Single-Investigator and Small-Group Research in Basic Energy Sciences

Tackling Our Energy Challenges in a New Era of Science

The Department of Energy's Office of Science, Office of Basic Energy Sciences (BES) announces its interest in receiving proposals from individual investigators and small groups of investigators for basic scientific research needed to create advanced energy technologies for the 21st century. These efforts will significantly enhance the core research programs in BES and pursue the fundamental understanding necessary to meet the global need for abundant, clean, and economical energy.

Background Information

Establishing the Energy Research Directions. In 2001, the Basic Energy Sciences Advisory Committee (BESAC) conducted a far reaching study to assess the scope of fundamental scientific research that must be considered to address the DOE missions in energy efficiency, renewable energy resources, improved use of fossil fuels, safe and publicly acceptable nuclear energy, future energy sources, and reduced environmental impacts of energy production and use.

The scientific community responded to this BESAC study with enthusiasm through participation in a week-long workshop, whose results were published in early 2003 in the report, *Basic Research Needs to Assure a Secure Energy Future*. That report inspired a series of ten follow-on "*Basic Research Needs*" workshops over the next five years, which together attracted more than 1,500 participants from universities, industry, and DOE laboratories. Topics included the hydrogen economy; solar energy utilization; superconductivity; solid-state lighting; advanced nuclear energy systems; combustion of 21st century transportation fuels; electrical-energy storage; geosciences as it relates to the storage of energy wastes (the long-term storage of both nuclear waste and CO_2); materials under extreme environments; and catalysis for energy-related processes. Amongst these reports, research needs in theory, modeling, and simulation have been a central theme, in which the BESAC report, *Opportunities for Discovery: Theory and Computation in Basic Energy Sciences*, captures major highlights.

The New Era of Science. Together, these workshop reports highlighted the remarkable scientific journey that has taken place during the past few decades. The resulting scientific challenges, which no longer were discussed in terms of traditional scientific disciplines, described a new era of science – an era in which materials functionalities are designed to specifications and chemical transformations are manipulated at will. Over and over, the recommendations from the workshops described similar themes – that in this new era of science, we would design, discover, and synthesize new materials and molecular assemblies through atomic scale control; probe and control photon, phonon, electron, and ion interactions with matter; perform multi-scale modeling that bridges the multiple length and time scales; and use the collective efforts of condensed matter and materials physicists, chemists, biologists, molecular engineers, and those skilled in applied mathematics and computer science.

The Grand Science Challenges. To accomplish this—to direct and control matter at the quantum, atomic, and molecular levels—requires a change in our fundamental understanding of how nature works. A BESAC Grand Challenges subcommittee was convened, which examined the roadblocks to progress, and the opportunities for truly transformational new understanding. The results of that examination were presented in the report, *Directing Matter and Energy: Five Challenges for Science and the Imagination*. This new era of energy science poses five challenges:

- How do we control materials processes at the level of electrons?
- How do we design and perfect atom- and energy-efficient syntheses of revolutionary new forms of matter with tailored properties?
- How do remarkable properties of matter emerge from the complex correlations of atomic or electronic constituents and how can we control these properties?
- How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?
- How do we characterize and control matter away—especially very far away—from equilibrium?

Addressing these grand challenges is key to making the transition from observation to control of matter.

Single-Investigator and Small-Group Research in BES

To implement the collective recommendations of these twelve workshops, the Office of Basic Energy Sciences is using two complementary approaches: multi-investigator research via the Energy Frontier Research Centers (http://www.sc.doe.gov/bes/EFRC.html) and a significant enhancement in single-investigator and small-group projects that currently form the bulk of the BES core research portfolio. These single-investigator and small-group research projects have long been recognized as a critically important engine for scientific discovery and BES is committed to their continued strong support. It is anticipated that approximately $60 million will be available for single-investigator and small-group awards starting in FY 2009, pending appropriations. The initial award period is expected to be 3 years. Single-investigator awards are expected to be in the range of $150–$300 thousand per year; small-group awards are expected to be in the range of $500–$1,500 thousand per year. No award will be funded at more than $1.5 million per year, with the specific exception of awards made in Midscale Instrumentation and Accelerator and Detector Research (see below).

Research Areas of Interest:

BES seeks applications in two broad areas of fundamental scientific research:

Grand Challenge Science

The proposed research program should lie at the forefront of one or more of the challenges described in the BESAC report *Directing Matter and Energy: Five Challenges for Science and the Imagination*
(http://www.sc.doe.gov/bes/reports/files/GC_rpt.pdf).
Within this broad framework, several key research areas are identified:

- Ultrafast Science

  Basic research to observe, control and understand chemical and material dynamic phenomena occurring on the inherent time scales of the fundamental components of matter, *viz.* electrons, atoms and molecules. These ultrafast time scales range from attoseconds to picoseconds. Research may also include the development and application of new tools for ultrafast science, particularly utilizing short x-ray pulses, and for theoretical approaches to better understand how ultrashort laser and x-ray pulses interact with matter.
  BES contacts:
  Jeff Krause, 301-903-5827, jeff.krause@science.doe.gov
  James Glownia, 301-903-2411, james.glownia@science.doe.gov

- Chemical Imaging

  Research to develop and apply new methods to measure the chemical behavior of individual molecules and reactions, with high resolution in both space and time in order to elucidate fundamental principles of chemical and material processes at the nanoscale level. The research will build on current single-molecule spectroscopies and microscopies by adding simultaneous time-dependent characterization of evolving chemical and material processes, ultimately with femtosecond time resolution.
  BES contacts:
  Bill Millman, 301-903-5805, william.millman@science.doe.gov
  James Glownia, 301-903-2411, james.glownia@science.doe.gov

- Complex Systems or Emergent Behavior

  Research aimed at understanding emergent behaviors arising from the collective, cooperative behavior of individual components of a system. This challenge of understanding how emergent behavior results from the complexity of competing interactions is among the most compelling of our time, spanning physical phenomena as diverse as phase transitions, high temperature superconductivity, colossal magneto resistance, random field magnets, and spin liquids and glasses.
  BES contacts:
  Greg Fiechtner, 301-903-5809, gregory.fiechtner@science.doe.gov
  James Horwitz, 301-903-4894, james.horwitz@science.doe.gov

Progress toward achieving the scientific grand challenges requires the building of improved tools. The following areas of interest address research designed to provide such enabling tools. Awards in these two areas are expected to include both equipment acquisition and instrument development. Awards are capped at a total project cost of $5 million over the three-year project period.

- Midscale Instrumentation

  There is a significant national need for new small to midsize, multi-user instruments designed to probe the detailed nature of materials using capabilities that are ever more subtle, sensitive and precise. Primarily multi-user in nature but at a scale below that of major BES facilities, high priority mid-scale instrumentation needs include end stations at the synchrotron light sources and neutron scattering facilities; laser systems for ultrafast studies; micro- and atomic-scale characterization tools such as electron micro-characterization and scanning probe microscopy; high-field magnets; facilities for providing large crystals and other unique materials; and computer clusters or midrange servers for support of local group production computing.

  Applications in this area are restricted to principal investigators currently supported by BES, and the instrumentation requested must be utilized in conjunction with BES-funded projects.
  BES contacts:
  Michael Casassa, 301-903-0448, michael.cassasa@science.doe.gov
  James Glownia, 301-903-2411, james.glownia@science.doe.gov

- Accelerator and Detector Research

  Basic research in accelerator physics and x-ray and neutron detectors are essential to the efficient operation and use of present BES x-ray and neutron scattering facilities and to the design of future facilities. Areas of interest include studies of ultra-high brightness electron beams to drive self amplified spontaneous emission free electron lasers, such as the Linac Coherent Light Source (LCLS); collective electron effects, such as micro-bunch instabilities from coherent synchrotron and edge radiation; beam bunching techniques, such as magnetic compression or velocity bunching; fast instruments to determine the structure of femtosecond electron bunches; and detectors capable of acquiring data at very high collection rates. Specific topics of current interest include: physics of gain mechanisms in free-electron lasers (FELs), rapid electron bunch diagnostics, and advanced x-ray and neutron detectors.
  BES contact:
  Roger Klaffky, 301-903-1873, roger.klaffky@science.doe.gov

Use-Inspired Discovery Science
The proposed research should address one of the energy challenges described in the ten BES workshop reports in the *Basic Research Needs* series

(http://www.sc.doe.gov/bes/reports/list.html).
These consist of:

- Solar Energy Utilization

  Research is sought in two major areas: solar-to-electric and solar-to-fuel conversions. Many of the proposed research directions identified in the BES workshop report *Basic Research Needs for Solar Energy Utilization* (http://www.sc.doe.gov/bes/reports/files/SEU_rpt.pdf) concern important cross-cutting issues, including: (1) coaxing cheap materials to perform as well as expensive materials in terms of their electrical, optical, chemical, and physical properties; (2) developing new paradigms for solar cell design that surpass traditional efficiency limits; (3) finding catalysts that enable inexpensive, efficient conversion of solar energy into chemical fuels; (4) identifying novel methods for self-assembly of molecular components into functionally integrated systems; and (5) developing materials for solar energy conversion infrastructure.
  BES contacts:
  Mark Spitler, 301-903-4568, mark.spitler@science.doe.gov
  James Horwitz, 301-903-4894; james.horwitz@science.doe.gov

- Hydrogen Fuel Initiative

  Research is sought to strengthen the scientific basis that will allow comprehensive understanding of the physical and chemical processes that lead to the extraction of hydrogen from its natural environments, storage and distribution of hydrogen, and the efficient energy conversion, all in a safe as well as economically and environmentally sustainable manner. Particular emphasis will be given to novel materials for hydrogen storage, functional membranes, and nanoscale catalysis, as described in the BES workshop report, *Basic Research Needs for the Hydrogen Economy* (http://www.sc.doe.gov/bes/reports/files/NHE_rpt.pdf).
  BES contacts:
  Raul Miranda, 301-903-8014, raul.miranda@science.doe.gov
  John Vetrano, 301-903-5976, john.vetrano@science.doe.gov

- Advanced Nuclear Energy Systems

  Basic research related to systems utilizing advanced fuel cycles is sought in areas described in the BES workshop report *Basic Research Needs for Advanced Nuclear Energy Systems* (http://www.sc.doe.gov/bes/reports/files/ANES_rpt.pdf), including: (1) understanding the fundamentals of radiation resistance and corrosion tolerance in materials; (2) fundamental principles to guide ligand design; (3) investigation of new separations approaches based on magnetic and electronic differences; (4) development of separations processes models to optimize waste minimization and minimize opportunities for diversion of nuclear materials; and (5) solution and interfacial behavior under extreme radiation flux and elevated temperatures.

BES contacts:
Lester Morss, 301-903-9311, lester.morss@science.doe.gov
John Vetrano, 301-903-5976, john.vetrano@science.doe.gov

- Electrical Energy Storage

  The use of electricity generated from intermittent, renewable sources requires efficient EES in order to effectively integrate it into the baseload grid system and to use it in transportation applications. A number of specific areas of research for both batteries and electrochemical capacitors have been identified in the BES workshop report *Basic Research Needs for Electrical Energy Storage* (http://www.sc.doe.gov/bes/reports/files/EES_rpt.pdf). These include: (1) Efficacy of structure in energy storage—new approaches combining theory and synthesis for the design and optimization of materials architectures including self-healing, self-regulation, failure-tolerance, and impurity sequestration. (2) Charge transfer and transport—molecular scale understanding of interfacial electron transfer. (3) Electrolytes—electrolytes with strong ionic solvation, yet weak ion-ion interactions, high fluidity, and controlled reactivity. (4) Probes of energy storage chemistry and physics at all time and length scales—analytical tools capable of monitoring changes in structure and composition at interfaces and in bulk phases with spatial resolution from atomic to mesoscopic levels and temporal resolution down to femtoseconds. (5) Multi-scale modeling—computational tools with improved integration of length and time scales to understand the complex physical and chemical processes that occur in EES from the molecular to system scales.
  BES contacts:
  Paul Maupin, 301-903-4355, paul.maupin@science.doe.gov
  John Vetrano, 301-903-5976, john.vetrano@science.doe.gov

- Geological Sequestration of Carbon Dioxide

  Research is sought to develop the scientific understanding that will underpin novel technological approaches to deep underground carbon sequestration. Research directions identified in the 2007 BES workshop report *Basic Research Needs for Geosciences* (http://www.sc.doe.gov/bes/reports/files/GEO_rpt.pdf) include: (1) understanding geochemical processes relevant to the dimensions of subsurface sequestration sites and incorporating realistic chemistry of reacting flowing fluids into predictive models of geological formations; (2) development of critical geophysical measurement techniques to enable remote probing and tracking of important chemical and physical processes within rock formations at depth, including capture of rock heterogeneity; and (3) development and application of fluid-flow measurement approaches and simulation tools that can link, and explicitly couple, chemical and physical processes at multiple scales.
  BES contact:
  Nick Woodward, 301-903-4061, nick.woodward@science.doe.gov

- Catalysis for Energy

  Basic research related to catalysis is sought in areas described in the BES workshop report *Basic Research Needs: Catalysis for Energy* (http://www.sc.doe.gov/bes/reports/files/CAT_rpt.pdf). The workshop sought to identify basic research needs and opportunities in catalysis to meet the nation's energy needs. The workshop identified three priority research directions for advancing catalysis science: advanced catalysts for the conversion of heavy fossil energy feedstocks; understanding the chemistry of lignocellulosic biomass deconstruction and conversion to fuels; photo- and electro-driven conversions of carbon dioxide and water. The grand challenge identified at the core of all of these areas was to achieve detailed understanding of mechanisms and dynamics of catalyzed reactions, and controlled synthesis of nanostructures and interfaces. Such understanding would allow scientists to build effective catalysts with atom-by-atom precision and convert complex reactants to energy-storing products with molecular precision. The means to resolve this challenge is several-fold: creating new and expanding current fundamental theories of chemical kinetics that effectively take into account the dynamics and statistical fluctuations of structurally complex and diverse feedstocks; creating and advancing instrumentation that permit real-time high-resolution chemical imaging of reacting species and catalysts; synthesizing new and more complex catalyst structures that exploit multifunctionality and versatility in order to guide reactions through highly selective pathways.
  BES contacts:
  Raul Miranda, 301-903-8014; raul.miranda@science.doe.gov
  Richard Kelley, 301-903-6051; richard.kelley@science.doe.gov

- Clean and Efficient Combustion

  Basic research related to clean and efficient combustion is sought in areas described in the BES workshop report *Basic Research Needs for Clean and Efficient Combustion of 21st Century Transportation Fuels* (http://www.sc.doe.gov/bes/reports/files/CTF_rpt.pdf). This workshop was charged with exploring basic research needs in the areas of gas-phase chemistry, combustion diagnostics, and combustion simulation that will enable the use of transportation fuels derived from non-traditional sources (oil shale, tar sands, coal, biomass) in a manner that optimizes engine efficiency and minimizes pollutant formation. Eight priority research directions were identified, two of which were devoted to a focus on engines or fuels and were similar in their strategy of working backward from technology drivers to scientific research needs. A third panel explored crosscutting science themes and identified critical gaps in our scientific understanding of 21st-century fuel combustion. The workshop identified a single, overarching grand challenge: The development of a validated, predictive, multi-scale, combustion modeling capability to optimize the design and operation of evolving fuels in advanced engines for transportation applications. The

workshop produced a keen sense of urgency and opportunity for the development of revolutionary combustion technology for transportation based upon fundamental combustion science.
BES contacts:
Michael Casassa, 301-903-0448; michael.casassa@science.doe.gov
Jeff Krause, 301-903-5827; jeff.krause@science.doe.gov

- Materials under Extreme Environments

  Basic research related to materials under extreme environments is sought in areas described in the BES workshop report *Basic Research Needs for Materials under Extreme Environments* (http://www.sc.doe.gov/bes/reports/files/MUEE_rpt.pdf). Reaching the intrinsic limit of materials performance is a key challenge, and solutions to this challenge require new understanding regarding the most fundamental atomic and molecular origins of material failure. In particular, ultra-high spatial and ultrafast temporal resolution characterization tools are needed to observe and follow the initiation and evolution of atomic-scale to cascading macroscale damage events. Complementary advanced computational capabilities to simulate and predict multiscale damage from atomic to macroscopic dimensions are also needed. Such new understanding of damage and failure will underpin research to discover how atomic and molecular structures could be manipulated in a predicable manner to enable development of new materials having an extraordinary tolerance to function within an extreme environment without property degradation, or even with the ability for self-repair.
  BES contacts:
  Lane Wilson, 301-903-5877; lane.wilson@science.doe.gov
  John Vetrano, 301-903-5976, john.vetrano@science.doe.gov

- Solid-State Lighting

  Basic research related to solid-state lighting is sought in areas identified in the BES workshop report *Basic Research Needs for Solid-State Lighting* (SSL) (http://www.sc.doe.gov/bes/reports/files/SSL_rpt.pdf). Broad areas of discovery research and scientific inquiry were identified as the required groundwork for the future of SSL, which were condensed into the following two primary challenges. One broad research challenge aims to change the very paradigm by which SSL structures are designed, moving from serendipitous discovery towards rational design. The other challenge aims to understand and control the microscopic pathways through which losses occur as electrons produce light, which is identified as a primary roadblock to SSL. By developing a fundamental understanding of the processes that mediate the competing conversion of electrons to light and heat, the challenge of converting every injected electron into useful photons will be addressed. The anticipated outcomes are ultra-high-efficiency light-emitting materials and nanostructures, and a deep scientific understanding of how light interacts with matter, with broad impact on science and technology areas beyond SSL.

BES contact:
Arvind Kini, 301-903-3565; a.kini@science.doe.gov

- Superconductivity

  Basic research related to superconductivity is sought in areas identified in the BES workshop report *Basic Research Needs for Superconductivity* (http://www.sc.doe.gov/bes/reports/files/SC_rpt.pdf). Many of the proposed research directions identified in the concern important cross-cutting issues. A central challenge with the biggest impact is the need to understand the fundamental mechanisms of high-temperature superconductivity. This is difficult precisely because the mechanisms are entangled with many anomalous normal state effects. Another primary scientific opportunity is rooted in nanoscale phenomenon as superconductivity's two composite building blocks have dimensions ranging from a tenth of a nanometer to a hundred nanometers. Unraveling superconductivity's mechanism with the promise of nanoscale fabrication, characterization, and simulation will provide a pathway for the rational design of and production of functional superconducting materials required for next-generation grid technology.
  BES contacts:
  Andrew Schwartz, 301-903-3535; andrew.schwartz@science.doe.gov
  Refik Kortan, 301-903-3308; refik.kortan@science.doe.gov

Application Procedures

Universities and Other Research Institutions:
Potential applicants are ***strongly encouraged*** to follow the BES guidelines for grant applications: http://www.sc.doe.gov/bes/grants.html . These guidelines include an initial contact with a suitable BES program manager (see contacts above) and submission of a pre-application. A pre-application will be evaluated by the BES program manager(s) for relevance to this expression of interest and to the existing BES research portfolio. A pre-application will either be encouraged for a full application or discouraged, in which case a full application will not be accepted. Full applications must be submitted in response to the Office of Science Financial Assistance Funding Opportunity Announcement DE-PS02-08ER08-01 (http://www.sc.doe.gov/grants/FAPN08-01.html).

DOE/NNSA FFRDCs (National Laboratories):
All potential proposals must be communicated to the appropriate BES program manager (see contacts above) by an approved BES laboratory coordinator. Only potential proposals communicated to BES via approved laboratory contacts will be considered. The BES program manager may request the submission of a pre-proposal for evaluation for its relevance to this expression of interest and to the existing BES research portfolio. A pre-proposal will either be encouraged for a full proposal or discouraged, in which case a full proposal will not be accepted. Full proposals must be submitted via the normal Field Work Proposal process for DOE/NNSA FFRDCs and should follow the

BES guidelines for preparation of proposals
(http://www.sc.doe.gov/bes/Guide_for_Lab_Rev_Docs.pdf).

Special Note:
The application guidance given above also applies to the resubmission of a proposal based upon a revision or update of a proposal declined under Office of Science Notice 06-13, *Basic Research for Midscale Instrumentation*; Notice 06-15, *Basic Research for Solar Energy Utilization*; Notice 06-17, *Basic Research for the Hydrogen Fuel Initiative*; and Notice 07-04, *Basic Research for Advanced Nuclear Energy Systems*. In particular, DOE laboratory principal investigators must work through the appropriate laboratory management and communicate with BES only via approved laboratory coordinators. And both laboratory coordinators and university investigators are ***strongly encouraged*** to contact the appropriate BES program manager to discuss a potential resubmission of a proposal declined under one of the above-named Notices.