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

Division:Materials Sciences and EngineeringPrimary Contact:Aravinda M. Kini (Aravinda.Kini@science.doe.gov; 301-903-3565) (Acting)Team Leader:Harriet Kung (Acting)Division Director:Harriet Kung

# **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 manpower 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 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 manpower 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.

## Basic Energy Sciences

• Neutron Scattering of Thin Films and Interfaces: Neutron scattering is undergoing a revolution due to vast improvements in sensitivity and resolution made possible with upgrades at the High Flux Isotope Reactor (HFIR) and the construction of the Spallation Neutron Source (SNS). Neutrons make it possible to make unique measurements of magnetic materials which are inaccessible with other techniques. Magnetic materials are currently used in the information storage industry for hard drives and in the near future for nonvolatile magnetic random access memories. Neutron scattering techniques are necessary for understanding the

fundamental properties of the materials. To improve these techniques a neutron analyzer with horizontal focusing was developed at the University of Alabama.

- This focusing analyzer is being implemented in a neutron spectrometer at HFIR. The spin structure of antiferromagnetic films and oxide materials was studied with neutron scattering techniques. Improvements in sample fabrication and characterization techniques are resulting in a more comprehensive understanding of the relationship between structure and magnetism in epitaxial antiferromagnetic films. This type of fundamental materials science research should aid in increasing the storage density, miniaturizing storage units, increasing data rates, and reducing the cost per bit in storage devices (Gary Mankey, University of Alabama).
- Enhanced Chemical Ordering in Ilmenite-Hematite Magnetic Semiconductors: This study demonstrated the enhancement of the magnetic moments of FeTiO3(1-x)/Fe2O3(x) semiconductor ceramic samples through irradiation with 40 MeV protons. The magnetic moment is directly related to the chemical order in the crystal structure. Thus, it is inferred that the proton irradiation reduces defects in these semiconductor ceramics. This effect allows for production of high-moment magnetic semiconductors for spin electronic applications. Moreover, this technique could lead to improved material properties in other systems, such as composite materials with thermally sensitive components like organic layers or metallic multilayers (R. K. Pandey, University of Alabama).
- Carbon nanotube-supported nanoparticle catalysts: Nanometer-sized metal particles are extremely active chemically because of their high surface-to-volume ratios. Scientists at the University of Idaho have developed methods of depositing and stabilizing nanometer-sized platinum group metals on surfaces of carbon nanotubes in supercritical fluid carbon dioxide. Uniformly distributed monometallic and bimetallic nanoparticles with narrow size distributions are formed on surfaces of carbon nanotubes using this method. The carbon nanotube-supported palladium (Pd) and rhodium (Rh) nanoparticles are far more effective than commercial carbon-based Pd and Rh catalysts for hydrogenation of olefins and aromatic compounds. These new nanoscale catalysts are currently being tested as electrocatalysts for low temperature polymer electrode fuel cells applications.

#### **Biological and Environmental Research**

Structural Biology and Computational Biology: The ability of an individual to form a clot primarily depends on the generation of a protein called thrombin. The process is aided by another protein called factor Va. Faculty and students at the University of Vermont have recently solved the 3-dimensional structure of bovine factor Va<sub>i</sub>, a fragment of factor Va, which provides an essential look at how this protein may function to regulate thrombin production. Due to its similarity to factor VIII, one of the proteins responsible for hemophilia, knowledge of this structure may lead to the development of new pharmaceuticals for the treatment of this devastating disease as well as other thrombotic disorders such as stroke.

#### Advanced Scientific Computing Research

High performance anisotropic diffusion equation solver: Members of this project have 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.

## Nuclear Physics

Designing and building a polarized frozen spin target at Thomas Jefferson National Laboratory (JLab): Ordinary matter is made of protons and neutrons called nucleons, and their exact structure is still unknown. Polarized beams and targets are essential tools in the study of the nucleon. Nucleons are like small magnets and can be collectively oriented by strong magnetic fields (~5T) at low temperatures (<1K). A state of the art polarized frozen spin target has been designed and being built at JLab. It will be used to look for so called "missing resonances" (nucleon states which are predicted but have not been seen so far). This target will assist in conducting cutting edge research in nuclear physics (C. Djalali, University of South Carolina).

## 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

Distributed Generators: Research by West Virginia University's Advanced Power and Electricity Research Center (APERC) shows that distributed generators (DGs) such as fuel cells and microturbines can be used to "balance" electricity supply and demand at the distribution network level, opening the possibility for distribution networks to operate autonomously from the transmission system, in effect becoming "microgrids." For such microgrids to work, the DG must be able to track electricity demand in real time, producing more or less electricity to exactly meet the current demand or risk losing the network causing a blackout. Today's DGs are not able to continuously vary the amount of electricity they produce. To address this issue, APERC researchers have developed control design algorithms that would allow DGs to adjust their output and provide energy balancing in a distribution system (Richard Bajura, West Virginia University).

### **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 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 2005 | FY 2006 Estimate | FY 2007 Estimate |
|---------------------|---------|------------------|------------------|
| Alabama             | 695     | 685              | 258              |
| Alaska              | 0       | 0                | 0                |
| Arkansas            | 145     | 135              | 139              |
| Delaware            | 0       | 0                | 0                |
| Hawaii              | 0       | 0                | 0                |
| Idaho               | 476     | 375              | 375              |
| Kansas              | 626     | 135              | 0                |
| Kentucky            | 224     | 0                | 0                |
| Louisiana           | 660     | 462              | 375              |
| Maine               | 0       | 0                | 0                |
| Mississippi         | 667     | 132              | 0                |
| Montana             | 375     | 455              | 133              |
| Nebraska            | 120     | 265              | 269              |
| Nevada              | 0       | 90               | 105              |
| New Hampshire*      | -       | 0                | 0                |
| New Mexico          | 135     | 135              | 0                |
| North Dakota        | 406     | 273              | 0                |
| Oklahoma            | 485     | 350              | 350              |
| Puerto Rico         | 375     | 375              | 0                |
| Rhode Island*       | -       | 0                | 0                |
| South Carolina      | 716     | 660              | 525              |
| South Dakota        | 125     | 125              | 0                |
| Tennessee           | 0       | 140              | 140              |
| Vermont             | 705     | 0                | 0                |
| U.S. Virgin Islands | 0       | 0                | 0                |
| West Virginia       | 315     | 225              | 135              |
| Wyoming             | 270     | 140              | 140              |
| Technical Support   | 123     | 60               | 110              |
| Other**             | 0       | 2,063            | 4,946            |
| Total               | 7,643   | 7,280            | 8,000            |

\*New Hampshire and Rhode Island became eligible for funding in FY 2006. \*\*Uncommitted funds in FY 2006 and FY 2007 will be competed among all EPSCoR states.

# **Projected Evolution:**

A solicitation for Implementation awards was issued in FY 2005, and 13 formal proposals were submitted and are under review. The program continues to meet the challenge of providing a balance between the Implementation awards and the Laboratory-State Partnership awards.