DEPARTMENT OF ENERGY OFFICE OF SCIENCE



## FY 2018 CONTINUATION OF SOLICITATION FOR THE OFFICE OF SCIENCE FINANCIAL ASSISTANCE PROGRAM

# FUNDING OPPORTUNITY ANNOUNCEMENT (FOA) NUMBER: DE-FOA-0001820

## FOA Type: Amendment 000002 CFDA Number: 81.049

| FOA Issue Date:                            | May 25, 2018                                  |
|--|---|
| Submission Deadline for Letters of Intent: | N/A   |
| Submission Deadline for Pre-Applications:  | A pre-application is optional                 |
| <b>Pre-Application Response Date:</b>      | N/A   |
| Submission Deadline for Applications:      | N/A   |
|  | This FOA will remain open until March 1, 2019 |
|  | or until replaced by a successor FOA.         |
|  | Applications may be submitted any time during |
|  | this period.                                  |

Amendment 2: The amendment will change the close date to March 1, 2019.

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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.

## 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/applicants/workspace</a>.

#### **RENEWAL APPLICATIONS**

The Principal Investigator (PI) for any application submitted for a **renewal** (an addition of a project period) of an existing award will be required to submit a Renewal Proposal Products section through the PAMS website at <u>https://pamspublic.science.energy.gov</u>. The submitted product list will be sent for merit review as part of the application. The application will not be considered complete and cannot be sent for review until the product list has been submitted.

#### 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 Section 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 program technical requirements must be directed to the point of contact listed for each program area within this FOA.

## 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

The Department of Energy (DOE)'s Office of Science (SC) hereby announces its continuing interest in receiving grant applications for support of work in the following program areas: Advanced Scientific Computing Research, Basic Energy Sciences, Biological and Environmental Research, Fusion Energy Sciences, High Energy Physics, and Nuclear Physics. On September 3, 1992, DOE published in the Federal Register the Office of Energy Research Financial Assistance Program (now called the Office of Science Financial Assistance Program), 10 CFR 605, as a Final Rule, which contained a solicitation for this program. Information about submission of applications, eligibility, limitations, evaluation and selection processes and other policies and procedures are specified in 10 CFR 605.

This FOA, DE-FOA-0001820, is our annual, broad, open solicitation that covers all of the research areas in SC and is open throughout the Fiscal Year.

This FOA will remain open until March 1, 2019, 11:59 PM Eastern Time, or until it is succeeded by another issuance, whichever occurs first. This annual FOA DE-FOA-0001820 succeeds FOA DE-FOA-0001664, which was published October 1, 2016.

## SUPPLEMENTARY INFORMATION

The SC mission is to deliver 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.

SC manages its research portfolio through six scientific program offices. The following program descriptions, websites, and technical points of contact are offered to provide more in-depth information on scientific and technical areas of interest to SC:

#### 1. Advanced Scientific Computing Research (ASCR)

- (a) Applied Mathematics
- (b) Computer Science
- (c) Computational Partnerships

#### 2. Basic Energy Sciences (BES)

- (a) Materials Chemistry
- (b) Biomolecular Materials
- (c) Synthesis and Processing Science
- (d) Experimental Condensed Matter Physics
- (e) Theoretical Condensed Matter Physics
- (f) Physical Behavior of Materials
- (g) Mechanical Behavior and Radiation Effects
- (h) X-ray Scattering

- (i) Neutron Scattering
- (j) Electron and Scanning Probe Microscopies
- (k) Atomic, Molecular, and Optical Sciences
- (1) Gas Phase Chemical Physics
- (m) Computation and Theoretical Chemistry
- (n) Condensed Phase and Interfacial Molecular Science
- (o) Catalysis Science
- (p) Separations and Analysis
- (q) Heavy Element Chemistry
- (r) Geosciences
- (s) Solar Photochemistry
- (t) Photosynthetic Systems
- (u) Physical Biosciences
- (v) BES Accelerator and Detector Research

## 3. Biological and Environmental Research (BER)

- (a) Biological Systems Science
- (b) Earth and Environmental Systems Sciences

## 4. Fusion Energy Sciences (FES)

- (a) Burning Plasma Science: Foundations—Advanced Tokamak and Spherical Tokamak
- (b) Burning Plasma Science: Foundations—Theory & Simulation
- (c) Burning Plasma Science: Long Pulse—Tokamak & Stellarator
- (d) Burning Plasma Science: Long Pulse—Materials & Fusion Nuclear Science
- (e) Discovery Plasma Science: Plasma Science Frontiers
- (f) Discovery Plasma Science: Measurement Innovation

## 5. High Energy Physics (HEP)

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

#### 6. Nuclear Physics (NP)

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

## 1. Advanced Scientific Computing Research (ASCR)

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

The mission of the Advanced Scientific Computing Research (ASCR) program is to advance applied mathematics and computer science; deliver the most advanced computational scientific applications in partnership with disciplinary science; advance computing and networking capabilities; and develop future generations of computing hardware and software tools for science, in partnership with the research community, including U.S. industry. The strategy to accomplish this has two thrusts: developing and maintaining world-class computing and network facilities for science; and advancing research in applied mathematics, computer science and advanced networking.

The priority areas for ASCR include the following:

- Develop mathematical models, methods and algorithms to accurately describe and predict the behavior of complex systems involving processes that span vastly different time and/or length scales.
- Advance key areas of computer science that:
  - Enable the design and development of extreme scale computing systems and their effective use in the path to scientific discoveries; and
  - Transform extreme scale data from experiments and simulations into scientific insight.
- Advance key areas of computational science and discovery that support SC's missions through mutually beneficial partnerships.
- Develop and deliver forefront computational, networking and collaboration tools and facilities that enable scientists worldwide to work together to extend the frontiers of science.

The computing resources and high-speed networks required to meet SC needs exceed the stateof- the-art by a significant margin. Furthermore, the system software, algorithms, software tools and libraries, programming models and the distributed software environments needed to accelerate scientific discovery through modeling and simulation are beyond the realm of commercial interest. To establish and maintain DOE's modeling and simulation leadership in scientific areas that are important to its mission, ASCR operates Leadership Computing facilities a high-performance production computing center, and a high-speed network, implementing a broad base research portfolio in applied mathematics, computer and network sciences, and computational science to solve complex problems on computational resources that are on a trajectory to reach exascale within a few years.

The ASCR subprograms and their objectives follow:

#### (a) Applied Mathematics

This subprogram supports research and development of applied mathematical models, methods, and algorithms for understanding complex natural and engineered systems related to DOE's mission. Important areas of supported research include: (1) novel numerical methods for the

scalable solution of large-scale, linear and nonlinear systems of equations, including those solution methods that take into consideration the possibilities brought about by future HPC architectures; (2) optimization techniques and next-generation solvers; (3) numerical methods for modeling multiscale, multi-physics or multi-component continuous or discrete systems that span a wide range of time and length scales; (4) methods of simulation and analysis of systems that account for the uncertainties of the systems, or are inherently stochastic or uncertain; and (5) innovative approaches for analyzing and extracting insight from large-scale data sets. Submission of preliminary research descriptions (e.g., preproposals, preapplications) is strongly encouraged. They will be reviewed for responsiveness of the proposed work to the research topics. Send e-mail to the Subprogram Contact for information regarding format and content.

#### Subprogram Contact:

• Steven Lee, (301) 903-5710, <u>Steven.Lee@science.doe.gov</u> Website: <u>http://science.energy.gov/ascr/research/applied-mathematics/</u>

## (b) Computer Science

This subprogram supports basic research to utilize computing at extreme scales, including distributed computing and science instruments, and to understand extreme scale data from both simulations and experiments. It also supports research in computer science that enables scientific applications and data-driven computational science through advances in computing systems, including systems in the Beyond Moore's Law era.

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

- Data analysis and visualization: techniques for deriving and visualizing insights from large scale and/or high dimensional simulation, experimental, or observational data or combinations of these as relevant to SC and DOE priority applications; visual analysis of uncertainty and the sources thereof; visual analytic approaches to understanding the state and behavior of a supercomputing system at scale.
- Techniques for insitu data analysis and workflow management in high performance computing environments;
- Techniques and tools for advancing fundamental practices of management, archiving, curation, and/or reuse, of data generated by experimental, observational, and simulation data relevant to SC mission areas.
- Knowledge representation and machine learning for analysis of extreme scale scientific data from simulations and/or experiments.
- Storage system software and/or scientific databases for extreme scale data that support scientists' models of their data and the use thereof.
- Programming models, environments and tools that increase code portability, increase levels of abstraction, increase developer productivity, and/or make programming for HPC more accessible for newcomers to the field.
- Operating and runtime systems, including intelligent resource management, and workflow management systems, that support use of heterogeneous computing

technologies, including diverse processors, accelerators, and memory and storage systems.

- Execution models and metrics to guide development and evaluation of software systems and applications for heterogeneous hardware environments.
- Research focused on information processing and computation systems for neuromorphic computing including hardware architectures, development of programming environments, languages, libraries, compilers, simulators, and research and development on their algorithms for physical simulation.
- Cybersecurity for scientific computing integrity: research on security techniques appropriate for open scientific environments, with a focus on ensuring scientific integrity in the context of extreme scale high performance computing and to deliver means that assure trustworthiness within open high-end networking and data centers.
- Machine learning in the narrow context of high performance computing, relevant to SC user facilities including those supported by ASCR, and extreme scale applications for the acceleration of scientific discovery and its applications.
- Autonomic computing and communication systems that integrate advances in applied artificial intelligence, Software Defined Networks (SDN), Science Internet of Things (S-IoT), and network analytics to support a new generation smart science facilities.

Topics that are out of scope for Computer Science include:

- Proposals that address topics not covered in the Computer Science Topics of Interest above, except with the specific encouragement of a Computer Science program manager in response to a preproposal;
- Proposals with primary emphasis on hardware design, resilient solvers, and/or new development of machine probabilistic methods and their mathematical formalisms;
- All aspects of computer-supported collaboration, social computing, natural language processing / understanding / generation and/or analysis, and generalized research in human-computer interaction;
- Discipline-specific data analytics and informatics;
- Research focused on the World Wide Web, the dark web, and/or data about it;
- Research that is primarily to advance cloud computing, and/or hand-held, portable, desktop, and/or embedded computing; and
- Research and applications not motivated and justified in the context of current and future SC user facilities, including those supported by ASCR (i.e., Argonne Leadership Computing Facility or ALCF, Oak Ridge Leadership Computing Facility or OLCF, and National Energy Research Scientific Computing Center or NERSC): <u>https://science.energy.gov/ascr/facilities/</u>

Subprogram Contacts:

- Laura Biven (301) 903-9556, <u>Laura.Biven@science.doe.gov</u>, data management, analysis and visualization; in-situ workflow management systems;
- Thomas Ndousse-Fetter, (301) 903-9960, <u>Thomas.Ndousse-Fetter@science.doe.gov</u>, network science and the Science Internet of Things;
- Lucy Nowell, (301) 903-3191, Lucy.Nowell@science.doe.gov, system software stack,

systems software aspects of support for in-situ workflow management, and programming environments, languages and tools; and

• Robinson Pino, (301) 903-1263, <u>Robinson.Pino@science.doe.gov</u>, machine learning, neuromorphic computing, and cybersecurity.

Website: http://science.energy.gov/ascr/research/computer-science/

## (c) Computational Partnerships

This subprogram supports research that will utilize or lead to partnerships with SC, National Nuclear Security Administration (NNSA), or other DOE programs. This includes research in pioneering science applications for the next generation of high-performance computing and research that incorporates and integrates applied mathematics, computer science, and computational sciences, to enable scientists to exploit effectively extreme

scale computers in their pursuit of transformational scientific discovery through simulation and modeling.

For examples of SciDAC partnerships, refer to the website <u>https://www.scidac.gov</u>. For examples of extreme scale computing systems, refer to the website: <u>https://science.energy.gov/~/media/ascr/pdf/facilities/ASCR\_Computing\_Facility\_Upgrades.pdf</u>

Additionally, this subprogram supports basic research to enable scientists to easily find and interact with unique scientific facilities and data, and to work with peers or facilities staff involved in a scientific discovery process. Research topics of interest include: Theories, algorithms, tools, and services needed to create diverse computing environments where multiple resources can be combined in unique ways to suit the needs of the science community, mechanisms and theories to enable scientists to interact with their peers and technical staff that operate a distributed scientific facility and tools and services needed to support physical experiments in testbeds and production networks.

Subprogram Contacts:

- Randall Laviolette, (301) 903-5195, <u>Randall.Laviolette@science.doe.gov</u> and Ceren Susut, (301)903-0366, <u>Ceren.Susut-Bennett@science.doe.gov</u>, SciDAC Partnerships;
- Richard Carlson, (301) 903-9486, <u>Richard.Carlson@science.doe.gov</u>, Partnerships that enable scientists to easily find and interact with unique scientific facilities.

Website: http://science.energy.gov/ascr/research/scidac/

## 2. Basic Energy Sciences (BES)

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

The mission of the Basic Energy Sciences (BES) program is to support fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security. The portfolio supports work in the natural sciences by emphasizing fundamental research in materials sciences, chemistry, geosciences, and biosciences. BES-supported scientific user facilities provide specialized instrumentation and expertise that enable scientists to carry out experiments not possible at individual laboratories.

The BES divisions, program areas, and their objectives follow:

## **Materials Sciences and Engineering**

The Materials Sciences and Engineering (MSE) Division supports fundamental experimental and theoretical research to provide the knowledge base for the discovery and design of new materials with novel structures, functions, and properties. This knowledge serves as a basis for the development of new materials for the generation, storage, and use of energy and for mitigation of the environmental impacts of energy use. The MSE research portfolio consists of the research program areas listed below.

## MSE Division Website: http://science.energy.gov/bes/mse/

## (a) Materials Chemistry

This program supports research on materials with a focus on the role of chemical reactivity, chemical transformation, and chemical dynamics on the material composition, structure, function, and lifetime across the range of length scales from atomic to mesoscopic. The program emphasis is on hypothesis-driven research on the chemistry-based synthesis of materials compositions and/or morphologies and on the chemical transformations that occur in functional materials in operating environments related to DOE's energy mission. Included are covalent and non-covalent assembly of materials, discovery of the mechanistic detail of chemical transformations and dynamics, utilization of chemistry to control interfacial properties and interactions, and new approaches involving the integration of theory and experiment.

Major scientific areas of interest include: (1) Fundamental aspects of the chemical synthesis and assembly of material structures and control of multi-scale morphology; (2) Synthesis and characterization of new classes of materials including hierarchical materials or otherwise innovative assemblies of matter with novel functionality; (3) Exploitation of extreme conditions, complex chemistries and molecules, or non-equilibrium conditions to accelerate new materials discovery; (4) Control of interphase chemistry and morphology; (5) Fundamental electrochemistry of solid state materials; (6) Chemical dynamics and transformations of functional materials in operational environments; and (7) Development of new tools and techniques for the elucidation of chemical processes in materials, particularly *in situ* or *operando* studies of materials in energy-relevant applications.

Research will not be supported if it is primarily aimed at optimization of properties of materials for applications, optimization of synthetic methods (including scale-up), device fabrication and testing, or synthesis of small molecules or nanoparticles. Proposals focused on the elucidation of mechanisms of catalytic reactions, particularly with single-site or single-atom catalysts, will not be supported.

Subprogram Contacts:

• Michael Sennett, (301) 903-6051, <u>michael.sennett@science.doe.gov</u>; and

• Craig Henderson, (301) 903-0805, <u>craig.henderson@science.doe.gov</u>

Website: http://science.energy.gov/bes/mse/research-areas/materials-chemistry/

## (b) Biomolecular Materials

This activity supports fundamental research in the discovery, design and synthesis of functional materials and complex structures, and materials aspects of energy conversion processes 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 science-driven creation of energy-relevant versions of these materials capable of functioning under harsher, non-biological environments. Within this context, new fundamental science approaches for predictive, scalable assembly incorporating error-correcting and defect-managing mechanisms via spatial and temporal control of energy-efficient assembly and synthetic pathways will be emphasized. Included are self-, directed-, and dissipative-assembly to form adaptive, resilient materials with self-repairing capabilities; materials that display novel, unexpected properties that are far from equilibrium; development of science-driven tools and techniques to achieve real-time understanding and control of assembly; and integrated theory and experiment approaches to attain these goals.

Major scientific areas of interest are: Mesoscale materials that can coordinate collective behavior, function autonomously, respond to stresses without losing function, reconfigure and reroute energy transfer, transport, and communication pathways, rebuild structure, and selfreplicate; Understanding and precisely controlling bioinspired synthesis and function at organicinorganic interfaces; Achieving targeted functionality and precise functional group positioning; and, Design and creation of next-generation materials for energy with programmable selectivity and transport based on biological gating and pumping functions.

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. Research that does not have a clear focus on materials science or is aimed at optimization of materials properties for any applications, device fabrication, sensor development, tissue engineering, and biomedical research will not be supported in this program.

Subprogram Contact:

• Michael Markowitz, (301) 903-6779, <u>mike.markowitz@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/mse/research-areas/biomolecular-materials/</u>

#### (c) Synthesis and Processing Science

This program supports research to understand the physical phenomena and unifying principles in different classes of materials that underpin their synthesis including diffusion, nucleation, and

phase transitions, often using *in situ* diagnostics, and development of new techniques to synthesize materials with tailored structure and desired function. An important element is the development of real-time monitoring tools, diagnostic techniques, and instrumentation that can provide information on the progression of structure and properties as a material is formed to understand the underlying physical pathways and to gain atomic level control. The emphasis is on fundamental research to enable discovery of new functional materials and development of new crystal growth methods and thin-film deposition techniques to create complex materials, perhaps in new states of matter and under non-equilibrium conditions, with targeted structure and function.

This activity focuses on predictive design and synthesis of materials across multiple length scales, with a particular emphasis on the mesoscale, and the role imperfections and interfaces can play in the emergence of materials' functionality. Proposals are encouraged that will accelerate progress in understanding synthesis pathways and discovery of new materials through coupling creative physical experimental synthesis and processing techniques, computational approaches, and/or *in situ* diagnostic tools and characterization techniques. The program is emphasizing innovative research in understanding kinetics and mechanisms of materials growth including: bulk material processes, organic and inorganic film deposition, and the organization of mesoscopic hierarchical assemblies across a range of length scales, especially underpinning energy-related areas.

Projects aimed at controlling synthesis to direct materials properties, including optimization of properties, will be de-emphasized. In addition, research will not be supported that focuses primarily on engineering scale-up, device fabrication, or device development.

Subprogram Contact:

• Bonnie Gersten, (301) 903-0002, <u>bonnie.gersten@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/mse/research-areas/synthesis-and-processing-science/</u>

#### (d) Experimental Condensed Matter Physics

The Experimental Condensed Matter Physics program supports research that will advance our fundamental understanding of the relationships between intrinsic electronic structure and properties of complex materials. Research supported by the program focuses on systems whose behavior derives from strong electron correlation, competing or coherent quantum interactions, topology, and effects of interfaces, defects, spin-orbit coupling, and reduced dimensionality. Scientific themes include charge, spin, and orbit degrees of freedom that result in phenomena such as superconductivity, magnetism, and topological protection, and the interactions of these in bulk and reduced-dimensional systems. The program supports synthesis and characterization of new material systems required to explore the central scientific themes. This includes development of experimental techniques that enable such research.

Growth areas include new and emergent quantum phenomena in topological materials, lowdimensional materials including proximity effects, and materials with targeted functionality (e.g., quantum information science and neuromorphic computing). Areas of decreasing emphasis include heavy fermion superconductivity, fractional quantum Hall physics, and cold atom physics. The program will not consider proposals on conventional superconductivity, bulk semiconductor physics (e.g., Si, GaAs), device development, and/or materials property optimization.

Subprogram Contact:

• Michael (Mick) Pechan, (301) 903-0540, <u>michael.pechan@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/mse/research-areas/experimental-condensed-matter-physics/</u>

#### (e) Theoretical Condensed Matter Physics

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 or driven response), and fundamental research in materials related to energy technologies. Examples of current research include strongly correlated electron systems, quantum phase transitions, topological states, magnetism, superconductivity, wide bandgap semiconductors, thermoelectric materials, computational and data-driven materials design, and neutron and photon scattering. Approaches from purely analytical to computational are supported, as are methods that incorporate multiple length and time scales. Development of validated, open-source codes and data analytics, as well as high throughput computations, is also supported.

Research in predictive theory and modeling on novel materials and theory for quantum information science will include disruptive physics-based computational techniques, data-driven approaches, and machine learning. These increases will be offset by decreases in long-standing research challenges including heavy fermion superconductivity, compound semiconductor physics, surface chemistry, piezoelectrics, and plasmonics. The program will continue to emphasize basic research on matter at the atomic, nano, and meso length scales to advance the understanding of fundamental physics and materials phenomena relevant to DOE's missions.

Soft matter and biomolecular physics, polymers, ionic liquids, granular materials, and Bose-Einstein condensates are not current priorities.

Subprogram Contacts:

- James Davenport, (301) 903-0035, james.davenport@science.doe.gov; and
- Matthias Graf, (301) 903-0874, <u>matthias.graf@science.doe.gov</u>

Website: http://science.energy.gov/bes/mse/research-areas/theoretical-condensed-matter-physics/

#### (f) Physical Behavior of Materials

This program supports basic research to advance our knowledge and understanding of fundamental processes that take place in materials in response to external stimuli, such as temperature, electromagnetic fields, chemical environments, and the proximity effects of surfaces and interfaces. The program emphasizes research on the structure-property relationships to physical behavior of materials, such as the relationship of atomic structure and crystal defects

to semiconducting, superconducting, and magnetic properties; and, diffusion and transport phenomena.

The research is necessary to understand how materials generate, transmit, and store energy. A detailed understanding of how materials behavior can be influenced by the surroundings is critical to the understanding of photo-induced charge transport, fast-ion conducting electrolytes, novel magnetic materials, magnetocaloric materials, and research on new energy-relevant materials. Areas targeted for increased emphasis include light-matter interactions in the fields of excitonics, plasmonics, metamaterials and the coherent interactions of quantum states in materials. Areas targeted for decreased emphasis in this program include conventional semiconductor physics and research focused on theory and modeling of defects in crystals and their influence on the structural properties of materials.

Subprogram Contact:

• Refik Kortan, (301) 903-3308, <u>refik.kortan@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/mse/research-areas/physical-behavior-of-materials/</u>

## (g) Mechanical Behavior and Radiation Effects

This activity supports 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 include deformation of ultra-fine scale materials, radiation-resistant material fundamentals, corrosion/stress-corrosion cracking in conjunction with radiation or stress, and research that would lead to microstructural design for increased strength, formability, and fracture resistance in energy-relevant materials. In addition to traditional structural materials, it is also important to understand deformation and failure mechanisms in other materials used in energy systems (e.g. membranes, coating materials, electrodes). Within these areas, research on topics such as driven systems, mesoscale science and non-linear cooperative phenomena (multiple inputs, e.g. radiation + stress + corrosion) are of interest. There will be an increased emphasis in the program for research on understanding defect evolution in materials in radiation environments. 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

The long-term goal of this program is to develop the scientific underpinning of defect behavior that will allow the development of predictive models for the design of materials having tailored mechanical properties and radiation resistance. Towards this goal, research that takes advantage of the new capabilities to fabricate and test tailored structures down to the nanoscale, as well as utilizing newly developed and more powerful leadership-class computational platforms and experimental tools, will be emphasized.

Proposals emphasizing mechanics of materials, rather than materials science, will not be considered responsive.

Subprogram Contact:

• John Vetrano, (301) 903-5976, john.vetrano@science.doe.gov Website: <u>http://science.energy.gov/bes/mse/research-areas/mechanical-behavior-and-radiation-</u> effects/

#### (h) X-Ray Scattering

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 in ultrafast materials science, across the full electromagnetic spectrum, including research aimed at manipulating and detecting ultrafast transient physical phenomena in materials (especially at excitation levels consistent with energy conversion and transport), is an integral part of the portfolio.

Advances in x-ray scattering and ultrafast sciences will continue to be driven by scientific opportunities presented by improved source performance and optimized instrumentation, especially with the advent of improved synchrotron coherence and free electron laser sources. The x-ray scattering activity will expand current capabilities at the DOE facilities by providing support for independent external researchers who motivate and lead new instrumentation and technique development at those facilities. A continuing theme in the scattering program will be the integration and support of materials preparation, especially when coupled to operational investigation of materials processing and realistic, energy-related materials environments. New investments in ultrafast science will focus on research that uses radiation sources associated with BES facilities and beam lines but also includes research performed with ultra-short pulse radiation probes created by tabletop laser sources.

The program will not support research considered "mature use" of existing x-ray or ultrafast techniques. Typically, the emphasis on new techniques enables new access to inhomogeneous and dynamic systems and therefore the program will de-emphasize steady-state research of bulk and equilibrium systems.

Subprogram Contact:

• Lane Wilson, (301) 903-5877, <u>lane.wilson@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/mse/research-areas/x-ray-scattering/</u>

#### (i) Neutron Scattering

This activity supports basic research on the unique interactions of neutrons with matter to achieve a fundamental understanding of the atomic, electronic, and magnetic structures and excitations of materials and their relationship to macroscopic properties. The program will develop novel approaches that will exploit the unique aspects of neutron scattering and the advanced neutron scattering capabilities to investigate materials with hierarchical structures and excitations in a wide range of length and time scales. It will focus on transformational research that uniquely requires neutron scattering as a major tool and that could serve as a driver for the

concomitant advancement of neutron scattering techniques and instruments for materials research. It will continue its stewardship role in fostering growth of the US neutron scattering community by developing innovative, time-of-flight neutron scattering instrumentation concepts and their effective utilization for materials research at the BES user facilities.

Topics emphasized in FY 2018 are new states of matter and phenomena in hard and soft condensed matter, emergent quantum phenomena at interfaces and in the bulk, design principles and collective behavior of multi-component systems, and the science at the mesoscale where macroscopic properties manifest. Major emphasis is to foster strong coupling among synthesis, neutron scattering experiments, theory and simulations that will enable a deeper understanding of the new states of matter and provide the knowledge needed for predictive design of advanced materials for future energy needs.

The program will not support research considered "minimal or peripheral use" of neutron scattering techniques. It will deemphasize applications with a major focus on conventional and high temperature superconductivity, single molecule magnets, organic photovoltaics, spintronics, and thermoelectrics.

Subprogram Contact:

• P. Thiyagarajan (Thiyaga), (301) 903-9706, <u>p.thiyagarajan@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/mse/research-areas/neutron-scattering/</u>

## (j) Electron and Scanning Probe Microscopies

This activity supports basic research in materials sciences using advanced electron and scanning probe microscopy and related spectroscopy techniques to understand the atomic, electronic, and magnetic structures and properties of materials. This activity also supports the development of new instrumentation concepts and quantitative techniques, including ultrafast electron diffraction and imaging techniques and the associated theoretical tools, 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.

New methods and approaches could provide an array of opportunities for groundbreaking science. These include understanding and controlling nano- or meso-scale inhomogeneity as well as the interplay between charge, orbital, spin, and lattice degrees of freedom. Other areas of emphasis are imaging the functionality of materials; investigation of the electronic structure, spin dynamics, magnetism, phase transition, and transport properties from atomistic to mesoscopic scales; and development of advanced *in situ* analysis capabilities for study of quantum materials.

The program will not support research considered to be "mature use" of microscopy techniques. Lower time resolution, dynamic electron scattering techniques will be deemphasized.

Subprogram Contact:

• Jane Zhu, (301) 903-3811, jane.zhu@science.doe.gov Website: <u>http://science.energy.gov/bes/mse/research-areas/electron-and-scanning-probe-microscopies/</u>

#### **Chemical Sciences, Geosciences, and Biosciences**

The Chemical Sciences, Geosciences, and Biosciences (CSGB) Division supports experimental, theoretical, and computational research to provide fundamental understanding of chemical transformations and energy flow in systems relevant to DOE missions. This knowledge serves as a basis for the development of new processes for the generation, storage, and use of energy and for mitigation of the environmental impacts of energy use.

Five synergistic, fundamental research themes are at the intersection of multiple CSGB research focus areas: Ultrafast Chemistry develops and applies approaches to probe the dynamics of electrons that control chemical bonding and reactivity; to understand energy flow underlying energy conversions in molecular, condensed phase, and interfacial systems; and to elucidate structural dynamics accompanying bond breaking and bond making in chemical transformations. Chemistry at Complex Interfaces addresses the challenge of understanding how the complex environment created at interfaces influences chemical phenomena such as reactivity and transport that are important in photochemical, catalytic, separations, biochemical and geochemical systems. These complex interfaces occur between phases with disparate properties, are structurally and functionally disordered, and exhibit dynamics on timescales commensurate with those of the chemical phenomena of interest. Charge Transport and Reactivity explores how the dynamics of charges contribute to energy flow and conversion and how the charge transport and reactivity are coupled. Reaction Pathways in Diverse Environments discovers the influence of nonequilibrium, heterogeneous, nanoscale environments on complex reaction mechanisms in chemical conversions. Research in this area increases understanding of the factors controlling chemical processes and provides mechanistic insights into the efficiency, control, and selectivity of reaction pathways. Chemistry in Aqueous Environments addresses the unique properties of water, particularly how they manifest in extreme environments such as confinement (e.g., nanoscale pores) and complex multi-component, multi-phase solutions (e.g., concentrated electrolytes), and the role aqueous systems play in energy and chemical conversions. Priority will be given to proposals in the CSGB research focus areas listed below that address one or more of the above synergistic research themes.

#### CSGB Division Website: http://science.energy.gov/bes/csgb/

#### (k) Atomic, Molecular, and Optical Sciences

This program supports basic experimental and theoretical research aimed at understanding the structural and dynamical properties of atomic and molecular systems. The research focuses on fundamental interactions of these systems with photons and electrons 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 probes of matter; the interactions of atoms and molecules with intense electromagnetic fields; and quantum control of atomic and molecular systems.

The program emphasizes ultrafast, strong-field, short-wavelength science, and correlated dynamics in atoms and molecules. The AMOS Program will continue to have a prominent role at

BES facilities in understanding and controlling the interaction of intense, ultrafast x-ray pulses with matter. 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; and development and characterization of femtosecond and attosecond pulses of x-rays produced by accelerator-based and table-top sources. Applications at 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. Experimental and theoretical tools will be used to study low-energy electron-molecule interactions in the gas and condensed phases. Key targets for greater investment include attosecond science, ultrafast x-ray science, and ultrafast electron diffraction from molecular systems.

The Atomic, Molecular, and Optical Sciences program **is not** accepting applications in the areas of nanoscience, bioscience, and science of ultracold systems.

#### Subprogram Contact:

• Thomas (Tom) Settersten, (301) 903-8428, <u>thomas.settersten@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/csgb/research-areas/atomic-molecular-and-optical-science/</u>

#### (l) Gas Phase Chemical Physics

This program supports research on gas-phase chemical processes important in energy applications. In the past, clean and efficient use of chemical energy was the major focus, such as in combustion processes, and it continues to be a significant driver. The overall goal of this program is to understand energy flow and reaction mechanisms in complex, nonequilibrium, gas-phase environments in which the coupling of chemical and transport processes is poorly understood, such as those encountered in combustion.

The major focus of research in this area is in four thrust areas. *Light-Matter Interactions* includes research in molecular spectroscopy and diagnostics development to probe molecular structure, dynamics and interactions in complex gas-phase systems to enable chemical and physical analysis of heterogeneous and dynamic gas-phase environments. *Chemical Reactivity* comprises research in chemical kinetics and mechanisms, chemical dynamics, collisional energy transfer, and construction of, and calculations on, molecular potential energy surfaces to develop fundamental insight into energy flow and chemical reactions. *Chemistry-Transport Interactions* consists of multidimensional, multi-scalar measurements in reacting flows and modeling of turbulent reacting flow to gain understanding of the influence of heterogeneous and dynamic environments on chemical reaction pathways. *Gas-Particle Interconversions* comprises research on the chemistry of small gas-phase particles, including their interactions with gas-phase molecules and dynamic evolution to understand the molecular mechanisms of formation, growth and transformation (such as evaporation, phase transition, and reactive processing) of small particles.

Currently, increased emphasis in gas-phase chemical physics is on experimental and theoretical investigations of the effect of non-thermal initial distributions on the reactions of radicals, experimental investigations of radical-radical reactions, better insight into reactions at high pressures, and approaches to expedite gas phase chemical physics calculations via computer automation. The Gas Phase Chemical Physics program does *not* support research in 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.

Subprogram Contact:

• Wade Sisk, (301) 903-5692, <u>wade.sisk@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/csgb/research-areas/gas-phase-chemical-physics/</u>

#### (m) Computational and Theoretical Chemistry

The Computational and Theoretical Chemistry program supports development, improvement and integration of new and existing theoretical and massively parallel computational or data-driven strategies for the accurate and efficient prediction or simulation of processes and mechanisms relevant to the BES mission. Focus is on non-empirical next-generation simulation of complex processes that require simultaneous computational implementation, testing, and development of new theories and algorithms. Efforts should provide fundamental solutions to problems associated with efficient conversion to clean, sustainable, renewable, novel or highly efficient energy use. Efforts must, directly or as part of multi-scale simulation methods, improve the ability to simulate processes at the molecular- and nano- scales. This includes computational and theoretical tools that enhance, or lead, analysis of spectroscopic measurements, especially in situ non-destructive techniques, or efforts aimed at enhancing accuracy, precision, applicability, scalability, or the fundamental basis of all variants of quantum-mechanical simulation methods. Developments of spatial and temporal multi-scale/multistage methodologies that allow for timedependent simulations of resonant, non-resonant and dissipative processes as well as rare events are encouraged. Developments of capabilities for simulation of light-matter interactions, bond breaking, conversion of light to chemical energy or electricity, and the ability to model and control externally driven electronic, charge, magnetic and spin-dependent transport processes in laboratory or natural/solvated environments are encouraged. Computational chemical science developments are expected to lead to discovery by rigorous and efficient prediction of fundamental phenomena that are not immediately quantified by experiment. Efforts that reliably calibrate prospects for emerging energy and computing technologies are encouraged. Machine learning and data-enabled open source computational chemical software, as well as deep learning techniques, especially when aimed at reducing parameterization in theories, are also supported.

Topics of interest include practical predictive methods for (1) excited-state or collective phenomena in complex molecular systems, (2) nontraditional or novel basis sets, meshes or representation of quantum-mechanical degrees of freedom, and (3) simulation and coupling of all interactions/scales that depend upon electronic, vibrational and atomistic structure to improve descriptions of dissipative interactions due to weak and strong interactions among matter, radiation, fields, environment, and solvents.

Methods for or applications to systems that do not explicitly consider rearrangements of quantum-mechanical degrees of freedom are not supported.

Subprogram Contact:

• Mark Pederson, (301) 903-9956, <u>mark.pederson@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/csgb/research-areas/computational-and-theoretical-chemistry/</u>

#### (n) Condensed Phase and Interfacial Molecular Science (CPIMS)

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, chemical synthesis, energy storage, and subsurface chemical and transport processes. Experimental and theoretical investigations in the condensed phase and at interfaces aim at elucidating the molecular-scale chemical and physical properties and interactions that govern chemical reactivity, solute/solvent structure and transport. Studies of reaction dynamics at well-characterized surfaces and clusters lead to the development of theories on the molecular origins of surface-mediated catalysis and heterogeneous chemistry. Studies of model condensed-phase systems target first-principles understanding of molecular reactivity and dynamical processes in solution and at 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.

Some examples of recent awards managed in the CPIMS portfolio: (1) Studies of how applied electric fields influence ion hydration properties and water organization at the air/aqueous interface; (2) research that pushes accurate quantum simulations toward large mesoscale systems; (3) explorations of multidimensional infrared microscopy for visualizing chemical dynamics in heterogeneous environments; (4) investigations of photochemical reactions of relevance to chemical synthesis in charged micro-droplets; (5) theoretical studies of rare events in molecular simulations in aqueous systems, such as heterogeneous nucleation; (6) studies of ion solvation and charge transfer at complex interfaces using nonlinear soft x-ray spectroscopy; and (7) research on understanding chemical bond dynamics in solution using mixed quantum/classical molecular dynamics simulations. Descriptions of all awards are found in

CPIMS Meeting Reports at the link <u>http://science.energy.gov/bes/csgb/principal-investigators-meetings/</u>, under "Condensed-Phase and Interfacial Molecular Science".

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

Subprogram Contact:

• Gregory Fiechtner, (301) 903-5809, <u>gregory.fiechtner@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/csgb/research-areas/condensed-phase-and-interfacial-molecular-sciences/</u>

#### (o) Catalysis Science

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 reaction mechanisms in diverse chemical environments comprises a central component of the program, with specific focus areas involving: (1) study of structure-reactivity relationships of solid and molecular catalysts, including *chemistry in aqueous environments* and *chemistry at complex interfaces*; (2) 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; (3) 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; (4) examination of the dynamics of catalyst and electronic structures occurring during catalytic cycles and deactivation; (5) investigation of emerging approaches to direct catalytic transformations in multicomponent mixtures, multiple reactions, and integrated processes; and (6) advanced theory, modeling, and data-science approaches to mechanism identification, catalyst discovery and development.

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. 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 in complex reaction networks. It also encourages integrated theory-experiment and predictive theoretical catalysis supported by dataintensive strategies. This program does not support: (1) the study of transformations appropriate for pharmaceutical applications; (2) non-catalytic stoichiometric reactions; (3) whole cell or organismal catalysis; (4) process or reactor design and optimization; or (5) the development of specific energy technologies.

Subprogram Contacts:

- Viviane Schwartz, (301) 903-0448, viviane.schwartz@science.doe.gov; and
- Chris Bradley, (301) 903-2047, chris.bradley@science.doe.gov

Website: http://science.energy.gov/bes/csgb/research-areas/catalysis-science/

#### (p) Separation Science

This program supports fundamental research to predict and control the atomic and molecular interactions toward all manner of chemical separations. This basic research is motivated by a desire to advance discovery and predictive design of future chemical separations utilizing novel, multifunctional, and/or energy- and atom-efficient methods; as well as the development and investigation of novel molecular structures with the desired dynamic and kinetic transport properties; and nano-, meso-, and macroscopic functionality. Research topics include, but are not limited to: inorganic and organic/hybrid membrane science; soft, hard, or hybrid membranes; ultraselective separations in diverse aqueous environments; reactive separations involving charge transport, complex mixture and complex interface separations; electrochemical processes, and non-traditional solvents such as ionic liquids and deep eutectic solvents. A range of basic research multidisciplinary experimental and computational approaches are employed, inspired by the multidimensional and time-dependent complexity of chemical separation problems.

Research that is responsive to the *Basic Research Needs for Environmental Management* report, and in particular, speciation and reactivity of non-equilibrium separation systems, is well-aligned with the goals of this program. Also well aligned are separation science topics associated with Future Nuclear Energy technologies, in particular those involving non-aqueous fluids. However, research focused on understanding the chemical and physical properties of actinide and transactinide elements is better covered under topic (q) Heavy Element Chemistry.

Of current interest are projects that include, but are not limited to, the structural and molecular dynamics of elementary separation steps at complex solid-fluid interfaces utilizing fast and ultrafast spectroscopy; the influence of nanoscale environments, such as ligands, electrolytes, confining structures, solvation or ionic spheres, etc., on separation mechanisms and kinetics at the molecular level; the role of amorphous, disordered, and non-equilibrium heterogeneous structures in separation mechanisms and efficiency; the influence of electromagnetic or other fields affecting transport and bonding of charged or neutral species; the mechanisms of energy absorption and dissipation in separating systems; and novel mechanisms of reactive separations.

The Separation Science program does not support engineering or scale up of processes, devices or sensors, microfluidics, or research directed toward medical or analytical applications; nor does the program support applied research, research focused on materials synthesis or materials processing, or research focusing on mineral processes, or classification of carbon nanotubes, nanoparticles, etc.

Subprogram Contact:

• Philip Wilk, (301) 903-4537, <u>philip.wilk@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/csgb/research-areas/separation-science/</u>

## (q) Heavy Element Chemistry

The Heavy Element Chemistry (HEC) program supports actinide and transactinide fundamental chemical research that underpins the DOE missions in energy, environment, and national security. The unique molecular bonding of these elements is explored using experiment and theory to elucidate electronic and molecular structure as well as reaction thermodynamics. Emphasis is on determining the chemical and physical properties of these elements – particularly those elements that are least understood – to identify solution, interfacial and solid-state bonding and reactivity, and to resolve the quantum-mechanical behavior of the 5f-electrons. Synthetic inorganic research is pursued within this program on molecules that contain heavy elements, with a focus on gaining a fundamental understanding of how the f-electrons participate in bonding. Ligand synthesis is supported only with an aim toward the discovery of novel interactions, complex reaction mechanisms, or to determine electronic structure. Spectroscopic research on the bonding and chemical reactivity of heavy-element-containing molecules is emphasized, particularly those explored in aqueous environments, utilizing national user facilities, and ultrafast techniques.

Resolving the role of the f-electrons is one of the three grand challenges identified in *Basic Research Needs for Advanced Nuclear Energy Systems*, the DOE report of the Basic Energy Sciences Workshop on this topic. Research to address this challenge is a central goal of this program and includes efforts aimed at implementing for actinide and transactinide elements, quantum-mechanical theories that correctly describe spin-orbit interactions and relativistic effects, which will expand our ability to predict heavy element chemical behavior.

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 using 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 focused primarily on separations that does not address the unique properties of the heavy elements is better aligned with the BES Separation Science program, which is described in section (p).

Subprogram Contact:

• Philip Wilk, (301) 903-4537, <u>Philip.Wilk@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/csgb/research-areas/heavy-element-chemistry/</u>

#### (r) Geosciences

The Geosciences program supports basic experimental, theoretical and computational research in geochemistry and geophysics. Geochemical research emphasizes fundamental molecular level understanding of phase equilibria, reaction mechanisms and rates associated with aqueous

geochemical processes, focusing on nanoscale materials and interfaces, and on the molecular origins of isotopic distributions and migration pathways in interfacial systems. Geophysical research focuses on fundamental mechanistic understanding of the origins of subsurface physical properties and material response of earth materials associated with processes such as strain localization and chemo-mechanical stress corrosion.

In both geophysics and geochemistry, the emphasis is on pushing the boundaries of current measurement techniques and modeling approaches and on designing experiments and models that connect with one another in transformative ways.

Basic Energy Sciences funding is only appropriate to research that has multiple potential application areas. Projects focused on particular applications should contact the appropriate technology program.

Subprogram Contact:

• James Rustad, (301) 903-1717, james.rustad@science.doe.gov Website: <u>http://science.energy.gov/bes/csgb/research-areas/geosciences/</u>

## (s) Solar Photochemistry

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

Among the challenges in catalytic fuels production, knowledge gained in 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, the fixation of N<sub>2</sub>, and H<sub>2</sub>O 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.

Another regime of interest is the chemistry initiated through creation of excited states with 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, solutions, and interfaces.

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

Subprogram Contact:

• Christopher Fecko, (301) 903-1303, <u>christopher.fecko@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/csgb/research-areas/solar-photochemistry/</u>

#### (t) Photosynthetic Systems

This program supports basic research on the capture of light energy and its conversion to and storage as chemical energy in plants, algae, and photosynthetic prokaryotes. Research topics supported include, but are not limited to, light harvesting, photosynthetic electron and proton transport, photosynthetic reduction of carbon dioxide into organic compounds, and the self-assembly, dynamics, and self-repair of photosynthetic proteins, complexes and membranes. The primary goal of the program is to foster greater mechanistic understanding of the diverse photosynthetic systems that occur in nature.

Projects funded by the program combine biochemistry, biophysics, molecular biology, computational chemistry, and other approaches to understand biological capture and utilization of light energy. Combining approaches supports a multidimensional mechanistic understanding of photosynthetic structures and processes that can guide the future development of bio-inspired, bio-hybrid, and biomimetic energy systems and inform strategies for genetic improvement of natural photosynthesis.

All submitted applications must clearly state how the knowledge gained from the proposed research is relevant to greater mechanistic understanding of the capture, conversion, and storage of energy in plants, algae, and photosynthetic prokaryotes. Consistent with this goal, Photosynthetic Systems does not fund: 1) development or optimization of energy 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.

Subprogram Contact:

• Stephen Herbert, (301) 903-0383, <u>stephen.herbert@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/csgb/research-areas/photosynthetic-systems/</u>

#### (u) Physical Biosciences

This program supports basic research that combines tools from the physical sciences with biochemical, chemical and molecular biological approaches to further our understanding of the ways plants and non-medical microbes capture, convert, and store energy. Research supported includes, but is not limited to, 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<sub>2</sub>/CH<sub>4</sub>, N<sub>2</sub>/NH<sub>3</sub>, and H<sup>+</sup>/H<sub>2</sub>), 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 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. Limited support is provided for basic research on the biosynthesis and structure of important electron stores in biological systems (such as plant cell walls, lipids, and terpenes), studies that provide insight into the assembly and maintenance of biological energy transduction systems, and research to understand the roles played by ion gradients in storing energy and driving transport processes. Please note that the program is not considering new projects in plant cell wall biosynthesis and structure in FY 2018.

Projects funded by the program combine biochemistry, biophysics, molecular biology, computation, and other approaches to understand structural, functional and mechanistic properties of enzymes, enzyme systems, and energy-relevant biological reactions. Such studies will lead to the identification of principles that will, for example, provide a basis for the design and synthesis of highly selective and efficient bioinspired catalysts, allow us to carefully control the flow of electrons in biological systems to achieve desired metabolic outcomes (e.g. enhance lipid or terpene production), and give us an unprecedented architectural and mechanistic understanding of such systems.

All submitted applications must clearly state the energy relevance of the proposed research: How will the knowledge gained from the proposed work better our understanding of the ways plants, algae, and non-medical microbes capture, convert, and/or store energy? Consistent with this focus, Physical Biosciences does not fund research in: 1) animal systems; 2) prokaryotic systems related to human/animal health or disease; 3) development or optimization of energy devices or processes; 4) development or optimization of microbial strains or plant varieties for biofuel/biomass production; 5) cell wall breakdown or deconstruction; 6) transcriptional or translational regulatory mechanisms or processes; 7) environmental remediation or identification of environmental hazards; 8) genomic or other "omic" data acquisition that does not test specific hypotheses relevant to the program; and 9) projects that are primarily computational in nature..

Subprogram Contact:

• Robert Stack, (301) 903-5652, <u>robert.stack@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/csgb/research-areas/physical-biosciences/</u>

## **Scientific User Facilities**

The Scientific User Facilities (SUF) Division supports the research and development, planning, construction, and operation of scientific user facilities for a vast range of science spanning the fields of biology, chemistry, geoscience, material science, and the physical sciences using x-ray, neutron, and electron beam scattering as fundamental probes of matter. These facilities provide unique capabilities to the scientific community and are a critical component of maintaining U.S. leadership in this diverse range of scientific disciplines. The SUF Division also supports research activities leading to the improvement of today's facilities, and research that lays the foundation for the development of the next generation of facilities.

SUF Division Website: http://science.energy.gov/bes/suf/

## (v) BES Accelerator and Detector Research

This program supports research that advances the instruments, techniques, and capabilities of the existing and/or future scientific user facilities. Research includes studies on creating, manipulating, transporting, and performing diagnostics of ultrahigh brightness electron beams, studies of the properties of cathodes materials and factors that limit cathode lifetime, and modeling of ultrashort electron beam dynamics. Research is supported that aims at developing techniques that will strongly benefit the next generation of free electron lasers (FELs). Development studies of beam dynamics in high-intensity proton sources used for neutron spallation facilities are also supported.

Major areas of interest include: Development of novel high-brightness electron sources, innovative methods of beam acceleration, seeding and beam manipulation techniques that enhance temporal control of x-ray FELs, and lead to higher peak and average brightness, enhanced energy stability, and reduction of temporal and intensity fluctuations. Methods to control and shape the spectrum of x-ray FELs, such as the generation of controlled multi-color (multi-frequency) photon beams that will enable many experimental techniques in ultrafast chemical and material dynamics studies. High-precision timing techniques for synchronization of accelerator and laser systems and for high-resolution measurements of electron and sub-femtosecond photon beam pulses. Methods to stimulate electron-photon conversion efficiency leading to enhanced output beam power. Development of advanced instrumentation for beam characterization, control, and optimization to enable the full utilization of the high flux, brilliance, and ultra-short pulses provided by the new light sources, and increased intensity at the neutron sources.

Also of interest are detector developments that will allow efficient use of the high-intensity xrays and neutrons produced by the new sources. Improved detectors are especially important in the study of multi-length-scale systems such as protein-membrane interactions as well as nucleation and crystallization in nanophase materials.

Advanced x-ray and neutron optics developments are needed to respond to increasing demands for higher energy resolution, focusing, and preservation of coherence. Innovative and precise optical elements are required to transport and manipulate x-ray beams possessing varying degrees of both longitudinal and transverse coherence.

New developments in data resource management techniques are sought to address the increasing volume and complexity of experimental data generated at the BES light sources and neutron scattering facilities.

Research aimed at the optimization of materials properties for accelerator, detector, and optics components, device fabrication, and sensor development will be discouraged.

Subprogram Contact:

• Eliane Lessner, (301) 903-9365, <u>eliane.lessner@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/suf/accelerator-and-detector-research/</u>

#### 3. Biological and Environmental Research (BER)

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

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

The BER subprograms and their objectives follow:

#### (a) Biological Systems Science

Research is focused on using DOE's unique resources and facilities to achieve a predictive systems-level understanding of complex biological systems to advance DOE missions in energy and the environment. By integrating genome science with advanced computational and experimental approaches, the Division seeks to gain a predictive understanding of living systems, from microbes and microbial communities to plants and ecosystems. This foundational knowledge enables design and reengineering of microbes and plants underpinning energy independence and a broad clean energy portfolio, including improved biofuels and bioproducts, improved carbon storage capabilities, and controlled biological transformation of materials such as nutrients and contaminants in the environment.

The major research objectives are:

- to determine the molecular mechanisms, regulatory elements, and integrated networks needed to understand genome-scale functional properties of microbes, plants, and communities (including the study of natural microbiomes and model microbiomes in targeted field environments relevant to BER's research efforts); develop "-omics" experimental capabilities and enabling technologies needed to achieve a dynamic, system-level understanding of organism and community functions; and develop the knowledgebase, computational infrastructure, and modeling capabilities to advance predictive understanding, manipulation and design of biological systems as they respond to biotic and abiotic stressors (such as nutrient and water availability or radiation exposure); and
- 2. to develop advanced measurement and imaging technologies to visualize the spatial and temporal relationships of key metabolic processes governing phenotypic expression in plants and microbes, information crucial for developing an understanding of the impact of various environmental and/or biosystems designs on whole cell or community function.

Subprogram Contact:

• Robert (Todd) Anderson, (301) 903-3213, <u>todd.anderson@science.doe.gov</u>, Website: <u>http://science.energy.gov/ber/research/bssd/</u>

#### (b) 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. This includes research on components such as clouds, aerosols, and the terrestrial ecology; modeling of component interdependencies under a variety of forcing conditions; interdependence of climate and ecosystem variabilities; vulnerability, and resilience of the full suite of energy and related infrastructures to extreme events, and uncertainty quantification.

The major research objectives are:

- 1. understand the physics, chemistry, and dynamics governing clouds, aerosols, and precipitation interactions, with a goal to advance the predictive understanding of the earth system;
- 2. improve the understanding and representation of physical and hydro-biogeochemical processes that govern terrestrial surface and subsurface ecosystems, that in turn can be represented in system models to improve confidence in the models; and
- 3. develop, evaluate and analyze complex models of the earth and environmental systems, in order to understand variability, environmental change, and system interactions and co-evolution of the systems.

Subprogram Contact:

• Gerald (Gary) Geernaert, (301) 903-3281, <u>Gerald.Geernaert@science.doe.gov</u> Website: <u>http://science.energy.gov/ber/research/cesd/</u>

#### 4. Fusion Energy Sciences (FES)

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

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

The next frontier 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.

FES also supports discovery plasma science, including research in laboratory plasma astrophysics, low-temperature plasmas, small-scale magnetized plasma experimental platforms, and high-energy-density laboratory plasmas.

To accomplish its mission, the FES program is organized into four subprograms.

• The *Burning Plasma Science: Foundations* subprogram supports foundational experimental and theoretical research aimed at resolving magnetic-confinement plasma science issues for the next generations of machines. The key objectives of this

subprogram are to establish the scientific basis for the optimization of the advanced tokamak and spherical tokamak approaches to magnetic confinement fusion, develop a predictive understanding of burning plasma behavior, develop technologies that will enhance the performance of existing and next-step machines, and provide necessary infrastructure improvements.

- The *Burning Plasma Science: Long Pulse* subprogram supports experimental research in new scientific regimes achievable with long-duration superconducting international machines and research in the development of materials to withstand the harsh conditions in a burning plasma environment. The key objectives of this subprogram are to utilize these new long-pulse capabilities to accelerate our scientific understanding of how to control and operate burning plasmas, as well as to develop the basis for future experiments.
- The *Burning Plasma Science: High Power* subprogram supports the U.S. Contributions to the ITER Project. These activities are performed by the U.S. ITER Program Office and therefore are not part of this Open Solicitation.
- The *Discovery Plasma Science* subprogram supports investigations into fundamental plasma properties and processes and the development of innovative diagnostic techniques, on small- and intermediate-scale, single-purpose experimental platforms. The key objectives of this subprogram are to expand the knowledge base of general plasma physics and to uncover directions for future plasma-related contributions to the DOE missions.

FES research is guided by the priorities in the "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>), and the research opportunities identified in a series of recently held community engagement workshops. The final reports from these workshops can be found in http://science.energy.gov/fes/community-resources/workshop-reports/.

Specific information about FES program areas is as follows:

#### (a) Burning Plasma Science: Foundations—Advanced Tokamak and Spherical Tokamak

This program element uses magnetic confinement fusion research facilities in the U.S. to develop the physics understanding needed to advance the FES mission and demonstrate the ultimate potential of the tokamak for fusion energy production. The FES large-scale experimental facilities provide essential tools to explore and solve many fundamental issues of fusion plasma physics in integrated systems at fusion-relevant parameters. Research at small-scale facilities addresses critical issues that may affect the tokamak concept. This program element also includes research and development in technology areas that enable improvements in tokamak plasma performance.. Major themes of this program element are (1) the physics basis for the spherical tokamak (ST) and the advanced tokamak (AT) concepts as candidates to support a fusion nuclear science program; (2) techniques to minimize the impact of transient plasma events; (3) solutions to the tokamak divertor and plasma-material interface (PMI) challenge; and (4) toroidal confinement physics understanding for ITER and beyond. Subprogram Contacts:

- Mark Foster, (858) 455-3360, <u>Mark.Foster@science.doe.gov</u>
- Matthew Lanctot, (301) 903-1972, <u>Matthew.Lanctot@science.doe.gov</u>
- Joshua (Josh) King, (301) 903-9707, Josh.King@science.doe.gov
- Barry Sullivan, (301) 903-8438, Barry.Sullivan@science.doe.gov

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

## (b) Burning Plasma Science: Foundations—Theory & Simulation

This program element focuses on advancing the scientific understanding of the fundamental physical processes governing the behavior of magnetically confined plasmas. 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;
- 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 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 whole-device modeling 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 emerging high-performance computing systems.

Subprogram Contact:

• John Mandrekas, (301) 903-0552, <u>John.Mandrekas@science.doe.gov</u> Website: <u>http://science.energy.gov/fes/research/</u>

## (c) Burning Plasma Science: Long Pulse—Tokamak & Stellarator

This program element supports research conducted by U.S. teams on long pulse superconducting international tokamaks as well as unique short pulse international tokamaks and stellarators that are currently operating or will be operating in the near future. These teams build on the experience gained from U.S. fusion facilities to conduct research on these international machines. This research will enable the exploration of scientific regimes that cannot be sustained for long duration on domestic machines, which will allow the U.S. fusion program to gain the knowledge needed to control and sustain plasma discharges in future burning plasma devices. In

addition, this category includes the U.S. stellarator domestic research program focused on optimization of confinement through quasi-symmetric shaping of the toroidal magnetic field.

Subprogram Contacts:

• Tokamaks: Matthew Lanctot, (301) 903-1972, Matthew.Lanctot@science.doe.gov

• Stellarators: Samuel (Sam) Barish, (301) 903-2917, <u>Sam.Barish@science.doe.gov</u> Website: <u>http://science.energy.gov/fes/research/</u>

## (d) Burning Plasma Science: Long Pulse—Materials & Fusion Nuclear Science

This program element focuses on advancing the scientific understanding required to design and deploy the materials and technologies needed to support a steady-state burning plasma device. The main technical issues of interest stem largely from the uniquely extreme operating environment associate with future fusion reactors. There are three broad research topics of interest: (1) taming the plasma-material interface, (2) conquering nuclear degradation of materials and structures, and (3) harnessing fusion power (fuel cycle, chamber technology, and systems studies). Scientific proposals of interest are those aimed at resolving key hurdles in order to establish the scientific proof of principle for fusion energy from a materials science and engineering perspective.

Subprogram Contacts:

- Daniel Clark, (301) 903-4883, Daniel.Clark@science.doe.gov
- Barry Sullivan, (301) 903-8438, <u>Barry.Sullivan@science.doe.gov</u> Website: <u>http://science.energy.gov/fes/research/</u>

## (e) Discovery Plasma Science: Plasma Science Frontiers

*General plasma science* supports research in the frontier areas of fundamental plasma science and engineering. The program is focused on advancing the understanding of the behavior of nonneutral and single-component plasmas, ultra-cold neutral plasmas, dusty plasmas, and microplasmas, as well as the study of dynamical processes in classical plasmas including turbulence, thermal, radiative and particle transport, waves, structures, flows, and their interactions. Research topics responsive to this subprogram may include: (1) energization and magnetic selforganization (dynamo, reconnection, and turbulent cascade) processes, (2) electric selforganization and the control of pattern formation, and (3) low-temperature plasma processes at the interface of chemistry and biology. Excluded from this call is research on low-energy nuclear reactions and relevant activities.

For more information, please see the recent 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>).

Since many of the topics are included in the NSF/DOE joint program, applicants are strongly encouraged to submit their proposals in response to the annual solicitation of the DOE/National Science Foundation Partnership in Basic Plasma Science and Engineering: http://www.nsf.gov/funding/pgm\_summ.jsp?pims\_id=5602 Subprogram Contacts:

- Nirmol Podder, (301) 903-9536, <u>Nirmol.Podder@science.doe.gov</u>
- Curtis (Curt) Bolton, (301) 903-4914, <u>Curt.Bolton@science.doe.gov</u>

Website: <u>http://science.energy.gov/fes/research/</u>

*High Energy Density Laboratory Plasmas* supports 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, corresponding to a pressure of approximately 1 million atmospheres. 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 electron volts) can have pressures as low as 0.1 Mbar and are also considered high-energy-density plasmas.

Subprogram Contact:

• Kramer Akli, (301) 903-2943, <u>Kramer.Akli@science.doe.gov</u> Website: <u>http://science.energy.gov/fes/research/</u>

*Exploratory Magnetized Plasma* supports basic and applied research directed at developing the understanding of magnetized plasma behavior necessary to advance capabilities for the creation, control, and manipulation of magnetically confined plasmas for both terrestrial and space applications.

Subprogram Contact:

• Nirmol Podder, (301) 903-9536, <u>Nirmol.Podder@science.doe.gov;</u> Website: <u>http://science.energy.gov/fes/research/</u>

## (f) Discovery Plasma Science: Measurement Innovation

This program element supports the development of innovative diagnostics to make detailed measurements of the behavior of plasmas. Advances in diagnostic systems with higher resolution, higher reliability, reduced complexity, or access to previously unmeasured parameters enable breakthroughs in scientific understanding, the linking of theory/computation with experiments, and active control of plasma properties to optimize device operation and plasma performance in a variety of device configurations.

Subprogram Contact:

• Mark Foster, (858) 455-3360, <u>Mark.Foster@science.doe.gov</u> Website: <u>http://science.energy.gov/fes/research/</u>

## 5. High Energy Physics (HEP)

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

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

The scientific objectives and priorities for the field recommended by the High Energy Physics Advisory Panel (HEPAP) are detailed in its recent long-range strategic plan, developed by the Particle Physics Project Prioritization Panel (P5) and available at: https://science.energy.gov/~/media/hep/hepap/pdf/May-2014/FINAL\_P5\_Report\_053014.pdf.

The HEP program focuses on three experimental scientific frontiers:

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

Together, these three interrelated and complementary discovery frontiers offer the opportunity to answer some of the most basic questions about the world around us. Also integral to the mission of HEP are four cross-cutting research areas that enable new scientific opportunities by developing the necessary tools and methods for discoveries:

- *Theoretical Particle Physics*, where the vision and mathematical framework for understanding and extending the knowledge of particles, forces, space-time, and the universe are developed;
- *Computational Particle Physics,* where the framework of simulation and computational techniques are developed for advancing the HEP mission;
- Accelerator Science and Technology Research and Development, where the technologies and basic science needed to design, build, and operate the accelerator facilities essential for making new discoveries are developed; and
- *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.

Applications in response to this FOA may propose activities *in support of* HEP research, which include, but are not limited to: conferences, experimental operations, conceptual research and development (R&D), design or fabrication directed towards a specific project within the HEP scientific program.

Applicants addressing *specific HEP research or technology development* activities in one or more of the six research subprograms (as in the examples given below, excluding Computational Research in High Energy Physics), are *strongly encouraged* to submit applications to either the annual HEP Comparative Review Funding Opportunity Announcement and/or to the annual Early Career Research Program Funding Opportunity Announcement, each available through <u>https://www.grants.gov</u>. Applications that are in direct support of HEP research activities in the six subprograms may be submitted to this open solicitation but will likely be assigned a lower programmatic priority than those from the comparative review process. Prior to any submission to this Funding Opportunity Announcement, applicants are *strongly encouraged* to contact the relevant HEP subprogram managers listed below to develop applications that address proper program goals.

Additional information about the HEP research subprogram areas described above, and in areas (a) through (g) below, may be found at <u>https://science.energy.gov/hep/research/</u>. Each of the research frontiers is described with a list of currently-supported experiments and facilities. Furthermore, applications submitted to this FOA for support of *generic particle 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 to the research area efforts and pre-conceptual R&D efforts directed to the relevant HEP scientific frontier research area.

#### (a) Experimental Research at the Energy Frontier in High Energy Physics

This research area seeks to support studies of fundamental particles and their interactions using proton-(anti)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 and CMS experiments. This research area also provides graduate and postdoctoral research training for the next generation of scientists, and equipment and computational support for physics research activities. Applications addressing physics studies and pre-conceptual R&D directed towards specific future Energy Frontier experiments are also accepted. Support for Heavy Ion Physics research is <u>not</u> provided under this research area.

Subprogram Contact:

• Abid Patwa, (301) 903-0408, <u>abid.patwa@science.doe.gov</u> Website: <u>http://science.energy.gov/hep/research</u>

#### (b) Experimental Research at the Intensity Frontier in High Energy Physics

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 LHCb research or studies of neutrinoless double beta decay is <u>not</u> provided under this research area.

Subprogram Contact:

• Glen Crawford, (301) 903-4829, <u>glen.crawford@science.doe.gov</u> Website: <u>http://science.energy.gov/hep/research</u>

#### (c) Experimental Research at the Cosmic Frontier in High Energy Physics

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 in High Energy Physics 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.

Subprogram Contact:

• Kathleen (Kathy) Turner, (301) 903-1759, <u>kathy.turner@science.doe.gov</u> Website: <u>http://science.energy.gov/hep/research</u>

#### (d) Theoretical Research in High Energy Physics

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.

Subprogram Contact:

• William (Bill) Kilgore, (301) 903-3711, <u>william.kilgore@science.doe.gov</u> Website: <u>http://science.energy.gov/hep/research</u>

#### (e) Computational Research in High Energy Physics

This research area supports computational, data management, and simulation techniques and tools that target the cross-cutting needs of HEP. Sponsored support within this area focuses on new technologies and methods, including areas of Quantum Information Science and quantum computing, that broadly advance scientific discovery aligned with the HEP mission and benefit multiple parts of the program.

This subprogram does <u>not</u> support computing research and/or activities specific to individual projects in any of the other six research and technology R&D subprograms described in this open solicitation. Support for specific operation efforts and/or hardware requests in each of the other subprograms are also outside the scope of this area. Applicants proposing such activities should submit their application to the relevant subprogram.

Subprogram Contact:

• Lali Chatterjee, (301) 903-0435, <u>lali.chatterjee@science.doe.gov</u> Website: <u>http://science.energy.gov/hep/research</u>

#### (f) Accelerator Science and Technology Research & Development in High Energy Physics

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-power targets; 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 proposals, 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.

Subprogram Contact:

• Lek (L. K.) Len, (301) 903-3233, <u>lk.len@science.doe.gov</u> Website: <u>http://science.energy.gov/hep/research</u>

## (g) Detector Research and Development in High Energy Physics

The detector R&D subprogram develops the next generation of instrumentation for HEP. It supports research leading to fundamental advances in the science of particle and radiation detection, and the development of new experimental techniques. This is typically long-term, "generic" R&D that may be high-risk, but has the potential for wide applicability and/or high-impact. Proposals for "Blue-Sky" scientific research on innovative technologies not already in contention for implementation in future DOE HEP projects are specifically encouraged.

Topics studied in the detector R&D research area include, but are not limited to: low-mass, high channel density charged particle tracking detectors; high resolution, fast-readout calorimeters and particle identification detectors; techniques for improving the radiation tolerance of particle detectors; detectors for photons from ultraviolet to infrared wavelengths; detectors for cosmic microwave background radiation; detectors and experimental techniques for ultralow-background experiments; and advanced electronics and data acquisition systems. Support for graduate and postdoctoral research training, engineering and other technical efforts, and equipment and computational efforts required for experimental detector R&D and fabrication *is* included in this research area.

Subprogram Contact:

• Helmut Marsiske, (301) 903-6989, <u>helmut.marsiske@science.doe.gov</u> Website: <u>http://science.energy.gov/hep/research</u>

#### 6. Nuclear Physics (NP)

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

The mission of the Nuclear Physics (NP) program is to discover, explore, and understand all forms of nuclear matter.

One of the enduring mysteries of the universe is the nature of matter—what are its basic constituents and how do they interact to form the properties we observe? The largest contribution by far to the mass of the matter we are familiar with comes from protons and heavier nuclei. 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.

The priority areas for NP include the following:

- Understand how nucleons—protons and neutrons—combine to form atomic nuclei and how these nuclei have emerged since the origin of the cosmos.
- Using particle accelerators, illuminate the structure of the nucleon—the core building block of matter; understand how quarks and gluons assemble to form matter's core; and search for undiscovered forms of matter.
- Penetrate mysteries surrounding the fundamental properties of the neutron and the neutrino.
- Conceive, construct, and operate national scientific user facilities.
- Steward isotope development, production, and technologies for research and applications.

To carry out its mission and address these priorities, the NP program addresses three broad, yet tightly interrelated, scientific thrusts:, Quantum Chromodynamics; Nuclei and Nuclear Astrophysics; and Fundamental Symmetries. NP supports basic research in six subprograms or areas: Medium Energy, Heavy Ion, Low Energy, Nuclear Theory, and Nuclear Data and Nuclear Theory Computing (a through e). The program is the steward of the DOE Isotope Program for the nation (f) and supports basic research in the development of the tools and capabilities to produce and process isotopes (g).

To advance knowledge in nuclear science and effectively train and mentor the next generation of nuclear scientists, NP places a priority on supporting Program Directors and Principle Investigators who are active-career tenured or tenure-track faculty researchers.

The NP subprograms and their objectives follow:

#### (a) Medium Energy Nuclear Physics

The Medium Energy Nuclear Physics subprogram focuses primarily on understanding the structure of hadrons, how quarks move within a hadron and tests of the theory of the strong interaction, known as Quantum Chromodynamics (QCD). According to QCD, all observed

nuclear particles, collectively known as hadrons, arise from the strong interaction of quarks, antiquarks, and gluons. The protons and neutrons inside nuclei are the best known examples of hadrons. QCD, although difficult to solve computationally, predicts what hadrons exist in nature, and how they interact and decay. Specific questions addressed include: What is the internal landscape of the protons and neutrons (collectively known as nucleons)? What does QCD predict for the properties of strongly interacting matter? What governs the transition of quarks and gluons into pions (hadronic subatomic particle) and nucleons? What is the role of gluons and gluon self-interactions in nucleons and nuclei? The objectives of this subprogram are to develop a comprehensive picture of the spatial, momentum and angular momentum structure of the nucleon, elucidate quark confinement and hadron excitations, and understand the strong interaction in nuclei. Various experimental approaches are used to determine the distribution of "up", "down", and "strange" quarks, their antiquarks, and gluons within protons and neutrons, as well as clarifying the role of gluons in confining the quarks and antiquarks within hadrons. Polarized electron and proton beams are typically used to study the effects of the quark and gluon spins within nucleons, and the effect of the nuclear environment on the quarks and gluons. The subprogram also supports experimental searches for higher-mass "excited state" and exotic hadrons predicted by QCD, as well as studies of their various production mechanisms and decay properties. In pursuing these topics, the Medium Energy subprogram supports experimental research at the subprogram's primary research facility, the Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF), and at other facilities, including the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory (BNL) and the High Intensity Gamma Source (HIGS) at the Triangle Universities Nuclear Laboratory (TUNL).

Subprogram Contact:

• Gulshan Rai, (301) 903-4702, <u>Gulshan.Rai@science.doe.gov</u> Website: <u>http://science.energy.gov/np/research/</u>

#### (b) Heavy Ion Nuclear Physics

The Heavy Ion Nuclear Physics subprogram focuses on studies of condensed quark-gluon matter at extremely high densities and temperatures characteristic of the infant universe. In the aftermath of collisions at RHIC and at the LHC, researchers have seen signs of the same 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. Relativistic Heavy Ion Collider (RHIC) facility and the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN).

Subprogram Contact:

• James Sowinski, (301) 903-7587, james.sowinski@science.doe.gov Website: <u>http://science.energy.gov/np/research/</u>

#### (c) Low Energy Nuclear Physics

The Low Energy subprogram addresses frontiers identified in the 2015 Long Range Plan for Nuclear Science: Nuclear Structure and Reactions, and Nuclear Astrophysics.

The atomic nucleus is at the core of all visible matter and comprises 99.9 % of its mass. Its relevance spans dimensions from the proton radius to objects as large as stars, and covers the evolutionary history of the universe from fractions of a second after the Big Bang to today, 13.8 billion years later. The subfield of nuclear structure and reactions strives to measure, explain, and use nuclei to meet society's scientific interests and needs. The research addresses the underlying nature of atomic nuclei and the limits to their existence. It also aims to describe dynamical processes such as nuclear reactions and fission. The ultimate goal is to develop a predictive understanding of nuclei and their interactions grounded in fundamental QCD and electroweak theory; furthermore, this understanding must be based on experimental data from a wide variety of nuclei.

Nuclear astrophysics addresses the role of nuclear physics in our universe. As a field at the interface of astrophysics and nuclear physics, it is concerned with the impact of nuclear processes on the evolution of the universe, the development of structure, and the build-up of the chemical elements that are the building blocks of life. It is a broad discipline that can identify new observational signatures probing our universe. Nuclear astrophysics can identify the conditions at the very core of stars and provide a record of the violent history of the universe.

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.

Subprogram Contact:

• Chris Gould, (301) 903-1963, <u>Chris.Gould@science.doe.gov</u> Website: <u>http://science.energy.gov/np/research/</u>

#### (d) Fundamental Symmetries

This subprogram investigates aspects of the third frontier of 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 seeks to measure 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.

Subprogram Contact:

• Paul Sorensen, (301) 903-1952, <u>Paul.Sorensen@science.doe.gov</u> Website: <u>http://science.energy.gov/np/research/</u>

#### (e) Nuclear Theory

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

Subprogram Contact:

• George Fai, (301) 903-8954, <u>george.fai@science.doe.gov</u> Website: <u>http://science.energy.gov/np/research/</u>

#### (f) Nuclear Data and Nuclear Theory Computing

The mission of the United States Nuclear Data Program (USNDP) is to provide current, accurate, authoritative data for workers in pure and applied areas of nuclear science and engineering. This is accomplished primarily through the compilation, evaluation, dissemination, and archiving of extensive nuclear datasets. The USNDP also addresses gaps in the data, through targeted experimental studies and the use of theoretical models. A new interagency program of experiments intended to address gaps in nuclear data was announced in FY 2017, with the first set of experiments planned for FY 2018. The USNDP involves the efforts of ~ 50 nuclear physicists at ~ 15 national labs, research centers, institutes and universities, and is an important resource for workers in a wide range of pure and applied topics in nuclear physics. Research opportunities in Nuclear Data include both experimental and theoretical work.

Nuclear Theory Computing supports research in nuclear physics with "extreme" computational requirements, which has been enabled by the advent of high performance computing (HPC). Funding for HPC-driven NP research is provided primarily through the programs Scientific Discovery through Advanced Computation (SciDAC) and the new Exascale Computing Project

(ECP), through joint projects with the Office of Advanced Scientific Computing Research (ASCR). There are currently three NP SciDAC projects, which are five-year multisite collaborations on specific projects in computational nuclear physics, funded jointly by NP and ASCR, and closely aligned with the needs of the NP experimental program. These projects investigate 1) the properties of nuclei, using state-of-the-art models and numerical techniques; 2) the properties of strongly interacting particles (hadrons) composed of quarks and gluons, as predicted by the fundamental theory QCD; and 3) computational nuclear astrophysics, including the synthesis of the heavier elements in supernovae and neutron star mergers, and their observables effects. The two current NP ECP projects are addressing changes needed in computational NP practice in the Exascale Era, in the areas of 1) lattice QCD, and 2) nuclear astrophysics. Some computational resources needed for HPC research on NP problems are also provided by the National Energy Research Scientific Computing center (NERSC).

Subprogram Contact:

• Frank E. (Ted) Barnes, (301) 903-3212, <u>ted.barnes@science.doe.gov</u> Website: <u>http://science.energy.gov/np/research/</u>

#### (g) Isotope Development and Production for Research and Applications

The mission of the Isotope Development and Production for Research and Applications subprogram (DOE Isotope Program) is to support isotope production and research into novel technologies for production of isotopes to assure availability of critical isotopes that are in short supply to address the needs of the Nation. The program provides facilities and capabilities for the production and/or distribution of research and commercial stable and radioactive isotopes. Support is also provided for the scientific and technical staff associated with general isotope production and isotope production research. Isotopes are made available by using unique facilities stewarded by the DOE Isotope Program at Brookhaven National Laboratory, Los Alamos 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 the production, processing, recycling and distribution of isotopes in short supply. This includes technologies for production of radioisotopes using reactor and accelerator facilities. Excluded from this solicitation are proposals related to the production of Mo-99, as this isotope is under the purview of the NNSA Office of Materials Management and Minimization. A primary document currently guiding Isotope Program priorities is entitled "Meeting Isotope Needs and Capturing Opportunities for the Future: The 2015 Long Range Plan for the DOE-NP Isotope Program." This document may be accessed at http://science.energy.gov/~/media/np/nsac/pdf/docs/2015/2015\_NSACI\_Report\_to\_NSAC\_Final .pdf.

Subprogram Contact:

• Ethan Balkin, (301) 903-1861, <u>ethan.balkin@science.doe.gov</u> Website: <u>http://science.energy.gov/np/research/</u>

## (h) Accelerator Research and Development for Current and Future Nuclear Physics Facilities

The Nuclear Physics program supports a broad range of activities aimed at research and development related to the science, engineering, and technology of heavy-ion, electron, and proton accelerators and associated systems. Areas of interest include R&D of technologies for the Brookhaven National Laboratory's Relativistic Heavy Ion Collider (RHIC), with heavy ion and polarized proton beams; linear accelerators such as the Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF); development of devices and/or methods that would be useful in the generation of intense rare isotope beams for the Facility for Rare Isotope Beams (FRIB) currently under construction at Michigan State University, and R&D in accelerator science and technology in support of next generation Nuclear Physics accelerator facilities such as an electron-ion collider (EIC).

#### Subprogram Contact:

• Manouchehr Farkhondeh, (301) 903-4398, <u>manouchehr.farkhondeh@science.doe.gov</u> Website: <u>http://science.energy.gov/np/research/</u>

## Section II – AWARD INFORMATION

## A. TYPE OF AWARD INSTRUMENT

DOE anticipates awarding grants and cooperative agreements under this FOA. If it is determined that a cooperative agreement is the appropriate award instrument, the nature of the Federal involvement will be included in a special award condition.

DOE will consider funding multi-institution collaborations under this FOA.

## **B. ESTIMATED FUNDING**

It is anticipated that approximately \$250 million will be available for DOE SC new, renewal, and supplemental grant and cooperative agreement awards under this and other, more targeted FOAs in FY 2018, subject to the availability of FY 2018 appropriated funds. The amount of funding allocated under this specific FOA will be decided based on a number of factors, including peer review, the number and contents of applications received, and the availability of appropriated funds.

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

The largest award made under the Fiscal Year 2017 version of this FOA received no more than \$4,000,000 in annual funding.

## Floor

The smallest award made under the Fiscal Year 2017 version of this FOA received \$2,000 in annual funding.

The ceiling and floor described in this FOA represent historical experience. Past practice is not an obligation to stay within the historic ceiling and floor for this open solicitation.

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

The number of awards is subject to availability of FY 2018 appropriated funds. Historically, applications that arrive in response to the FOA have resulted in 200 to 350 new awards per year.

The exact number of awards will depend on the number of meritorious applications and the availability of appropriated funds.

## E. ANTICIPATED AWARD SIZE

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

## F. PERIOD OF PERFORMANCE

Awards are expected to be made for a project period of six months to five years as befitting the project, with the most common project period being three years in duration.

Continuation funding (funding for the second and subsequent budget periods) is contingent on: (1) availability of funds appropriated by Congress and future year budget authority; (2) progress towards meeting the objectives of the approved application; (3) submission of required reports; and (4) compliance with the terms and conditions of the award.

## G. TYPE OF APPLICATION

DOE will accept new, renewal, and supplemental applications under this FOA.

For renewal applications only, the Principal Investigator is required to submit a Renewal Proposal Products section through the SC's PAMS website at <u>https://pamspublic.science.energy.gov</u>. The Principal Investigator must enter into PAMS each product created during the course of the previous project period. Types of products include publications, intellectual property, technologies or techniques, and other products such as databases or software. As soon as the renewal application is assigned to a program manager, the Principal Investigator will receive an automated email from PAMS (<<u>PAMS.Autoreply@science.doe.gov</u>>) instructing him or her to navigate to the PAMS Task tab to complete and submit the Renewal Proposal Products. The submitted product list will be sent for merit review as part of the application. The application will not be considered complete and

cannot be sent for review until the product list has been submitted. H. VALUE/FUNDING FOR DOE/NNSA NATIONAL LABORATORY CONTRACTORS

# AND NON-DOE/NNSA FFRDC CONTRACTORS

For grant awards, the value of, and funding for, a DOE/NNSA National Laboratory contractor, a non-DOE/NNSA FFRDC contractor, or another Federal agency's portion of the work will not be included in the award to the successful applicant. DOE will fund a DOE/NNSA National Laboratory contractor through the DOE field work authorization system or other appropriate process and will fund non-DOE/NNSA FFRDC contractors and other Federal agencies through an interagency agreement in accordance with the Economy Act, 31 U.S.C. 1535, or other statutory authority.

## I. RESPONSIBILITY

The successful prime applicant/awardee (lead organization) will be the responsible authority regarding the settlement and satisfaction of all contractual and administrative issues, including

but not limited to, disputes and claims arising out of any agreement between the applicant and any team member, and/or subawardee.

If an award is made to another Federal agency or its FFRDC contractor, all Disputes and Claims will be resolved in accordance with the terms and conditions of the interagency agreement in consultation between DOE and the prime awardee.

## Section III – ELIGIBILITY INFORMATION

## A. ELIGIBLE APPLICANTS

All types of applicants are eligible to apply, except 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.

Applicants that are not domestic organizations should be advised that:

- Individual applicants are unlikely to possess the skills, abilities, and resources to successfully accomplish the objectives of this FOA. Individual applicants are encouraged to address this concern in their applications and to demonstrate how they will accomplish the objectives of this FOA.
- Non-domestic applicants are advised that successful applications from non-domestic applicants include a detailed demonstration of how the applicant possesses skills, resources, and abilities that do not exist among potential domestic applicants.

## **B. COST SHARING**

Cost sharing is not required.

## **C. ELIGIBLE INDIVIDUALS**

Individuals with the skills, knowledge, and resources necessary to carry out the proposed research as a Program Director/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.

## 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>http://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-0001820) 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**

Letters of intent are not required.

#### 2. Pre-application

A pre-application (also called a white paper) is recommended but optional. Before submitting a pre-application, read the information in Section I of this FOA carefully to make sure your idea is responsive and to select the topical subprogram most relevant to your idea.

The pre-application should be concise (up to three pages), provide a summary of the proposed research, provide a list of proposed collaborators/co-investigators/consultants with their institutions, and contain brief biographical information of the principal investigator(s). Please also include an order-of-magnitude estimate of the proposed work's total cost.

You will be required to select a program manager when you submit your pre-application using the DOE SC Portfolio Analysis and Management System (PAMS) website. Choose the subprogram contact for the topical area most relevant to your idea from those listed in Section I of this FOA.

Feedback from DOE to the principal investigator is optional, but you are encouraged to use your submitted pre-application/white paper to initiate a discussion with the listed program manager about the appropriateness of the proposed research for this solicitation.

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

Title of Pre-application Principal Investigator Name, Job Title Institution PI Phone Number, PI Email Address DOE/SC Program Office: Funding Opportunity Announcement Number: DE-FOA-0001820 The absence of a pre-application will not negatively affect a thorough evaluation of a responsive full application submitted in a timely fashion.

It is important that the pre-application be a single file with extension .pdf, .docx, or .doc. The filename should 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 Principal Investigator and anyone submitting on behalf of the Principal Investigator must register for an account in PAMS before it will be possible to submit a 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. For best results, please use Internet Explorer.

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

#### **Create PAMS Account:**

To register, click the "Create New PAMS Account" link on the website <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.

#### **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.

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

- At the bottom of the screen, click the "Submit to DOE" button to save and submit the preproposal to DOE.
- Upon submission, the PI will receive an email from the PAMS system <<u>PAMS.Autoreply@science.doe.gov</u>> acknowledging receipt of the preproposal.

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 Funding Opportunity Announcement should reference **DE-FOA-0001820**.

## 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: https://www.grants.gov/web/grants/applicants/organization-registration.html

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: https://www.grants.gov/web/grants/applicants/apply-for-grants.html

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 download software page at <u>http://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 in Adobe Portable Document Format (PDF) unless otherwise specified in this announcement. 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 PDF-compatible 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.

## APPLICATIONS FOR NEW AWARDS

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

Applicants should contact the appropriate DOE Program Manager or see the SC Program Website to determine if additional, program-specific guidance and/or limitations exist for the submission of new applications.

## APPLICATIONS FOR RENEWAL AWARDS

Renewal applications are requests for additional funding for a period subsequent to that provided by a current award. In preparing a renewal application, applicants should assume that reviewers will not have access to previous applications. The application should be developed as fully as though the applicant were applying for the first time. The application must include all the information required for a new project; additionally, the project narrative section should discuss the results from prior work.

Renewal applications must include the same forms and information categories as a new application, except for the following changes:

- Include under the project description section information on any changes that affect the overall direction of the research being pursued.
- Include an estimate of anticipated unexpended funds that will remain at the end of the current project period.
- Include a progress report as a separate section that describes the results of work

accomplished through the date of the renewal application and how such results relate to the activities proposed to be undertaken in the renewal period.

A renewal application generally will be subjected to the SC merit review requirements. Should an application be approved and funded, the extended period of support is treated as an extension of the original project period.

Applicants should contact the appropriate DOE Program Manager or see the SC Program Website to determine if additional, program-specific guidance and/or limitations exist for the submission of renewal applications.

For renewal applications only, the Principal Investigator is required to submit a Renewal Proposal Products section through SC's PAMS website at <u>https://pamspublic.science.energy.gov</u>. The Principal Investigator must enter into PAMS each product created during the course of the previous project period. Types of products include publications, intellectual property, technologies or techniques, and other products such as databases or software. As soon as the renewal application is assigned to a program manager, the Principal Investigator will receive an automated email from PAMS (<<u>PAMS.Autoreply@science.doe.gov</u>>) instructing him or her to navigate to the PAMS Task tab to complete and submit the Renewal Proposal Products. The submitted product list will be sent for merit review as part of the application. The application will not be considered complete and cannot be sent for review until the product list has been submitted.

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 submitted into grants.gov: please refrain from attempting to submit the Renewal Proposal Products in PAMS until you receive an email with the subject line, "Receipt of Proposal 0000xxxxxx by the DOE Office of Science," providing the assignment of a program manager. Shortly thereafter, the PI will receive an email with the subject line, "DOE…Request to Submit Renewal Proposal Products for Proposal xxxxx," indicating that the Renewal Proposal Products task is available for completion in PAMS.

#### APPLICATIONS FOR SUPPLEMENTAL AWARDS

Two types of supplemental applications may be submitted:

- If the grantee is requesting support for a new task or activity to be added to the approved project, a supplemental application shall contain the same information categories as a new application. These applications will undergo merit review and will compete for funding with other new applications.
- If the awardee needs additional funds:
  - for increased costs that could not have been predicted when the application was originally approved; or
  - to increase the "level of effort" or accelerate the project with no change to the project description as contained in the approved application.

A supplemental application, completed and submitted by the appropriate official, shall contain forms as instructed in Grants.gov and an explanation of the need for the additional funding.

Applicants should contact the appropriate DOE Program Manager or see the SC Program Website to determine if additional, program-specific guidance and/or limitations exist for the submission of supplemental applications.

### COLLABORATIVE APPLICATIONS

Collaborative applications submitted from different institutions must clearly indicate they are part of a collaborative project/group. Every partner institution must submit an application through its own sponsored research office. Each collaborative group can have only one lead institution. Each application within the collaborative group, including the narrative and all required appendices and attachments, must be identical with the following exceptions:

- Each application must contain a correct SF-424 (R&R) cover page for the submitting institution only.
- Each application must contain a unique budget corresponding to the expenditures for that application's submitting institution only.
- Each application must contain a unique budget justification corresponding to the expenditures for that application's submitting institution only.

#### **RESUBMISSION OF APPLICATIONS**

Applications submitted under this FOA may be withdrawn from consideration by using SC's 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.

After an application is withdrawn, it may be resubmitted if this FOA is still open for the submission of applications.

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 <a href="http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms">http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms</a> under Certifications and Assurances.

#### DUNS AND EIN NUMBERS

The DUNS and EIN number 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. A **renewal** application requests additional funding for a period of time following a current award. If the application requests a significant change in the scope of work, please consult with the Program contact identified in this FOA to determine if the application should be considered new or a renewal.

SC does not make use of the Resubmission, Continuation, or Revision options.

Applications for supplemental support of an existing award should be marked as "New."

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.

#### PUBLIC POLICY REQUIREMENTS

The applicant is made aware of generally-applicable public policy requirements, including the following:

| Animal Welfare Act                                  | 7 USC 2131 et seq.,                          |
|---|--|
| Buy American Act                                    | 41 USC 10 et seq.                            |
| Cargo Preference Act                                | 46 USC 55305, 46 CFR 381.7                   |
| Civil Rights Protections                            | 10 CFR 1040                                  |
| Debarment and Suspension                            | 2 CFR 180, 2 CFR 901                         |
| Drug-Free Workplace Act                             | 41 USC 701, 10 CFR 607                       |
| Environmental Protections                           | 42 USC 7401, 33 USC 1251, 42 USC 4321        |
| False Claims Act                                    | 31 USC 3729, 18 USC 287, 18 USC 1001, 10 CFR |
|   | 1013   |
| Federal Funding Accountability and Transparency Act | P.L. 109-282, 2 CFR 170                      |
| Fly America Act                                     | 49 USC 40118                                 |
| Hatch Act   | 5 USC 1501 et seq.                           |
| Human Research Subjects Protections                 | 10 CFR 745                                   |
| Lobbying Disclosure Act                             | 2 USC 1601 et seq.                           |
| Lobbying Prohibitions                               | 31 USC 1352, 10 CFR 601                      |
| Metric System use                                   | EO 12770                                     |
| Non-delinquency on Federal Debt                     | 28 USC 3201                                  |
| Prohibition on benefitting Members of Congress      | 41 USC 6306                                  |
| Seat Belt Use                                       | EO 13043                                     |
| Terrorist Financing                                 | EO 13224, 66 FR 49079                        |
| Text Messaging While Driving                        | EO 13513, 74 FR 51225                        |
| Trafficking in Persons                              | 22 USC 7104, 2 CFR 175                       |

#### 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. (http://www.ecfr.gov)

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, if there would be 1) 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 1 through 6 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 project director/principal investigator(s) (PD/PI) and the PD/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."

- 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 should begin with a cover page. The cover page must include the following items:

- The project title
- Applicant/Institution:
- Street Address/City/State/Zip:

- Postal Address:
- Lead PI name, telephone number, email:
- Administrative Point of Contact name, telephone number, email:
- Funding Opportunity FOA Number: DE-FOA-0001820
- DOE/SC Program Office (ASCR, BER, BES, FES, HEP, or NP):
- Topic Area\*:
- Topic Area Program Manager (from Section I of this FOA):
- DOE Award Number (if Renewal or Supplemental Application):
- PAMS Preproposal tracking number (if applicable):

\*The topic area can be found in Section I, Supplementary Information, of this FOA. For example, the topic area might be Synthesis and Processing Science or Medium Energy Nuclear Physics. Please select from the list in Section I.

## **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.

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

Collaborative applications submitted from different institutions must clearly indicate they are part of a collaborative project/group. Every partner institution must submit an application through its own sponsored research office. Each collaborative group can have only one lead institution. Each application within the collaborative group, including the narrative and all required appendices and attachments, must be identical with the following exceptions:

- Each application must contain a correct SF-424 (R&R) cover page for the submitting institution only.
- Each application must contain a unique budget corresponding to the expenditures for that application's submitting institution only.
- Each application must contain a unique budget justification corresponding to the expenditures for that application's submitting institution only.

Each application belonging to a collaborative group should have the same title in Block 11 of the SF 424 (R&R) form.

SC will use the multiple applications associated with a collaborative group to create one consolidated document for merit review that consists of the common, identical application materials combined with a set of detailed budgets from the partner institutions. It is very important that every application in the collaborative group be identical (including the title) with the exception of the budget and budget justification pages.

If the project is a collaboration, provide the following information on a separate page as a supplement to the cover page.

- List all collaborating institutions by name with each institution's principal investigator on the same line.
- Indicate the lead PI who will be the point of contact and coordinator for the combined research activity.
- Provide a statement explaining the leadership structure of the collaboration.
- Include a description of each collaborating institution's facilities, equipment, and resources that will be made available to the collaborative group.
- If applicable, explain how students and junior researchers will be trained and mentored by the collaborators.
- Include a table modeled on the following chart providing summary budget information from all collaborating institutions. Provide the total costs of the budget request in each year for each institution and totals for all rows and columns.

| Collaborative Application Information |       |             |                  |  |                  |                 |
|---------------------------------------|-------|-------------|------------------|--|------------------|-----------------|
|                                       | Names | Institution | Year 1<br>Budget |  | Year 5<br>Budget | Total<br>Budget |
| Lead<br>PI                            |       |             |                  |  |                  |                 |
| Co-PI                                 |       |             |                  |  |                  |                 |
| Co-PI                                 |       |             |                  |  |                  |                 |
| Co-PI                                 |       |             |                  |  |                  |                 |

Example budget table (\$ in thousands)

\* Note that collaborating applications must be submitted separately.

PROJECT NARRATIVE (FIELD 8 ON THE FORM)

The project narrative consists 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.

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."

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 major part of the narrative should be devoted to a description and justification of the proposed project, including details of the method to be used. It should also include a timeline for the major activities of the proposed

project, and should indicate which project personnel will be responsible for which activities. There should be no ambiguity about which personnel will perform particular parts of the project or the time at which these activities will take place.

**For Collaborative Proposals Only**: Each collaborating institution must submit an identical common narrative. Collaborative proposals will necessarily be longer than single-institution proposals. The common narrative must identify which tasks and activities will be performed by which of the collaborating institutions in every budget period of the proposed project. The budget and the budget justification which are unique to each collaborating institution—may refer to parts of the common narrative to further identify each collaborating institution's activities in the joint project. There should be no ambiguity about each institution's role and participation in the collaborative group.

SC will use the multiple applications associated with a collaborative group to create one consolidated document for merit review that consists of the common, identical application materials combined with a set of detailed budgets from the partner institutions. It is very important that every application in the collaborative group be identical (including the title) with the exception of the budget and budget justification pages.

Do not attach any of the 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.

APPENDIX 1: BIOGRAPHICAL SKETCH

Provide a biographical sketch for the PI and each senior/key person listed in Section A on the R&R Budget form.

As part of the sketch, provide information that can be used by reviewers to evaluate the PI's potential for leadership within the scientific community. Examples of information of interest are invited and/or public lectures, awards received, scientific program committees, conference or workshop organization, professional society activities, special international or industrial partnerships, reviewing or editorship activities, or other scientific leadership experiences.

- Provide the biographical sketch information as an appendix to your project narrative.
- Do not attach a separate file.
- The biographical information (curriculum vitae) for each person must not exceed 2 pages when printed on 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 11 point and must include:

The biographical information (curriculum vitae) must include the following items within its page limit:

• **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 no more than 5 professional and scholarly activities related to the effort proposed.

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 Project Director/Principal Investigator(s) (PD/PI) and senior/key persons, including subawardees, for ongoing projects and pending applications. List all sponsored activities or awards requiring a measurable commitment of effort, whether paid or unpaid. For every activity, list the following items:

- The sponsor of the activity or the source of funding
- The award or other identifying number

- The title of the award or activity
- The total cost or value of the award or activity, including direct and indirect costs. For pending proposals, provide the total amount of requested funding.
- The person-months of effort per year being dedicated to the award or activity

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.

#### 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). For example, your paper may be listed as, "A Really Important New Result," A. Aardvark et. al. (MONGO Collaboration), PRL 999. 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.

## APPENDIX 4: FACILITIES & OTHER RESOURCES

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

• Do not attach a separate file.

#### **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.

#### APPENDIX 6: DATA MANAGEMENT PLAN

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

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

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>http://science.energy.gov/funding-opportunities/digital-data-management/</u>.

SC program offices may provide additional guidance, available through <a href="http://science.energy.gov/funding-opportunities/digital-data-management/">http://science.energy.gov/funding-opportunities/digital-data-management/</a>. Compliance with a program office's additional guidance will not be considered during merit review and award selection.

DMPs are NOT required for conference or workshop applications.

DMPs are required for all New and Renewal applications submitted to this FOA.

DMPS are required for supplemental applications that expand the scope of work beyond that of the originally funded project. Supplemental application DMPs should address the research products of the expanded, supplemental research scope.

- This appendix should not exceed 2 pages 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)
- Do not attach a separate file.

#### APPENDIX 7: OTHER ATTACHMENT

If you need to elaborate on your responses to questions 1-6 on the "Other Project Information" document, please provide the Other Attachment information as an appendix to your project narrative. Information not easily accessible to a reviewer may be included in this appendix. Reviewers are not required to consider information in this appendix.

- Do not attach a separate file.
- Do not attach any of the requested appendices described above as files for fields 9, 10, 11, and 12.
- Follow the above instructions to include the information as appendices to the project narrative file.
- 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).

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

- Funds requested for personnel (senior, key, and other) 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.

| Section A<br>Senior/Key Person | For each Senior/Key Person, enter the requested information. List<br>personnel, base salary, the number of months that person will be<br>allocated to the project, requested salary fringe benefits, and the total<br>funds requested for each person. The requested salary must be the<br>product of the base salary and the effort.<br>Include a written narrative in the budget justification that justifies the<br>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   |
|                                | requested for each person.   |
|                                | Include a written narrative in the budget justification that fully justifies the need for requested personnel.   |
| Section C                      | For the purpose of this budget, equipment is designated as an item of  |
| Equipment                      | 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<br>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  |

**Budget Fields** 

| Participant/Trainee<br>Support Costsintend to support trai<br>graduate) must list ea<br>amounts, cost of tuiti<br>same information as<br>costs for any related<br>associated with confe<br>breakout items shoul<br>participant, purpose of<br>any related administri<br>Indicate the basis for<br>suppliers, past experi-<br>Section F<br>Other Direct Costs• Materials and S<br>materials and sup<br>justification, indic<br>chemicals, include<br>identified under 'not required to be | the cost estimate (quotes from vendors or<br>ience of similar items, or some other basis).<br><b>upplies:</b> Enter total funds requested for<br>oplies in the appropriate fields. In the budget  |
|--|---|
| Section F<br>Other Direct Costs<br>Other Direct Costs<br>Other Direct Costs<br>Other Direct Costs<br>Other Direct Costs<br>Section F<br>Materials and Section<br>justification, indi<br>chemicals, include<br>identified under '<br>not required to be   | <b>upplies:</b> Enter total funds requested for pplies in the appropriate fields. In the budget   |
| <ul> <li>similar items, or it</li> <li>Publication Cost<br/>The proposal bud<br/>documenting, preavailable to other<br/>conducted under<br/>supporting inform<br/>(quotes from ven<br/>items, or some of</li> <li>Consultant Service<br/>consultant, the set<br/>travel costs, and to<br/>cost estimate (quoties)<br/>of similar items, or</li> <li>ADP/Computer<br/>ADP/Computer S<br/>including compute<br/>education inform<br/>justification, inclu-<br/>proposing organi</li> </ul> | rices: Enter total funds requested for all<br>es. In the budget justification, identify each<br>ervices he/she will perform, total number of days,<br>total estimated costs. Indicate the basis for the<br>otes from vendors or suppliers, past experience<br>or some other basis).<br>Services: Enter total funds requested for<br>Services. The cost of computer services,<br>ter-based retrieval of scientific, technical and<br>ation may be requested. In the budget<br>ude the established computer service rates at the<br>zation if applicable. Indicate the basis for the<br>otes from vendors or suppliers, past experience |

|                      | <ul> <li>for all subawards/consortium organizations and other contractual costs proposed for the project. In the budget justification, justify the details.</li> <li>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).</li> <li>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.</li> <li>Other: Add text to describe any other Direct Costs not</li> </ul> |
|----------------------|---|
|                      | requested above. Enter costs associated with "Other" item(s).<br>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 through F)   |
| Section H            | Enter the Indirect Cost information for each field. Only four general   |
| Other Indirect Costs | categories of indirect costs are allowed/requested on this form, so   |
|                      | please consolidate if needed. Include the cognizant Federal agency and 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 K. 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

**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 K.

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

Your application must include the following items:

| Name of Document                                  | Format | Attach to |
|---|--------|-----------|
| SF 424 (R&R)                                      | Form   | N/A       |
| RESEARCH AND RELATED Other<br>Project Information | 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 K   |
| PROJECT/PERFORMANCE SITE                          | Form   | N/A       |

| LOCATION(S)                   |      |      |
|-------------------------------|------|------|
| SF-LLL Disclosure of Lobbying | Form | NI/A |
| 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.

# **E. SUBMISSION DATES AND TIMES**

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

None

# 2. Pre-application Due Date

None

# **3. Application Due Date**

This FOA will remain open until March 1, 2019, 11:59 PM Eastern Time, or until it is succeeded by another issuance, whichever occurs first. This Annual FOA DE-FOA-0001820 succeeds FOA DE-FOA-0001664, which was published October 1, 2016.

Applications for conference or workshop support must be submitted at least six months before the meeting date.

Renewal applications compete with all other applications and must be submitted through Grants.gov at least six months before the scheduled expiration of the current award's project period. Earlier submission is strongly encouraged to allow for timely processing.

# F. INTERGOVERNMENTAL REVIEW

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

# G. 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.

**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.

# H. 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 http://fedgov.dnb.com/webform.

Applicants must register with the System for Award Management (SAM) at <u>http://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

https://www.sam.gov/sam/transcript/Quick\_Guide\_for\_Grants\_Registrations.pdf. 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 Employer Identification Number (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 <u>http://www.irs.gov/Businesses/Small-Businesses-%26-Self-</u> Employed/Apply-for-an-Employer-Identification-Number-(EIN)-Online.

DOE discourages the use of a SSN as a TIN. You are encouraged to obtain a TIN from the Internal Revenue Service (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 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 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. For best results, please use Internet Explorer.

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.

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

For help with PAMS, click the "External User Guide" link on the PAMS website, <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 Funding Opportunity Announcement should reference DE-FOA-0001820.

#### 5. Viewing Submitted Applications

Each grants.gov application submitted to 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 0000xxxxxx by the DOE Office of Science." These three people are the Principal Investigator (Block 14), Authorized Representative (Block 19), and Point of Contact (Block 5). In PAMS notation, applications are known as proposals, the Principal Investigator 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 submitted into 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. For best results, please use Internet Explorer.

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 submission and inquiries about this Funding Opportunity Announcement should reference **DE-FOA-0001820**.

# 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; (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.

# 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.

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

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

SCIENTIFIC AND/OR TECHNICAL MERIT OF THE PROPOSED RESEARCH

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

#### APPROPRIATENESS OF THE PROPOSED METHOD OR APPROACH

- How logical and feasible are the research approaches?
- Does the proposed research employ innovative concepts or methods?
- 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?

COMPETENCY OF APPLICANT'S PERSONNEL AND ADEQUACY OF PROPOSED RESOURCES

- What is 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?

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?

# **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>http://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:

- Availability of funds
- Relevance of the proposed activity to SC priorities
- Ensuring an appropriate balance of activities within SC programs
- Performance under current awards

# 3. Selection

The Selection Officials 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

SC aims to make award selection within six months. The time interval begins on the date the application is received.

# Section VI - AWARD ADMINISTRATION INFORMATION

# A. AWARD NOTICES

## **1. Notice of Selection**

**Selected Applicants Notification**: DOE will notify applicants selected for award. This notice of selection is not an authorization to begin performance. (See Section IV. Part G 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; and (7) 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 https://www.nsf.gov/pubs/policydocs/rtc/rtcoverlay\_march17.pdf and the DOE Agency Specific Standard Research Terms and Conditions published at https://www.nsf.gov/pubs/policydocs/rtc/agencyspecifics/doe\_417.pdf. 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>http://www.ecfr.gov</u>). Prime awardees must keep their data at the System for Award Management (SAM) current at <u>http://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>http://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 the System for Award Management (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>http://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: http://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>http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms</u> under Award Terms.

# 4. Statement of Substantial Involvement

Either a grant or cooperative agreement may be awarded under this FOA. If the award is a cooperative agreement, the DOE contract specialist and DOE project officer will negotiate a Statement of Substantial Involvement prior to award.

# **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 Funding Opportunity Announcement. Publications and other methods of public communication describing any work based on or developed under an award resulting from this Funding Opportunity Announcement must contain an acknowledgment of DOE SC support. The format for such acknowledgments is provided at <a href="http://science.energy.gov/funding-opportunities/acknowledgements/">http://science.energy.gov/funding-opportunities/acknowledgements/</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 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="http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance/financial-assistance-forms">http://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 Funding Opportunity Announcement should reference **DE-FOA-0001820**. 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                               |
| Program Manager    | Questions regarding the specific program areas/technical       |
| Scientific Contact | requirements should be directed to the point of contact listed |
|                    | for each program office 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="http://www.fedconnect.net">http://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="http://energy.gov/gc/services/technology-transfer-and-procurement/office-assistant-general-counsel-technology-transf-1">http://energy.gov/gc/services/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 OF WORK 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. 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."