Program Announcement
To DOE National Laboratories

LAB 11-572

Office of Science
Early Career Research Program

GENERAL INQUIRES ABOUT THIS PROGRAM ANNOUNCEMENT SHOULD BE DIRECTED TO:

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

Technical Contact: Questions regarding the specific program areas/technical requirements can be directed to the technical contacts listed for each program within the Announcement.

LETTER OF INTENT:

A Letter of Intent is not required.

PREPROPOSAL:

PREPROPOSALS ARE REQUIRED.

Preproposals are **REQUIRED** and must be submitted by Thursday, September 1, 2011, 11:59 P.M. Eastern Time. The preproposal should be uploaded as a Word or Portable Document Format (pdf) attachment and submitted through the website https://EarlyCareerPreapp.science.doe.gov. Preproposals will be reviewed for responsiveness of the proposed work to the research topics identified in this Program Announcement. DOE will send a response by email to each proposer encouraging or discouraging the submission of a formal proposal by Monday, October 3, 2011. **Only those proposers that receive notification from DOE encouraging a formal proposal may submit full proposals.** No other formal proposals will be considered. Each laboratory is responsible for ensuring that the research ideas submitted in its preproposals fit within the scope of Office-of-Science-funded programs at the national laboratory.

The preproposal attachment should include, at the top of the first page, the following information:

Title of Preproposal
Principal Investigator Name, Job Title
National Laboratory
PI Phone Number, PI Email Address
Year Doctorate Awarded: XXXX
Program Announcement Number: LAB 11-572

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

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

Only one preproposal per Principal Investigator is allowed.

Note: The website, https://EarlyCareerPreapp.science.doe.gov, is designed for submission of one preproposal at a time.

PROPOSAL DUE DATE: Formal proposals submitted in response to this Progam Announcement must be submitted from the laboratory to the site office through Searchable FWP by Tuesday, November 29, 2011, 11:59 P.M. Eastern Time, to permit timely consideration of awards. **Each proposal should be in a single PDF file. The first few pages of the PDF should be the Field Work Proposal followed in the same PDF by the full technical proposal. You are encouraged to transmit your proposal well before the deadline. Only those proposers that receive notification from DOE encouraging a formal proposal may submit full proposals. PROPOSALS RECEIVED AFTER THE DEADLINE WILL NOT BE REVIEWED OR CONSIDERED FOR AWARD.**

SUMMARY:

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

SUPPLEMENTARY INFORMATION:
Office of Science Website: http://science.energy.gov/

The mission of the DOE Office of Science is to deliver scientific discoveries and major scientific tools to transform our understanding of nature and to advance the energy, economic, and national security of the United States.

The following program descriptions are offered to provide more in-depth information on scientific and technical areas of interest to the Office of Science:

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

I. Advanced Scientific Computing Research (ASCR)
(a) Applied Mathematics
(b) Computer Science

II. Biological and Environmental Research (BER)
(a) Microbial Systems Biology Design for Bioenergy Production
(b) Arctic Terrestrial Ecosystem Science
(c) Subsurface Biogeochemistry
(d) Uncertainty Characterization for Integrated Earth System Modeling

III. Basic Energy Sciences (BES)
(a) Materials Chemistry
(b) Biomolecular Materials
(c) Synthesis and Processing Science
(d) Experimental Condensed Matter Physics
(e) Theoretical Condensed Matter Physics
(f) Physical Behavior of Materials
(g) Mechanical Behavior and Radiation Effects
(h) X-ray Scattering
(i) Neutron Scattering
(j) Electron and Scanning Probe Microscopies
(k) Atomic, Molecular, and Optical Sciences (AMOS)
(l) Gas Phase Chemical Physics (GPCP)
(m) Computation and Theoretical Chemistry
(n) Condensed Phase and Interfacial Molecular Science (CPIMS)
(o) Catalysis Science
(p) Separations and Analysis
(q) Heavy Element Chemistry (HEC)
(r) Geosciences Research
(s) Solar Photochemistry
(t) Photosynthetic Systems
(u) Physical Biosciences

(v) BES Nanoscale Science Research Centers and Electron-Beam Microcharacterization Centers Research
(w) BES Accelerator and Detector Research
(x) BES X-ray and Neutron Scattering Instrumentation and Technique Development

IV. Fusion Energy Sciences (FES)
(a) Magnetic Fusion Energy Science Experimental Research
(b) Magnetic Fusion Energy Science Theory and Simulation
(c) High-Energy-Density Plasma Science and Inertial Fusion Energy Science
(d) General Plasma Science Experiment and Theory
(e) Materials Science and Enabling Technologies for Fusion

V. High Energy Physics (HEP)
(a) Experimental High Energy Physics Research
(b) Theoretical High Energy Physics Research
(c) Advanced Technology Research and Development

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

I. Advanced Scientific Computing Research (ASCR)
Program Website: http://science.energy.gov/ascr/

The mission of the Advanced Scientific Computing Research (ASCR) program is to discover, develop, and deploy computational and networking capabilities to analyze, model, simulate, and predict complex phenomena important to the Department of Energy. A particular challenge of this program is fulfilling the science potential of emerging computing systems and other novel computing architectures, which will require numerous significant modifications to today's tools and techniques to deliver on the promise of exascale science.

Some priority areas for ASCR are listed below:
- To develop mathematical descriptions, models, methods and algorithms to accurately describe and understand the behavior of complex systems involving processes that span vastly different time and/or length scales.
- To develop the underlying understanding and software to make effective use of computers at extreme scales
- To transform extreme scale data from experiments and simulations into scientific insight.

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

For the purposes of the Early Career Research Program, proposed research must be in either Applied Mathematics or Computer Science and be responsive to their respectively specified topic areas.

(a) Applied Mathematics
Technical Contact: Sandy Landsberg, 301-903-8507, sandy.landsberg@science.doe.gov

This program supports basic research leading to fundamental mathematical advances and computational breakthroughs across DOE and Office of Science missions. Applied Mathematics research includes and supports efforts to develop robust mathematical models, algorithms and numerical software for enabling predictive scientific simulations of DOE-relevant complex systems. For this solicitation, the specific topic areas of interest are listed here:

1. Numerical methods for the scalable solutions of linear and/or nonlinear systems on advanced high-concurrency, memory-bound high-performance computer architectures, such as communication-avoiding solvers, alternative PDE solvers that may take advantage of advanced architectures, or analysis and modifications of today’s popular linear solvers for high-concurrency computing systems;
2. Rigorous mathematical and computationally efficient approaches for analyzing and extracting information and insight from large-scale scientific datasets;
3. Mathematical development and efficient numerical algorithms for optimization under uncertainty, including stochastic programming, stochastic optimization, robust optimization, and nonlinear programming under uncertainty, for DOE mission-relevant applications; and
4. Innovative mathematical approaches to improve the fidelity and predictability of continuous and/or distributed complex systems that accurately capture the physics and/or subcomponent interactions across vastly different time and length scales. Approaches that address hierarchical models as well as new methodologies for understanding the impact on system behavior are encouraged.

The proposal’s responsiveness to this solicitation in these topic areas will be based on addressing all of the following criteria: (a) advances and innovations in mathematical models, methods and/or numerical algorithms, (b) applicability to advanced high-concurrency, memory-bound high-performance computer architectures, (c) relevance of proposed research to DOE missions and/or scientific grand challenges, and (d) mathematical and algorithmic challenges arising in computational simulations at scale. Furthermore, proposals that are limited to a specific scientific discipline, or the development and implementation of existing numerical methods, are out of scope for this solicitation.

(b) Computer Science
Technical Contact: Sonia R. Sachs, 301-903-0060, sonia.sachs@science.doe.gov

This program supports research to advance the development, operation and systems management of Leadership Class and production high performance computing facilities at DOE National Labs, application software development for scientific modeling and simulation at petascale to exascale, high performance computing systems architecture and software, and scientific data management and analysis at scale.

Research topics of interest for this solicitation are focused on three key software challenges for exascale platforms, namely:

1. Novel methods and abstract machines to analyze and understand common memory access patterns to improve data locality, minimize excessive data movement and reduce power requirements. Machine abstractions should provide a theoretical framework to reason about exascale architectures and their idealized software boundary.
2. Programming models, language constructs, compilers and runtime systems that address the challenges of programming applications that are characterized by computations on irregular data structures and with unstructured and dynamic communication patterns.
3. Scientific data management; data integration/fusion; data interoperability; and data analysis and visualization for petabyte to exabyte data sets, both static and streaming, including in-situ and remote-access methods.

Proposals must explain their relevance to current and future high performance computing platforms as well as their relevance to the mission of the Office of Science. Topics which are out of scope for this program include hardware architecture, and performance modeling and assessment tools, software development tools and methods (e.g., debuggers, integrated development environments, etc.), scientific workflows, interoperability at the application level, quantum computing, networking, computer-supported collaboration, social computing, natural language processing / understanding / generation, generalized research in human-computer interaction, discipline-specific data analytics and informatics, and research which is only applicable to hand-held, portable, desktop, cluster or cloud computing.

II. Biological and Environmental Research (BER)
Program Website: http://science.energy.gov/ber/

The mission of the Biological and Environmental Research (BER) program is to understand complex biological, climatic, and environmental systems across spatial and temporal scales ranging from sub-micron to the global, from individual molecules to ecosystems, and from nanoseconds to millennia. This is accomplished by exploring the frontiers of genome-enabled biology; discovering the physical, chemical and biological drivers of climate change; and seeking the geochemical, hydrological, and biological determinants of environmental sustainability and stewardship.

Biological Systems Science
Research is focused on using DOE's unique resources and facilities to develop fundamental knowledge of biological systems that can be used to address DOE needs in clean energy, carbon sequestration, and environmental cleanup and that will underpin biotechnology-based solutions to energy challenges. The objectives are: (1) to develop the experimental and computational resources needed to understand and predict complex behavior of complete biological systems, principally plants, microbes, and microbial communities; (2) to take advantage of the remarkable high throughput DNA sequencing capacity at the Joint Genome Institute to meet the genome sequencing and analysis needs of the scientific community; (3) to understand and characterize the risks to human health from exposures to low levels of ionizing radiation; (4) to operate experimental biological stations at synchrotron and neutron sources; and (5) to develop radiochemistry and advanced technologies for imaging and high throughput characterization and analysis for BER missions in bioenergy, subsurface, and climate change.

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

(a) Microbial Systems Biology Design for Bioenergy Production
Technical Contact: Pablo Rabinowicz, 301-903-0379, pablo.rabinowicz@science.doe.gov

Research aimed at understanding metabolic and regulatory networks of microbes or microbial consortia relevant to production of advanced biofuels, with the goal of identifying underlying biological design principles that govern critical functional properties and enable functional redesign. Proposals should contain predictive approaches validated by experimental systems biology to relate key biological parts to their functional and dynamic operation in living microbial systems.

Climate and Environmental Sciences
The program seeks to understand the basic physical, chemical, and biological processes of the Earth's System and how these processes may be affected by energy production and use. Research is designed to provide data to enable an objective, scientifically based assessment of the potential for, and the consequences of, human-induced climate change at global and regional scales. The program also provides data and models to enable assessments of mitigation options to prevent such change. The program is comprehensive with emphasis on: (1) understanding and simulating the radiation balance from the surface of the Earth to the top of the atmosphere, including the effect of clouds, water vapor, trace gases, and aerosols. (The Atmospheric Radiation Measurement Climate Research Facility provides key observational data to the climate research community on the radiative properties of the atmosphere, especially clouds and aerosols. This national user facility includes highly instrumented ground stations, a mobile facility, and an aerial vehicles program.); (2) enhancing and evaluating the quantitative models necessary to predict natural climatic variability and possible human-caused climate change at global and regional scales; (3) understanding and simulating the net exchange of carbon dioxide between the atmosphere, and terrestrial systems, as well as the effects of climate change on the global carbon cycle; (4) understanding ecological effects of climate change; (5) improving approaches to integrated assessments of effects of, and options to mitigate, climatic change; (6) basic

research directed at understanding options for sequestering excess atmospheric carbon dioxide in terrestrial ecosystems, including potential environmental implications of such sequestration; (7) subsurface biogeochemical research to understand and predict subsurface contaminant fate and transport; and (8) take advantage of the national user facility, the Environmental Molecular Sciences Laboratory (EMSL) that houses an unparalleled collection of state-of-the-art capabilities, including a supercomputer and over 60 major instruments, providing integrated experimental and computational resources for discovery and technological innovation in the environmental molecular sciences. EMSL also contributes to systems biology by providing leading edge capabilities in proteomics.

BER is only seeking Climate and Environmental Sciences research in the following three areas:

(b) Arctic Terrestrial Ecosystem Science
Technical Contact: Mike Kuperberg, 301-903-3511, michael.kuperberg@science.doe.gov

Research that combines measurements, experiments, and modeling that provide improved quantitative and predictive understanding of the arctic terrestrial carbon cycle processes that in turn influence the directions of arctic and global climate change. The goal should be to understand the impacts of, and feed backs from a changing climate on non-managed arctic terrestrial ecosystems, that contain permafrost and dynamically changing conditions. Research should be posed in the context of representing terrestrial carbon cycle processes in earth system models.

(c) Subsurface Biogeochemistry
Technical Contact: David Lesmes, 301-903-2977, david.lesmes@science.doe.gov

Investigations of the coupled physical, chemical, and biological processes affecting the transport of subsurface contaminants at DOE sites emphasizing critical knowledge gaps and hypothesis-driven research to better understand the significant physical, chemical, and biological processes influencing the form and mobility of DOE contaminants in the subsurface. The environment of interest is the terrestrial subsurface including the vadose zone, the saturated zone and key groundwater-surface water interfaces.

(d) Uncertainty Characterization for Integrated Earth System Modeling
Technical Contact: Dorothy Koch, 301-903-0105, Dorothy.koch@science.doe.gov

Development of methodologies that characterize uncertainties in integrated earth system models, by examining the various components that contribute to uncertainties. It is expected that proposed research will include novel approaches that examine nonlinear relationships between different component level uncertainties, due to e.g. data limitations associated with initial and boundary conditions, biogeophysical simplifications of parameterizations and submodel codes, resolution, correlated error analyses across system components, numerical methods, and validation.

BER EXCLUSIONS: Proposals for BER research should specifically identify which of the four topics listed above, (a) Microbial Systems Biology Design for Bioenergy Production, (b) Arctic

Terrestrial Ecosystem Science, (c) Subsurface Biogeochemistry, (4) Uncertainty Characterization for Integrated Earth System Modeling, is the focus of the proposed research and how the proposed research will address the stated aims. Proposals that address other BER-related topics or that do not make specific reference to the stated aims of these four topics will not be accepted.

III. Basic Energy Sciences (BES)

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

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

The four long-term goals in scientific advancement that the BES program is committed to and against which progress can be measured are:

- Design, model, fabricate, characterize, analyze, assemble, and use a variety of new materials and structures, including metals, alloys, ceramics, polymers, bioinspired and biomimetic materials and more-particularly at the nanoscale-for energy-related applications.
- Understand, model, and control chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic and biological systems.
- Develop new concepts and improve existing methods to assure a secure energy future, e.g., for solar energy conversion and for other energy sources.
- Conceive, design, fabricate, and use new scientific instruments to characterize and ultimately control materials, especially instruments for x-ray, neutron, and electron beam scattering and for use with high magnetic and electric fields.

More detailed information about BES sponsored research can be found at the BES website listed above. There you will find BES-sponsored workshop reports that address the current status and possible future directions of some important research areas. Also, Principal Investigators' Meetings Reports contain abstracts of BES supported research in topical areas associated with Division-sponsored technical conferences. Finally, the websites of individual BES Divisions may also be helpful. The following web pages are listed for convenience:

Basic Research Needs Reports:
http://science.energy.gov/bes/news-and-resources/reports/basic-research-needs/
BES Workshop Reports:
http://science.energy.gov/bes/news-and-resources/reports/workshop-reports/
Materials Sciences and Engineering Division Principal Investigators' Meetings:
http://science.energy.gov/bes/mse/principal-investigators-meetings/
Chemical Sciences, Geosciences, & Biosciences Division Principal Investigators' Meetings:

http://science.energy.gov/bes/csgb/principal-investigators-meetings/
Scientific User Facilities Division web page:
http://science.energy.gov/bes/suf/

Proposed research must be directed to one of the core research areas listed below:

(a) Materials Chemistry
Technical Contact: Aravinda Kini, 301-903-3565, a.kini@science.doe.gov

This research activity supports basic research in chemical synthesis and discovery of new materials. The major programmatic focus is on the discovery, design and synthesis of novel materials with an emphasis on the chemistry and chemical control of structure and collective properties. Major scientific areas include: nanoscale chemical synthesis and assembly; solid state chemistry for exploratory synthesis and tailored reactivities; novel polymeric materials and complex fluids; and surface and interfacial chemistry including electrochemistry.

With the completion of the recent cycle of BES Basic Research Needs (and other) workshops and reports, the scientific community has articulated very clearly those areas of science and materials which are most relevant to energy. All of the reports variously identify the overarching goal of materials chemistry research as providing the knowledge needed to design and produce new materials with tailored properties from first principles. This program will make progress towards that goal by emphasizing the following areas: (1) Development of new chemical means to direct and control the non-covalent assembly of materials, such as strategies to organize electron donors and acceptors; (2) Creation of ways to tailor the symmetry and dimensionality of crystalline lattices; (3) Utilization of chemistry to control and design interfaces between dissimilar materials. All of these activities will be conducted in order to develop and/or discover new materials that have the potential for use in next generation energy technologies, including solar energy conversion, electrical energy storage and transport, solid-state lighting, fuel cells, and carbon capture.

The program **will not** support projects aimed at optimization of materials properties or device fabrication.

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

This activity supports basic research in the discovery, design and synthesis of functional materials and complex structures based on principles and concepts of biology. The major programmatic focus is on the creation of robust, scalable, energy-relevant materials and systems with emergent behavior that work with the extraordinary effectiveness of molecules and processes of the biological world. Major scientific areas include: Bioinspired materials discovery by linking physical and chemical synthesis with the synthesis strategies of biology to create new materials *in vitro* with altered morphologies and desired materials properties; self-assembly inspired by biological processes that yields complex structures that are far from equilibrium and exhibiting emergent behaviors; and design and synthesis of adaptive, self-healing materials.

Recent BES Basic Research Needs (and other) workshops and reports have clearly identified mastering the capabilities of living systems as a Grand Challenge that could provide the knowledge base to discover, design, and synthesize new materials with totally new properties for next-generation energy technologies. This program will make progress towards that goal by emphasizing the following areas: (1) Enhanced integration of theory and experiment leading to new design ideas and opportunities for discovery; (2) Bioinspired synthesis of inorganic materials and polymers; (3) Dynamically adaptive and self-repairing materials; (4) Functional structures that take inspiration from biological membranes and motors..

The program **will not** support projects aimed at optimization of materials properties, device fabrication, and development of sensors, tissue engineering and biomedical research.

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

This activity supports basic research for developing new techniques to synthesize materials with desired structure and properties; to understand the physical mechanisms that underpin materials synthesis often using *in situ* monitoring. The emphasis is on the synthesis of complex thin films and nanoscale materials with atomic layer-by-layer control; preparation techniques for pristine single crystal and bulk materials with novel physical properties; understanding the contributions of precursor states to the processing of bulk nanoscale materials; and processing techniques for scalable nanostructured materials. The focus of this activity on bulk synthesis and crystal and thin films growth via physical means is complementary to the BES Materials Chemistry and Biomolecular Materials research activities.

Over the past few years, the activity has evolved an increasing interest in understanding nanoscale morphology, defect control in deposition processes, and complex chemical and structural materials growth. Over the next several years, these directions are expected to continue with a stronger focus on research in bulk materials growth, deposition, and sintering and added emphasis in mechanisms for interfacing soft-hard hybrid materials and their organization. Expansion is planned in research for discovery of novel synthesis methods, especially using extreme environments of high pressure and field, and research to forge new understanding in synthesis and processing related to use-inspired technologies including solid-state lighting, solar energy conversion, and electrical energy storage. This activity will continue to support hypothesis-driven fundamental science in synthesis and processing with a particular interest in high-risk, high-impact, and imaginative projects. The activity continues to support and encourages natural collaboration between theorists and experimentalists.

Synthesis and Processing **does not** fund research on device fabrication or optimization of material properties.

(d) Experimental Condensed Matter Physics
Technical Contact: Andrew Schwartz, 301-903-3535, andrew.schwartz@science.doe.gov

This program supports experimental research aimed at gaining fundamental understanding of the relationships between intrinsic electronic structure, particularly strong electron correlation effects, and the properties of complex materials such as superconductors, magnetic materials, and two-dimensional electron or hole gases. A particular emphasis is placed on investigating the physics of low-dimensional systems, including nanostructures, as well as studies of electronic structure under extreme conditions such as low temperatures and high magnetic fields. The program will continue a longstanding investment in research to understand unconventional superconductors, including the high-temperature cuprate family and the recently discovered class of iron-based superconductors. In the last few years the program has increased support for studies of spin physics and nanomagnetism, and has begun to explore whether cold atom research can provide insight into open questions about correlated electron behavior in hard condensed matter systems. The program does not support research in electrochemistry, thermoelectric materials, or mechanical properties of materials.

(e) Theoretical Condensed Matter Physics
Technical Contact: James Davenport, 301-903-0035, james.davenport@science.doe.gov

This activity supports Theoretical Condensed Matter Physics with emphasis on the theory, modeling, and simulation of electronic correlations. A major thrust is nanoscale science, where links between the electronic, optical, mechanical, and magnetic properties of nanostructures and their size, shape, topology, and composition are poorly understood. Other major research areas include strongly correlated electron systems, quantum transport, superconductivity, magnetism, and optics. Development of theory targeted at aiding experimental technique design and interpretation of experimental results is also emphasized.

The program will continue to emphasize the development of our understanding of matter on the atomic scale and expanding to add the capability of addressing length scales both larger and smaller than the nanoscale is part of the scientific future of theory, modeling and simulation for condensed matter and materials. A rich future exists in basic science and applications surrounding highly correlated materials as well as novel superconductors. This research is motivated by the newest science of materials, as well as by the potential for impact on longstanding problems for energy technologies and for fundamental physics, including understanding of the physics of microstructure and granular material. Computationally enabled science is simultaneously growing in maturity and seeing dramatic advances. Those advances, which further the basic research and mission of BES, have a natural home in this program.

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

This activity supports basic research on the behavior of materials in response to external stimuli, such as temperature, electromagnetic fields, chemical environments, and the proximity effects of surfaces and interfaces. Emphasis is on the relationships between performance, such as electrical, magnetic, optical, electrochemical, and thermal performance, and the microstructure and defects in the material. Included within the activity are research to establish the relationship of crystal defects to semiconducting, superconducting, and magnetic properties; phase equilibria and kinetics of reactions in materials in hostile environments; and diffusion and transport phenomena. Basic research is also supported to develop new instrumentation, including *in situ* experimental tools, and to probe the physical behavior in real environments encountered in energy applications.

In the near term, four central topics define the current program: electronic and magnetic behavior of materials; corrosion and electrochemistry science; nano-scale phenomena; and multiscale modeling of materials behaviors. Major efforts in these areas will continue. Increased investment in plasmonics, metamaterials and organic electronic materials will be considered. In addition, focus in theory and modeling at universities and national laboratories, taking advantage of the vast advances in computing speed and power, will be emphasized.

The long term goals of this program to understand the macroscopic behavior of materials it is important to understand the relationship between a material's properties and its response to external stimuli. This can be achieved by determining structure over multiple length scales, with emphasis at the atomic level, and by understanding the response of the nanometer and larger features of the material to those external stimuli. Studies of the physical response of a single nanometer-scale feature needs to be related to the macroscopic behavior of the material. This can often be done with modeling, but further advances are necessary to fully couple the length scales from atomic to macroscopic. Currently, atomistic simulation methods can be used to study systems containing hundreds of thousands of atoms, but these systems are still orders of magnitude too small to describe macroscopic behavior. Continuum methods, typically using finite element methods, fail to adequately describe many important properties because they use phenomenology that has little connection to the real processes that govern physical interactions. Modeling at an intermediate length scale, the mesoscale, where many defects can be included and from which predictive models at the continuum scale can be developed is required for advances in materials science. At this intermediate length-scale it is necessary to model the collective phenomena that include well over a billion atoms. Developing and applying novel techniques to these problems will be emphasized in coordination with the investment in theory and modeling. This program also seeks to foster theory, modeling, and simulation activities that address the following key topics in organic electronic materials: charge and energy transfer; electronic structure calculation; exciton dynamics and transport; and spin dynamics.

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

This activity supports hypothesis-driven basic research to understand defects in materials and their effects on the properties of strength, structure, deformation, and failure. Defect formation, growth, migration, and propagation are examined by coordinated experimental and modeling efforts over a wide range of spatial and temporal scales. Topics include fundamental studies of deformation of ultra-fine scale materials, radiation resistant of structural materials, and intelligent microstructural design for increased strength, formability, and fracture resistance in energy relevant materials. The goals are to develop the scientific underpinning for predictive models for the design of materials having superior mechanical properties and radiation resistance.

Research opportunities that can be realized by the application of mechanics fundamentals to the general area of self-assembly, physical behavior, and behavior under extreme environments (primarily environments that are experienced in current or future fission reactors) will constitute an increasingly significant part of the development of devices that harvest energy, sense trace amounts of matter, and manipulate information. With the emerging importance of nanoscale structures with high surface-to-volume ratios, it is appropriate to take advantage of the new, unprecedented capabilities to fabricate and test tailored structures down to the nanoscale, taking advantage of more powerful parallel computational platforms and new experimental tools. High-strain rate deformation **will not** be explored in this program at this time.

Radiation is increasingly being used as a tool and a probe to gain a greater understanding of fundamental atomistic behavior of materials. Incoming fluxes can be uniquely tuned to generate a materials response that can be detected *in situ* over moderate length and time scales. Materials also sustain damage after long times in high-radiation environments typical of current and projected nuclear energy reactors and in geological waste storage. As nuclear energy is projected to play a larger role in U.S. energy production, these are issues that need to be addressed at a fundamental level. High-dose studies **will not** be explored in this program at this time.

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

This activity supports basic research on the fundamental interactions of photons with matter to achieve an understanding of atomic, electronic, and magnetic structures and excitations and their relationships to materials properties. The main emphasis is on x-ray scattering, spectroscopy, and imaging research, primarily at major BES-supported user facilities. Instrumentation development and experimental research directed at the study of ultrafast physical phenomena in materials, is an integral part of the portfolio. Based on programmatic priorities, this activity **will not** support ultra-fast source development in the FY 2012 Early Career Program, but will focus on the application of ultra-fast probe interactions with materials and the resulting connection to materials dynamics.

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

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

This activity supports basic research on the fundamental interactions of neutrons with matter to achieve an understanding of the atomic, electronic, and magnetic structures and excitations of materials and their relationship to materials properties. Major emphasis is on the application of neutron scattering and spectroscopy for materials research, primarily at BES-supported user facilities. A continuing theme of this program is the integration of material synthesis, neutron scattering experiments and computational modeling as this is vital to obtain controlled samples for careful neutron scattering measurements and modeling for in-depth understanding of the structure and dynamics. Development of innovative focusing optics for time-of-flight instruments and application of polarized neutrons are distinct aspects of this activity.

Research at the intersection of hard and soft condensed matter sciences will be high priority as polymers, biomaterials and hybrid nanocomposites are ubiquitous in various advanced applications. *In situ* research can measure properties dynamically, during synthesis and use of materials in appropriate environments and operational conditions, yielding direct data for comparison to predictions. Proposals that take advantage of the *in situ* capabilities and unique aspects of neutron scattering that can lead to the discovery of advanced materials for efficient photovoltaics, electrodes and electrolytes for the next generation energy storage systems, thermoelectrics, fuel cell membranes, carbon dioxide sequestration and radiation resistant self healing materials are encouraged. The goal will be to facilitate stronger interaction between the neutron scattering experiments and theory coupled with high performance computation to ensure that the experimental and computational data on structure and dynamics of functional materials are available to accelerate development and enable validation of the software.

Elastic and inelastic neutron scattering techniques will remain as essential tools for the investigation of complex correlated electron systems. This program will support research on materials for such applications including thermoelectics and energy storage, but NOT on superconductivity and magnetism, based on programmatic priorities in the 2012 Early Career Program.

(j) Electron and Scanning Probe Microscopies
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This activity supports basic research in condensed matter physics and materials science using electron and scanning probe microscopy and spectroscopy techniques. The research includes experiments and theory to understand the atomic, electronic, and magnetic structures and properties of materials. This activity also supports the development of new instrumentation and techniques, including ultrafast diffraction and imaging techniques, to advance basic science and materials characterizations for energy applications. The goal is to develop a fundamental understanding of materials through advanced microscopy and spectroscopy.

This program will build upon the tremendous advancements in electron and scanning probe microscopy capabilities in the last decade and use scattering, imaging and spectroscopy methods to understand functionality and fundamental processes at the atomic or nanometer scale. Characterization of semiconducting, superconducting, magnetic, and ferroelectric materials benefits greatly from these abilities and from other research supported in this program. Concurrently, new frontiers in fundamental understanding of materials are being opened with the creation of novel characterization techniques.

Development of advanced electron and scanning probe microscopy techniques will be continued in order to meet our energy and basic science challenges. Significant improvements in resolution and sensitivity will provide an array of opportunities for groundbreaking science. These include the possibilities of understanding and controlling nanoscale inhomogeneity, new phenomena emerging at nanoscale, atomic-scale tomography, probing magnetism at the atomic scale with spin excitation spectroscopy, imaging spin density and spin waves, imaging functionality at the atomic scale, combination of multiple probes, and *in situ* analysis capabilities (under perturbing parameters such as temperature, irradiation, stress, magnetic field, and chemical environment). New methods and approaches addressing the scientific challenges will lead to the development of unique new analysis tools and breakthroughs in materials. The combined new experimental and theoretical capabilities will enable the fundamental understanding of atomic origins of materials properties. Significant advances will be made in the fundamental understanding of the mechanisms by which electrons, individual atoms, surface/interfaces and defects influence the properties and behavior of materials.

(k) Atomic, Molecular, and Optical Sciences (AMOS)
Technical Contact: Jeffrey Krause, 301-903-5827, jeff.krause@science.doe.gov

This program supports experimental and theoretical research aimed at understanding the structural and dynamical properties of atoms, molecules and nanostructures. The research emphasizes 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, electron correlation, ultracold chemistry, and light-matter interactions in nanoscale structures. Topics of interest include the development and application of novel, ultrafast optical probes of matter; the interactions of atoms and molecules with intense electromagnetic fields; and studies of collisions and many-body cooperative interactions in atomic and molecular systems.

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

The program emphasizes ultrafast, ultra-intense, short-wavelength science, and correlated dynamics in atoms and molecules. Examples are the use of high-harmonic generation or its variants as soft x-ray sources, intense, ultrafast x-ray science at the Linac Coherent Light Source (LCLS), development and characterization of femtosecond and attosecond pulses of x-rays at synchrotrons as well as accelerator-based and table-top sources. Applications of these light sources include ultrafast imaging of chemical reactions, diffraction and harmonic generation from aligned molecules, and atomic and molecular inner-shell photoionization. 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 in the study of low-energy electron-molecule interactions in the gas and condensed phases, and collisions of ultracold molecules.

The AMOS program **does not** support research in quantum information science, ultracold quantum gases, condensates, or plasmas.

(l) Gas Phase Chemical Physics (GPCP)
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The Gas Phase Chemical Physics (GPCP) Program supports research that improves our understanding of the dynamics and rates of chemical reactions at energies characteristic of combustion and the chemical and physical properties of key combustion intermediates. The overall aim is the development of a fundamental understanding of chemical reactivity enabling validated theories, models and computational tools for predicting rates, products, and dynamics of chemical processes involved in energy utilization by combustion devices. Important to this aim is the development of experimental tools for discovery of fundamental dynamics and processes affecting chemical reactivity. Combustion models using this input are developed that incorporate complex chemistry with the turbulent flow and energy transport characteristics of real combustion processes.

Major thrust areas supported by the GPCP program include: quantum chemistry, reactive molecule dynamics, chemical kinetics, spectroscopy, predictive combustion models, combustion diagnostics, and soot formation & growth. The GPCP program **does *not*** support research in the following areas: non-reacting fluid dynamics and spray dynamics, data-sharing software development, end-use combustion device development, and characterization or optimization of end-use combustion devices.

The focus of the GPCP program is the development of a molecular-level understanding of gas-phase chemical reactivity of importance to combustion. The desired evolution is to multi-phase predictive capabilities that span the microscopic to macroscopic domains enabling the computation of individual molecular interactions as well as their role in complex, collective behavior in real-world devices. Currently, increased emphasis in gas-phase chemical physics is on validated theories and computational approaches for the structure, dynamics, and kinetics of open shell systems, experimental measurements of combustion reactions at high pressures, better insight into soot particle growth and an improved understanding of the interaction of chemistry with fluid dynamics.

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

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

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

Current interest includes applications to (i) energy storage, (ii) solar light harvesting including sunlight-to-fuel, (iii) interfacial phenomena, (iv) selective carbon-dioxide/gas separation, storage and capture (v) next-generation combustion modeling, (vi) reactivity and catalysis (vii) molecular and nano- scale electronic and energy transport (ix) quantum simulation of biologically inspired mechanisms for energy management and (x) alternative fuel.

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

This activity emphasizes molecular understanding of chemical, physical, and electron- and photon-driven processes in aqueous media and at interfaces. Studies of reaction dynamics at well-characterized metal and metal-oxide 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 understandings of molecular reactivity and dynamical processes in solution and at interfaces. The approach confronts the transition from molecular-scale chemistry to collective phenomena in complex systems, such as the effects of solvation on chemical structure and reactivity. Fundamental studies of reactive processes driven by radiolysis in condensed phases and at interfaces provide improved understanding of radiolysis effects and radiation-driven chemistry in nuclear fuel and waste environments.

Research in CPIMS is fundamental to meeting the grand challenges for basic energy sciences, as identified in the report from the Basic Energy Sciences Advisory Committee: *Directing Matter and Energy: Five Challenges for Science and the Imagination.* This activity supports experimental and theoretical investigations in the gas phase, condensed phase, and at interfaces aimed at elucidating the molecular-scale chemical and physical properties and interactions that govern chemical reactivity, solute/solvent structure, and transport. The impact of this cross-cutting program on DOE missions is far reaching, including energy utilization, catalytic and separation processes, energy storage, and environmental chemical and transport processes.

The desired evolution for CPIMS research is toward predictive capabilities that span the microscopic to macroscopic domains enabling the computation of individual molecular interactions as well as their role in complex, collective behavior in real-world devices. In surface chemistry, continued emphasis is on the development of a structural basis for gas/surface interactions, encouraging site-specific studies that measure local behavior at defined sites. At interfaces, emphasis is on aqueous systems and the role of solvents in mediating solute reactivity. Future emphasis includes the need to probe the chemical physics of energy transfer and reactivity in large molecules, to explore the molecular origins of condensed phase behavior and the nature and effects of non-covalent interactions including hydrogen bonding, and to investigate temporally resolved interfacial chemical dynamics and charge transfer using advances in chemical imaging. Renewed emphasis is anticipated in areas such as emergent behavior in condensed phase systems and for interfacial science relevant to electrical energy storage, including studies for electrode-electrolyte interfaces.

The CPIMS program **does not** fund research in bulk fluid dynamics, such as studies of laminar or turbulent flows. In addition, the program does not support applications such as micro-scale devices, and the CPIMS program **does not** support research of molecules and/or cells that is directed toward medical applications.

The abstracts from the Seventh Research Meeting of the CPIMS Program can be found on the web page link labeled 'Chemical Sciences, Geosciences, & Biosciences Division Principal Investigators' Meetings' at the beginning of this section, under III. Basic Energy Sciences (BES). The most recent report is labeled 'June 12-15, 2011'.

(o) Catalysis Science
Technical Contact: Raul Miranda, 301-903-8014, raul.miranda@science.doe.gov

This activity develops the fundamental scientific principles enabling rational catalyst design and chemical transformation control. Research includes the identification of the elementary steps of catalytic reaction mechanisms and their kinetics; construction of catalytic sites at the atomic level; synthesis of ligands, metal clusters, and bio-inspired reaction centers designed to tune molecular-level catalytic activity and selectivity; the study of structure-reactivity relationships of inorganic, organic, or hybrid catalytic materials in solution or supported on solids; the dynamics of catalyst structure relevant to catalyst stability; the experimental determination of potential energy landscapes for catalytic reactions; the development of novel spectroscopic techniques and structural probes for *in situ* characterization of catalytic processes; and the development of theory, modeling, and simulation of catalytic pathways. A wealth of experimental information has been accumulated relating catalytic structure, activity, selectivity, and reaction mechanisms. However, for phenomenological catalysis to evolve into predictive catalysis, the principles connecting kinetic phenomena must be more clearly and thoroughly identified. Better understanding of catalysis will result from synthesis of catalyst structures that are stable and reproducible under working conditions; fast and ultrafast characterization of intermediate and transition states; and hybrid quantum/classical mechanics and microkinetics analysis of complex reactions.

The convergence of heterogeneous, homogeneous, and biocatalysis is emerging and being used to derive new biomimetic catalysts. Designed secondary and tertiary structures add structural flexibility and chemical specificity that affect catalytic properties of inorganic catalysts. In terms of applications, the research will focus on understanding and controlling the synthesis and chemistry of novel inorganic, organic, and hybrid catalysts. New strategies for design of selective catalysts for fuel and chemical production from both fossil and renewable biomass feedstocks will be explored. Selective and low-temperature activation of alkanes, CO_2, and multifunctional molecules will continue to receive attention. Increased emphasis will be placed on the use of theory, spectroscopy and microscopy to probe and understand catalytic systems under realistic working conditions. Emphasis will also be placed on the investigation of catalytic mechanisms, pathways, and bond rearrangements under electrochemical and photoelectrochemical conversion of small as well as complex molecules into chemicals and fuels.

Examples of research funded in this category can be found in Catalysis Science Program Meeting Reports at the link labeled ‘Chemical Sciences, Geosciences, & Biosciences Division Principal Investigators' Meetings’ at the beginning of this section, under <u>III. Basic Energy Sciences (BES)</u>. For molecular and homogeneous catalysis, see the catalysis science meeting report labeled ‘June 1-4, 2010’. For interfacial, heterogeneous and electro catalysis, see the catalysis science meeting report labeled ‘May 31-June 3, 2009’. A recent BESAC-sponsored workshop, Basic Research Needs: Catalysis for Energy, outlining the current challenges and needs in this field can also be found on the ‘Basic Research Needs Reports’ web page link at the beginning of this section.

(p) Separations and Analysis
Technical Contact: Larry Rahn, 301-903-2508, larry.rahn@science.doe.gov

This activity supports fundamental research focused at the molecular and nanoscale related to a broad spectrum of separation concepts, including membrane processes, extraction under both standard and supercritical conditions, adsorption, chromatography, and complexation. Also supported is work to improve the sensitivity, reliability, and productivity of analytical determinations and to develop new approaches to analysis in complex, heterogeneous environments, including techniques that combine chemical selectivity and spatial resolution to achieve chemical imaging. The separations and analysis activity is inspired by the common, and often tightly coupled, fundamental underpinnings associated with a wide range of energy related chemical recognition, separation, and analysis problems. These include processing and utilization of current and future petroleum, bio, solar, and nuclear fuels including carbon capture, needed efficiency and/or selectivity improvements for chemical processing, and production of strategic energy-relevant materials. The overall goal is to obtain a predictive understanding, at molecular and nanoscale dimensions, of the basic chemical and physical principles involved in separations systems and analytical tools so that innovative approaches to these problems may be discovered and advanced.

Separations research will continue to advance the understanding of and control of the atomic and molecular interactions between target species and separations media; multifunction separations media; supramolecular recognition (using designed, multi-molecule assemblies to attract specific target species); synthesis of new porous/hierarchical materials, understanding and control of interface properties at the molecular/nanoscale; ligand design and synthesis of extractant molecules; mechanisms of transport and fouling in polymer and inorganic membranes; and relevant solvation in supercritical and ionic liquids. Analytical research will pursue the elucidation of ionization, ion chemistry, and excitation mechanisms for optical and mass spectrometry; single molecule detection, characterization, and observation; nano- and molecular-scale analytical methods including biomolecules relevant to DOE's bioenergy interests; laser and tip-enhanced methods for high-resolution spectroscopy and for presentation of samples for mass spectrometry; characterization of interfacial phenomena with emphasis on chromatography; and surface-enhanced Raman spectroscopy. This research will also pursue the underlying science needed to achieve true chemical imaging, i.e., the ability to selectively image selected chemical moieties at the molecular scale and to do so with temporal resolution that allows one to follow physical and chemical processes relevant to energy science.

This activity **does not** support engineering or scale up of particular processes or devices. Research that is directed toward medical applications **is not** supported.

Examples of research funded in this category can be found in Separations and Analysis Meeting Reports at the link labeled 'Chemical Sciences, Geosciences, & Biosciences Division Principal Investigators' Meetings' at the beginning of this section, under III. Basic Energy Sciences (BES). The most recent one is labeled 'April 25-28, 2010'. For actinide related separations, see the description below of BES Heavy Element Chemistry.

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

This activity supports basic research in the chemistry of the heavy elements, focused on the actinides, but also includes the transactinide elements and some fission products. 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 placed on resolving the f-electron challenge; the chemical and physical properties of these elements to determine solution, interfacial and solid-state bonding and reactivity; fundamental transactinide chemical properties; fundamental science underpinning the extraction and separation of the actinides; and on bonding relationships among the actinides, lanthanides, and transition metals.

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 report of the Basic Energy Sciences Workshop (July 31 – August 3, 2006) on this topic, and echoed in the report from the Basic

Energy Sciences Advisory Committee: *Science for Energy Technology: Strengthening the Link between Basic Research and Industry* (August 2010). Research to meet this challenge is pursued in the HEC program and includes efforts aimed at implementing quantum-mechanical theories that more adequately describe spin-orbit interactions and relativistic effects, and efforts to expand our ability to predict actinide and fission product chemical behavior under conditions relevant to all stages of fuel reprocessing.

Synthetic and spectroscopic research is pursued within the HEC program on chemical bonding and reactivity of molecules that contain heavy elements and of actinides in environmentally relevant species, with a focus on gaining a fundamental understanding of separations processes and aiding the development of ligands to sequester actinides. Better characterization and modeling of the interactions of actinides at liquid-solid and liquid-liquid interfaces, including mineral surfaces under environmentally relevant conditions and as colloids, is motivated by improving the separations processes that are essential for advanced nuclear fuel cycles and improving models of actinide environmental transport.

The abstracts from the 2011 Separations and Heavy Element Chemistry Research Meeting can be found on the web page link labeled ‘Chemical Sciences, Geosciences, & Biosciences Division Principal Investigators' Meetings’ at the beginning of this section, under III. Basic Energy Sciences (BES). The report is labeled ‘April 26-29, 2011’.

* This workshop report can be found on the ‘Basic Research Needs Reports’ page link at the beginning of this section, III. Basic Energy Sciences (BES).

(r) Geosciences Research
Technical Contact: Nicholas Woodward, 301-903-4061, nick.woodward@science.doe.gov

This activity supports basic experimental and theoretical research in geochemistry and geophysics. Geochemical research emphasizes fundamental understanding of geochemical processes and reaction rates, focusing on aqueous solution chemistry, mineral-fluid interactions, and isotopic distributions and migration in natural systems. Geophysical research focuses on new approaches to understand the subsurface physical properties of fluids, rocks, and minerals and develops techniques for determining such properties at a distance; it seeks fundamental understanding of wave propagation physics in complex media and the fluid dynamics of complex fluids through porous and fractured subsurface rock units. Geosciences research seeks to better understand the significance of commonly observed natural nanophases and nanoparticles in shallow earth systems and how they contribute to mineral-fluid interactions, hydrologic flow dynamics, and geophysical responses.

The activity seeks new research efforts on imaging of earth processes with attention devoted both to improved small-scale imaging (geochemistry focus) using x-ray sources, neutron sources, and scanning microscopies, and large-scale imaging (geophysics focus) of physical properties. New energy waste storage options will require high-resolution measurements, monitoring and verification at a new level of sophistication. Geosciences activities will link analytical capabilities with computational capabilities to provide improved understanding of geochemical and geophysical processes occurring at natural time and length scales.

(s) Solar Photochemistry
Technical Contact: Mark Spitler, 301-903-4568, mark.spitler@science.doe.gov

This activity supports fundamental, molecular-level research on solar energy capture and conversion in the condensed phase and at interfaces. These investigations of solar photochemical energy conversion focus on the elementary steps of light absorption, charge separation, and charge transport within a number of chemical systems, including those with significant nanostructured composition. Although the long term mission of this Program is an understanding of the science behind solar-driven production of fuels and electricity, it is recognized that fundamental research in the interaction of light, matter and electrons in these systems is essential to the achievement of Program goals.

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

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

Research areas concerned with separation of charge that might result in electricity include multibandgap, multilayer cascade-type semiconductors, photosensitized nanoparticulate solids, and the study of the mechanism of multiple exciton generation within nanoparticles. There are also challenges in fundamental understanding of photoconversion processes – energy transfer and the generation, separation, and recombination of charge carriers – in organic-based molecular semiconductors, which could lead to a new type of inexpensive and flexible solar cell Another regime of chemistry initiated through creation of high energy excited states is highly ionizing radiation, as can be produced through electron pulse radiolysis, to investigate reaction dynamics, structure, and energetics of short-lived transient intermediates in the condensed phase. Among many topics, fundamental research is of interest in areas which have a long term impact upon the understanding of radiolytic degradation of nuclear tank waste, the reactivity of solid surfaces in reactor coolant systems, and the chemistry of reagents used in separations processes in nuclear cycles.

Solar Photochemistry **does not** fund research on device development or optimization. Not of interest during FY 2012 are proposals that involve the assembly of dye sensitized solar cells with TiO_2.

(t) Photosynthetic Systems
Technical Contact: Gail McLean, 301-903-7807, gail.mclean@science.doe.gov

This activity supports basic research on the biological conversion of solar energy to chemically stored forms of energy. Topics of study include but are not limited to light harvesting, exciton transfer, charge separation, transfer of reductant to carbon dioxide, as well as the biochemistry of carbon fixation, metabolism, and storage. Such research will enhance understanding and control of the weak intermolecular forces governing molecular assembly in photosynthetic systems; understanding the biological machinery for cofactor insertion into proteins and protein subunit assemblies; adapting combinatorial, directed evolution, and high-throughput screening methods to enhance energy production in photosynthetic systems; characterizing the structural and mechanistic features of photosynthetic complexes; and determining the physical and chemical rules that underlie biological mechanisms of repair and photo-protection.

Photosynthetic Systems **does not** fund research: 1) in prokaryotic systems related to human/animal health or disease; 2) on development or optimization of devices/processes; 3) on development or optimization of microbial strains or plant varieties for biofuel/biomass production. Projects should ideally be hypothesis-driven; projects that develop high-throughput screening approaches **will not** be supported.

All submitted proposals 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 and/or non-medical microbes capture, transduce, and store energy?

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

This activity supports basic research that combines the tools of the physical sciences with biochemical and molecular biological approaches to further our understanding of the ways plants and/or non-medical microbes capture, transduce, and store energy. Research supported includes studies that investigate the mechanisms by which energy transduction systems are assembled and maintained, the processes that regulate energy-relevant chemical reactions within the cell, the underlying biochemical and biophysical principles determining the architecture of biopolymers and the plant cell wall, and active site protein chemistry that provides a basis for highly selective and efficient bioinspired catalysts.

Future impact is, in general, envisioned through increased use of physical science and computational tools (ultrafast laser spectroscopy, current and future x-ray light sources, and quantum chemistry) to probe spatial and temporal properties of biological systems. For instance, the application of such tools to the study of individual enzymes (and multi-enzyme complexes) will enable the design of improved industrial catalysts and processes (e.g. more cost-effective, highly-efficient, etc) through a more complete understanding of structure and mechanistic principles. One such priority area for the program is achieving a greater understanding of the active site chemistries of multi-electron redox reactions (e.g. CO2 reduction). Another unique aspect of biological systems is their ability to self-assemble and self-repair. These capabilities occur via complex processes that are not well-understood, and enhanced efforts will be devoted to the identification of the underlying chemical/physical principles that govern such behaviors.

Physical Biosciences **does not** fund research: 1) in animal systems; 2) in prokaryotic systems related to human/animal health or disease; 3) development or optimization of devices/processes; 4) development or optimization of microbial strains or plant varieties for biofuel/biomass production. Projects should ideally be hypothesis-driven; projects that develop or rely primarily on high-throughput screening approaches **will not** be supported.

All submitted proposals 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 and/or non-medical microbes capture, transduce, and store energy?

(v) BES Nanoscale Science Research Centers and Electron-Beam Microcharacterization Centers Research
Technical Contact: Mihal Gross, 301-903-6827, mihal.gross@science.doe.gov

This research area supports work that advances the instruments, techniques, and capabilities of the existing BES Scientific User Facilities and/or contributes to capabilities of future facilities in this area. We do not intend to support proposals to establish new, unrelated types of facilities or to develop techniques that do not relate to the missions of the nanoscale science research centers or electron beam microcharacterization facilities.

Five Nanoscale Science Research Centers (NSRCs) support the synthesis, processing, fabrication, and analysis of materials at the nanoscale: the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory (ORNL), the Molecular Foundry at Lawrence Berkley National Laboratory (LBNL), the Center for Integrated Nanotechnologies at Sandia National Laboratory (SNL)/Los Alamos National Laboratory (LANL), the Center for Nanoscale Materials at Argonne National Laboratory (ANL), and the Center for Functional Nanomaterials at Brookhaven National Laboratory (BNL). These centers are the Department of Energy's premier user facilities for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools for synthesis, fabrication, and analysis, and new computing approaches and capabilities. As such, research is supported across the spectrum of scientific and engineering disciplines to understand and exploit unique and phenomena materials at the nanoscale, including materials for energy conversion, structured materials derived from or inspired by nature, hard and crystalline materials (including the structure of macromolecules), magnetic and soft materials (including polymers and ordered structures in fluids), and nanoscale materials integration. Tools for probing nanoscale materials and phenomena are increasingly multi-modal, to enable characterization of electrical, optical, and/or magnetic properties on the same sample with high resolution over a range of length scales. The ability to characterize functional nanoscale materials in-situ, under operating conditions, is also increasingly important, from, for example, battery electrode charging/discharging, to catalysts at high pressures and temperatures, to biologically-inspired, soft, and/or hybrid materials in liquid environments. New approaches to probe at the nanoscale also frequently leverage complementary electron-beam, x-ray, and neutron facilities. Theory and modeling are closely coupled with experiment to advance the understanding of nanoscale phenomena, provide insights to inform materials by design, and develop and implement new capabilities leveraging the most advanced computational resources.

In the area of electron-beam microcharacterization the focus is on the development of next generation electron-beam instrumentation and on conducting corresponding research. Electron scattering has key attributes that give such approaches unique advantages and make them complementary to x-ray and neutron beam techniques. These characteristics include strong interactions with matter (allowing the capture of meaningful signals from very small amounts of material, including single atoms under some circumstances) and the ability to readily focus the charged electron beams using electromagnetic lenses. The net result is unsurpassed spatial resolution and the ability to simultaneously get structural, chemical, and other types of information from sub-nanometer regions, allowing study of the fundamental mechanisms of catalysis, energy conversion, corrosion, charge transfer, magnetic behavior, and many other processes. All of these are fundamental to understanding and improving materials for energy applications and the associated physical characteristics and changes that govern performance. Instrumentation and technique development efforts are supported in areas including scanning, transmission, and scanning transmission electron microscopes, atom probes and related field ion instruments, related surface characterization apparatus and scanning probe microscopes, and ancillary tools such as spectrometers, detectors, and advanced sample preparation equipment.

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

This research area supports work that advances the instruments, techniques, and capabilities of the existing BES Scientific User Facilities and/or contributes to capabilities of future facilities in this area. We **do not** intend to support proposals to establish new, unrelated types of facilities or to develop techniques that do not relate to the missions of the light sources and neutron scattering centers.

BES supports five light sources whose unique properties of continuous spectrum, high flux, and brightness make them indispensable tools for exploration of matter: the National Synchrotron Light Source, the Stanford Synchrotron Radiation Light Source, the Advanced Light Source, the Advanced Photon Source, and the first hard x-ray free electron laser, the Linac Coherent Light Source.

BES also supports three neutron scattering facilities: the Spallation Neutron Source, the High Flux Isotope Reactor, and the Manuel Lujan Jr. Neutron Scattering Center. Their output beams are particularly well-suited for measurement of the positions as well as the fluctuations in the positions of atoms (phonons), and the structure (position and direction) of atomic magnetic moments in solids and the excitations in their magnetic structure (spin waves).

In this accelerator and detector research program, the objective is to improve the output and capabilities of light sources and neutron scattering facilities that are the most advanced of their kind in the world. This program supports basic research in accelerator physics and x-ray and neutron detectors. Research is supported that seeks to achieve a fundamental understanding beyond the traditional accelerator science and technology to develop new concepts for the design of accelerator facilities.

To fully exploit the fluxes delivered by all these sources, new detectors capable of acquiring data several orders of magnitude faster than current rates are required. 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. They will also enable real-time kinetic studies and studies of weak scattering samples.

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

(x) BES X-ray and Neutron Scattering Instrumentation and Technique Development
Technical Contact: David L. Price, 301-903-4591, david.price@science.doe.gov

This research area supports work that advances the instruments, techniques, and capabilities of the existing BES Scientific User Facilities and/or contributes to capabilities of future facilities in this area. We **do not** intend to support proposals to establish new, unrelated types of facilities or to develop techniques that do not relate to the missions of the light sources and neutron scattering centers.

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

Neutrons are a unique and effective tool for probing the structure of matter, particularly the positions, as well as the fluctuations in the positions of atoms (phonons), and the structure (position and direction) of atomic magnetic moments in solids and the excitations in their magnetic structure (spin waves). Such studies increase the understanding of phenomena such as melting, magnetic order, and superconductivity. At the three BES neutron facilities, measurements of structure and dynamics can cover length scales of 0.01 to 10 nm and time scales of 10 fs to 1 µs.

To fully exploit the wide range of capabilities of these sources, imaginative concepts for new types of scattering instruments are needed, as well as innovative uses of existing instruments, including sample environments, use of different wavelength ranges and time structures, and novel approaches to data visualization and analysis.

IV. Fusion Energy Sciences (FES)

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

The mission of the Fusion Energy Sciences (FES) program is to expand the fundamental understanding of matter at very high temperature and density and to build the scientific foundation needed to develop a fusion energy source. This is accomplished by studying plasma and its interaction with its surroundings across wide ranges of temperature and density, developing advanced diagnostics to make detailed measurements of its properties and dynamics, and creating theoretical and computational models to resolve the essential physics principles.

Plasma science is at the center of the research needed to be able to harness the power of the stars on earth. Plasma science has advanced to the point where we are ready to explore the regime of self-sustaining, or burning plasmas. The key activity in this exploration is the U.S. participation in ITER, an experiment to study and demonstrate the sustained burning of fusion fuel. ITER will provide an unparalleled scientific research opportunity and will test the scientific and technical feasibility of magnetic fusion power. Currently FES scientists and engineers are supporting the design activities, technical R&D, hardware procurement and other construction activities which support our share of the project. In addition, the FES program supports research in high-energy-density laboratory plasma (HEDLP) science.

The National Research Council report *Plasma Science: Advancing Knowledge in the National Interest* has recognized that plasma science has a coherent intellectual framework unified by physical processes that are common to many subfields. Because of the wide range of plasma densities and temperatures encountered in fusion applications, it is valuable to support plasma science across many of its subfields in order to advance the fusion energy mission. Accordingly, the FES program has four strategic goals:

- Advance the fundamental science of magnetically confined plasmas to develop the predictive capability needed for a sustainable fusion energy source;
- Pursue scientific opportunities and grand challenges in high-energy-density plasma science to explore the feasibility of the inertial confinement approach as a fusion energy source, to better understand our universe, and to enhance national security and economic competitiveness;
- Support the development of the scientific understanding required to design and deploy the materials needed to support a burning plasma environment; and
- Increase the fundamental understanding of basic plasma science, including both burning plasma and low temperature plasma science and engineering, to enhance economic competiveness and to create opportunities for a broader range of science-based applications.

To address these strategic goals, research on the specific topics below is supported by the Fusion Energy Sciences program. Proposals are sought in all areas of plasma science listed below, but priority will be given to plasma theory and modeling to provide the foundations for integrated simulation of fusion systems, experimental research advancing the magnetic fusion energy science; high-energy-density plasma science, general plasma processes and low temperature plasma science, and development of materials and technologies that will allow fusion facilities to enter new regimes of plasma science.

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

This Experimental Research program seeks to utilize unique magnetic fusion research facilities to develop the physics knowledge needed to advance the FES energy mission and fulfill the FES's role as federal steward for basic plasma science. The effort requires operation of a set of diversified experimental facilities, ranging from smaller-scale university experiments to large national facilities that involve extensive collaborations. The extensive plasma diagnostic systems operating on these facilities provide the experimental data required to study fusion science, basic plasma physics, and fusion energy production and to validate theoretical understanding and computer models, leading ultimately to a predictive understanding of plasma properties, including their dynamics and interactions with surrounding materials. Operation of major fusion facilities will be focused on science issues relevant to ITER design and operation, burning plasma physics, magnetic confinement, and other high priority plasma physics issues. The research needs of the magnetic fusion energy sciences component of this program were detailed in the report of a community-wide Research Needs Workshop (ReNeW) *Research Needs for Magnetic Fusion Energy Sciences* (http://science.energy.gov/~/media/fes/pdf/workshop-reports/Res_needs_mag_fusion_report_june_2009.pdf). This report describes the scientific research required during the ITER era to develop the knowledge needed for a practical fusion power source. Research in this area also involves small-scale facilities that explore emerging concepts for plasma confinement and stability, address critical issues that may affect the tokamak concept (e.g. plasma disruptions, impulsive heat loads, and operational maintenance and complexity), and investigate topics common to all fusion power plant concepts (e.g. interactions between plasma and material surfaces, and material science issues associated with the high fluxes of heat, charged-particles, and neutrons in a fusion power plant). The program also supports development of ITER-relevant diagnostic systems, advanced diagnostic capabilities to enable close coupling of experiments and theory/computations, and sensors or actuators required for active control of plasma properties to optimize device operation and plasma performance. Scientists from the U.S. also participate in leading experiments on fusion facilities abroad and conduct comparative studies to supplement the scientific understanding they can obtain from domestic facilities.

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

The Plasma Theory and Modeling program focuses on advancing the scientific understanding of the fundamental physical processes governing the behavior of magnetically confined plasmas and on using this knowledge to improve the design and performance of future fusion power reactors. Among the fundamental problems addressed by this program are the macroscopic stability and dynamics of fusion plasmas, with a strong focus on the prediction, avoidance, control and mitigation of deleterious or performance-limiting macroinstabilities; the understanding and controlling of the multiscale, collisional, and turbulent physical mechanisms responsible for the loss of heat, momentum, and particles from the confining region; the interaction of externally launched radiofrequency waves designed to heat and drive current with the background plasma and surrounding structures; the 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 edge on the plasma performance and on the interaction and interface of the hot plasma boundary with the material walls. The efforts supported by this program provide the foundations for integrated simulations of fusion systems and range from analytical work to the development and application of advanced simulation codes capable of exploiting the potential of next generation high performance computers. Strong synergies and connections with other program elements exist, from the crosscutting plasma science of magnetic reconnection and plasma turbulence to the experimental validation of theoretical models and codes enabled by collaborations with the experimental plasma science and plasma diagnostics development programs.

(c) High-Energy-Density Plasma Science and Inertial Fusion Energy Science
Technical Contact: Sean Finnegan, 301-903-4920, sean.finnegan@science.doe.gov

High-energy-density laboratory plasma (HEDLP) physics is the study of ionized matter at extremely high density and temperature, specifically when matter is heated and compressed to a point that the stored energy in the matter reaches approximately 100 billion Joules per cubic meter (the energy density of a hydrogen molecule). This corresponds to a pressure of approximately 1 million atmospheres or 1 Mbar. Systems in which free electrons play a significant role in the dynamics and for which the underlying assumptions and methods of traditional ideal-plasma theory and standard condensed matter theory do not apply (e.g., Warm Dense Matter at temperatures of a few eV) can have pressures as low as 0.1 Mbar and are also considered HED plasmas. Discovery-driven and use-inspired scientific explorations of high-energy-density states of matter are being supported in this program. Topical examples being emphasized include (1) high-energy-density hydrodynamics, (2) radiation-dominated dynamics and material properties, (3) magnetized high-energy-density plasmas, (4) nonlinear optics of plasmas and laser-plasma interactions, (5) relativistic HED plasmas and intense beam physics, and (6) warm dense matter.

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

The General Plasma Science program is directed toward research that addresses fundamental issues in plasma science and engineering not directly related to fusion energy. This research strengthens the fundamental underpinnings of the discipline of plasma physics that complements burning plasma science and reaches beyond into many basic and applied physics areas. The focus of the initiative continues to be fundamental issues of plasma science and engineering that can have impact in other areas or disciplines in which improved understanding of the plasma state is needed. Dynamic growth in new research areas, fostered by the development of new investigative techniques and tools, continues to present exciting opportunities for fundamental studies in basic plasma science and engineering. At the same time, economic forces are driving the need for more fundamental knowledge for the many applications of low temperature plasmas in modern technology. General plasma science is truly a broad, multidisciplinary field that spans many science issues such as interaction of waves with plasmas, magnetic reconnection and particle acceleration, physics of non-neutral plasmas and antimatter, chaos, turbulence, and structure in plasmas. Topics being encouraged include but not limited to: (1) astrophysical, solar, and space plasmas, (2) plasmas in biological and environmental science, (3) plasma modification, synthesis and processing of materials, (4) dusty, non-neutral and antimatter plasmas, (5) advanced plasma diagnostics, and (6) advanced methods for plasma modeling and simulation.

(e) Materials Science and Enabling Technologies for Fusion
Technical Contact: Peter Pappano, 301-903-4883, peter.pappano@science.doe.gov

The Enabling Technology R&D program supports the advancement of fusion science for both the near and long-term by carrying out research on technological topics that: (1) enable domestic experiments to achieve their full performance potential and scientific research goals; (2) permit scientific exploitation of the performance gains being sought from physics concept improvements; (3) allow the U.S. to enter into international collaborations, thus gaining access to experimental conditions not available domestically; (4) develop the technology and materials required for future fusion facilities, and (5) explore the science underlying these technological advances. Due to the harshness of the fusion environment and the significant challenge to overcome it, one of the four major goals of the FES program is to support the development of the scientific understanding required to design and deploy the materials needed to support a burning plasma environment. Given this goal, the Enabling Technology R&D program is interested in research that addresses the development of materials for use in fusion. This includes, but is not limited to, the following research topics: development of tungsten as a plasma facing material, plasma material interactions, fabrication, joining and cooling of plasma facing materials, development of both solid and liquid blanket concepts that can breed tritium and provide necessary heat transfer capabilities, and development of ferritic steels and oxide-dispersion strengthened steels as first wall structural materials.

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

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

The HEP program focuses on three scientific frontiers:

- *The Energy Frontier,* where powerful accelerators are used to create new particles, reveal their interactions, and investigate fundamental forces;
- *The Intensity Frontier,* where intense particle beams and highly sensitive detectors are used

to pursue alternate pathways to investigate fundamental forces and particle interactions by studying events that occur rarely in nature; and

- *The Cosmic Frontier,* where ground and space-based experiments and telescopes are used to make measurements that will offer new insight and information about the nature of dark matter and dark energy to understand fundamental particle properties and discover new phenomena.

Together, these three interrelated and complementary discovery frontiers offer the opportunity to answer some of the most basic questions about the world around us. All proposals should address specific research goals in one or more of these frontiers (as in the examples given below), and explain how the proposed research or technology development supports the broad scientific objectives and mission of the HEP program.

There are three broad areas within the Office of High Energy Physics that support research and technology development aimed at these objectives. New proposals should generally focus on one of these areas.

(a) Experimental High Energy Physics Research
Technical Contact: Eli Rosenberg, 301-903-3711, eli.rosenberg@science.doe.gov

The experimental HEP research effort supports experiments that utilize man-made and natural particle sources to study fundamental particles and their interactions as well as explore the basic nature of space and time.

This is accomplished through direct detection of new phenomena or through sensitive measurements that probe the Standard Model and new physics beyond it. This subprogram also provides graduate and postdoctoral research training for the next generation of scientists, equipment for experiments, and related computational support.

Topics studied in the experimental research program include, but are not limited to: fundamental particles and their interactions using proton-(anti)proton collisions at the highest possible energies and high intensity electron-positron collisions; studies of the properties of neutrinos produced by accelerators and nuclear reactors; studies of rare processes using high intensity proton beams on fixed targets; searches for proton decay; measurements of dark energy properties; studies of primordial antimatter; and detection of the particles constituting dark matter. Studies of gravitational phenomena are not included in this subprogram.

(b) Theoretical High Energy Physics Research
Technical Contact: Laurence Yaffe, 301-903-3715, laurence.yaffe@science.doe.gov

The theoretical HEP research subprogram provides the vision and mathematical framework for understanding and extending the knowledge of particles, forces, space-time, and the universe. This subprogram also provides graduate and postdoctoral research training for the next generation of scientists and computational resources needed for theoretical calculations.

Topics studied in the theoretical research program include, but are not limited to: phenomenological and theoretical studies that support the experimental research program, both in understanding the data and in finding new directions for experimental exploration; developing analytical and numerical computational techniques for these studies; and to find theoretical frameworks for understanding fundamental particles and forces at the deepest level possible.

(c) Advanced Technology Research and Development
Technical Contact: L.K. Len, 301-903-3233, lk.len@science.doe.gov

The advanced technology R&D subprogram develops the next generation of particle accelerators, detectors, and computing technologies for the future advancement of high-energy physics and other sciences, supporting world-leading research in the physics of particle beams and fundamental advances in particle detection. This subprogram supports long-range, exploratory research aimed at developing new concepts. This subprogram also provides graduate and postdoctoral research training, equipment for experiments and related computational efforts. Topics studied in the accelerator science program include, but are not limited to: analytic and computational techniques for modeling particle beams; novel acceleration concepts; muon colliders and neutrino factories; the science of high gradients in room-temperature accelerating cavities; high-brightness beam sources; and cutting-edge beam diagnostic techniques. Topics studied in the detector R&D program include, but are not limited to: low-mass, high channel density charged particle tracking detectors; high resolution, fast-readout calorimeters and particle identification detectors; techniques for improving the radiation tolerance of particle detectors; and advanced electronics and data acquisition systems. In addition, this subprogram develops next-generation computational tools and techniques to complement the experimental and theoretical physics research programs.

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

The mission of the Nuclear Physics (NP) program is to discover, explore, and understand all forms of nuclear matter. The fundamental particles that compose nuclear matter—quarks and gluons—are relatively well understood, but exactly how they fit together and interact to create different types of matter in the universe is still largely not understood. To solve this mystery, the NP program supports experimental and theoretical research—along with the development and operation of particle accelerators and advanced technologies—to create, detect, and describe the different forms and complexities of nuclear matter that can exist, including those that are no longer commonly found in our universe.

The NP program also produces and/or distributes stable and radioactive isotopes that are critical for the Nation.

To carry out this research, nuclear physics focuses on three broad yet tightly interrelated areas of inquiry. These areas are described in *The Frontiers of Nuclear Science* (http://science.energy.gov/np/nsac/), a long range plan for nuclear science released in 2007 by the Nuclear Science Advisory Committee (NSAC). The three frontiers are: Quantum Chromodynamics, Nuclei and Nuclear Astrophysics, and Fundamental Symmetries and

Neutrinos. To address these frontiers, specific questions are addressed by the research activities of each subprogram supported by the Office of Nuclear Physics:

(a) Medium Energy Nuclear Physics
Technical Contact: Before 8/31/11: E. A. Henry, 301-903-3614, gene.henry@science.doe.gov; After 8/31/11: T. Hallman, 301-903-3613, timothy.hallman@science.doe.gov

The Medium Energy subprogram focuses primarily on questions having to do with Quantum Chromodynamics (QCD), especially the behavior of quarks inside protons and neutrons and the spectrum of excited mesons and baryons. Specific questions that are being addressed include: *What is the internal landscape of the nucleons? What does QCD predict for the properties of excited mesons and baryons? What governs the transition of quarks and gluons into pions and nucleons? What is the role of gluons and gluon self-interactions in nucleons and nuclei?* One major goal of the Jefferson Laboratory (JLAB) program is to achieve an experimental description of the substructure of the proton and the neutron. Another is to identify "exotic mesons" which carry gluonic excitations. This subprogram also supports investigations of some aspects of the second frontier, Nuclei and Nuclear Astrophysics, including the question: *What is the nature of the nuclear force that binds protons and neutrons into stable nuclei?* The Medium Energy subprogram also addresses aspects of the third area, Fundamental Symmetries and Nuclei, including the questions: *Why is there now more visible 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 it evolved?* In pursuing these topics the Medium Energy subprogram supports several experimental research programs, notably at the Thomas Jefferson National Accelerator Facility and the Relativistic Heavy Ion Collider.

(b) Heavy Ion Nuclear Physics
Technical Contact: G. Rai, 301-903-4702, gulshan.rai@science.doe.gov

The Heavy Ion subprogram supports experimental research that investigates the frontier of Quantum Chromodynamics (QCD) by attempting to recreate and characterize new and predicted forms of matter and other new phenomena that might occur in extremely hot, dense nuclear matter and which have not existed since the Big Bang. This subprogram addresses what happens when nucleons "melt." QCD predicts that nuclear matter can change its state in somewhat the same way that ordinary matter can change from solid to liquid to gas. The fundamental questions addressed include: *What are the phases of strongly interacting matter, and what roles do they play in the cosmos? What governs the transition of quarks and gluons into pions and nucleons? What determines the key features of QCD, and what is their relation to the nature of gravity and spacetime?* Experimental research is carried out primarily using the U.S. Relativistic Heavy Ion Collider (RHIC) facility and the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN).

(c) Low Energy Nuclear Physics
Technical Contact: C. Baktash, 301-903-0258, cyrus.baktash@science.doe.gov

The Low Energy subprogram aims primarily at answering the overarching questions associated with the second frontier identified by NSAC— Nuclei and Nuclear Astrophysics. These questions include: *What is the nature of the nucleonic matter? What is the origin of simple patterns in complex nuclei? What is the nature of neutron stars and dense nuclear matter? What is the origin of the elements in the cosmos? What are the nuclear reactions that drive stars and stellar explosions?* Major goals of this subprogram are to develop a comprehensive description of nuclei across the entire nuclear chart, to utilize rare isotope beams to reveal new nuclear phenomena and structures unlike those that are derived from studies using stable ion beams, and to measure the cross sections of nuclear reactions that power stars and spectacular stellar explosions and are responsible for the synthesis of the elements. The subprogram also 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, or set a limit on, the neutrino mass and to determine if the neutrino is its own antiparticle. Experiments with cold neutrons also investigate the dominance of matter over antimatter in the universe, as well as other aspects of Fundamental Symmetries and Interactions.

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

The Nuclear Theory subprogram supports theoretical research at universities and DOE national laboratories with the goal of improving our fundamental understanding of nuclear physics, interpreting the results of experiments, and identifying and exploring important new areas of research. This subprogram addresses all of the field's scientific frontiers 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 phenomena 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. 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 aspects of the Standard Model can be explored through nuclear physics experiments, including the interactions of neutrinos, unusual nuclear transitions, rare decays, and high-precision studies of cold neutrons.

(e) Nuclear Data and Nuclear Theory Computing
Technical Contact: T. Barnes, 301-903-3212, ted.barnes@science.doe.gov

This subprogram supports the National Nuclear Data effort, as well as several activities that facilitate the application of high performance computing to Nuclear Theory. The Nuclear Data program collects, evaluates, and disseminates nuclear physics data for basic nuclear research and for applied nuclear technologies through the National Nuclear Data Center (NNDC), which maintains open databases of scientific information gathered over the past 100+ years of nuclear physics research. This subprogram also supports Nuclear Theory Computing, which includes the NP portion of the Scientific Discovery through Advanced Computing (SciDAC) program. SciDAC promotes the use of supercomputers at national laboratories and universities to solve problems of current interest in the sciences; in nuclear physics this involves computational studies of various topics, including in recent work the theory of quarks and gluons on a lattice (LQCD), models of the properties of nuclei and nuclear matter, nuclear astrophysics, and studies of novel high tech approaches to particle acceleration.

The NP program also supports the development of the tools and capabilities that make fundamental research possible, and is responsible for developing new isotope production techniques, and producing isotopes that are in short supply. These components of NP are represented by the following two subareas.

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

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

(g) Isotope Development and Production for Research and Applications
Technical Contact: D. Phillips, 301-903-7866, dennis.phillips@science.doe.gov

The Isotope Development and Production for Research and Applications subprogram supports the production and development of production techniques of radioactive and stable isotopes that are in short supply. The program provides facilities and capabilities for the production and/or distribution of research and commercial stable and radioactive isotopes, scientific and technical staff associated with general isotope research and production, and a supply of critical isotopes to address the needs of the Nation. Isotopes are made available by using the Department's unique facilities, the Brookhaven Linear Isotope Producer (BLIP) at BNL and the Isotope Production Facility (IPF) at LANL, of which the subprogram has stewardship responsibilities. The Program also coordinates and supports isotope production at a suite of university, national laboratory, and other federal accelerator and reactor facilities throughout the Nation to promote a reliable supply of isotopes domestically. Topics of interest include research that is focused on the development of advanced, cost-effective and efficient technologies for producing, processing, recycling and distributing isotopes in short supply. This includes innovative approaches to model and predict behavior and yields of targets undergoing irradiation in order to minimize target failures during routine isotope production.

Under this Program Announcement, NP does not support investigations in nuclear reactor studies or nuclear reactor modeling.

ADDITIONAL INFORMATION:

DOE anticipates awarding laboratory work authorization awards under this Program Announcement. DOE will accept new proposals through the Searchable FWP system (https://www.osti.gov/fwp/) under this Announcement.

A single Portable Document Format (PDF) file should be submitted from the laboratory to DOE. Please have your Searchable FWP Laboratory Administrator submit a Field Work Proposal (FWP) via Searchable FWP (https://www.osti.gov/fwp). The FWP and proposal should be combined into a single PDF file and uploaded into Searchable FWP. The words "**Early Career:**" should be placed at the beginning of the FWP Title listed in Searchable FWP (for example, the title might be "Early Career: Experimental Study of Scientific Information"). When using Searchable FWP, please use the **exact** Program Announcement Title **Office of Science Early Career Research Program** and the **exact** Program Announcement Number **LAB 11-572**. Failure to enter the **exact** program announcement title and number into Searchable FWP will put the proposal at risk of not being considered in the competition. If you need contact information for your Laboratory Administrator, please contact the Searchable FWP Support Center. The Searchable FWP Support Center can be reached Monday-Friday 8:00 a.m.-5:00 p.m. ET. Telephone: 865-241-1844, Email: FWPSupport@osti.gov.

PROGRAM FUNDING: It is anticipated that up to $10M will be available for laboratory work authorization awards in FY 2012. This amount is approximate and subject to availability of funds. It is anticipated that 15-35 awards will be made in Fiscal Year 2012. The number of awards is subject to availability of funds. The typical award size is expected to be $2,500,000 over five years. The minimum award size is $500,000 per year over five years. DOE national laboratories are encouraged to propose research expenditures as close to this funding minimum as possible. The size of a national laboratory award is commensurate with the requirement to charge twelve-month annual salaries (compared with professors, who are partially paid by academic institutions). Thus, a minimum of 50% and up to 100% of the principal investigator's salary should be proposed.

ELIGIBLE INVESTIGATORS: The Principal Investigator must be a full-time, permanent, non-postdoctoral national laboratory employee as of the deadline for the proposal. No more than ten (10) years can have passed between the year the Principal Investigator's Ph.D. was awarded and the year of the deadline for the proposal (for the present competition, those who received doctorates no earlier than 2001 are eligible). Each Principal Investigator may only submit one

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

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

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

There can be no co-Principal Investigators.

There is no limit on the number of preproposals from a DOE national laboratory in a given year. Each laboratory is responsible for ensuring that the research ideas submitted in its preproposals fit within the scope of Office-of-Science-funded programs at the national laboratory. Only those Principal Investigators that receive notification from DOE encouraging a formal proposal may submit full proposals.

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

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

Principal Investigators of early career awards from other agencies or entities are eligible.

Principal Investigators who received awards in FY 2010 or FY2011 under the Office of Science Early Career Research Program are not eligible.

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

If an investigator is a current recipient of one of the following awards and is selected for an award under this announcement, the institution must forgo any remaining years of funding for the current award when the new award begins. The previous awards covered by this condition are (1) Office of Advanced Scientific Computing Research Early Career Principal Investigator Program; (2) Office of Fusion Energy Sciences Plasma Physics Junior Faculty Award Program; (3) Office of High Energy Physics Outstanding Junior Investigator Program; (4) Office of Nuclear Physics Outstanding Junior Investigator Program; and (5) DOE Presidential Early Career Award for Scientists and Engineers (PECASE).

Eligibility exemptions will not be granted.

Letters of recommendation are not allowed.

AWARD ADMINISTRATION INFORMATION

Annual progress reports from the award investigators will be required and will be due 90 days before the end of each budget year.

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

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

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

AWARD NOTICES: DOE will notify proposers selected for award. This notice of selection is not an authorization to begin performance. Organizations whose proposals have not been selected will be advised as promptly as possible. This notice will explain why the proposal was not selected.

The instructions and format described below should be followed. You must reference Program Announcement LAB 11-572 on all submissions and inquiries about this program.

OFFICE OF SCIENCE
GUIDE FOR PREPARATION OF SCIENTIFIC/TECHNICAL PROPOSALS TO BE SUBMITTED BY NATIONAL LABORATORIES

Proposals from National Laboratories submitted to the Office of Science (SC) as a result of this Program Announcement will follow the Department of Energy Field Work Proposal process with additional information requested to allow for scientific/technical merit review. The following guidelines for content and format are intended to facilitate an understanding of the requirements necessary for SC to conduct a merit review of a proposal. Please follow the guidelines carefully, as deviations could be cause for declination of a proposal without merit review.

1. Review Criteria: Prior to a comprehensive merit evaluation, DOE staff will perform an initial evaluation of each proposal to ensure that the information required is provided, that the proposed effort is technically sound and feasible, and that the effort is consistent with program funding priorities. For proposals that pass the initial evaluation, DOE shall review and evaluate them based on the criteria set forth below.

Proposals will be subjected to scientific merit review (peer review) and will be evaluated against the following evaluation criteria which are listed in descending order of importance:

1. Scientific and/or technical merit of the project.
2. Appropriateness of the proposed method or approach.
3. Competency of applicant's personnel and adequacy of proposed resources.
4. Reasonableness and appropriateness of the proposed budget.

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

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

The evaluation process will include program policy factors such as the relevance of the proposed research to the terms of the announcement and the programmatic needs of the DOE Office of Science. Note that external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Both Federal and non-Federal reviewers may be used, and submission of a proposal constitutes agreement that this is acceptable to the investigator and the submitting institution.

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

1. Scientific and/or Technical Merit of the Project.
What is the scientific innovation of proposed research? What is the likelihood of achieving valuable results? How might the results of the proposed research impact the direction, progress, and thinking in relevant scientific fields of research? How does the proposed research compare with other research in its field, both in terms of scientific and/or technical merit and originality?

2. 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?

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

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

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

6. Potential for leadership within the scientific community.
What has the Principal Investigator (PI) done to serve others in the scientific community outside of direct research contributions? How has the PI demonstrated the potential for scientific leadership and vision?

<u>For criterion 5, the missions of the program areas are:</u>

Advanced Scientific Computing Research (ASCR): To discover, develop, and deploy computational and networking capabilities to analyze, model, simulate, and predict complex phenomena important to the Department of Energy (DOE). A particular challenge of this program is fulfilling the science potential of emerging computing systems and other novel computing architectures, which will require numerous significant modifications to today's tools and techniques to deliver on the promise of exascale science.

Biological and Environment Research (BER): To understand complex biological, climatic, and environmental systems across spatial and temporal scales ranging from sub-micron to global, from individual molecules to ecosystems, and from nanoseconds to millennia. This is accomplished by exploring the frontiers of genome-enabled biology; discovering the physical, chemical, and biological drivers of climate change; and seeking the geochemical, hydrological, and biological determinants of environmental sustainability and stewardship.

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

Fusion Energy Sciences: To expand the fundamental understanding of matter at very high temperature and density and to build the scientific foundation needed to develop a fusion energy source. This is accomplished by studying plasma and its interactions with its surroundings across wide ranges of temperature and density, developing advanced diagnostics to make detailed measurements of its properties and dynamics, and creating theoretical and computational models to resolve the essential physics principles.

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

Nuclear Physics (NP): To discover, explore, and understand all forms of nuclear matter. The fundamental particles that compose nuclear matter—quarks and gluons—are relatively well understood, but exactly how they fit together and interact to create different types of matter in the universe is still largely not understood. To solve this mystery, NP supports experimental and theoretical research—along with the development and operation of particle accelerators and advanced technologies—to create, detect, and describe the different forms and complexities of nuclear matter that can exist, including those that are no longer commonly found in the universe.

The selection official will consider the merit review recommendation, program policy factors, and the amount of funds available.

DOE is striving to make awards within seven months. The time interval begins on the date proposals are due or the date the proposal is received. **Awards will be made in Fiscal Year 2012.**

2. Summary of Proposal Contents

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

Optional letters of collaboration for unfunded or funded collaborations may be placed in Appendix 6 (Other Attachments). Letters of collaboration should state the intention to participate, but they should not be written as recommendation or endorsement letters, which are not allowed.

- Field Work Proposal (FWP) Format (Reference DOE Order 412.1A)
- Proposal Cover Page
- Budget (DOE Form 4620.1) and Budget Explanation
- Project Summary/Abstract (no more than one page)
- Project Narrative (**No more than 15 pages long**)
- Appendix 1: Biographical Sketch
- Appendix 2: Current and Pending Support

- Appendix 3: Bibliography and References Cited
- Appendix 4: Facilities and Other Resources
- Appendix 5: Equipment
- Appendix 6: Other Attachment (optional)

3. Detailed Contents of the Proposal

Proposals must have 1-inch margins at the top, bottom, and on each side. Type sizes must be at least 11 point. Line spacing is at the discretion of the researcher, but there must be no more than 6 lines per vertical inch of text. Pages should be standard 8 1/2" x 11" (or metric A4, i.e., 210 mm x 297 mm).

Field Work Proposal Format (Reference DOE Order 412.1A) (DOE ONLY)

The Field Work Proposal (FWP) is to be prepared and submitted consistent with policies of the investigator's laboratory and the local DOE Operations Office. Additional information is also requested to allow for scientific/technical merit review.   The table at the end of this document lists by topic the appropriate B&R codes for national laboratory Field Work Proposals (FWPs).

Proposal Cover Page

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

> **The cover page must also include the following information (this page will not count in the project narrative page limitation):**
>
> **DOE National Laboratory:**
> **Street Address/City/State/Zip:**
> **Principal Investigator (PI):**
> **Position Title of PI:**
> **Business Mailing Address of PI:**
> **Telephone Number of PI:**
> **Email of PI:**
> **Program Announcement Number: LAB 11-572**
> **DOE/Office of Science Program Office (ASCR, BER, BES, FES, HEP, or NP):**
> **Topic Area*:**
> **Topic Area Technical Contact:**
> **Year Doctorate Awarded:**
> **Number of Times Previously Applied[†]: (0, 1, or 2)**
> **PECASE Eligible**: (Yes or No)?**

* The topic area can be found in the summary section of this Program Announcement. For example, the topic area might be Applied Mathematics or Theoretical High Energy Physics Research. Please select from the list in the summary section.

† Indicate how many times the PI has previously submitted a full proposal in the Office of Science Early Career Research Program. The program has been offered in two previous years, FY 2010 and FY 2011. Participation in the competition is defined as submission of a full, formal proposal.

** The White House Office of Science and Technology Policy may ask the agencies each year to nominate candidates for the Presidential Early Career Awards for Scientists and Engineers (PECASE). A Principal Investigator is PECASE-eligible if he or she is a U.S. citizen, U.S. national, or permanent resident and if she or he has not received a PECASE previously through any agency. Investigators from the top proposals in the Office of Science Early Career Research Award competition may be nominated for PECASE.

Budget and Budget Explanation

The size of a national laboratory award is commensurate with the requirement to charge twelve-month annual salaries (compared with professors, who are partially paid by academic institutions). Thus, a minimum of 50% and up to 100% of the principal investigator's salary should be proposed.

Budgets are required for the entire five year project period. The DOE's budget page, Form 4620.1 (http://www.science.doe.gov/grants/budgetform.pdf), should be used. A budget form should be completed for each of the five years of the award, and a cumulative budget form for the entire five year period should also be included. A detailed budget justification narrative should be included after the budget pages. The justification should cover labor, domestic and foreign travel, equipment, materials and supplies, and anything else that will be covered with project funds.

Project Summary/Abstract (no more than one page)

The project summary/abstract must contain a summary of the proposed activity suitable for public dissemination. It should be a single page that identifies the national laboratory, the principal investigator, the project title, 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). The document should be written to appeal to a general audience and not just scientific experts in the specialty of the proposed research. This document must not include any proprietary or sensitive business information as the Department may make it available to the public. The project summary must not exceed one 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.

Project Narrative (No more than 15 pages long)

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

The body of the Project Narrative should not exceed 15 pages 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 information necessary to review the proposal, because the information contained in these sites will not be reviewed. Each proposal should be in a single PDF file.

Appendix 1: Biographical Sketch

This information is required for the Principal Investigator submitting the proposal. **This appendix will not count in the project narrative page limitation.** The biographical sketch is limited to a maximum of three pages when printed on 8.5” by 11” paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 11 point and must include:

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

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

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

Synergistic Activities. List no more than 5 professional and scholarly activities related to the effort proposed. Some examples might be invited and/or public lectures, awards received, scientific program committees, conference or workshop organization, professional society membership and/or activities, special international or industrial partnerships, reviewing or editorship activities, or other scientific leadership experiences.

Collaborators and Co-editors: A list of all persons in alphabetical order (including their current organizational affiliations) who are currently, or who have been, collaborators or co-authors with the Principal Investigator on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of the proposal. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the Principal Investigator interacted on a regular basis while the research was being done. Also, include those individuals who are currently or have been co-editors with the Principal Investigator of a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of the proposal. If there are no collaborators or co-editors to report, this should be so indicated.

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

Appendix 2: Current and Pending Support

Provide a list of all current and pending support (both Federal and non-Federal) for the Principal Investigator (PI) for ongoing projects and pending proposals. For each organization providing support, show the total award amount for the entire award period (including indirect costs) and the number of person-months per year to be devoted to the project by the PI. If the PI has submitted a similar research proposal to an early career program at another agency or foundation, she or he should provide a few sentences explaining the similarities and/or differences with the current Early Career Research Program proposal. Concurrent submission of a proposal to other organizations for simultaneous consideration will not prejudice its review. **This appendix will not count in the project narrative page limitation.**

Appendix 3: Bibliography and References Cited

Give full bibliographic entries for each publication cited in the 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. Include only bibliographic citations. Principal investigators should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the proposal. 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. **This appendix will not count in the project narrative page limitation.**

Appendix 4: Facilities and Other Resources

This information is used to assess the capability of the organizational 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. **This appendix will not count in the project narrative page limitation.**

Appendix 5: Equipment

List major items of equipment already available for this project and, if appropriate, identify location and pertinent capabilities. **This appendix will not count in the project narrative page limitation.**

Appendix 6: Other Attachments

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

4. Detailed Instructions for the Budget

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

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

4.1 Salaries and Wages

List the names of the principal investigator and other key personnel and the estimated number of person-months for which DOE funding is requested. Proposers should list the number of postdoctoral associates and other professional positions included in the proposal and indicate the number of full-time-equivalent (FTE) person-months and rate of pay (hourly, monthly or annually). For graduate and undergraduate students and all other personnel categories such as secretarial, clerical, technical, etc., show the total number of people needed in each job title and total salaries needed. Salaries requested must be consistent with the institution's regular practices. The budget explanation should define concisely the role of each position in the overall project.

4.2 Equipment

DOE defines equipment as "an item of tangible personal property that has a useful life of more than two years and an acquisition cost of $50,000 or more." Special purpose equipment means equipment which is used only for research, scientific or other technical activities. Items of needed equipment should be individually listed by description and estimated cost, including tax, and adequately justified. Allowable items ordinarily will be limited to scientific equipment that is not already available for the conduct of the work. General purpose office equipment normally will not be considered eligible for support.

4.3 Domestic Travel

The type and extent of travel and its relation to the research should be specified. Funds may be requested for attendance at meetings and conferences, other travel associated with the work and subsistence. In order to qualify for support, attendance at meetings or conferences must enhance the investigator's capability to perform the research, plan extensions of it, or disseminate its results.

4.4 Foreign Travel

Foreign travel may be approved only if it is directly related to project objectives.

4.5 Other Direct Costs

The budget should itemize other anticipated direct costs not included under the headings above, including materials and supplies, publication costs, computer services, and consultant services (which are discussed below). Other examples are: aircraft rental, space rental at research establishments away from the institution, minor building alterations, service charges, and fabrication of equipment or systems not available off- the-shelf. Reference books and periodicals may be charged to the project only if they are specifically related to the research.

a. Materials and Supplies

The budget should indicate in general terms the type of required expendable materials and supplies with their estimated costs. The breakdown should be more detailed when the cost is substantial.

b. Publication Costs/Page Charges

The budget may request funds for the costs of preparing and publishing the results of research, including costs of reports, reprints page charges, or other journal costs (except costs for prior or early publication), and necessary illustrations.

c. Consultant Services

Consultant services are not allowed.

d. Computer Services

The cost of computer services, including computer-based retrieval of scientific and technical information, may be requested. A justification based on the established computer service rates should be included.

e. Subcontracts

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

Subcontracts that fit the above description should be listed so that they can be properly evaluated. There should be an anticipated cost and an explanation of that cost for each subcontract. The total amount of each subcontract should also appear as a budget item.

4.6 Indirect Costs

Explain the basis for each overhead and indirect cost. Include the current rates.

TABLE: Budget & Reporting (B&R) Codes for DOE National Laboratory Field Work Proposal Submission

I. Advanced Scientific Computing Research (ASCR)	
(a) Applied Mathematics	KJ0401
(b) Computer Science	KJ0402
II. Biological and Environmental Research (BER)	
(a) Microbial Systems Biology Design for Bioenergy Production	KP160101
(b) Arctic Terrestrial Ecosystem Science	KP160101
(c) Subsurface Biogeochemistry	KP160101
(d) Uncertainty Characterization for Integrated Earth System Modeling	KP160101
III. Basic Energy Sciences (BES)	
(a) Materials Chemistry	KC020301
(b) Biomolecular Materials	KC020301
(c) Synthesis and Processing Science	KC020105
(d) Experimental Condensed Matter Physics	KC020202
(e) Theoretical Condensed Matter Physics	KC020203
(f) Physical Behavior of Materials	KC020103
(g) Mechanical Behavior and Radiation Effects	KC020102
(h) X-ray Scattering	KC020201
(i) Neutron Scattering	KC020201
(j) Electron and Scanning Probe Microscopies	KC020101
(k) Atomic, Molecular, and Optical Sciences	KC030103
(l) Gas Phase Chemical Physics	KC030102
(m) Computation and Theoretical Chemistry	KC030102
(n) Condensed Phase and Interfacial Molecular Science (CPIMS)	KC030102
(o) Catalysis Science	KC030201
(p) Separations and Analysis	KC030202
(q) Heavy Element Chemistry	KC030203
(r) Geosciences Research	KC030301, KC030302
(s) Solar Photochemistry	KC030101
(t) Photosynthetic Systems	KC0304

(u) Physical Biosciences	KC0304
(v) BES Nanoscale Science Research Center and Electron-Beam Microcharacterization Research	KC0407
(w) BES Accelerator and Detector Research	KC0407
(x) BES X-ray and Neutron Scattering Instrumentation and Technique Development	KC0407
IV. Fusion Energy Sciences (FES)	
(a) Magnetic Fusion Energy Science Experimental Research	AT501090
(b) Magnetic Fusion Energy Science Theory and Simulation	AT501090
(c) High-Energy-Density Plasma Science and Inertial Fusion Energy Science	AT501090
(d) General Plasma Science Experiment and Theory	AT501090
(e) Materials Science and Enabling Technologies for Fusion	AT501090
V. High Energy Physics (HEP)	
(a) Experimental High Energy Physics Research	KA110102, KA120102, KA130102
(b) Theoretical High Energy Physics Research	KA140102
(c) Advanced Technology Research and Development	KA150102, KA150302, KA140105
VI. Nuclear Physics (NP)	
(a) Medium Energy Nuclear Physics	KB010102
(b) Heavy Ion Nuclear Physics	KB020102
(c) Low Energy Nuclear Physics	KB040102
(d) Nuclear Theory	KB030102
(e) Nuclear Data and Nuclear Theory Computing	KB030102
(f) Accelerator Research and Development for Current and Future Nuclear Physics Facilities	KB010105-2
(g) Isotope Development and Production for Research and Applications	ST5002