in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation).

**Pre-award Costs**: Recipients may charge to an award resulting from this FOA pre-award costs that were incurred within the ninety (90) calendar day period immediately preceding the effective date of the award, if the costs are allowable in accordance with the applicable Federal cost principles referenced in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation). Recipients must obtain the prior approval of the contracting officer for any pre-award costs that are for periods greater than this 90 day calendar period.

Pre-award costs are incurred at the applicant's risk. DOE is under no obligation to reimburse such costs if for any reason the applicant does not receive an award or if the award is made for a lesser amount than the applicant expected.

## I. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS

## 1. Systems to Register In

Applicants must complete a series of registrations and enrollments to submit applications in

response to this FOA. Applicants not currently registered with SAM and Grants.gov should allow **at least 4 weeks** to complete these requirements.

You should start the process as soon as possible.

You may not be able to use your preferred Internet browser: Each system has its own requirements.

Applicants must obtain a DUNS number at https://fedgov.dnb.com/webform.

Applicants must register with SAM at <u>https://www.sam.gov/</u>. If you had an active registration in the Central Contractor Registry (CCR), you should have an active registration in SAM. More information about SAM registration for applicants is found at <u>https://www.sam.gov/sam/transcript/Quick\_Guide\_for\_Grants\_Registrations.pdf</u>. SAM maintains a complete user guide at <u>https://www.sam.gov/sam/SAM\_Guide/SAM\_User\_Guide.htm</u>.

Applicants must provide a Taxpayer Identification Number (TIN) to complete their registration in SAM.gov. An applicant's TIN is an EIN assigned by the Internal Revenue Service (IRS). In limited circumstances, a Social Security Number (SSN) assigned by the Social Security Administration (SSA) may be used as a TIN. You may obtain an EIN from the IRS at <a href="https://www.irs.gov/businesses/small-businesses-self-employed/apply-for-an-employer-identification-number-ein-online">https://www.irs.gov/businesses/small-businesses-self-employed/apply-for-an-employer-identification-number-ein-online</a>.

DOE discourages the use of a SSN as a TIN. You are encouraged to obtain a TIN from the IRS using the website listed above.

Applicants must register with FedConnect at <u>www.fedconnect.net</u>. The full, binding version of assistance agreements will be posted to FedConnect.

Recipients must register with the Federal Funding Accountability and Transparency Act Subaward Reporting System at <u>https://www.fsrs.gov</u>. This registration must be completed before an award may be made: you are advised to register while preparing your application.

## 2. Registering in Grants.gov

Applicants must register with Grants.gov, following the instructions at <u>https://www.grants.gov/web/grants/applicants/registration.html</u>.

## 3. Where to Submit an Application

You must submit the application through Grants.gov at <u>https://www.grants.gov/</u>, using either the online webforms or downloaded forms. (Additional instructions are provided in Section IV Part A of this FOA.)

Submit electronic applications through the "Apply for Grants" function at <u>www.grants.gov</u>. If

you have problems completing the registration process or submitting your application, call Grants.gov at 1-800-518-4726 or send an email to <u>support@grants.gov</u>.

Please ensure that you have read the applicable instructions, guides, help notices, frequently asked questions, and other forms of technical support on Grants.gov.

## 4. DOE SC Portfolio Analysis and Management System (PAMS)

After you submit your application through Grants.gov, the application will automatically transfer into the Portfolio Analysis and Management System (PAMS) for processing by the DOE SC. Many functions for grants and cooperative agreements can be done in PAMS, which is available at <u>https://pamspublic.science.energy.gov</u>.

You will want to "register to" your application: a process of linking yourself to the application after it has been submitted through Grants.gov and processed by DOE.

You must register in PAMS to submit a pre-application or a letter of intent.

You may use the Internet Explorer, Firefox, Google Chrome, or Safari browsers to access PAMS.

Notifications sent from the PAMS system will come from the PAMS email address <<u>PAMS.Autoreply@science.doe.gov</u>>. 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 <u>https://pamspublic.science.energy.gov/</u>.

- 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 to the "Having Trouble Logging In?" page. (If you have been an SC merit reviewer or if you have previously submitted an application, you may already be linked to an institution in PAMS. If this happens, you will be taken 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 do not need to enter the exact name of the institution, but you should enter a word or phrase contained within the institution name. (If your institution has a frequently used acronym, such as ANL for Argonne National Laboratory or UCLA for the Regents of the University of California, Los Angeles, you may find it easiest to 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.
- If, after searching, you think your institution is not currently in the database, click the "Cannot Find My Institution" button and enter the requested institution information into PAMS. Click the "Create Institution" button. PAMS will add the institution to the system, associate your profile with the new institution, and return you to the "Institutions List" page when you are finished.

For help with PAMS, click the "External User Guide" link on the PAMS website, <u>https://pamspublic.science.energy.gov/</u>. 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: <u>sc.pams-helpdesk@science.doe.gov</u>. All submission and inquiries about this FOA should reference DE-FOA-0002019.

#### 5. Viewing Submitted Applications

Each Grants.gov application submitted to the DOE SC automatically transfers into PAMS and is subsequently assigned to a program manager. At the time of program manager assignment, the three people listed on the SF-424 (R&R) cover page will receive an email with the subject line, "Receipt of Proposal 0000xxxxx by the DOE Office of Science." These three people are the PI (Block 14), Authorized Representative (Block 19), and Point of Contact (Block 5). In PAMS notation, applications are known as proposals, the PI is known as the PI, the Authorized Representative is known as the Sponsored Research Officer/Business Officer/Administrative Officer (SRO/BO/AO), and the Point of Contact is known as the POC.

There will be a period of time between the application's receipt at Grants.gov and its assignment to a DOE SC program manager. Program managers are typically assigned two weeks after

applications are due at Grants.gov: please refrain from attempting to view the proposal in PAMS until you receive an email providing the assignment of a program manager.

Once the email is sent, the PI, SRO/BO/PO, and POC will each be able to view the submitted proposal in PAMS. Viewing the proposal is optional.

You may use the Internet Explorer, Firefox, Google Chrome, or Safari browsers to access PAMS.

Following are two sets of instructions for viewing the submitted proposal, one for individuals who already have PAMS accounts and one for those who do not.

If you already have a PAMS account, follow these instructions:

- 1. Log in to PAMS at <u>https://pamspublic.science.energy.gov/</u>.
- 2. Click the "Proposals" tab and click "Access Previously Submitted Grants.gov Proposal."
- 3. Enter the following information:
  - Proposal ID: Enter the ten-digit PAMS proposal ID, including the leading zeros (e.g., 00002xxxx). Do not use the Grants.gov proposal number. Use the PAMS number previously sent to you in the email with subject line, "Receipt of Proposal ...".
  - Email (as entered in Grants.gov application): Enter your email address as it appears on the SF424(R&R) Cover Page.
  - Choose Role: Select the radio button in front of the role corresponding to the SF-424 (R&R) cover page. If your name appears in block 19 of the SF-424 (R&R) cover page as the authorizing representative, select "SRO/BO/AO (Sponsored Research Officer/Business Officer/Administrative Officer)." If your name appears in block 14 of the SF424 R&R cover page as the PI, select "Principal Investigator (PI)." If your name appears in block 5 of the SF424 R&R as the point of contact, select "Other (POC)."
- 4. Click the "Save and Continue" button. You will be taken to your "My Proposals" page. The Grants.gov proposal will now appear in your list of proposals. Click the "Actions/Views" link in the options column next to this proposal to obtain a dropdown list. Select "Proposal" from the dropdown to see the proposal. Note that the steps above will work only for proposals submitted to the DOE SC since May 2012.

If you do not already have a PAMS account, follow these instructions:

- 1. To register, click the "Create New PAMS Account" link on the website <u>https://pamspublic.science.energy.gov/.</u>
- 2. Click the "No, I have never had an account" link and then the "Create Account" button.
- 3. 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.
- 4. 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.
- 5. 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.

- 6. You will be taken to the Register to Institution page. Select the link labeled, "Option 1: My institution has submitted a proposal in Grants.gov. I am here to register as an SRO, PI, or POC (Sponsored Research Officer, Principal Investigator, or Point of Contact)."
- 7. Enter the following information:
  - Proposal ID: Enter the ten-digit PAMS proposal ID, including the leading zeros (e.g., 00002xxxx). Do not use the Grants.gov proposal number. Use the PAMS number previously sent to you in the email with subject line, "Receipt of Proposal ...".
  - Email (as entered in Grants.gov proposal): Enter your email address as it appears on the SF424(R&R) Cover Page.
  - Choose Role: Select the radio button in front of the role corresponding to the SF-424 (R&R) cover page. If your name appears in block 19 of the SF-424 (R&R) cover page as the authorizing representative, select "SRO/BO/AO (Sponsored Research Officer/Business Officer/Administrative Officer)." If your name appears in block 14 of the SF424 R&R cover page as the PI, select "Principal Investigator (PI)." If your name appears in block 5 of the SF424 R&R as the point of contact, select "Other (POC)."
- 8. Click the "Save and Continue" button. You will be taken to your "My Proposals" page. The Grants.gov proposal will now appear in your list of proposals. Click the "Actions/Views" link in the options column next to this proposal to obtain a dropdown list. Select "Proposal" from the dropdown to see the proposal.

If you were listed as the PI on a prior submission but you have not previously created an account, you may already be listed in PAMS. If this is the case, you will be taken to the PAMS home page after agreeing to the Rules of Behavior. If that happens, follow the instructions listed above under "If you already have a PAMS account..." to access your Grants.gov proposal.

The steps above will work only for proposals submitted to the DOE SC since May 2012.

For help with PAMS, click the "External User Guide" link on the PAMS website, <u>https://pamspublic.science.energy.gov/.</u> 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: <u>sc.pams-helpdesk@science.doe.gov.</u> All submissions and inquiries about this FOA should reference **DE-FOA-0002019**.

# Section V - APPLICATION REVIEW INFORMATION

# A. CRITERIA

## **1. Initial Review Criteria**

Prior to a comprehensive merit evaluation, DOE will perform an initial review in accordance with 10 CFR 605.10(b) to determine that (1) the applicant is eligible for the award; (2) the information required by the FOA has been submitted; (3) all mandatory requirements are satisfied including having an approved pre-application and attachment of a biographical sketch, current and pending support, and data management plan; (4) the proposed project is responsive to the objectives of the funding opportunity announcement; and (5) the proposed project is not duplicative of programmatic work. Applications that fail to pass the initial review will not be forwarded for merit review and will be eliminated from further consideration.

An application declined without merit review by the DOE SC will not count as one of the three allowed submissions to the Early Career Research Program. Likewise, an application withdrawn prior to being sent for merit review by the DOE SC will not count as one of the three allowed submissions.

## 2. Merit Review Criteria

Applications will be subjected to scientific merit review (peer review) and will be evaluated against the following criteria, listed in descending order of importance as found in 10 CFR 605.10 (d), the Office of Science Financial Assistance Program Rule.

- 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 FOA-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 application is submitted.
- 6. Potential for leadership within the scientific community.

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 an application constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

The questions below are provided to the merit reviewers to elaborate the criteria established by regulation:

#### 1. SCIENTIFIC AND/OR TECHNICAL MERIT OF THE PROPOSED RESEARCH

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 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? Does the proposed work take advantage of unique facilities and capabilities?

#### 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 APPLICATION IS SUBMITTED

How does the proposed research contribute to the mission of the program in which the application is being evaluated? Is the proposed research aligned with the program office's priorities as described in advisory committee reports?

#### 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

Applications that pass the initial review will be subjected to a formal merit review and will be evaluated based on the criteria codified at 10 CFR 605.10(d) in accordance with the guidance provided in the "Office of Science Merit Review System for Financial Assistance," which is available at: <u>https://science.energy.gov/grants/policy-and-guidance/merit-review-system/</u>.

## 2. Program Policy Factors

The Selection Official may consider any of the following program policy factors in making the selection, listed in no order of significance:

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

- Institutional history of training and mentoring early-career researchers
- Providing career pathways for the next generation of researchers
- Ensuring opportunities to investigators not currently supported by DOE
- Commitment to sharing the results of research

## 3. Selection

The Selection Official will consider the findings of the merit review and may consider any of the Program Policy Factors described above.

## 4. Review of Risk

Pursuant to 2 CFR 200.205, DOE will conduct an additional review of the risk posed by applications submitted under this FOA. Such review of risk will include:

- Technical merit of the application,
- Reports and findings from audits performed under 2 CFR 200 or OMB Circular A-133, and
- Systems maintained under 2 CFR 180.

DOE may make use of other publicly available information and the history of an applicant's performance under DOE or other Federal agency awards.

Applicants with no prior performance of DOE awards may be asked to provide information about their financial stability and or their ability to comply with the management standards of 2 CFR 200.

REPORTING OF MATTERS RELATED TO RECIPIENT INTEGRITY AND PERFORMANCE (DECEMBER 2015)

DOE, prior to making a Federal award with a total amount of Federal share greater than the simplified acquisition threshold, is required to review and consider any information about the applicant that is in the designated integrity and performance system accessible through SAM (currently FAPIIS) (see 41 U.S.C. 2313); The applicant, at its option, may review information in the designated integrity and performance systems accessible through SAM and comment on any information about itself that a Federal awarding agency previously entered and is currently in the designated integrity and performance system accessible through SAM; DOE will consider any written comments by the applicant, in addition to the other information in the designated integrity, business ethics, and record of performance under Federal awards when completing the review of risk posed by applicants as described in §200.205 Federal awarding agency review of risk posed by applicants.

## 5. Discussions and Award

The Government may enter into discussions with a selected applicant for any reason deemed necessary, including but not limited to the following: (1) the budget is not appropriate or reasonable for the requirement; (2) only a portion of the application is selected for award; (3) the

Government needs additional information to determine that the recipient is capable of complying with the requirements in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation); and/or (4) special terms and conditions are required. Failure to resolve satisfactorily the issues identified by the Government will preclude award to the applicant.

## C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES

It is anticipated that the award selection will be completed by September 30, 2019. It is expected that awards will be made in Fiscal Year 2019.

## Section VI - AWARD ADMINISTRATION INFORMATION

#### A. AWARD NOTICES

SC Early Career Research Program investigators intending to transfer to a new institution must submit a request for transfer along with a new application. If the scope of work has not changed, the award may be transferred. If the scope of work has changed, the new application will be subject to merit review as described above. Transfer awards will be for the remaining award period only, and the requested budget cannot exceed the remaining budget for the original award. While a transfer application 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 application must be accompanied by a letter from the national laboratory director to the technical point of contact confirming that the proposed research 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. The DOE national laboratory employing the principal investigator has the primary responsibility to address funding transition issues that arise when the award ends.

To retain an award at an academic institution, the investigator must remain on the tenure track (e.g., be either tenured or untenured but on the tenure track).

#### **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. (See Section IV, PartG with respect to the allowability of pre-award costs.)

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

#### 2. Notice of Award

An Assistance Agreement issued by the contracting officer is the authorizing award document. It normally includes, either as an attachment or by reference, the following items: (1) Special Terms and Conditions; (2) Applicable program regulations, if any; (3) Application as approved by DOE; (4) 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation); (5) National Policy Assurances To Be Incorporated As Award Terms; (6) Budget Summary; (7)

General Terms and Conditions; and (8) Federal Assistance Reporting Checklist, which identifies the reporting requirements.

For grants and cooperative agreements made to universities, non-profits and other entities subject to Title 2 CFR, research awards made under this funding opportunity will be subject to the government-wide Research Terms and Conditions published at <a href="https://www.nsf.gov/pubs/policydocs/rtc/rtcoverlay\_march17.pdf">https://www.nsf.gov/pubs/policydocs/rtc/rtcoverlay\_march17.pdf</a> and the DOE Agency Specific Standard Research Terms and Conditions published at <a href="https://www.nsf.gov/pubs/policydocs/rtc/rtcoverlay\_march17.pdf">https://www.nsf.gov/pubs/policydocs/rtc/rtcoverlay\_march17.pdf</a> and the DOE Agency Specific Standard Research Terms and Conditions published at <a href="https://www.nsf.gov/pubs/policydocs/rtc/agencyspecifics/doe\_417.pdf">https://www.nsf.gov/pubs/policydocs/rtc/rtcoverlay\_march17.pdf</a>. These Terms and Conditions published at <a href="https://www.nsf.gov/pubs/policydocs/rtc/agencyspecifics/doe\_417.pdf">https://www.nsf.gov/pubs/policydocs/rtc/agencyspecifics/doe\_417.pdf</a>. These Terms and Conditions will be incorporated in the award by reference.

## **B. ADMINISTRATIVE AND NATIONAL POLICY REQUIREMENTS**

#### 1. Administrative Requirements

The administrative requirements for DOE grants and cooperative agreements are contained in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation).

NONDISCLOSURE AND CONFIDENTIALITY AGREEMENTS REPRESENTATIONS (JUNE 2015)

In submitting an application in response to this FOA the Applicant represents that: (1) It **does not and will not** require its employees or contractors to sign internal nondisclosure or confidentiality agreements or statements prohibiting or otherwise restricting its employees or contactors from lawfully reporting waste, fraud, or abuse to a designated investigative or law enforcement representative of a Federal department or agency authorized to receive such information.

(2) It **does not and will not** use any Federal funds to implement or enforce any nondisclosure and/or confidentiality policy, form, or agreement it uses unless it contains the following provisions:

a. "These provisions are consistent with and do not supersede, conflict with, or otherwise alter the employee obligations, rights, or liabilities created by existing statute or Executive order relating to (1) classified information, (2) communications to Congress, (3) the reporting to an Inspector General of a violation of any law, rule, or regulation, or mismanagement, a gross waste of funds, an abuse of authority, or a substantial and specific danger to public health or safety, or (4) any other whistleblower protection. The definitions, requirements, obligations, rights, sanctions, and liabilities created by controlling Executive orders and statutory provisions are incorporated into this agreement and are controlling."

b. The limitation above shall not contravene requirements applicable to Standard Form 312, Form 4414, or any other form issued by a Federal department or agency governing the nondisclosure of classified information.

c. Notwithstanding provision listed in paragraph (a), a nondisclosure or confidentiality policy form or agreement that is to be executed by a person connected with the conduct of an intelligence or intelligence-related activity, other than an employee or officer of the United States Government, may contain provisions appropriate to the particular activity for which such document is to be used. Such form or agreement shall, at a minimum,

require that the person will not disclose any classified information received in the course of such activity unless specifically authorized to do so by the United States Government. Such nondisclosure or confidentiality forms shall also make it clear that they do not bar disclosures to Congress, or to an authorized official of an executive agency or the Department of Justice, that are essential to reporting a substantial violation of law.

#### **REGISTRATION REQUIREMENTS**

Additional administrative requirements for DOE grants and cooperative agreements are contained in 2 CFR 25 (See: <u>https://www.ecfr.gov</u>). Prime awardees must keep their data in SAM current at <u>https://www.sam.gov</u>. SAM is the government-wide system that replaced the Central Contractor Registry (CCR). If you had an active registration in the CCR, you have an active registration in SAM. Subawardees at all tiers must obtain DUNS numbers and provide the DUNS to the prime awardee before the subaward can be issued.

#### SUBAWARD AND EXECUTIVE REPORTING

Additional administrative requirements necessary for DOE grants and cooperative agreements to comply with the Federal Funding and Transparency Act of 2006 (FFATA) are contained in 2 CFR 170. (See: <u>https://www.ecfr.gov</u>). Prime awardees must register with the new FSRS database and report the required data on their first tier subawardees. Prime awardees must report the executive compensation for their own executives as part of their registration profile in SAM.

#### PROHIBITION ON LOBBYING ACTIVITY

By accepting funds under this award, you agree that none of the funds obligated on the award shall be expended, directly or indirectly, to influence congressional action on any legislation or appropriation matters pending before Congress, other than to communicate to Members of Congress as described in 18 USC 1913. This restriction is in addition to those prescribed elsewhere in statute and regulation.

#### 2. Terms and Conditions

The DOE Special Terms and Conditions for Use in Most Grants and Cooperative Agreements are located at <u>https://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms</u> under Award Terms.

The standard DOE financial assistance intellectual property provisions applicable to various types of recipients are located at: https://energy.gov/gc/standard-intellectual-property-ip-provisions-financial-assistance-awards

#### **3. National Policy Assurances**

The National Policy Assurances To Be Incorporated As Award Terms are located at <u>https://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms</u> under Award Terms.

## 4. Statement of Substantial Involvement

Not applicable.

#### 5. Additional Conditions

#### CONFERENCE SPENDING (FEBRUARY 2015)

The recipient shall not expend any funds on a conference not directly and programmatically related to the purpose for which the grant or cooperative agreement was awarded that would defray the cost to the United States Government of a conference held by any Executive branch department, agency, board, commission, or office for which the cost to the United States Government would otherwise exceed \$20,000, thereby circumventing the required notification by the head of any such Executive Branch department, agency, board, commission, or office to the Inspector General (or senior ethics official for any entity without an Inspector General), of the date, location, and number of employees attending such conference.

CORPORATE FELONY CONVICTION AND FEDERAL TAX LIABILITY REPRESENTATIONS (MARCH 2014)

In submitting an application in response to this FOA the Applicant represents that:

- It is **not** a corporation that has been convicted of a felony criminal violation under any Federal law within the preceding 24 months,
- It is **not** a corporation that has any unpaid Federal tax liability that has been assessed, for which all judicial and administrative remedies have been exhausted or have lapsed, and that is not being paid in a timely manner pursuant to an agreement with the authority responsible for collecting the tax liability.

For purposes of these representations the following definitions apply:

• A Corporation includes any entity that has filed articles of incorporation in any of the 50 states, the District of Columbia, or the various territories of the United States [but not foreign corporations]. It includes both for-profit and non-profit organizations.

#### PUBLICATIONS

The recipient is expected to publish or otherwise make publicly available the results of the work conducted under any award resulting from this FOA. Publications and other methods of public communication describing any work based on or developed under an award resulting from this FOA must contain an acknowledgment of SC support. The format for such acknowledgments is provided at <a href="https://science.energy.gov/funding-opportunities/acknowledgments/">https://science.energy.gov/funding-opportunities/acknowledgments/</a>. The author's copy of any peer-reviewed manuscript accepted for funding must be announced to DOE's Office of Scientific and Technical Information (OSTI) and made publicly available in accordance with the instructions contained in the Reporting Requirements Checklist incorporated in all Assistance Agreements.

# **C. REPORTING**

Reporting requirements are identified on the Federal Assistance Reporting Checklist, DOE F 4600.2, attached to the award agreement. The checklist is available at <a href="https://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms">https://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms</a> under Award Forms.

## Section VII - QUESTIONS/AGENCY CONTACTS

#### A. QUESTIONS

Questions relating to the Grants.gov registration process, system requirements, how an application form works, or the submittal process must be directed to Grants.gov at 1-800-518-4726 or <u>support@grants.gov</u>. DOE cannot answer these questions.

Please only contact the Grants.gov help desk for questions related to Grants.gov.

For help with PAMS, click the "External User Guide" link on the PAMS website, <u>https://pamspublic.science.energy.gov/</u>. 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: <u>sc.pams-helpdesk@science.doe.gov</u>. All submission and inquiries about this FOA should reference **DE-FOA-0002019**.

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 FOA or below. Please contact the program staff with all questions not directly related to the Grants.gov or PAMS systems.

Grants.gov	800-518-4726 (toll-free)	
Customer Support	support@grants.gov	
PAMS	855-818-1846 (toll-free)	
Customer Support	301-903-9610	
	sc.pams-helpdesk@science.doe.gov	
Administrative Contact	Questions about program rules should be sent to	
	SC.Early@science.doe.gov	
Program Manager	Questions regarding the specific program areas/technical	
Scientific Contact	requirements can be directed to the program managers /	
	technical contacts listed for each program within the FOA.	

## **B. AGENCY CONTACTS**

# Section VIII - OTHER INFORMATION

## A. MODIFICATIONS

Notices of any modifications to this FOA will be posted on Grants.gov and the FedConnect portal. You can receive an email when a modification or an FOA message is posted by registering with FedConnect as an interested party for this FOA. It is recommended that you register as soon after release of the FOA as possible to ensure you receive timely notice of any modifications or other FOAs. More information is available at <a href="https://www.fedconnect.net">https://www.fedconnect.net</a>.

# **B. GOVERNMENT RIGHT TO REJECT OR NEGOTIATE**

DOE reserves the right, without qualification, to reject any or all applications received in response to this FOA and to select any application, in whole or in part, as a basis for negotiation and/or award.

# C. COMMITMENT OF PUBLIC FUNDS

(a) A DOE financial assistance award is valid only if it is in writing and is signed, either in writing or electronically, by a DOE Contracting Officer.

(b) Recipients are free to accept or reject the award. A request to draw down DOE funds constitutes the Recipient's acceptance of the terms and conditions of this Award.

# **D. PROPRIETARY APPLICATION INFORMATION**

Patentable ideas, trade secrets, proprietary or confidential commercial or financial information, disclosure of which may harm the applicant, should be included in an application 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 application which are to be restricted:

"The data contained in pages \_\_\_\_\_\_ of this application have been submitted in confidence and contain trade secrets or proprietary information, and such data shall be used or disclosed only for evaluation purposes, provided that if this applicant receives an award as a result of or in connection with the submission of this application, DOE shall have the right to use or disclose the data herein to the extent provided in the award. This restriction does not limit the government's right to use or disclose data obtained without restriction from any source, including the applicant."

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. Non-Federal reviewers must sign conflict of interest agreement prior to reviewing an application. Non-Federal personnel conducting administrative activities must sign a non-disclosure agreement.

# F. INTELLECTUAL PROPERTY DEVELOPED UNDER THIS PROGRAM

**Patent Rights:** The government will have certain statutory rights in an invention that is conceived or first actually reduced to practice under a DOE award. 42 USC 5908 provides that title to such inventions vests in the United States, except where 35 USC 202 provides otherwise for nonprofit organizations or small business firms. However, the Secretary of Energy may waive all or any part of the rights of the United States subject to certain conditions. (See "Notice of Right to Request Patent Waiver" in paragraph G below.)

**Rights in Technical Data**: Normally, the government has unlimited rights in technical data created under a DOE agreement. Delivery or third party licensing of proprietary software or data developed solely at private expense will not normally be required except as specifically negotiated in a particular agreement to satisfy DOE's own needs or to insure the commercialization of technology developed under a DOE agreement.

# G. NOTICE OF RIGHT TO REQUEST PATENT WAIVER

Applicants may request a waiver of all or any part of the rights of the United States in inventions conceived or first actually reduced to practice in performance of an agreement as a result of this FOA, in advance of or within 30 days after the effective date of the award. Even if such advance waiver is not requested or the request is denied, the recipient will have a continuing right under the award to request a waiver of the rights of the United States in identified inventions, i.e., individual inventions conceived or first actually reduced to practice in performance of the award. Any patent waiver that may be granted is subject to certain terms and conditions in 10 CFR 784. For more information, see <a href="https://energy.gov/gc/services/technology-transfer-and-procurement/office-assistant-general-counsel-technology-transf-1">https://energy.gov/gc/services/technology-transfer-and-procurement/office-assistant-general-counsel-technology-transf-1</a>

Domestic small businesses and domestic nonprofit organizations will receive the patent rights clause at 37 CFR 401.14, i.e., the implementation of the Bayh-Dole Act. This clause permits domestic small business and domestic nonprofit organizations to retain title to subject inventions. Therefore, small businesses and nonprofit organizations do not need to request a waiver.

## H. NOTICE REGARDING ELIGIBLE/INELIGIBLE ACTIVITIES

Eligible activities under this program include those which describe and promote the understanding of scientific and technical aspects of specific energy technologies, but not those

which encourage or support political activities such as the collection and dissemination of information related to potential, planned or pending legislation.

# I. 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.

# J. ENVIRONMENTAL, SAFETY AND HEALTH (ES&H) PERFORMANCE OFWORK AT DOE FACILITIES

With respect to the performance of any portion of the work under this award which is performed at a DOE-owned or controlled site, the recipient agrees to comply with all state and Federal ES&H regulations, and with all other ES&H requirements of the operator of such site.

Prior to the performance on any work at a DOE-Owned or controlled site, the recipient shall contact the site facility manager for information on DOE and site specific ES&H requirements.

The recipient shall apply this provision to all subawardees at any tier.

# K. FEDERAL, STATE, AND LOCAL REQUIREMENTS

With respect to the performance of any portion of the work under this award, the recipient agrees to comply with all applicable local, state, and Federal ES&H regulations. The recipient shall apply this provision to all sub awardees at any tier.

## L. NATIONAL ENVIRONMENTAL POLICY ACT (NEPA) COMPLIANCE

If question 4.a. on the "Research and Related Other Project Information" document indicates "potential impact on the environment", or if DOE's own review indicates it, DOE may ask the applicant to provide additional information on those impacts in order to prepare an environmental critique/synopsis per 10 CFR 1021.216. Note that this pre-award environmental critique/synopsis process would be separate from the preparation of a NEPA document such as an environmental impact statement (EIS) or an environmental assessment (EA). If DOE determines the latter documentation is necessary, this process would need to be completed, funded by and with the participation of the awardee, prior to them taking any action on the proposed project that could have adverse environmental effects or that could limit the choice of reasonable alternatives. The inability to satisfy the NEPA requirements after an award would result in cancellation of the award. Note that in most cases, even where potential impact on the environment exists, preparation of such NEPA documents is rarely necessary, but DOE has the expectation that the Applicant will disclose the potential, which would serve to initiate dialog with DOE if necessary. Should the applicant have any uncertainty, they should check "yes."