## Research Activity: Experimental Program to Stimulate Competitive Research (EPSCoR)

Division: Materials Sciences and Engineering
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## Portfolio Description:

The Department of Energy (DOE) Experimental Program to Stimulate Competitive Research (EPSCoR) activity supports basic research spanning the broad range of science and technology programs within DOE in states that have historically received relatively less federal research funding. EPSCoR includes the states of Alabama, Alaska, Arkansas, Delaware, Hawaii, Idaho, Kansas, Kentucky, Louisiana, Maine, Mississippi, Montana, Nebraska, Nevada, New Hampshire, New Mexico, North Dakota, Oklahoma, Rhode Island, South Carolina, South Dakota, Tennessee, Vermont, West Virginia, and Wyoming, as well as the Commonwealth of Puerto Rico and the U.S. Virgin Islands. The work supported by EPSCoR includes research in materials sciences, chemical sciences, biological and environmental sciences, high energy and nuclear physics, fusion energy sciences, computational sciences, fossil energy sciences, and energy efficiency and renewable energy sciences.

## Unique Aspects:

The program objective is accomplished by sponsoring two types of grants: (1) Implementation Grants and (2) Laboratory-State Partnership Grants. Implementation grants are for a maximum period of six years with an initial grant period of three years. Maximum funding for these grants is $750,000 per year. Fifty percent state matching funds are required. The Laboratory-State partnership grants are for a period of one to three years. Maximum funding for these grants is $150,000 per year. Ten percent state matching funds are required. EPSCoR has placed a high priority on integrating the scientific workforce development component with the research component of the program. In addition, it is promoting strong research collaboration and training of students at the DOE national laboratories where unique and world-class facilities are available. This program is science-driven and supports the most meritorious proposals based on peer and merit review. Workshops and discussions are regularly held with representative scientists from EPSCoR states to acquaint them with the facilities and personnel at the DOE national laboratories.

## Relationship to Other Programs:

The activity interfaces with all other research activities within BES. In addition, it is responsive to programmatic needs of other program offices within DOE. The principal objective of the DOE EPSCoR program is to enhance the abilities of the designated states to conduct nationally competitive energy-related research and to develop science and engineering workforce to meet current and future needs in energy related areas. Most of the research clusters that have graduated from the DOE EPSCoR program after six years of funding have found alternate funding for continuing the research activity. This demonstrates that the research clusters funded by EPSCoR are becoming competitive. In addition, EPSCoR grants are supporting graduate students, undergraduates, and postdoctoral associates, and encouraging them to be trained in frontier research areas by making use of world-class research facilities at the national laboratories. The work supported by the EPSCoR program impacts all DOE mission areas including research in materials sciences, chemical sciences, biological and environmental sciences, high energy and nuclear physics, fusion energy sciences, advanced computer sciences, fossil energy sciences, and energy efficiency and renewable energy sciences.

## Significant Accomplishments:

The EPSCoR program funds basic research in support of all programmatic needs of DOE. The accomplishments are grouped according to the relevant DOE program office.

<u>Basic Energy Sciences</u>

- Palladium complexes are among the most powerful and versatile catalysts for a variety of chemical reactions including the delivery and release of hydrogen, the chemical transformations of hydrocarbons, and the production of pharmaceuticals and industrial chemicals. Knowledge of the fundamental steps involved in these reactions is vital for the design and improvement of these important processes. Studies of these steps using both fast laser spectroscopy (taking a snapshot of the reaction) and low temperature methods (freezing the reaction midstream) have led researchers to the identification of a number of new palladium species with very short lifetimes. These species are chemically important because of their exceptionally high reactivity. Investigation of these species are leading to the production of new and more efficient catalysts for chemical processes important to energy as well as other sectors of our economy (M.J. Fink, Tulane University). Together with researchers and tools at Brookhaven National Laboratory, investigators in Louisiana are taking snapshots of catalysis processes to reveal new palladium species.

- An ever-increasing demand for portable electronic devices is driving technological improvements in rechargeable solid-state batteries. Lithium-ion batteries, with their high energy density and design flexibility, are the systems of choice. They are lightweight and have longer lifespans than other batteries. Current research in this area is aimed towards achieving higher capacity, better cycleability, and reduced "fading" by synthesizing new materials and improving existing ones. Researchers at the University of Puerto Rico are taking a new approach of replacing the liquid electrolyte with flexible polymer electrolytes in order to increase the energy density of the Li-ion batteries, looking for suitable conductivities (better than $10^{-3}$ S/cm) for practical energy applications. By synthesizing novel nanoparticles in polymer salt complexes, they are investigating fundamental crystalline dynamics that are leading to improved control of ion transport in these novel polymer electrolyte systems. Together with researchers from Argonne National Laboratory, their theoretical predictions of the structure and physical properties of the electrodes and electrolyte materials are being used to guide the development and synthesis of high performance materials for these applications (R. K. Katiyar, U. Puerto Rico).
- Photovoltaic devices are the most direct ways to convert solar energy to electricity. At present, photovoltaic devices based on inorganic semiconductors are efficient, but the high cost of manufacturing silicon-based devices makes the cost per watt too high to be competitive with fossil fuels. Novel photovoltaic devices based on organic, carbon-based nanostructures offer the possibility of developing low cost, easily processed thin films of polymeric materials which function as photovoltaic cells. Such devices could be competitive with other sources of energy if power efficiencies even as low as 10% can be attained. Investigators at Oklahoma State University are using first-principle, theoretical studies to investigate the electronic and structural properties of relevant conjugated polymers and carbon nanotubes. Such studies are facilitating the design and fabrication of new carbon-based materials for use in photovoltaic devices and improved renewable energy source devices (J. W. Mintmire, Oklahoma State University).
- Thermal energy exists in many forms ranging from solar energy to waste heat from existing power sources. For example, over 70% of the input power into an automobile engine is lost, a large majority of the loss in the form of waste heat. One way to harness thermal energy is through the use of thermoelectric materials and devices that enable us to transform this thermal energy into usable high quality electrical energy. Research in current thermoelectric materials is attempting to significantly increasing their efficiency. Over the past decade, significant advances have been achieved in low dimensional structures such as superlattices and quantum dots. New investigations by researchers in South Carolina using novel nanostructures and nanocomposites including exotic "cage structure" materials consist of matrices of bulk and nanomaterials are offering to nearly double the performance of low-dimensional materials. Such improved performance and continued development of high efficiency thermoelectric nanocomposites may provide environmentally safe and reliable power sources to sustain the nation's future (T. M. Tritt, Clemson University).

Biological and Environmental Research

Most doses of radiation exposures associated with human activity are predicted low dose in nature. These may arise from medical diagnostics, hazardous waste abatement, power systems operation, and even terrorist acts such as dirty bombs. While the precise risk of exposure continues to be debated, recent findings indicate that a measurable risk exists even at very low doses. By measuring gene activity before and after exposure, researchers in Tennessee are working to identify biological pathways that are activated or repressed in response to the radiation insult. Work at the University of Tennessee on in situ gene expression is enhancing our understanding of low dose radiation's effects at all levels of biological organization, from genes to cells to tissues and finally to complex organisms such as humans. Understanding the risks to human health associated with low dose radiation is critical if we are to protect the nation's workforce while making the most effective use of national resources (M. A. Langston, U. Tennessee).

Advanced Scientific Computing Research

High performance anisotropic diffusion equation solver: Members of this project have [who? at what institutions?] developed a unique algorithm that, when used in conjunction with advanced medical images, can predict communication pathways in the brain. In particular, the algorithm uses solutions of the anisotropic diffusion equation to help predict converging or branching fiber tracts. Prior methods for predicting pathways stall when they reach branch points (or at the very best do not proceed down all the branches). The new algorithm easily predicts and proceeds down all branches, and could prove crucial in helping to non-invasively diagnose the onset of various brain disorders. The anisotropic diffusion equation solver requires modules from a specialized toolkit, a set of high performance computational routines developed at various DOE national laboratories.

High Energy Physics

- Discovering the Higgs Bosons: The most important goal for the Fermilab Tevatron Run II and the CERN Large Hadron Collider (LHC) is the investigation of the mechanism by which elementary particles acquire mass—the discovery of the favored Higgs bosons or another mechanism. A research group at the University of Oklahoma has investigated the prospects for the discovery of a neutral Higgs boson ($\phi 0$) produced with one bottom quark bg $\rightarrow$ b$\phi$0 followed by Higgs decays into muon pairs within the framework of the minimal supersymmetric standard model. Promising results are found for the CP-odd (A0) and the heavier CP-even (H0) Higgs bosons. This discovery channel with one bottom quark greatly improves the LHC discovery potential beyond the inclusive channel pp $\rightarrow \phi 0 \rightarrow \mu+\mu- +X$. The muon discovery channel will provide a good opportunity for a precise reconstruction of the Higgs boson masses.
- Another group at the University of Oklahoma is in the race to measure the electric dipole moment of the electron. Approximately 20 groups world wide are seeking to measure this important fundamental property that will allow the world to assign a size to the electron. Current experimental limits already show that the ratio of size of an electron to the size of a proton is less than the ratio of the size of an ant to the distance between the Earth and Sun. Specifically, the size of the electron differentiates between many competing models of how particles interact. These models include the venerable Standard Model of Physics and the newer Super Symmetric Theories. Using a lead fluoride molecule researchers at the University of Oklahoma are helping to differentiate these models (N. Shafer-Ray, U. Oklahoma).

Nuclear Energy

Gas-cooled fast reactors have the potential to use a wide range of fuel including recycled, spent nuclear fuel. Because of their high temperature operation, gas-cooled fast reactors can be used for the future production of hydrogen to replace fossil fuels for transportation. Key to the realization of the gas-cooled fast reactor is the development of a robust fuel. This fuel form must accommodate a wide variety of elements including, those in recycled fuels, and must also perform safely at very high temperatures. Researchers at the University of South Carolina are developing a composite fuel system consisting of uranium carbide microspheres contained in a zirconium carbide matrix for potential use in these reactors. This work on these fuels contributes to the safety, sustainability, and security of our energy supply for both electricity and transportation. As an additional environmental plus, use of such fuels in nuclear reactors would provide safe energy without the production of greenhouse gases (T. W. Knight, U. South Carolina).

Nuclear Physics

Magneto-inertial fusion (MIF) is an advanced form of fusion which holds the promise for safe, clean, affordable energy for the 21$^{st}$ century. It combines the favorable attributes of other fusion concepts currently supported by the U.S. Department of Energy, and has recently been shown to be the most economically viable way of using fusion energy for production of electricity. The University of Alabama in Huntsville is collaborating with Los Alamos National Laboratory and other institutions around the country to model the physical processes involved in MIF so that we may understand how to build a working reactor. The Huntsville group has verified that a new, advanced modeling technique called smooth particle hydrodynamics can accurately capture the physics of converging and reflecting shock waves, which is necessary for reaching fusion ignition temperatures and densities. This modeling is an important step along the road to a sustainable energy source that has the potential to liberate the United States, and the world, from its dependence on fossil fuels. Further, fusion reactors are free from many of the objectionable aspects of current nuclear power reactors and offer a more environmentally friendly alternative (J. Cassibry, U. Alabama Huntsville).

Renewable Energy and Efficiency

Use of Biomass: Researchers at Jackson State University are improving the amount of ethanol that can be produced from Southern pines. Acid hydrolysis is being developed for conversion of biomass into a liquid process stream (hydrolyzate) that can be either directly fermented into ethanol or further processed by enzymatic conversion into a then more fermentable stream used to make ethanol. Southern pine acid hydrolyzate containing sugars and inhibitors, such as furans and phenolics, was treated with a weak anion resin and laccase immobilized on kaolinite. Fermentation of the sugars in the treated hydrolyzate resulted in significantly higher ethanol production levels than those achieved with the untreated hydrolyzate.

Defense Programs

Robust Radiography Devices: Development of robust x-ray radiographic devices is an important need for many DOE national security applications, which require an improved understanding of electrical breakdown in high voltage insulators. To address this challenge, the Nevada Shocker (a 540,000 V pulse power machine) has been developed, and is now in operation, at the Pulsed Power Laboratory at the University of Nevada, Las Vegas. Also developed were a number of sensors and a novel calibration technique to absolutely quantify the sensor data, which measures the strength and motion of the radially propagating electromagnetic pulse interrogating the insulator under test. This will lead to basic understanding of electrical properties of insulators that are used in nuclear weapons program.

Fossil Energy

- Fuel cells offer the promise of increasing the net efficiency of central electric coal generation plants from the present level of 30% to 35% (for conventional coal combustion systems) to levels approaching 60% to 70% (in advanced gasification systems using fuel cell, gas turbine, and steam turbine generation cycles). This increased efficiency and the attendant reduction in carbon emissions require the development of high temperature fuel cells which operate on “synthesis” gas generated from coal. However, one difficulty in using syngas in fuel cells is that it contains undesirable species such as arsenic, mercury, and nickel. A group of researchers at West Virginia University is focused on improving the reliability and life expectancy of solid oxide fuel cells in the presence of these trace contaminants. They are using atomic scale computational models to guide the development of new anode materials and macro scale modeling to predict the performance of integrated system designs for coal syngas. Industrial team members provide technical support and ensure that these results will actually be transferred to the electric power generation industry (R. Bajura, West Virginia University).
- Coal has a wide variety of trace elements such as arsenic, selenium and antimony that can have undesirable environmental consequences. In order to mitigate this potential hazard, it is important to develop a fundamental understanding of how these trace elements are partitioned in the combustion products between the gas phase and particulate matter. To correctly predict how this partitioning occurs, the generation of currently unavailable thermodynamic and kinetic data is required. Researchers in North Dakota are performing novel experiments to generate this data for these hazardous trace elements as well as for major elements, such as calcium, iron, and aluminum, over melts that replicate the solid surfaces of ash particles. Computational calculations have also been performed to compare the thermodynamic stabilities of compounds of these trace elements. Ab initio calculations suggest that oxygen-rich compounds of the trace elements are preferred to the simple oxide forms predicted by classical thermodynamic calculations. Such results are helping researchers envision the reduction of the environmental impact of burning coal (W. Seames, U. North Dakota).

## Mission Relevance:

The principal objective of the DOE EPSCoR program is to enhance the abilities of the designated states to conduct nationally competitive energy-related research and to develop science and engineering human resources to meet current and future needs in energy related areas. In addition, EPSCoR grants are supporting graduate students, undergraduates, and postdoctoral associates, and encouraging them to be trained in world-class research at DOE national laboratories.

## Scientific Challenges:

The DOE EPSCoR activity will continue to support basic research spanning the broad range of science and technology programs within DOE.

**Funding Summary: BY EPSCoR STATES**

(**Dollars in Thousands)**

| | FY 2007 | FY 2008 | FY 2009 |
|---|---|---|---|
| Alabama | 393 | 264 | 0 |
| Alaska | 0 | 0 | 0 |
| Arkansas | 139 | 0 | 0 |
| Delaware | 629 | 980 | 980 |
| Hawaii | 0 | 0 | 0 |
| Idaho | 400 | 400 | 400 |
| Kansas | 0 | 0 | 0 |
| Kentucky | 450 | 650 | 650 |
| Louisiana | 440 | 440 | 440 |
| Maine | 450 | 650 | 650 |
| Mississippi | 0 | 0 | 0 |
| Montana | 134 | 131 | 0 |
| Nebraska | 269 | 140 | 0 |
| Nevada | 455 | 468 | 0 |
| New Hampshire* | 498 | 545 | 569 |
| New Mexico | 0 | 0 | 0 |
| North Dakota | 350 | 350 | 0 |
| Oklahoma | 713 | 661 | 681 |
| Puerto Rico | 0 | 0 | 0 |
| Rhode Island | 0 | 0 | 0 |
| South Carolina | 939 | 910 | 785 |
| South Dakota | 0 | 0 | 0 |
| Tennessee** | 275 | 275 | 135 |
| Vermont | 0 | 0 | 0 |
| US Virgin Islands | - | - | 0 |
| West Virginia | 495 | 495 | 0 |
| Wyoming | 140 | 0 | 0 |
| Technical Support | 111 | 0 | 110 |
| Other*** | 0 | 7,321 | 2,840 |
| Total | 7,280 | 14,680 | 8,240 |

*Became eligible in FY2006.
**Became ineligible in April 2006. Amounts shown represent continuation funds.
***Uncommitted funds in FY 2008 and FY 2009 will be competed among all EPSCoR states.

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SBIR contribution is not included in the Funding Summary Total above.

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|---|---|---|---|
| SBIR | 321 | 222 | 222 |

## Projected Evolution:

A solicitation for Implementation awards was issued in FY 2007 with a due date for formal application in January 2008. A solicitation for Laboratory-State Partnership awards was issued in April 2007, and 197 pre-applications were received. Of these, 80 were invited for full proposal. Proposals were peer reviewed, and 12 University/ National Laboratory pairs selected in April 2008 for negotiation of final awards. The program continues to meet the challenge of providing a balance between the Implementation awards and the Laboratory-State Partnership awards.