This is a summary of
Funding Opportunity Announcement
DE-FOA-0000395

The full announcement is located on FedConnect under reference number DE-FOA-0000395.

Office of Science
Financial Assistance
Funding Opportunity Announcement

DE-FOA-0000395

Early Career Research Program

SUMMARY:

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

PREAPPLICATIONS

PREAPPLICATIONS ARE REQUIRED.

Preapplications are **REQUIRED** and must be submitted by Friday, August 13, 2010, 4:00 AM Eastern Time. The preapplication should be uploaded as a Word or Portable Document Format (pdf) attachment and submitted through the website https://EarlyCareerPreapp.science.doe.gov. Preapplications will be reviewed for responsiveness of the proposed work to the research topics identified in this funding announcement. DOE will send a response by email to each applicant encouraging or discouraging the submission of a formal application by Tuesday, September 14, 2010. **Only those applicants that receive notification from DOE encouraging a formal application may submit full applications.** No other formal applications will be considered.

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

Title of Preapplication
Principal Investigator Name, Job Title
Institution
PI Phone Number, PI Email Address
Year Doctorate Awarded: XXXX
Funding Announcement Number: DE-FOA-0000395

This information should be followed by a clear and concise description of the objectives and technical approach of the proposed research. The preapplication 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.

Those preapplications that are encouraged will be used to help the Office of Science begin planning for the formal application peer review process. The intent of the Office of Science in discouraging submission of certain full applications is to save the time and effort of applicants in preparing and submitting formal applications not responsive to this funding announcement.

Only one preapplication per Principal Investigator is allowed.

APPLICATION DUE DATE: November 9, 2010, 11:59 p.m. Eastern Time

Formal applications submitted in response to this Funding Opportunity Announcement must be received by **November 9, 2010**, 11:59 p.m. Eastern time, to permit timely consideration of awards in **Fiscal Year 2011. You are encouraged to transmit your application well before the deadline. APPLICATIONS RECEIVED AFTER THE DEADLINE WILL NOT BE REVIEWED OR CONSIDERED FOR AWARD.**

IMPORTANT SUBMISSION INFORMATION:

The full text of the Funding Opportunity Announcement (FOA) is located on FedConnect. Instructions for completing the Grant Application Package are contained in the full text of the FOA which can be obtained at: https://www.fedconnect.net/FedConnect/?doc=DE-FOA-0000395&agency=DOE . To search for the FOA in FedConnect click on “Search Public Opportunities”. Under “Search Criteria”, select “Advanced Options”, enter a portion of the title “Early Career Research Program”, then click on “Search”. Once the screen comes up, locate the appropriate FOA.

In order to be considered for award, applicants must follow the instructions contained in the Funding Opportunity Announcement.

WHERE TO SUBMIT: Applications must be submitted through Grants.gov to be considered for award.

You cannot submit an application through Grants.gov unless you are registered. Please read the registration requirements carefully and start the process immediately. Remember you have to update your CCR registration annually. If you have any questions about your registration, you should contact the Grants.gov Helpdesk at 1-800-518-4726 to verify that you are still registered in Grants.gov.

Registration Requirements: There are several one-time actions you must complete in order to submit an application through Grants.gov (e.g., obtain a Dun and Bradstreet Data Universal Numbering System (DUNS) number, register with the Central Contract Registry (CCR), register with the credential provider, and register with Grants.gov). See http://www.grants.gov/GetStarted. Use the Grants.gov Organization Registration Checklist at http://www.grants.gov/assets/OrganizationRegCheck.pdf to guide you through the process. Designating an E-Business Point of Contact (EBiz POC) and obtaining a special password called an MPIN are important steps in the CCR registration process. Applicants, who are not registered with CCR and Grants.gov, should allow at least 21 days to complete these requirements. It is suggested that the process be started as soon as possible.

IMPORTANT NOTICE TO POTENTIAL APPLICANTS: When you have completed the process, you should call the Grants.gov Helpdesk at 1-800-518-4726 to verify that you have completed the final step (i.e. Grants.gov registration).

Questions: Questions relating to the registration process, system requirements, how an application form works, or the submittal process must be directed to Grants.gov at 1-800-518-4726 or support@grants.gov. Part VII of the FOA explains how to submit other questions to the Department of Energy (DOE).

GENERAL INQUIRIES ABOUT THIS FOA SHOULD BE DIRECTED TO:

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

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

ELIGIBLE APPLICANTS

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

The Principal Investigator must be an **untenured** Assistant Professor or an **untenured** Associate Professor on the tenure track at a U.S. academic institution as of the deadline for the application. 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 application. For the present competition, those who received doctorates no earlier than 2000 are eligible.

The act of submitting an application implies that the submitting institution has checked and confirmed that the Principal Investigator is eligible. No additional certifying documentation is required.

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

There can be no co-Principal Investigators.

Applications must be submitted through a U.S. academic institution. A companion announcement (LAB 10-395) describes the Early Career Research Program opportunity for full-time DOE national laboratory employees. An employee with a joint appointment between a university and a DOE national laboratory must apply through the institution that pays his or her salary and provides his or her benefits.

Eligibility exemptions will not be granted.

OTHER ELIGIBILITY REQUIREMENTS

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 under the Office of Science Early Career Research Program are not eligible.

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).

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

Letters of recommendation are not allowed. A department chair letter is not required and should not be included.

SUPPLEMENTARY INFORMATION:

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
(c) Computational Science
(d) Network Environment Research

II. Biological and Environmental Research (BER)

(a) Microbial Environmental Processes
(b) Microbial and Plant Processes for Bioenergy
(c) Characterizing Key Molecular Species, Events, and Multicellular Processes for Genomic Science
(d) Biomass and Plant Feedstock Genomics
(e) Radiochemistry and Radionuclide Imaging Instrumentation
(f) Low Dose Radiobiology
(g) Carbon Cycle Science
(h) Subsurface Biogeochemistry
(i) Simulation of Climate at Regional Scales
(j) Earth System Modeling
(k) Integrated Assessment Modeling
(l) Atmospheric Systems

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
(l) Gas Phase Chemical Physics
(m) Computation and Theoretical Chemistry
(n) Condensed Phase and Interfacial Molecular Science (CPIMS)

(o) Catalysis Science
(p) Separations and Analysis
(q) Heavy Element Chemistry
(r) Geosciences Research
(s) Solar Photochemistry
(t) Photosynthetic Systems
(u) Physical Biosciences
(v) Scientific User Facilities-Related Research

IV. Fusion Energy Sciences (FES)
(a) Experimental Plasma Science
(b) Plasma Theory and Modeling
(c) Development of Plasma Diagnostics
(d) Low-Temperature and High-Energy-Density Plasma Science
(e) Enabling Technology Research and Development

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 (including the Nuclear Data subprogram)
(e) Accelerator Research and Development for Current and Future Nuclear Physics Facilities
(f) Isotope Development and Production for Research and Applications

I. Advanced Scientific Computing Research (ASCR)
Program Website: http://www.sc.doe.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 multi-core computing systems and other novel "extreme-scale" computing architectures, which will require significant modifications to today's tools and techniques.

The priority areas for ASCR include:

- 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.
- To advance key areas of computational science and discovery that advance the missions of the Office of Science through mutually beneficial partnerships.
- To deliver the forefront computational and networking capabilities to extend the frontiers of science.
- To develop networking and collaboration tools and facilities that enable scientists worldwide to work together.

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 in applied mathematics, computer science, computational science and network research to solve complex problems on computational resources that are on a trajectory to reach well beyond a petascale within a few years.

Proposed research may include one or more of the areas listed below. Research areas of interest include:

(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. Important areas of supported research include: (1) novel numerical methods for the scalable solution of large-scale, linear and nonlinear systems of equations; (2) innovative approaches for analyzing and extracting insight from large-scale data sets; (3) efficient techniques for characterizing, propagating, and/or quantifying uncertainties and errors in next-generation solver, optimization, simulation, risk analysis, and other codes; (4) multiscale methods for continuous and/or discrete systems that efficiently account for physics and subcomponent interactions across vastly different time and length scales. Development and/or implementation of existing numerical methods to a specific application is not within the scope of this program, no matter how challenging the application.

(b) Computer Science
Technical Contact: Lucy Nowell, 301-903-3191, lucy.nowell@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 include advanced hardware and software architectures for exascale computing systems; hardware and software approaches to power/energy management for HPC systems; scalable and fault tolerant operating and runtime systems, including file systems and input/output bottlenecks; programming and execution models; programming environments and compilers; autotuning and performance modeling and assessment tools; software development tools and methods; scientific workflow systems; interoperability at the application level and/or the data level; and scientific data management, integration, analysis and visualization for petabyte to exabyte data sets, both static and streaming, including in-situ methods. Applications must explain their relevance to current and future high performance computing platforms as well as their relevance to the mission of the Office of Science. Quantum computing, networking, computer-supported collaboration, social computing, natural language processing/understanding/generation, generalized research in human-computer interaction; and research which is only applicable to hand-held, portable, desktop, cluster or cloud computing are out of scope for this program

(c) Computational Science
Technical Contact: Randall Laviolette, 301-903-5195, randall.laviolette@science.doe.gov

This program supports research in pioneering science application codes for the next generations of high performance computers. Research topics include the development of transformative new science application software, techniques and methods. The Computational Science program supports computational innovations to specific science applications as well as approaches that combine ideas from applied mathematics, computer science and network environment research. The development of new computational science techniques will allow scientists to tap the potential of extreme-scale computers to enable new discoveries and advance scientific knowledge. Proposed application codes should support core DOE mission areas such as materials sciences, chemical sciences, geosciences including climate and environmental impacts, biological sciences, nanoscale science, nuclear energy, superconductivity and transportation. Applications that address human, pharmaceutical or medical sciences, robotics, economics, or sociology are beyond the scope of this program.

(d) Network Environment Research
Technical Contact: Thomas Ndousse-Fetter, 301-903-9960, tndousse@ascr.doe.gov

This program conducts system level research and development in next-generation networking and scientific collaborations to support diverse types of distributed science activities in the Office of Science. Current areas of interest are 1) high-capacity optical networking technologies and 2) data-intensive scientific collaborations. High-capacity networking is focused on system level agile terabits networking that can deliver end-to-end throughput a thousand times (1000x) faster than today's commercial Internet. Potential research topics for high-capacity networks include, but are not limited to radically new architectures and protocols for hybrid terabits networking that support best-effort IP and dynamic circuits; composable and scalable transport protocols with end-to-end performance that far outstrip TCP/IP and its variants; storage and file systems extensions for 100 Gbps throughput and beyond. Data-intensive scientific collaboration is focused on advanced collaboration services that enable distributed science teams to work together and share enterprise-level science facilities. Potential topics of interest include, but are not limited to end-to-end performance analysis tools and services; scientific workflows for optimizing collaborative resources; and distributed data management toolkits. Respondents to both technical areas are encouraged to use component-based approaches to facilitate the adoption their proposed algorithms/software into DOE science infrastructures. Sensornets, wireless networks, device level (switches, routers, etc.), photonics, and low level chip design and research activities are beyond the scope of the program.

II. Biological and Environmental Research (BER)

Program Website: http://www.sc.doe.gov/ober

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

Technical Contact: Marvin Stodolsky, 301-903-4475, marvin.stodolsky@science.doe.gov

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, together with the ASCR program, the computational resources, tools, and technologies needed to understand and predict complex behavior of complete biological systems, principally microbes and microbial communities; (2) to take advantage of the remarkable high throughput and cost-effective DNA sequencing capacity at the Joint Genome Institute to meet the DNA sequencing needs of the scientific community through competitive, peer-reviewed nominations for DNA sequencing; (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; (5) to anticipate and address ethical, legal, and social implications arising from Office of Science-supported biological research, especially synthetic biology, sustainability, and nano technology and (6) to develop radiochemistry and advanced technologies for imaging and high through-put characterization and analysis for BER missions in bioenergy, subsurface, and climate change.

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

(a) Microbial Environmental Processes

Technical Contact: Joe Graber, 301-903-1239, joseph.graber@science.doe.gov

To develop a systems-level understanding of the functional processes used by microbes and microbial consortia that link the internal metabolic processes of microbial species to their external biogeochemical activities.

(b) Microbial and Plant Processes for Bioenergy
Technical Contact: Arthur Katz, 301-903-4932, arthur.katz@science.doe.gov

To develop new approaches that advance our understanding of the systems biology of plants and microbes in producing biofuels including the utilization of lignocellulosic biomass and microbial synthesis of advanced biofuel

(c) Characterizing Key Molecular Species, Events, and Multicellular Processes for Genomic Science
Technical Contact: Dean Cole, 301-903-3268, dean.cole@science.doe.gov

To develop innovative technology approaches to characterize biological processes and networks at the subcellular, cellular and multicellular levels.

(d) Biomass and Plant Feedstock Genomics
Technical Contact: Cathy Ronning, 301-903-9549, catherine.ronning@science.doe.gov

Genomics-based research that will lead to the improved use of biomass and plant feedstocks for the production of fuels such as ethanol or renewable chemical feedstocks, e.g., research to improve biomass characteristics, biomass yield, or sustainability. Systems biology approaches to identify genetic indicators or regulators of protein networks, proteins and metabolites, enabling plants to be efficiently bred or manipulated, or research that yields fundamental knowledge of the structure, function and organization of plant genomes leading to improved feedstock characterization and sustainability.

(e) Radiochemistry and Radionuclide Imaging Instrumentation
Technical Contact: Prem Srivastava, 301-903-4071, prem.srivastava@science.doe.gov

Development and use of highly innovative radiotracer chemistry or instrumentation technologies for quantitative *in vivo* or *in situ* measurement of site-specific chemical reactions, their spatial distributions and metabolic perturbations, and ensuing biological processes with a high degree of accuracy and sensitivity specifically focusing on plants, plant–microbe interactions, or complex microbial communities.

(f) Low Dose Radiobiology
Technical Contact: Noelle Metting, 301-903-8309, noelle.metting@science.doe.gov

New experimental radiobiology to underpin current and future regulatory decisions setting workplace exposure limits. Research should focus on molecular and cellular responses within tissue- and higher levels of mammalian biological organization. Topics include radio-adaptive responses; systems genetics of individual radiation sensitivity; low dose and/or low dose-rate effects on: a) the immune system, b) epigenetic regulation, and c) molecular and cellular hallmarks of aging. Low doses are defined as less than 10 rads (0.1 Gray); low dose rates should be less than 1 rad/day (0.001 Gray/day).

Climate and Environmental Sciences
Technical Contact: Bob Vallario, 301-903-5758, bob.vallario@science.doe.gov
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 areas:

(g) Carbon Cycle Science
Technical Contact: Mike Kuperberg, 301-903-3511, michael.kuperberg@science.doe.gov

Research on measurements, experiments, and modeling that provide improved quantitative and predictive understanding of the terrestrial carbon cycle processes that can affect atmospheric CO_2 concentration changes and thereby affect the CO_2 forcing of climate. The goal should be to understand the impacts of, and feed backs from a changing climate on non-managed terrestrial ecosystems. Research should be posed in the context of representing terrestrial carbon cycle processes in earth system models.

(h) 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.

(i) Simulation of Climate at Regional Scales
Technical Contact: Renu Joseph, 301-903-9237, renu.jospeh@science.doe.gov

Development of climate models for getting high fidelity simulations of regional climate including (a) evaluation of methods of climate modeling at regional scales and develop innovative concepts and modeling frameworks for integrating results across various spatial scales, and (b) development of insights on process feedbacks contained in both coupled-climate models and Earth System Models (ESMs) and characterize uncertainties associated with those processes.

(j) Earth System Modeling
Technical Contact: Renu Joseph, 301-903-9237, renu.jospeh@science.doe.gov

Development of next generation Earth System Models that incorporate biogeochemistry, atmospheric chemistry and dynamic vegetation into coupled models of the atmosphere, ocean, sea ice, and land surface, and provide improved simulations of temperature, precipitation, and extreme weather events, all at much finer scales.

(k) Integrated Assessment Modeling
Technical Contact: Bob Vallario, 301-903-5758, bob.vallario@science.doe.gov

Exploration of multi-scale phenomenon within Integrated Assessment models (IAMs) including: the types of varied systems interactions that dominate in higher resolution spatial and temporal regimes, specifically, in regional scale IAMs; new insights on the mitigation-adaptation interface; the influence and interactions of multiple stressors on human and natural systems; energy systems impacts and vulnerabilities; and broadly, sustainability at regional scales under global change. Applications should also explore issues of multi-scale, multi-model interactions at regional, national, and global scales.

(l) Atmospheric Systems
Technical Contact: Kiran Alapaty, 301-903-3175, kiran.alapaty@science.doe.gov

Use of innovative laboratory and observational data analyses to improve cloud and aerosol formulations in global climate models, improving understanding and modeling of cloud and aerosol properties and processes and their impact on the atmospheric radiation balance. Research can include development or improvement of algorithms for retrieving the required atmospheric parameters from Atmospheric Radiation Measurement (ARM) instruments; developing instrument simulators to facilitate more accurate intercomparison of measurements with modeling data; studies utilizing ARM data and Atmospheric Science Program (ASP) measurements to improve understanding of cloud, aerosol, and radiation physical processes; and, the translation of process study results to improve or develop formulations for the respective processes to improve climate model simulations.

EXCLUSIONS – BER will not fund research in the following areas or involving:

- Bioenergy from sewage processing;
- Bioremediation of organics;
- Phytoremediation;
- Marine biology;
- Oceanography;
- Existing or newly proposed processes for commercial, industrial, residential, and municipal solid and liquid waste management, even if those processes hold potential to positively impact the carbon cycle, nitrogen cycle, and more;
- Experimentation in support of industrial processes, including feedstock substitutions, emissions scrubbing, and other processes designed for greenhouse gas emissions;
- Policy and implementation studies related to climate change;
- General human behavioral research, even as it applies to such areas as biofuels acceptance and climate change; however, economic and risk research is very much on point and encouraged;
- Marine experimentation in support of climate research, including understanding of marine organisms and marine ecology even when it may impact carbon, nutrient, and other cycles and/or hold potential for marine carbon sequestration;
- Observations and experimentation on ocean currents, ocean heat transfer, and other physical ocean properties;
- Engineering of systems or instrumentation or deployment of innovative combinations of existing probes where basic research is not the main thrust;
- Technology development and testing for climate change mitigation or adaptation technology development;
- Air pollution measurements, control technology development or evaluation;
- Site-specific scientific studies of climate change where research may be focused on a particular community, localized resource, or region, but where more generalized extensions and interpretations of the research are not a central component;
- Medically related research;
- Plant pests;
- Biomass process engineering optimization;
- Climate effects on biomass production;
- Molecular dynamics simulations towards enzyme engineering; or
- DNA sequencing technology.

III. Basic Energy Sciences (BES)

Program Website: http://www.sc.doe.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.

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

(a) Materials Chemistry
Technical Contact: Mary Galvin, 301-903-8334, mary.galvin@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 thrust areas include: nanoscale chemical synthesis and assembly; solid state chemistry for exploratory synthesis and tailored reactivities; novel polymeric materials and complex fluids; surface and interfacial chemistry including electrochemistry; and the development of new, science-driven laboratory-based analytical tools and techniques.

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 increasing activity in 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 on materials that have potential for use in the next generation energy technologies, including research that underpins new approaches and chemistries related to carbon capture. The program will seek to increase the proportion of research in classes that demonstrate promise in providing the properties required for energy solutions. Some examples of these classes include complex inorganic oxides, metamaterials, and liquid crystals with novel electronic, magnetic, photonic and thermal properties.

(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 biomimetic and bioinspired functional materials and complex structures, and materials aspects of energy conversion processes based on principles and concepts of biology. The major program emphasis is 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 thrust areas include: understanding, controlling, and building complex hierarchical structures by mimicking nature's self- and directed-assembly approaches; design and synthesis of environmentally adaptive, self-healing multi-component, e.g., inorganic, polymeric, and biological, materials and systems that demonstrate energy conversion and storage capabilities found in nature; functional systems with collective properties not achievable by simply summing the individual components; biomimetic and/or bioinspired routes for the synthesis of energy relevant materials, e.g., semiconductor and magnetic materials under mild conditions; and development of science-driven tools and techniques for the characterization of biomolecular and soft materials.

This activity will continue to support curiosity-driven and multi-disciplinary approaches to model, design, and synthesize novel materials with unique functionalities. The program will continue to seek a fundamental understanding of thermodynamic, kinetic, and dynamical aspects of self-assembly processes to produce both equilibrium and far-from-equilibrium materials and systems like those found in nature. Enhanced integration of theory, computation, and experiment is sought to develop a more comprehensive understanding of the nanoscale structure and non-equilibrium behavior of bioinspired/bioderivative materials and systems leading to new design ideas and opportunities for discovery. In addition, the program will expand in the following areas: dynamically adaptive and self-repairing materials; low temperature synthesis of energy relevant materials; effective and unique strategies for interfacing biological and non-biological materials systems in search of emergent behavior; synthetic enzymes; material architectures for efficiently integrating light-harvesting, photo-redox, and catalytic functions; and biomolecular functional structures that take inspiration from biological gates, pores, channels, and motors.

(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 phenomena that underpin materials synthesis such as diffusion, nucleation, and phase transitions; and to develop *in situ* monitoring and diagnostic capabilities. 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 the liquid and other precursor states to the processing of bulk nanoscale materials; and low energy processing techniques for large-scale 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, which emphasize chemical and biomimetic routes to new materials synthesis and design.

Over the past few years, the activity has evolved an increasing interest in understanding nanoscale morphology through nucleation and growth kinetics and mechanisms, defect control in deposition processes, and complex chemical and structural materials growth. Over the next several years, these directions are expected to continue with strengthen research in bulk materials growth, deposition, and sintering and added emphasis in the fundamental understanding of the mechanisms for interfacing soft-hard hybrid materials and the organization of these structures. Expansion is planned in research for discovery of novel synthesis methods, especially using extreme environments of field and flux, and research to push the limits of our basic understanding in synthesis and processing related to use-inspired technologies including solid-state lighting, solar energy conversion, hydrogen storage, 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, innovative, and imaginative projects. The activity continues to support and encourages natural collaboration between theorists and experimentalists to address the opportunities described in the scientific challenges described above.

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

This activity supports Experimental Condensed Matter Physics emphasizing the relationship between the electronic structure and the properties of complex materials, often at the nanoscale. The focus is on systems whose behavior derives from strong correlation effects of electrons as manifested in superconducting, semi-conducting, magnetic, thermoelectric, and optical properties. Also supported is the development of new techniques and instruments for characterizing the electronic states and properties of materials under extreme conditions, such as in ultra low temperatures (millikelvin), in ultra-high magnetic fields (100 Tesla), and at ultra-fast time scales (femtosecond).

The Experimental Condensed Matter Physics activity will include further work at the nanoscale and at low temperatures, the development of a very high magnetic field research program, and continued development of the materials synthesis and crystal growth thrust. The portfolio can be expected to continue thrusts in electronic structure, new materials, surfaces/interfaces, and development of experimental techniques. Efforts will continue to strengthen research in unconventional superconductivity, including the high-temperature cuprate superconductors, first discovered nearly 25 years ago, and the recently discovered iron pnictide superconductors. In the last few years the program has increased support for spin physics and nanomagnetism, and new investigations of the Casimir force have been initiated. Recently the program has begun to explore whether cold atom research can provide insight into open questions about correlated electron behavior in condensed matter systems.

(e) Theoretical Condensed Matter Physics
Technical Contact: James Horwitz, 301-903-4894, james.horwitz@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 billions 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 basic research to understand defects in materials and their effects on the properties of strength, structure, deformation, and failure. Defect formation, growth, migration, and propagation are examined by coordinated experimental and modeling efforts over a wide range of spatial and temporal scales. Topics include deformation of ultra-fine scale materials, radiation-resistant material fundamentals, and intelligent microstructural design for increased strength, formability, and fracture resistance in energy relevant materials. The goals are to develop 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 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.

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 US energy production, these are issues that need to be addressed at a fundamental level.

(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 in ultrafast materials science, including research aimed at generating, manipulating, and detecting ultrashort and ultrahigh-peak-power electron, x-ray, and laser pulses to study ultrafast physical phenomena in materials, is an integral part of the portfolio.

Advances in x-ray scattering and ultrafast sciences will continue to be driven by scientific opportunities presented by improved source performance and optimized instrumentation. 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 develops and uses radiation sources associated with BES facilities and beam lines but also includes 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, spectroscopy, and imaging for materials research, primarily at BES-supported user facilities. Development of next-generation instrumentation concepts, innovative optics, novel detectors, advanced sample environments, data analysis tools and polarized neutrons are distinct aspects of this activity.

The neutron scattering activity will continue in fully developing the capabilities at the DOE facilities by providing instrumentation and research support. A continuing theme in the scattering program will be the integration and support of materials preparation as this is a core competency that is vital to careful structural measurements related to materials properties. This program will continue its stewardship role in fostering growth in the US neutron scattering community in the development of innovative time-of-flight neutron scattering instrumentation concepts and its effective utilization for high profile research.

Correlated and Complex Materials – Realization of the enormous potential in functionality of correlated electron systems requires a complete understanding of the underlying mechanisms and phenomena to ultimately control the complexities to achieve desired functionality. In addition to cuprates, the recently discovered iron pnictides family will provide as yet another platform to investigate high Tc superconductivity. Elastic and inelastic neutron scattering techniques will remain as essential tools for the investigation of complex correlated electron systems.

Research at the Intersection of Hard and Soft Condensed Matter Sciences – Polymers, biomaterials and hybrid nanocomposites are ubiquitous in the modern world. Surfaces and interfaces play strong roles in hybrid materials relevant to such applications as organic photovoltaics, thermoelectrics, fuel cells, Li-ion batteries, organic light emitting diodes, and materials for carbon sequestration and hydrogen storage. Neutron scattering will play a major role to understand the effects of interfaces on the collective behavior of these multi-component systems, enabling science in the emerging areas in soft condensed matter science.

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

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 and improvement of electron scattering and scanning probe instrumentation and techniques, including ultrafast diffraction and imaging techniques.

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
Technical Contact: Jeffrey Krause, 301-903-5827, jeff.krause@science.doe.gov

This activity supports theory and experiments to understand structural and dynamical properties of atoms, molecules, and nanostructures. The research emphasizes the fundamental interactions of these systems with photons and electrons to characterize and control their behavior. These efforts aim to develop accurate quantum mechanical descriptions of properties and dynamical processes of atoms, molecules, and nanoscale matter. For example, the study of energy transfer within isolated molecules provides the foundation for understanding chemical reactivity. Topics include the development and application of novel, ultrafast optical probes of matter with particular interest in x-ray sources; the interactions of atoms and molecules with intense electromagnetic fields; and studies of collisions and many-body cooperative interactions of atomic and molecular systems. The knowledge and techniques produced by this activity form a science base that underpins several aspects of the DOE mission. The AMOS activity provides new ways to control and probe interactions in the gas and condensed phases, and enhances our ability to understand materials. New methods for using photons, electrons, and ions to probe matter enable more effective use of BES light source, nanoscience, and microcharacterization facilities. This enabling aspect will continue to be emphasized, particularly with respect to research involving the generation and application of ultrafast, intense x-ray pulses. Similarly, the study of formation and evolution of energized states in atoms, molecules, and nanostructures provides a fundamental basis for understanding elementary processes in solar energy conversion and radiation-induced chemistry.

Research in AMO science 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.* In recent years, AMO science has transformed from a field in which the fundamental interactions of atoms, molecules, photons, and electrons are probed to one in which they are controlled. Systems studied are increasingly complex, and exhibit highly correlated, non-perturbative interactions. AMOS scientists can shape the quantum mechanical wave functions of atoms and small molecules using controllable laser fields, trap and cool atoms and molecules to ultracold temperatures, create nanoscale structures that manifest novel light-matter interactions and properties, and coherently drive electrons to generate ultrafast x-ray pulses. Theoretical advances are enabling modeling and simulation of increasingly complex systems to provide interpretation of existing data, and predictions for new experiments. These capabilities create opportunities to investigate chemical processes under conditions that are far from equilibrium, where complex phenomena are predominant and controllable, and on ultrafast timescales commensurate with the motions of atoms and electrons.

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

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 ineractions, 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 is to 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. Expanding into the future, plans are to probe the chemical physics of energy transfer 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 emphasis of research support toward the molecular level means that the CPIMS program does not fund research in bulk fluid dynamics, such as studies in laminar or turbulent flows or microfluidics. The relevance of research to the energy mission means that the CPIMS program does not support research on molecules or cells directed toward medical applications.

(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 those 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 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 and pathways bond rearrangements under electrochemical and photoelectrochemical conversion of small as well as complex molecules into chemicals and fuels.

(p) Separations and Analysis
Technical Contact: William Millman, 301-903-5805, william.millman@science.doe.gov

This activity supports fundamental research covering a broad spectrum of separation concepts, including membrane processes, extraction under both standard and supercritical conditions, adsorption, chromatography, photodissociation, 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. This activity is the nation's most significant long-term investment in the fundamental science underpinning actinide separations and mass spectrometry. The overall goal is to obtain a thorough understanding, at molecular and nanoscale dimensions, of the basic chemical and physical principles involved in separations systems and analytical tools so that their full utility can be realized.

Separations research will continue to advance the understanding of multifunction separations media; supramolecular recognition (using designed, multi-molecule assemblies to attract specific target species); synthesis of new porous materials and control of interface properties at the nanoscale; ligand design and synthesis of extractant molecules; mechanisms of transport and fouling in polymer and inorganic membranes; solvation in supercritical fluids; field-enhanced mixing; and drop formation. Analytical research will pursue the elucidation of ionization 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-based methods for high-resolution spectroscopy and for presentation of samples for mass spectrometry; characterization of interfacial phenomena, with emphasis on chromatography; surface-enhanced Raman spectroscopy; and use of quadrupole ion traps to study gas-phase ion chemistry. 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.

(q) Heavy Element Chemistry
Technical Contact: Larry Rahn, 301-903-2508, larry.rahn@science.doe.gov

This activity supports basic research in the chemistry of the heavy elements, including actinides and some fission products. The unique molecular bonding of the heavy elements is explored using theory and experiment to elucidate electronic and molecular structures, bond strengths, and chemical reaction rates. Additional emphasis is placed on the chemical and physical properties of actinides to determine solution, interfacial, and solid-state bonding and reactivity; on determining chemical properties of the heaviest actinide and transactinide elements; and on bonding relationships among the actinides, lanthanides, and transition metals.

Theoretical chemists predict the properties of actinides and transactinides in gaseous molecules, clusters in liquids, and solid species, using modern calculation tools such as density functional theory and sophisticated quantum mechanical calculations that include both spin-orbit and relativistic effects. Support of research to understand the chemical bonding of elements that have 5f electrons leads to fundamental understanding of separations processes and to the design and synthesis of preorganized chelating agents for the separations of particular actinide ions. Research in bonding, reactivity, and spectroscopic properties of molecules that contain heavy elements and of actinides in environmentally relevant species aids the development of ligands to sequester actinides in the environment and to remove toxic metals from the human body. Better characterization and modeling of the interactions of actinides at liquid-solid and liquid-liquid interfaces, including mineral surfaces under environmentally relevant conditions, improve separations processes that are essential for advanced nuclear fuel cycles.

(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 continues its basic activity understanding the significance of commonly observed natural nanophases and nanoparticles in shallow earth systems and how they contribute to mineral-fluid interactions.

The activity plans 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 microscopy, and large-scale imaging (geophysics focus) of physical properties. New energy waste storage options will require high-resolution monitoring and verification at a new level of sophistication. The GSECARS and BESSRC at the Advanced Photon Source (APS) begin their second decade as the premier synchrotron user facilities for the earth sciences community, pioneering approaches that can be exported to designing other facilities such as the National Synchrotron Light Source II (NSLS II). They will expand research efforts in nanogeosciences to understand the role of nanophases in geological systems and efforts on understanding the geophysical and geochemical challenges of predicting the fate and transport of CO_2 as sequestration in deep geological formations is tested as a technology option to mitigate greenhouse gas emissions.

Geosciences activities will link analytical capabilities with computational capabilities at the nano-, micro- and macro-scales to provide understanding of geochemical 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 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, electrical charge generation, and charge transport within a number of chemical systems, including those with significant nanostructured composition. Supported research areas include organic and inorganic photochemistry and photocatalysis, photoinduced electron and energy transfer in the condensed phase and across interfaces, photoelectrochemistry, and artificial assemblies for charge separation and transport that mimic natural photosynthetic systems.

In solar photochemistry, an increased emphasis on solar water splitting will explore new semiconductor and molecular systems for photoconversion. Also of emphasis are new hybrid systems that feature molecular catalysis at surfaces and new nanoscale structures for the photochemical generation of fuels. Modern combinatorial techniques will broaden and accelerate the search for new semiconductor and molecular structures. Novel quantum size structures, such as multiexciton generating quantum dots, hybrid semiconductor/carbon nanotube assemblies, fullerene-based linear and branched molecular arrays, and semiconductor/metal nanocomposites, will be examined that will allow for more complete and efficient use of the solar energy spectrum. Unresolved basic science issues in photocatalysis will be explored in coupling photoinduced charge separation to multielectron, energetically uphill redox reactions. Photoconversion systems will be investigated that are based on organic semiconductors and conducting polymers, which are inexpensive and easy to manufacture. An enhanced theory and modeling effort is needed for rational design of artificial solar conversion systems. Of particular interest is the calculation of factors controlling photoinduced long-range electron transfer, charge injection at the semiconductor/electrolyte interface, and photoconversion in biomimetic assemblies for solar photocatalytic water splitting.

Electron pulse radiolysis methods will investigate reaction dynamics, structure, and energetics of short-lived transient intermediates in the condensed phase. Fundamental studies on reactivity of nitrogen oxides in aqueous solution are pertinent to understanding radiolytic degradation of nuclear tank waste. Studies of solvent effects on free radical reaction rates in supercritical fluids are relevant to next-generation supercritical water-cooled nuclear power plants.

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

(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 light harvesting, exciton transfer, charge separation, transfer of reductant to carbon dioxide, as well as the biochemistry of carbon fixation, metabolism, and storage. Emphasized areas include those involving strong intersection between biological sciences and energy-relevant chemical sciences and physics, such as in self-assembly of nanoscale components, efficient photon capture and charge separation, predictive design of catalysts, and self-regulating/repairing systems.

Advances in genomics technologies such as metabolomics along with increased availability of plant genomic sequences provide new opportunities to leverage the strengths of the Photosynthetic Systems program in molecular biology and biochemistry with powerful capabilities in imaging and computation. This will allow an unprecedented biophysical understanding at the nanoscale of photosynthesis and related processes such as carbon fixation and metabolism. Research will continue to emphasize 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 fuel 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 in animal systems or prokaryotic systems related to human/animal health or disease.

All submitted applications must clearly state the energy relevance of the proposed research: How will the knowledge gained from the proposed work better our understanding of the ways plants 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 experimental and computational tools from the physical sciences with biochemistry and molecular biology. A fundamental understanding of the complex processes that convert and store energy in living systems is sought. 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. Combined with efforts in molecular biology and biochemistry, this will give us an unprecedented architectural and mechanistic understanding of such systems and allow the incorporation of identified principles into the design of bio-inspired synthetic or semi-synthetic energy systems. The application of such tools to the detailed 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. Still another area of emphasis for the program lies in the application of these same tools to achieve a more detailed understanding of the structure – and dynamics – of complex biological nanomaterials such as plant cell walls, biological motors, and cytoskeletal and other assemblies involved in energy capture, transduction, and storage.

Physical Biosciences does not fund research in animal systems or prokaryotic systems related to human/animal health or disease.

All submitted applications must clearly state the energy relevance of the proposed research: How will the knowledge gained from the proposed work better our understanding of the ways plants and/or non-medical microbes capture, transduce, and store energy?

(v) Scientific User Facilities-Related Research
Technical Contact: Eliane Lessner, 301-903-9365, eliane.lessner@science.doe.gov

This subprogram supports the R&D, planning, and operation of scientific user facilities for the development of novel nano-materials and for materials characterization through x-ray, neutron, and electron beam scattering. The main research elements of the subprogram are accelerator and detector research for light sources and neutron scattering facilities, electron-beam microcharacterization, nanoscale science and engineering, and the development and use of x-ray and neutron scattering to address scientific problems of interest to the study of nano materials and materials characterization. All of these research elements are in the context of serving the needs of the Scientific User Facilities.

In accelerator and detector research the objective is to improve the output and capabilities of synchrotron radiation 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 in order to develop new concepts to be used in the design of new accelerator facilities for synchrotron radiation and spallation neutron sources. To exploit fully the fluxes delivered by synchrotron radiation facilities and spallation neutron sources, new detectors capable of acquiring data several orders of magnitude faster 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.

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 subnanometer 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.

Nanoscience research is focused at the following five Nanoscale Science Research Centers, which support the synthesis, processing, fabrication, and analysis of materials at the nanoscale: the Center for Nanophase Materials Sciences at ORNL, the Molecular Foundry at LBNL, the Center for Integrated Nanotechnologies at SNL/LANL, the Center for Nanoscale Materials at ANL, and the Center for Functional Nanomaterials at BNL. These facilities are the Department of Energy's premier user centers for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. As such, research is supported in a wide variety of scientific disciplines including 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 nanotechnology integration.

For this research area, work that advances the instruments, techniques, and capabilities of the existing BES Scientific User Facilities, or contributes to those aspects of future facilities in these areas, is of particular interest. We do not intend to support applications to establish new, unrelated types of facilities or to develop techniques that do not relate to the missions of the light sources, neutron scattering centers, nanoscale science research centers, or electron beam microcharacterization facilities.

IV. Fusion Energy Sciences (FES)

Program Website: http://www.science.doe.gov/ofes/

The mission of the Fusion Energy Sciences (FES) program is to expand the fundamental understanding of matter at very high temperatures and densities and to build the scientific foundations needed to develop a fusion energy source. This is accomplished by studying plasmas under a wide range of temperature and density conditions, developing advanced diagnostics to make detailed measurements of plasma properties, and creating theoretical/computational models to resolve the essential physics ideas and 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 inertial fusion energy sciences (IFES) as part of our high-energy-density laboratory plasma program. For IFES, the National Ignition Facility (NIF) will be capable of producing conditions that could dramatically advance our understanding of plasmas, materials in extreme environments, nuclear processes, shocks and hydrodynamic flows, and will be possibly a demonstration of laboratory ignition.

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. Grant applications 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; development and application of new plasma diagnostic techniques with emphasis on validation of simulation; both low-temperature and high-energy-density plasma science and development of materials that will allow fusion facilities to enter new regimes of plasma science.

(a) Experimental Plasma Science
Technical Contact: Stephen Eckstrand, 301-903-5546, Steve.Eckstrand@science.doe.gov

The Experimental Plasma Science program seeks to utilize unique research facilities to develop the physics knowledge needed to advance the FES energy mission and serves to 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 apparatus 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 recently detailed in the report of a community-wide Research Needs Workshop (ReNeW) *Research Needs for Magnetic Fusion Energy Sciences* (http://www.science.doe.gov/ofes/ReNeW_report_press.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 compromises associated with the high fluxes of heat, charged-particles, and neutrons in a fusion power plant). 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) Plasma Theory and Modeling
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 performance of future fusion power plants. 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 performance of the confined plasma and on the interaction and interface of the hot plasma boundary with the cold 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) Development of Plasma Diagnostics
Technical Contact: Nirmol Podder, 301-903-9536, nirmol.podder@science.doe.gov

The purpose of the Plasma Diagnostics program is to develop advanced diagnostics to make detailed measurements of plasma properties and new techniques to measure quantities not previously accessible or at a level of detail greater than previously possible. The FES program continues to support the development of unique measurement capabilities and diagnostic instruments primarily to serve two important functions: to provide a link between theory/computation and experiments, thereby increasing the understanding of the complex behavior of the plasma in fusion research devices; and to provide sensory tools for feedback control of plasma properties in order to enhance device operation. Research supported under this program will include the development of diagnostics for fundamental plasma parameter measurements, state-of-the-art measurement techniques, and R&D for ITER-relevant diagnostic systems. Program priority is to provide data and analyses for validating theoretical models and fusion simulation codes in support of the FES goal to develop an experimentally validated predictive capability for magnetically confined fusion plasmas. Additionally, improved and sophisticated diagnostic systems are developed that are intended to be installed and operated on current experiments in the U.S. and, where appropriate, abroad through collaborative programs. The proposed measurement must be of benefit to the research program of the fusion facility on which the diagnostic system will be installed and tested. Note, stand-alone theory, modeling, computation, code development, and/or software development applications, or grant requests seeking funding for the application of proven diagnostic techniques to experimental facilities will not be considered.

(d) Low-Temperature and High-Energy-Density Plasma Science
Technical Contact: Mark Koepke, 301-903-9908, mark.koepke@science.doe.gov

Low-temperature plasmas can be nonlinear, internally complicated, and unusually coupled. Research is supported on their processes, structuring, and dynamics. Neutral-species chemistry adds enormous complexity to these plasmas, typically found outside of local thermodynamic equilibrium. This activity will expand in some areas represented in the research needs workshop report *Low-Temperature Plasma Science: Not only the Fourth State of Matter but All of Them* (http://www.science.doe.gov/ofes/Low_temp_plasma_workshop_report_final_Sept08.pdf) published in September 2008. Topics being encouraged include (1) selective and predictive control of interactions between plasma and material surfaces, (2) discovery of behavioral scaling laws beyond the empirical, conventional ones based on the product of plasma discharge pressure and the plasma spatial dimension over which the plasma density or electric field changes substantially, (3) new diagnostic methodologies for measuring essential plasma properties, three-dimensional structures with spatial resolution of 5 micrometers and time resolution of 5 nanoseconds, and the chemical composition of a material surface while it is immersed in a plasma, and (4) revolutionary modeling and simulation tools for predicting plasma physics and chemistry processes that encompass length scales from angstroms to meters and time scales from picoseconds to minutes.

Far from the low-temperature-plasma regime are environments having temperatures of millions of degrees and pressures of millions of atmospheres, where matter exhibits surprising and exotic properties. The ability to create and control stellar conditions in a terrestrial laboratory makes possible the investigation of a broad range of questions from the profound, addressing the very laws of nature themselves, to the most practical, dealing with the extraction of useful energy from matter under extreme conditions. 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) the rise of exotic behavior and self-organization in dense collections of electrons, ions, and photons, (2) the manipulation and control of intense transient flows of energy and particles, unconstrained by conventional material limits, and (3) the control of the interactions of matter under extreme conditions for enabling practical inertial fusion energy.

(e) Enabling Technology Research and Development
Technical Contact: Gene Nardella, 301-903-4956, gene.nardella@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://www.science.doe.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 grant applications should address specific research goals in one or more of these frontiers (as in the examples given below), or else explain how the proposed research or technology development supports the broad scientific objectives 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 applications 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: C.N. Leung, 301-903-3715, cn.leung@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 in support of the experimental and theoretical physics research programs.

VI. Nuclear Physics (NP)

Program Website: http://www.sc.doe.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 in the universe, including those that are no longer found naturally in our universe.

The NP program also produces 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://www.sc.doe.gov/np/nsac/nsac.html), 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: W. B. Tippens, 301-903-3904, brad.tippens@science.doe.gov; and E. A. Henry, 301-903-3614, gene.henry@science.doe.gov

The Medium Energy subprogram focuses primarily on questions having to do with Quantum Chromodynamics (QCD) and the behavior of quarks inside protons and neutrons. Specific questions that are being addressed include: *What is the internal landscape of the nucleons? What does QCD predict for the properties of strongly interacting matter? 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, for example, is to achieve an experimental description of the substructure of the proton and the neutron. The subprogram supports investigations into a few aspects of the second frontier, Nuclei and Nuclear Astrophysics, such as the question: *What is the nature of the nuclear force that binds protons and neutrons into stable nuclei?* The subprogram also examines 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 goals the Medium Energy subprogram supports different experimental approaches primarily 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 nuclei, 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 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 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 (including the Nuclear Data subprogram)
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 three of the field's scientific frontiers described in NSAC's long range plan, and the associated specific questions listed for the experimental subprograms above.

Theoretical research on QCD (the fundamental theory of quarks and gluons) addresses 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.

Nuclear Theory activities at DOE also include the Nuclear Data subprogram, which compiles, maintains and distributes a database of information on nuclear properties and reactions that is of critical interest both to researchers and to developers of industrial applications of nuclear technology.

The NP program also supports the development of the tools and capabilities that make the fundamental research possible, and is the steward of the isotopes program for the nation:

(e) 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 beam; the development of an electron-ion collider (EIC); 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 (FRIB).). Areas of interest also include accelerator R&D technologies in support of next generation Nuclear Physics accelerator facilities.

(f) 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 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 commercial accelerator and reactor facilities throughout the Nation to promote a reliable supply of domestic isotopes. 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 Funding Opportunity Announcement, NP does not support investigations in nuclear reactor studies or nuclear reactor modeling.

Program Funding

It is anticipated that up to $6,000,000 per year will be available under this FOA, contingent on satisfactory peer review and the availability of appropriated funds. Between 30 and 50 awards are anticipated, and applicants should request project support for five years, with out-year support contingent on the availability of funds, progress of the research, and programmatic needs. Awards are expected to begin in **FY 2011**.

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

While the minimum award size is $750,000, DOE expects the typical award size will be $750,000 over five years. Applicants are encouraged to propose research expenditures as close to the funding minimum as possible. Typical budgets will be $150,000 per year for five years.

Merit Review

Applications 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 codified at 10 CFR 605.10(d):

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

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

5. Relevance to the mission of the specific program (e.g., ASCR, BER, BES, FES, HEP, or NP) to which the application 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 FOA and the agency's programmatic needs. Note that external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Both Federal and non-Federal reviewers may be used, and submission of an application constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

The following questions will be posed to reviewers for each of the review criterion 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 the Research Team and Adequacy of Available Resources
What are the past performance and potential of the Principal Investigator (PI)? How well qualified is the research team to carry out the proposed research? Are the research environment and facilities adequate for performing the research? Does the proposed work take advantage of unique facilities and capabilities?

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

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

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 multi-core computing systems and other novel “extreme-scale” computing architectures, which will require significant modifications to today’s tools and techniques.

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 temperatures and densities and to develop the scientific foundations needed to develop a fusion energy source. This is accomplished by studying plasmas and their interactions with their surroundings under a wide range of temperature and density, developing advanced diagnostics to make detailed measurements of their properties, and creating theoretical and computational models to resolve the essential physics.

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 in the universe, including those that are no longer found naturally.

The Catalog of Federal Domestic Assistance (CFDA) number for this program is 81.049, and the solicitation control number is ERFAP 10 CFR Part 605.

Posted on the Office of Science Grants and Contracts Web Site July 1, 2010.