Basic Energy Sciences

Summary of FY 2012 President's Budget Request

(dollars in thousands)

	09 Recovery	10 Appr	12 Request	12 Request vs. 10	
Basic Energy Sciences	555,406	1,598,968	1,985,000	+386,032	+24.1%

Highlights

Energy Innovation Hubs

In FY 2012, BES will support the continuation of the Fuels from Sunlight Hub and will initiate a new Hub on Batteries and Energy Storage. The Hubs are aimed at assembling multidisciplinary teams to address the basic science and technology issues hindering the nation's secure and sustainable energy future. Because the components and processes of energy systems are highly interdependent, innovative solutions to real-world energy challenges will require concerted efforts that couple the various elements of the technology chain and combine the talents of universities, national laboratories, and the private sector. The Batteries and Energy Storage Hub is part of the proposed new basic research for clean energy technologies increases (see following) that will enhance the BES core program in energy research.

	10 Appr.	12 Request	12 Request vs. 10
Energy Innovation Hubs	0	58,320	+58,320

Basic Research for Clean Energy Technologies

In FY 2012, the BES program will support expanded efforts in basic research related to transformational clean energy technologies. These new directions derive from the series of "Basic Research Needs" workshop reports and the follow-on workshop reports by the Basic Energy Sciences Advisory Committee (BESAC). The requested increases are primarily guided by the recent BESAC report *Science for Energy Technology: Strengthening the Link between Basic Research and Industry*, which stresses the importance of sustained efforts of testing new concepts, identifying roadblocks, and pursuing scientific and technical solutions to accelerate transformative advances for targeted impact on cost, reliability, and performance.

The FY 2012 BES budget request includes funding for integrated R&D activities across the Department's technology programs and the Office of Science. The DOE technology programs will manage applied research, development, and deployment efforts to gain and apply knowledge to achieve identified near-to-mid-term goals. The basic research work within BES is selected in clean energy areas where an understanding of the fundamental phenomena is necessary to achieve game-changing discoveries for mid-to-longer-term technological innovation.

Our science based approach for creating transformational improvements in clean energy technologies consists of increasing basic research on a set of interrelated energy issues: non-carbon sources, carbon capture and sequestration, transportation and fuel switching, transmission and energy storage, and efficiency. These basic research efforts will be conducted in coordination with the complementary R&D activities in the following DOE programs: Office of Energy Efficiency and Renewable Energy, Office of Nuclear Energy, Office of Electricity Delivery and Energy Reliability, Office of Fossil Energy, and the

National Nuclear Security Administration. The FY 2012 budget contains increases to BES research in the areas summarized below.

Non-carbon Sources:

- *Solar Electricity from Photovoltaics – Fundamental Science of Interfaces and Degradation* (+$8,000,000). Many critical issues that surround the performance, cost, and reliability of solar photovoltaics (PV) are associated with interfaces: p-n junctions, device contacts, light and carrier reflectors, tunnel junctions, passivation and buffer layers, grain boundaries in polycrystalline semiconductors, and packaging materials. Technology development in PV interfaces has been largely empirical in nature. Greatly improved characterization tools provide a unique opportunity to probe PV interfaces in situ and enable new research opportunities for improved fundamental understanding of their behavior. Fundamental research is also required to improve the scientific basis for understanding the mechanisms by which PV modules are degraded. Particular emphasis will be place on degradation and the long-term effects of impurity diffusion processes.
- *Advanced Nuclear Energy – Basic Actinide Chemistry Research for Fuel Cycles* (+$8,000,000). New research is proposed to significantly advance fundamental understanding of actinide molecules and their chemistry, with broad impacts for nuclear reactor fuels, waste forms, and separations techniques. Proposed research includes development of more sophisticated theoretical and experimental tools for the understanding of the structure and bonding of actinide species with an emphasis on separation chemistry addressing the multiplicity of chemical forms and oxidation states for actinides in fuels, solutions, and waste forms. New characterization and computational tools can play particularly important roles in addressing these challenges. These tools offer the opportunity to transform and accelerate the fundamental chemistry that underpins technology development for advanced nuclear energy systems.
- *Materials under Extreme Environments* (+$15,000,000). The physical processes that occur in materials under extreme nuclear technology environments span time scales from femtoseconds to decades and proceed over length scales ranging from atomistic to meters. These processes must be understood for real, engineered materials including complex alloys, materials with defects and impurities, materials with complex microstructures, and ranging from actinides to metals to composites. Research in this area will focus on understanding, modeling, and designing radiation-resistant materials that maintain all of the required physical properties after prolonged exposure. Materials discovery will include nanoscale design of new materials, including self-healing potential to limit the impact of defects generated in the extreme exposures in reactors. In situ experiments will be closely integrated with theoretical/computational efforts to develop a fundamental understanding of degradation mechanisms and kinetics over multiple length and time scales.

Carbon Capture and Sequestration

- *Carbon Capture – Novel Molecular Design* (+$8,000,000). The objective of research in predictive modeling of carbon capture will be to gain significant advances in quantum chemical structure determination, intermolecular potentials, and molecular dynamics algorithms on CO_2 interactions with complex materials and minerals for efficient and cost-effect carbon capture and sequestration. Specific emphasis will be placed on the discovery and design of new materials that incorporate complex structures and functionalities tuned for optimum separation properties; understanding and controlling the atomic and molecular level interactions of the targeted species with the separation media; and tailored capture/release processes with alternative driving forces, taking advantage of a new generation of nanoscale materials.

- *Carbon Sequestration – Multiscale Dynamics of Flow and Plume Migration* (+$8,000,000). Permanent storage of captured CO_2 through injection into deep underground geologic formations has been proposed as the most practical approach to store captured industrial scale carbon emissions. Significant scientific and technical challenges must be overcome to scale up sequestration methodologies reliably and safely to effective operational levels. A critical current limitation is the inaccuracy of models that seek to describe the migration of CO_2 in the subsurface, which require characterization over vast spatial scales under multiple geological sites. New research to improve field-scale models will emphasize the improved understanding of geologic processes and rates relevant to subsurface sequestration sites, including better understanding of reservoir-scale geochemistry; reactive flow and transport processes and rates; higher resolution geophysical measurement techniques; and more accurate simulation approaches for linking geochemical processes and geophysical responses across multiple spatial scales.

Transportation and Fuel Switching

- *Energy Systems Simulation – Internal Combustion Engines (ESS-ICE).* (+$15,000,000). Research activities in this area will focus on predictive modeling of combustion in an evolving fuel environment, thus building on the science base for the development of simulation tools for advanced internal combustion engine design. Basic research in ESS-ICE will emphasize the development of two complementary, experimentally validated sets of codes: one for stochastic, in-cylinder engine processes and one that can reliably predict the temporal and spatial behavior of liquid fuel injection. These two areas have been identified as high priorities by the U.S. engine industry and lie on the critical path toward the complete transition from hardware-intensive, experience-based engine design to simulation-intensive, science-based design. This research will be particularly important for the economic design of high-efficiency, clean engines burning a variety of fuels, including biofuels.
- *Batteries and Energy Storage Hub* (+$34,020,000). Initiated in FY 2010, the Energy Innovation Hubs are designed as a multidisciplinary effort that addresses critical science and technology issues in an integrated manner. A Hub focuses teams of researchers in separate but collaborative research areas on overcoming scientific barriers to development of a complete energy system with potential for implementation into a transformative energy technology. In FY 2012, BES will support the continuation of the Fuels from Sunlight Hub and will initiate a new Hub on Batteries and Energy Storage. The Hub is aimed at developing electrochemical energy storage systems that safely approach theoretical energy and power densities with very high cycle life. These are systemic challenges, and the Hub will result in new materials, systems, and knowledge critical to developing a robust industrial base leading the next generation of energy storage technology, including that for transportation (e.g., batteries for plug-in hybrid and all electric vehicles). Knowledge gained in the Batteries and Energy Storage Hub could also contribute to grid-level or stationary energy storage, as noted in the *Transmission and Energy Storage* section below.

Transmission and Energy Storage

- *Electric Power Grid – Enabling Materials Sciences* (+$4,000,000). The research activities will include development of advanced materials for normal and superconducting power transmission lines and electronic components and devices to control and link complex high voltage direct current networks. Additional research will be initiated for developing nano-materials and novel deposition processes to achieve improved properties for cost-effective, high-capability electric power distribution.
- *Power Electronics* (+$3,500,000). The Nation's future electric systems will need cost-effective, reliable, high-capability power electronic components and devices to control and link complex high

voltage networks, measure and control flow, and reduce energy losses in long-distance transmission. Power electronics are particularly important in interfacing new, renewable electrical power sources to the existing grid distribution systems. In particular, wide bandgap materials that permit single devices to control current flows at higher voltages with high efficiency could make power electronics affordable and enable efficient tools to control and manage electricity. Focus areas in basic materials research will be initiated in low defect density, wide bandgap semiconductors; magnetic materials for high frequency inductors, including non-rare earth based materials; and next generation dielectrics.

- *Batteries and Energy Storage Hub* (same Hub as above). The Hub is aimed at developing electrochemical energy storage systems that safely approach theoretical energy and power densities with very high cycle life. These are systemic challenges, and the Hub will result in new materials, systems, and knowledge critical to developing a robust industrial base leading the next generation of energy storage technology, including that for grid and other stationary energy storage applications. Knowledge gained in this Hub could also contribute to electrical energy storage for vehicle applications as noted in the *Transportation and Fuel Switching* section above.

Efficiency

- *Advanced Solid-state Lighting – Novel Light Emitting Diodes* (+$8,000,000). Solid-state lighting is the direct conversion of electricity to visible white light using inorganic semiconductor materials, organic materials or hybrid combinations. By avoiding the indirect processes characteristic of traditional incandescent and fluorescent lighting that generate heat, solid state lighting can greatly improve the conversion efficiency. There is no known fundamental physical barrier to achieving ultrahigh efficiencies for visible white light. The proposed research will focus on the design of new materials to control the flow of electrons, including research on understanding light-emitting organic and inorganic (and hybrid) materials and nanostructures, control of the materials and nanostructure properties, research on interfacial issues between semiconductors, metals and organic materials and the development of a fundamental understanding of the processes that mediate the competing conversion of electrons to light and heat.
- *Energy Efficiency – Enabling Materials Sciences* (+$4,000,000). Buildings are responsible for nearly 40 percent of US primary energy use and 70 percent of electricity demand. Significant opportunities exist to improve building efficiencies. These include research on the development of novel building materials using nano-materials, novel deposition processes to achieve improved properties. Research on reducing electrical energy needs will include materials with optical and thermal properties that respond passively or controllably to external conditions for reducing heating and cooling demands, windows with controllable optical properties, and new lighting devices.

	10 Appr.	12 Request	12 Request vs. 10
Non-carbon Sources			
Solar Electricity from Photovoltaics	0	8,000	+8,000
Advanced Nuclear Energy	0	8,000	+8,000
Materials under Extreme Environments	0	15,000	+15,000
Carbon Capture and Sequestration			
Carbon Capture	0	8,000	+8,000
Carbon Sequestration	0	8,000	+8,000

Transportation and Fuel Switching			
Energy Systems Simulation	0	15,000	+15,000
Batteries and Energy Storage Hub	0	34,020	+34,020
Transmission and Energy Storage			
Electric Power Grid	0	4,000	+4,000
Power Electronics	0	3,500	+3,500
Batteries and Energy Storage Hub		See above	
Efficiency			
Advanced Solid-state Lighting	0	8,000	+8,000
Energy Efficiency – Enabling Materials Sciences	0	4,000	+4,000

Basic Research in Methane Hydrates

In addition to the aforementioned basic research opportunities in clean energy technologies, BES will initiate a new program in methane hydrates, which are naturally occurring combinations of methane and water that form at low temperatures and high pressures. The emphasis of this activity will be on expanding the research base to characterize the formation mechanisms of gas hydrates and to understand and ultimately predict the environmental stability of hydrates at the systems level. This activity supports theory, multi-scale modeling and simulation, and experimental research in areas such as: the intermolecular forces that govern the structure and properties of methane hydrates; multi-phase behavior of hydrate-sediment systems; and studies of methane hydrates in the natural environment.

	10 Appr.	12 Request	12 Request vs. 10
BES Methane Hydrates (basic research)	0	10,000	+10,000

Computational Materials and Chemistry by Design

Increases in research funding are requested as part of two inter-agency coordinated initiatives that will provide the broad knowledge foundations critical for clean energy and other advanced technologies. One of the two initiatives is the *Computational Materials and Chemistry by Design* effort. As described in the Office of Science Workshop on *Computational Materials Science and Chemistry for Innovation*, over the past two decades, the United States has developed and deployed the world's most powerful collection of tools for the synthesis, processing, characterization, and simulation and modeling of materials and chemical systems at the nanoscale, from dimensions of a few atoms to a few hundred atoms across. DOE will lead in the development of new software tools and data standards that catalyze a fully integrated approach from material discovery to applications. New research efforts will be initiated to design materials with targeted properties and advanced chemical processes with high efficiencies through theory, computation, and modeling, as validated by precise experimental characterization. The era of modern technology requires understanding the complexity of materials and chemical assemblies well beyond that of the past centuries and beyond the current capabilities offered by experimental approaches alone. The need to accelerate the innovation cycle by taking advantage of the significant growth in modeling and high performance computing, underscores the critical importance of this request. Coupled with the goal of materials and chemistry by design is another critical goal for accelerating advances in energy technologies—the ability to accurately predict changes in materials and their properties associated with their use in a specific application, incorporating the effects of fabrication of materials into system components, influence of the environment in which materials are used, and

extend the lifetime of their usage. Discovery of new materials and chemical assemblies with totally new properties and accurate lifetime predictions are crucial to generation, use, and advances in energy technologies, as well as to virtually all industries that use materials, both structural and functional, in their infrastructure and products—crossing the spectrum of transportation, electronics, buildings, chemicals and pharmaceuticals, health, and consumer products. This request envisions assembling integrated teams focused on key scientific knowledge gaps to develop new theoretical models, including their realization in reusable and broadly-disseminated software. Special attention will be paid to the development of powerful abstraction methods to enable the distillation of new physical laws bridging multiple length and temporal scales. The ultimate goal is to provide the Nation with a science-based computational tool set to rationally predict and design materials and chemical processes to gain a global competitive edge in scientific discovery and innovation.

	10 Appr.	12 Request	12 Request vs. 10
Computational Materials and Chemistry by Design	0	40,000	+40,000

Nanoelectronics

Increases in research funding are requested as part of two inter-agency coordinated initiatives that will provide the broad knowledge foundations critical for clean energy and other advanced technologies. One of the two initiatives is the *Nanoelectronics* effort. It is one of the signature activities of the National Nanotechnology Initiative coordinated by the National Science and Technology Council's subcommittee on Nanoscale Science, Engineering and Technology. BES research will focus on overcoming fundamental physics limitations of semiconductor processing and memory devices in two thrust areas: (1) exploring new or alternative "state variables" for computing, e.g., other alternatives to charge transfer exploited by conventional transistors such as spintronics, and (2) exploiting nanoscale processes and phenomena for quantum information science. These activities require the development of novel fabrication, processing, and instrumentation techniques, and new theoretical and modeling tools. This research will be informed by and coordinated with applied research in industries to identify the next generation of logic device beyond mainstream silicon-based Complementary Metal-Oxide Semiconductor (Si/CMOS) technology.

	10 Appr.	12 Request	12 Request vs. 10
Nanoelectronics	0	10,000	+10,000

Linac Coherent Light Source Expansion (LCLS-II)

The Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory completed construction in FY 2010 within budget, ahead of schedule, and with capabilities meeting—and in some aspects exceeding—the designed technical specifications. The LCLS is the world’s first hard X-ray free electron laser (FEL) and produces ultrafast pulses of X-rays millions of times brighter than even the most powerful synchrotron light sources. It provides scientists with a unique tool for studying the arrangement and motion of atoms and electrons in metals, semiconductors, ceramics, polymers, catalysts, plastics, and biological molecules with the potential to significantly impact advanced energy research and other fields. Capitalizing on LCLS’s success, a new MIE project for LCLS expansion (LCLS-II) is initiated in FY 2012 (+$30,000,000) to extend the x-ray spectral range at the LCLS and expand the experimentation capacity to accommodate the fast growing number of users. The LCLS-II MIE will enable the U.S. maintain leadership in FEL science and keep pace with facilities under construction elsewhere in the world.

(dollars in thousands)

	10 Appr.	12 Request	12 Request vs. 10
Linac Coherent Light Source Expansion (LCLS-II)	0	30,000	+30,000

National Synchrotron Light Source-II EXperimental Tools (NEXT)

Support is continued for construction and Other Project Costs (FY 2012 funding of $151,400,000 and $7,700,000, respectively) for the National Synchrotron Light Source-II (NSLS-II)—built as a replacement for NSLS—to enable the study of material properties and functions, particularly materials at the nanoscale, at a level of detail and precision never before possible. The NSLS-II project provides funding for six experimental beamlines, which is only a fraction of the total capacity. Although some of the equipment can be reused from the NSLS instruments, in order to make full use of the scientific capabilities of the new machine, new state of the art instruments need to be designed, constructed, and commissioned. A new MIE, the NSLS-II EXperimental Tools (NEXT), is requested in FY 2012 (+$12,000,000) to initiate the fabrication of approximately five to six additional instruments.

	10 Appr.	12 Request	12 Request vs. 10
National Synchrotron Light Source-II EXperimental Tools (NEXT)	0	12,000	+12,000

Advanced Photon Source Upgrade (APS-U)

The Advanced Photon Source (APS) at Argonne National Laboratory is one of the most productive light sources in the US, serving the largest number of users per year. It is a leading machine for physical sciences, having pioneered instruments and techniques in high-pressure science, x-ray photon correlation spectroscopy and inelastic x-ray scattering. Commissioned in 1996, many of the APS components—both accelerator and instruments—were designed in the early 1990s and are not optimized for today's needs. The Advanced Photon Source Upgrade (APS-U) project is to add new x-ray capabilities and increase the number of experiments that the APS can accommodate. The new APS-U MIE project (+$20,000,000) would provide significant technical enhancements in the source's entire hard x-ray range, particularly above 20 keV, both in source brightness and intensity. Such capabilities are critically needed to examine real materials, in real time, in real environments, especially in extreme conditions encountered in advanced energy applications.

	10 Appr.	12 Request	12 Request vs. 10
Advanced Photon Source Upgrade (APS-U)	0	20,000	+20,000

Transmission Electron Aberration-Corrected Microscope II (TEAM II)

Transmission Electron Aberration-Corrected Microscope II (TEAM II) will produce a new microscope that incorporates many of the component innovations in the initial TEAM instrument that was completed and made available to users in FY 2009. The TEAM instrument was designed with an emphasis on extending spatial resolution to new limits by fully integrating the correction of lens aberrations. The new TEAM-II MIE project (+$18,000,000) will be optimized differently to provide complementary functionality following the recommendations of a BES workshop on *Future Science Needs and Opportunities for Electron Scattering: Next-Generation Instrumentation and Beyond*. Approaches being considered include: dramatic expansion of the range of in-situ conditions (temperatures, pressures,

electromagnetic fields, fluid environments) under which materials can be studied, challenges of examining soft (such as polymeric and biological or biomimetic) materials and hard/soft interfaces, and improved temporal resolution for observation of dynamic processes. These capabilities will be especially critical for exploring the unit processes and phenomena involved in clean energy technologies.

	10 Appr.	12 Request	12 Request vs. 10
Transmission Electron Aberration-Corrected Microscope II (TEAM II)	0	18,000	+18,000

Facilities Instrumentation for Clean Energy Technologies

Funding is requested to upgrade, enhance, and procure beamlines and instruments at light sources, neutron sources, and nanoscale science research centers. The funding will be competed amongst BES scientific user facilities with the goal of significantly advancing the synthesis and characterization capabilities for clean energy technologi*es. This may include capabilities to collect data at high or low extremes of temperature, at high pressur*e, in the presence of gasses or liquid, and/or at operating voltages in a working device; to engage in materials synthesis, including high throughput combinatorial synthesis for nanoscale materials discovery and design; and for the facilities to handle full scale devices, ranging from a solar panel to a battery that powers an electric vehicle. This supports one of the key priority research directions of the BESAC Science for Energy Technology report, in which "at scale" experiments on commercial materials/devices in real-world environments is highlighted as a key enabling cross-cutting capability.

Facilities Instrumentation for Clean Energy Technologies	10 Appr.	12 Request	12 Request vs. 10
• Light Sources	0	24,000	+24,000
• Neutron Sources	0	8,000	+8,000
• Nanoscale Science Research Centers	0	15,000	+15,000
Total, BES User Facilities Instrumentation	0	47,000	+47,000

Core Research

In FY 2012, the BES program will continue support of principal investigator and small group projects in areas derived from the series of "Basic Research Needs" workshop reports and the workshop reports by the Basic Energy Sciences Advisory Committee. As recognized in the series of workshop reports, clean energy technologies are in their infancy compared to traditional fossil fuel-based technologies, and they have many scientific and technological challenges to overcome in order to operate at their full potential. The reports have defined the decadal science challenges whose solutions will create comprehensive understanding and control of clean energy phenomena; they have also been instrumental in guiding the establishment of the 46 Energy Frontier Research Centers (EFRCs), which exemplify the pursuits of the broad-based science challenges for energy applications. In FY 2012, the BES program will support expanded efforts in basic research related to transformational clean energy technologies and related topics itemized above and the continuation of the EFRCs.

	10 Appr.	12 Request	12 Request vs. 10	
Core Research	663,428	658,317	-5,111	-0.8%

Scientific User Facilities, Operations

Support is provided for the operation of the BES scientific user facilities, which consist of light sources, neutron sources, and nanoscale science research centers (NSRCs). The BES user facilities provide open access to specialized instrumentation and expertise that enable scientific users from universities, national laboratories, and industry to carry out experiments and develop theories that could not be done at their home institutions. In FY 2012, operation of these scientific user facilities is funded at a level that will permit optimal service to users. The request also includes additional funds for procurement of accelerator, beamline, and/or other capital equipment instrumentation to advance research capabilities for clean energy technologies as described above. The expansion of capabilities to examine and characterize materials "at scale" and under a wide range of operating conditions across the suite of BES facilities supports key priority research directions of the BESAC Science for Energy Technology report.

	10 Appr.	12 Request	12 Request vs. 10	
Scientific User Facilities, Operations	734,994	778,416	+43,422	+5.9%