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U. S. Department of Energy
Office of Science • Office of Basic Energy Sciences • Division of Materials Sciences

EPSCoR
Experimental Program to Stimulate Competitive Research

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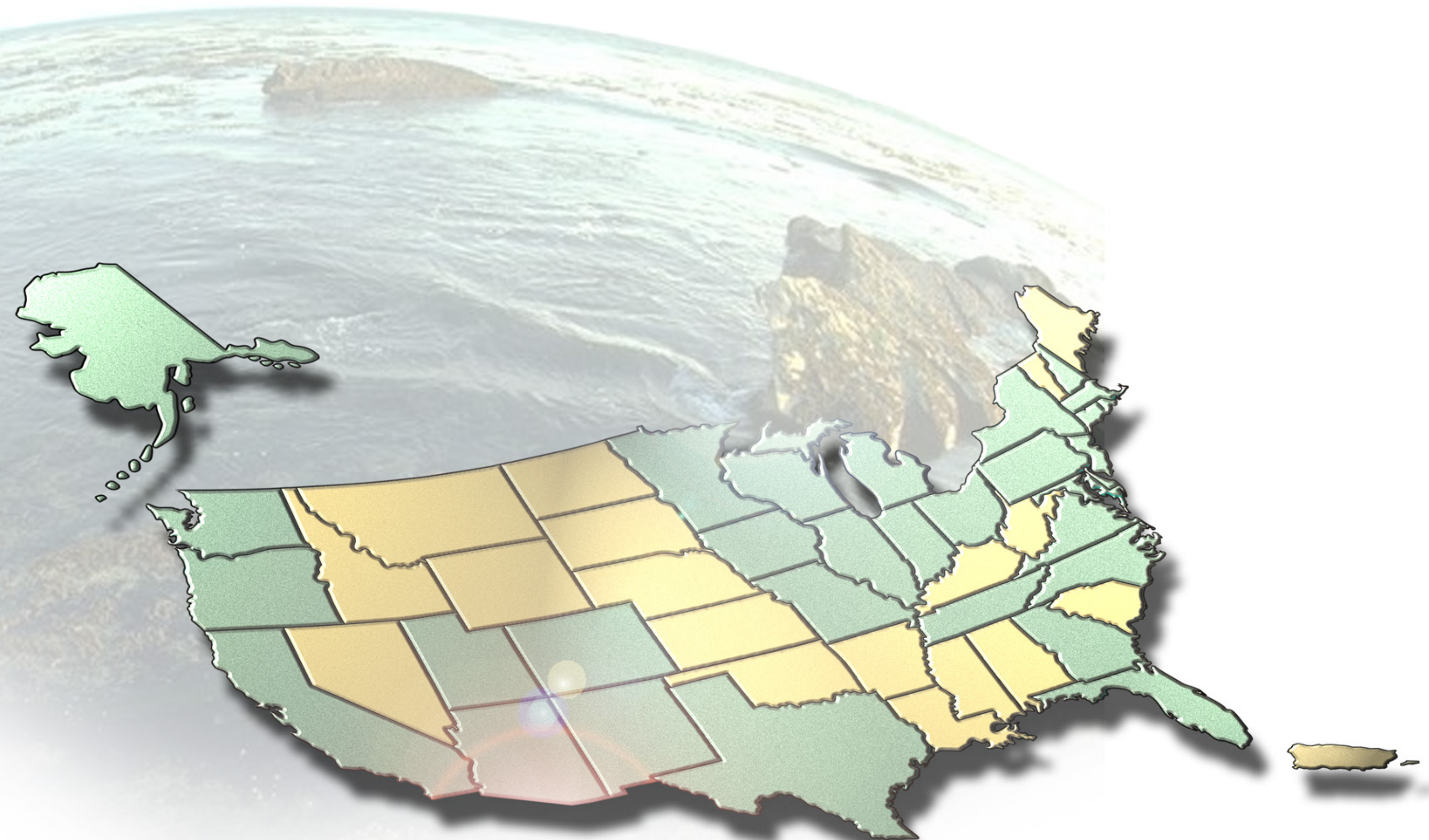

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Experimental Program to Stimulate Competitive Research

Summaries of Research Projects

Fiscal Year 1999

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Compiler and Editor

Prepared for the U.S. Department of Energy
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PREFACE

The Department of Energy's Experimental Program to Stimulate Competitive Research (EPSCoR) is managed by the Division of Materials Sciences within the Office of Basic Energy Sciences. The principal objective of the DOE/EPSCoR program is to enhance the capabilities 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. The DOE program is limited to the states of Alabama, Arkansas, Idaho, Kansas, Kentucky, Louisiana, Maine, Mississippi, Montana, Nebraska, Nevada, North Dakota, Oklahoma, South Carolina, South Dakota, Vermont, West Virginia, Wyoming and the Commonwealth of Puerto Rico. Particular emphasis is placed on exploiting the unique scientific and technical capabilities present at the DOE national laboratories to accomplish the objectives of this program. This program addresses research needs across all of the Department of Energy research interests. The aim of the program is facilitated by organizing workshops and meetings on targeted scientific areas, such as materials science, neutron science, environmental science, etc. These workshops provide a venue for indepth and effective interaction among the scientists at the national laboratories and the faculty and students from the EPSCoR states. These interactions should result in joint collaborative research projects between the laboratory scientists and the EPSCoR state personnel that in turn will lead to establishing nationally competitive scientific expertise at the home institutions of the EPSCoR states.

This summary book provides information on research supported in the designated EPSCoR states by the Office of Science during Fiscal Year 1999, including projects funded by EPSCoR and the regular grant program. The research summaries and other information in the main section of this publication are the most current ones available to the division, as provided by the principal investigators.

This publication also provides information on the wide range of research programs supported by the Department. In addition, information on the contact person for individual programs is listed. We hope that this publication will provide guidance to scientists both from the national laboratories and from EPSCoR states who may be considering submitting research proposals for financial support from the DOE EPSCoR program. The program is continually evaluated and adjusted, taking into account the advances in new technology, basic research needs and priorities of the Department. Thus, scientists are encouraged to contact the appropriate staff to determine the most current program priority and scope before submitting a proposal. New initiatives are generally announced in the *Federal Register*. These notices and other useful information are available on the World Wide Web at: http:/www.er.doe.gov.

Comments on this publication and suggestions to make it more effective and useful are welcome.

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PROGRAM SCOPE

The research within the Department of Energy is sponsored by a number of offices that are responsible for a specific mission of the Department. The Office of Science supports most of the basic research in the energy sciences, biological and environmental science, advanced computing, fusion energy, and high-energy and nuclear physics. The Defense Program funds research relevant to defense needs and nonproliferation and safety. The Environmental Management Program supports specific research needed for environmental remediation and improvement. The Fossil Energy Program funds research on coal and other fossil-related energy sources. The Nuclear Energy, Science and Technology Program supports basic research in nuclear energy. The Office of Civilian Radioactive Waste Management oversees the disposal of all spent nuclear fuel from commercial nuclear reactors and high-level radioactive waste resulting from atomic energy defense activities. The Office of Energy Efficiency and Renewable Energy develops and deploys efficient and clean energy technologies that meet our Nation's energy needs, enhance our environment and strengthen our national competitiveness. The Office of Fissile Materials Disposition strives to reduce the global nuclear danger associated with inventories of surplus weapons-usable fissile materials.

All programs strive to bring science, security, and energy to our Nation.

Additional descriptions of each of these research programs sponsored by the Department of Energy are provided in Appendix B.

ACKNOWLEDGMENTS

Suggestions and assistance from program managers in the Office of Science in the preparation of this manuscript are deeply appreciated. Substantial efforts by Melanie Becker and Christie Ashton, Division of Materials Science, in preparing the draft manuscript, are gratefully acknowledged. We appreciate the valuable contributions of Catherine H. Shappert, editor, Oak Ridge National Laboratory, to ensure the quality of this document.

LIST OF ACRONYMS

DOE	Department of Energy
DP	Office of Defense Programs
EERE	Office of Energy Efficiency and Renewable Energy
EM	Office of Environmental Management
EPSCOR	Experimental Program to Stimulate Competitive Research
FE	Office of Fossil Energy
HRD	Human Resources Development
MC	Office of Management and Coordination
MD	Office of Fissile Materials Disposition
NE	Office of Nuclear Energy, Science and Technology
NN	Office of Nonproliferation and National Security
NSF	National Science Foundation
OASCR	Office of Advanced Scientific Computing Research
OBER	Office of Biological and Environmental Research
OBES	Office of Basic Energy Sciences
OCRWM	Office of Civilian Radioactive Waste Management
OFES	Office of Fusion Energy Sciences
OHENP	Office of High-Energy and Nuclear Physics
PI	Principal Investigator
RC	Energy Research Cluster
SC	Office of Science

EPSCoR STATE PROGRAMS

STATE OF ALABAMA

A. Projects Supported by EPSCoR

1. Alabama DOE/EPSCoR Management and Coordination

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The Alabama DOE/EPSCoR Program is made up of three integrated components including Management and Coordination (MC), Human Resources Development (HRD) and Energy Research Clusters (RC). All programmatic elements are coordinated through a state-wide steering committee. Day-to-day management is provided by an Associate Director who has financial and operational authority for all elements of the program. Three Research Clusters involve highly interdisciplinary research in Petroleum Reservoir Characterization studies, highly focused research in Fusion Energy, and interdisciplinary/ intercampus research in Novel Organic Semiconducting Materials. Collectively, these programs include 21 PIs, 16 Postdoctoral Research Associates, 17 Graduate Students, and 17 Undergraduate Students, and are located at Auburn University (FE and NOSM) and The University of Alabama (PRC and NOSM). The HRD element is comprised of two DOE/ EPSCoR Partnerships: programs which have established track records for educational innovation and effectiveness. The Project Energy partnership brings energy education programs to primary- and secondary-education students and teachers through their own unique and highly successful programs. Project Energy develops lesson plans and projects related to energy-based subject matter for primary and secondary educators. The Young Investigator Enhancement (YIE) Partnership uses the past cooperative program with the Alabama Alliance for Minority Participation (AAMP), as well as other institutions to deliver research and education information to participating HBCU institutions. In addition, a general call for energy-related research, that supports the Research Clusters (RC) and that supports emerging energy areas important to Alabama, supplements these contacts. In its 4-year history, the Alabama DOE/EPSCoR program has generated: 368 publications, 230 presentations, 73 funded proposals, 6 patents, and 3 books published. These success stories are the type needed to self-sustain the research of these and other energy-related programs by selectively capturing the necessary financial assets from federal, state/institutional and industrial sponsors.

2. Fusion Energy

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As a part of the long-term effort to contribute to the National Stellarator Proof-of-Principle Program, the experimental torsatron group has started the upgrade to the Compact Auburn Torsatron (CAT), increasing the magnetic field strength by a factor of 5 to 0.5 T. This has involved an analysis of the increased stresses and the acquisition of a motor-generator set to provide the necessary DC power to the magnets. A new experimental wave study in cooperation with the RF theory group has given strong support for the description of the new stellarator wave that has the potential to impact the international stellarator effort. In addition to the discovery of an adequate theory for the stellarator wave, the RF group has also discovered a new and more general theory of linear wave coupling due to plasma inhomogeneities. The initial electron cyclotron emission (ECE) diagnostics have been installed on the Alcator C-Mod tokamak at MIT and recently tested. The complete diagnostic system is to be installed imminently and is expected to soon provide the principal source of information on the observed micro instabilities. The Atomic Physics group has completed the analysis of numerous special cases of electron-ion ionization, excitation, and recombination interactions, adding to the database for modeling and diagnosing high-temperature plasmas.

3. Novel Organic Semiconducting Materials

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The overall objectives of this program are: (1) design and syntheses of novel organic semiconducting materials, (2) preparation of single crystals, thin films, composite structures and various junction devices using the materials, (3) detailed investigation of the electronic and optical characteristics of the materials and devices, and (4) fundamental understanding of the correlations between the structures and electronic and optical properties. Our major objective is to select specific novel molecular and polymeric semiconductors that are most attractive from fundamental scientific and/or technological standpoints. The three areas that we will focus on include: (1) nonlinear optical and light emission measurements, (2) thin-film transistors, and (3) stress and strain sensors. We have reported large electro-optic modulation, picosecond all-optical switching and efficient photoluminescence characteristics in specific materials. Several of the new materials have shown excellent thin-film transistor characteristics or unimolecular rectification. Also, very recently we have demonstrated highly sensitive mechanical sensors based on polymer semiconductors. These results will guide us in the synthesis of materials with optimized structure and properties to impact the above three areas. Thus, the proposed research program will include efforts in materials synthesis, detailed time-resolved measurements of nonlinearities and photoluminescence using pico- and femtosecond pulses, electro-optic studies at higher frequencies (several GHz), studies of thin-film transistors, nanotransistors based on Langmuir-Blodgett multilayer films, more detailed studies of highly sensitive sensors of stress and strain and theoretical modeling to understand the materials, devices and processes.

4. Petroleum Reservoir Characterization

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Petroleum reservoir characterization is the process of identifying and quantifying those properties of a given petroleum reservoir which affect the distribution and migration of fluids within that reservoir. These aspects are controlled by the geological history of the reservoir. The ultimate goal of a hydrocarbon reservoir characterization study is the development of a reasonable physical description of a given reservoir. This physical description can then be used as a basis for simulation studies, which, in turn, are used to assess the effectiveness of various recovery strategies. An accurate physical description of the reservoir often will lead to the maximum production of hydrocarbons from the reservoir. A primary objective of this research is to develop an internationally recognized reservoir characterization research cluster, particularly for the analysis of carbonate reservoirs and for reservoir simulation. The achievement of this goal will require a comprehensive, multidisciplinary effort involving geologists, engineers, physicists, statisticians, and computer scientists. Reservoir characterization is a specialized application which acts as a focal point for involving fundamental research from all disciplines. The strong interaction that is promoted through this application enhances the ability to make advances in the fundamental research areas of science and engineering. These advances can then be applied to other research-related areas.

5. Alabama-ORNL Collaboration: Adaptation of Fast Multipole Code for Atomic-Scale Micromagnetics

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Understanding the molecular-scale dynamics of magnetic materials is a long-standing problem of fundamental physics, as well as being of great importance in the technology of information storage (tapes and disks). Disk capacity has increased rapidly in recent years, the most recent example being IBM's new 16-GB 3.5-in. disk drive for the PC. The new "GMR" read heads in these drives work because of the phenomenon of "exchange bias" at the interface between a ferromagnetic and antiferromagnetic material. The theory group headed by Dr. W. H. Butler at Oak Ridge National Laboratory has made recent progress in understanding the structures of these interfaces, but is limited by the fact that the computation of long-ranged magnetostatic interactions is extremely time-consuming, even on modern parallel computers, because the time required is proportional to the square of the number of particles. Professor Visscher's group at Alabama has developed improved hierarchical "fast-multipole" methods for dealing with this problem, in computation time that rises only linearly with the number of particles. Conventional methods are roughly analogous to delivering 100 million tax returns from the IRS to taxpayers by sending 100 million individual couriers from Washington, whereas the hierarchical method corresponds to sending 1 million to each of 100 distribution centers, which each send 10,000 to 100 sub-distribution centers, etc.

6. Advanced Design of a Novel Stellarator Using the Free-Boundary VMEC Code

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The Variational Moments Equilibrium Code (VMEC) is a complex computer program used to model the magnetic equilibrium of fully three-dimensional toroidal fusion research devices called stellarators. Developed by Dr. S. Hirshman of Oak Ridge National Laboratory and his co-workers, the VMEC code is an essential tool for the design of modern stellarators. Moreover, it has great potential as an interpretive tool that can be used to measure the experimental magnetic equilibrium parameters of a real stellarator plasma based on a finite number of measurements of the internal magnetic field in the stellarator plasma. This technique has been employed to model the plasma current profile in axisymmetric tokamak plasmas, but its application to stellarator configurations, which generally lack symmetry in the magnetic field strength along any axis, is novel. In collaboration with Dr. Hirshman, this capability of the VMEC code to reconstruct 3-D magnetic equilibria will be developed in this project to measure the magnetic equilibrium properties of the Compact Auburn Torsatron (CAT) plasma. The CAT device is the only operating stellarator in the U.S. at this time. It is being upgraded to be a lead element of the National Stellarator Proof-of Principle (PoP) Program, which also includes a new stellarator nearing completion at the University of Wisconsin, and two advanced stellarators being designed at Princeton Plasma Physics Laboratory and Oak Ridge National Laboratory. The major contribution of the CAT experiments will be a quantitative study of current-driven instabilities and disruptions in stellarator plasmas, which is a critical topic for the larger stellarators of the PoP program. The measurement and interpretation of the magnetic equilibrium through the use of the VMEC code will be key to understanding the results of this experiment. Moreover, the technique of 3-D magnetic equilibrium reconstruction developed in this project will in itself be a highly useful deliverable contribution to the PoP program.

B. Projects Supported by Office of Science

7. Carbon Storage and Cycling, Soil Microbiology, and Water Quality in CO_2-Enriched Agroecosystems

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A five-year study of belowground responses of the two-crop species is under way. An open-top chamber system was installed on an outdoor soil bin (7 m by 76 m by 2 m deep) filled, in 1966, with Blanton loamy sand (loamy, silicious, thermic Grossarenic Paleudults) supported on a tile-and-gravel drainage basin. Sorghum bicolor (L.) Moench and Glycine max (L.) Merr. are being grown. These species offer contrasting characteristics with respect to photosynthetic pathways, responses to CO_2, rooting patterns, nitrogen fixation, decomposition rates, and impact on soil carbon and nitrogen cycling; both are prominent the world over, including the Third World.

8. Radiopharmaceutical and Gene Therapy Program

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The objective of the project is to develop a new therapeutic strategy that combines the complimentary strengths of gene therapy and targeted radiotherapy into one unique methodology for treatment of human cancer.

9. Theoretical Atomic Collision Physics for Controlled Fusion

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Summary not available.

10. RF Heating and Diagnostics

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This project, part of the Fusion Energy Cluster of the Alabama DOE EPSCoR, has both an experimental part and a theoretical part, both involving waves in inhomogeneous plasmas. The experimental portion is under the direction of Christopher Watts and uses Electron Cyclotron Emission (ECE) to measure electron temperature and fluctuations. The system was developed on TEXT at the University of Texas and has been adapted and installed on CMOD at MIT. The theory portion of the project deals primarily with Mode Conversion theory, which describes resonance absorption, emission and conversion of waves in plasmas. Part of the effort is to design better numerical procedures for modeling purposes, and part of the effort is to refine the theory. The theory of another type of absorption, which is unique to stellarator devices, was discovered under this program and is being developed with improved numerical techniques for modeling realistic stellarator-like devices. This method heats stellarators at the fundamental ion cyclotron frequency, a phenomenon not observed on tokamaks, but which was observed on the L-2 stellarator.

11. Experimental Studies of Plasma Fluctuations Using Electron Cyclotron Emission on Alcator C-Mod

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Summary not available.

12. The Quasi-Toroidal Stellarator: An Innovative Confinement Experiment

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The goal of this experimental project is to complete a major upgrade to the existing Compact Auburn Torsatron (CAT) so that it will fulfill its role in the National Stellarator Proof-of-Principle Program Plan. This plan has been developed over the last year by a consortium of researchers from national labs and universities, including one of the PIs of this project's team. The upgraded CAT device will be used to investigate the magnetohydrodynamic stability of current-carrying stellarator plasmas. The results will contribute to the design of the National Compact Stellarator Experiment, the major element of the Proof-of-Principle program to be located at the Princeton Plasma Physics Laboratory. Furthermore, the project will continue fundamental studies of ICRF mode transformation motivated by theoretical investigations pioneered by the RF Theory project of this cluster. These wave studies are directly relevant to improved radio-frequency heating of stellarator plasmas. Encouraging preliminary results of mode transformation have recently been obtained in low-density, low-magnetic-field CAT plasmas; more definitive work will continue during the present and upcoming project periods. Quantitative measurements of direct-ion heating resulting from the mode transformation will be made in plasmas in the upgraded CAT device, which will be less dominated by ion-neutral collisions than present CAT plasmas. The project will use the

EPSCoR renewal grant mainly to educate and support personnel for this research, and to sustain the outside laboratory linkages key to the success of these efforts. The improvement of the infrastructure of the laboratory and the direct participation of the project in the National Stellarator Program Plan significantly improve the ability to develop new investigations of innovative magnetic confinement concepts, leading to long-term, self-sustained research activities at Auburn University, strengthened by linkages with other laboratories.

13. Joining of Dissimilar Materials for Fusion Reactor Applications

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The ability to join components of different materials is critical to the successful implementation of fusion systems. It is necessary to make transition joints from low-activation ferritic and vanadium alloys to stainless steel as well as to ceramic-based materials. Tuskegee University, in cooperation with Auburn University, is investigating issues related to the joining of dissimilar materials (metal-to-metal and metal-to-ceramic) in high-temperature fusion systems. The research program addresses both the scientific and the engineering aspects in the joining of dissimilar materials for fusion structures through three technical objectives: (1) predict, using finite-element methods, anticipated temperature and resulting stress distributions to be encountered during the joining of vanadium and low-activation ferritic steels to dissimilar metal and ceramic materials (2) experimentally investigate the feasibility of joining dissimilar metals and metal to ceramics for fusion device components, vanadium and low-activation ferritics being the base materials with the weld and/or braze material composed of low-activation constituents (3) experimentally investigate the thermal stability, microstructure evolution and failure mechanisms of these low-activation joints. Metal-to-metal joining techniques based on welding and brazing are being investigated to produce the desired interfacial structures and properties, which are crucial to the high-temperature performance and radiation resistance. Efforts are concentrated on low-activation ferritic steels and vanadium alloys. Both direct welding and the use of transition layers are being examined. Braze materials, based on thermodynamic compatibility with the metals and ceramics of interest, are being developed. Since cracks along dissimilar material joints intrinsically undergo mixed-mode deformation, interfacial-fracture-mechanics-based analysis is used for gaining insight into the failure process. The influence of thermal property mismatch on the fracture toughness characteristics of the bonds is also being investigated.

14. Alliance for Computational Science Collaboration HBCU Partnership at Alabama A&M University

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In October 1997, the Joint Institute for Computational Science (JICS) of Oak Ridge National Laboratory (ORNL) and the University of Tennessee, Knoxville (UTK), together with the Krell Institute, agreed to establish an alliance to support a comprehensive computational science program in collaboration with Historically Black Colleges and Universities (HBCUs). Initial HBCU partners were Tennessee State University (TSU) and Fisk University (Fisk), Both in Nashville, Tennessee. In early 1998, the program expanded to include Alabama A&M University (AAMU) in Huntsville, Alabama. The mission of the Alliance is to promote, encourage, and facilitate computational science activities and to use collaborative technologies to create an environment in which students and researchers from a wide variety of application areas can exchange ideas and share resources. The goals of this project are to involve HBCU students and faculty members in computational science projects at national laboratories and research institutions; to assist HBCU faculty members in integrating interdisciplinary computational science courses into their undergraduate curricula, involving freshmen to senior students; and to provide support and expertise to HBCU researchers using state-of-the-art computational science technologies and methodologies.

15. Experimental High-Energy-Physics Group

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The experimental high-energy-physics group at the University of South Alabama (USAHEP) is currently working on the HyperCP experiment (E-871) at Fermilab. This experiment has taken approximately 75 billion triggers in the last Fermilab fixed-target run. The HyperCP experiment has been approved to take more data in the upcoming fixed-target run scheduled for March through November 1999. The HyperCP experiment is searching for evidence of charge conjugation and parity (CP) violation in the decays of \XI and \LAM baryons and rare hyperon decays. The USAHEP group is responsible for the two trigger hodoscopes, the high-voltage power supplies, the event display program for this experiment and has contributed to the off-line analysis. Our group has also taken its fair share of shifts to collect data. Over the last summer the USAHEP group worked on the data analysis of the HyperCP experiment. The members of the USAHEP group are also part of Fermilab experiments E-705 and E-771. E-705 has completed publication of its results, and E-771 is in the publication process. In the next year, the USAHEP group will continue to work on the analysis of data collected in the last fix target run, build a new minimum bias trigger telescope for the HyperCP experiment, and help in the data collection in the second run of the HyperCP experiment.

16. Research in Elementary Particle Physics Theory (Task A) Research in Neutrino Physics (Task B)

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Theoretical high-energy physics areas include programs in quantum groups, quantum black holes, and the phenomenology of supersymmetry. Recent investigations include a hidden quantum group structure in general relativity, the effect of a light gluino on hadronic and leptonic processes, and the effect of a scalar (dilatonic) component of gravity on the propagation of electromagnetic waves near a Kerr-Newman dilaton black hole. Experimental high-energy-physics activities center on the L3 experiment at LEP (CERN), performing precision tests of the standard model and searching for new particles in e+ e- collisions at the highest available accelerator energies. In collaboration with Cal Tech, Stanford and Arizona State, the UA high-energy group has recently undertaken a new experiment to search for neutrino oscillations at the Palo Verde nuclear reactor in Arizona.

17. Study of Isospin Correlation in High-Energy Heavy-Ion Interactions with the RHIC PHENIX

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The University of Alabama, Huntsville, program studies the isospin correlation of mesons in ultra-relativistic heavy-ion collider experiments. The quest for high-density state of nuclear matter has a new era when the first operation of the Relativistic Heavy-Ion Collider (RHIC) will begin operation in 1999 at the Brookhaven National Laboratory. Among four prepared experiments, the PHENIX is expected to provide the most comprehensive set of the observable data that could characterize the possible phase of Quark-Gluon Plasma (QGP). PHENIX tries to incorporate measurements on electrons, photons and muons, as well as hadrons at the same time. The notable forte of the PHENIX, among others, is its versatile capability of cross-examination and correlated observation of various quanta. The UAH research program is to take a responsible part of the role to study the fluctuation of particle density and advance the study of the isospin correlation for observing the Disoriented Chiral Condensate (DCC). The MVD detector has specific roles in the PHENIX. It provides the event characterization, a centrality trigger, measures fluctuations of the charged particle density, and provides a collision vertex position. The charged particle density fluctuations will be obtained by the MVD itself, while the isospin fluctuations will be analyzed by correlating the MVD data (charged particles) with the EMCAL data (photons. Monte Carlo studies are required to characterize how high the detection efficiencies and particle composition are for the charged pions (in the MVD data) and neutral pions (in the EMCAL data). Isospin clustering might appear with significant anomalies in the heavy-ion collisions at RHIC, if several theoretical predictions being made are valid: (1) multiple Bose-Einstein interference (Zajc), (2) possible “Correlated Classical Pion Fields (Blaizot et al.),”Impulsive Twist of the Chiral Axis” (Bjorken) or “Disordered Chiral Condensate” (Taylor), and (3) “Coherent Long Wavelength Isospin Oscillations after a Chiral Quench” (Rajagapol and Wilczek) or in “Annealing During Expansion” (Asakawa et al.). The event-by-event measurement of gamma/charged ratio with high statistics allows an examination of the distribution of the isospins, albeit being much limited to the part of the segmented track densities. Some of the algorithms of finding DCC (isospin clusters) have been developed for use in the RHIC data analysis, and could also be applied to the pi-+ and pi-– multiparticle data expected from the STAR experiment.

18. Magnetic Resonance and Optical Spectroscopic Studies of Carotenoids

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The goal of this research is to evaluate the role of polar media in the mechanism of carotenoid radical cation and dication formation and decay and to determine the special properties of carotenoids bound to pigment-protein complexes in photosynthetic membranes that enable them to serve both as antennae and as photoprotective agents and as a possible component of electron transfer processes. Simultaneous electrochemical and electron spin resonance measurements, simultaneous electrochemical and optical measurements, and simultaneous electrochemical and resonant Raman measurements have been carried out. From these studies, the reason has been deduced for the observation of carotenoid radicals in some photosystems and not others. In the solid state, the energy of the cis isomers falls close enough to that of the all trans isomers that the solid host can stabilize higher-energy cis isomers. All trans or cisoidal carotenoid radical cations can exist on solid supports and in solution. Semiempirical molecular orbital (RHF-INDO/SP) calculations of the canthaxanthin cation radical in solution are in excellent agreement with the electron nuclear double resonance measurements. The host matrix is being manipulated in such a manner as to understand the carotenoid.

STATE OF ARKANSAS

A. Projects Supported by EPSCoR

19. Monitoring and Tracking in STAR's Main Time Projection Chamber

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STAR refers to the Solenoidal Tracking instrument At RHIC (the Relativistic Heavy Ion Collider). For momenta above 500 MeV/c, charged kaons are not separated from pions within STAR's Main TPC (Time Projection Chamber) by track density alone and they are poorly separated below 500 MeV/c, even when using information from other sources like the vertex tracker. Within the TPC, large numbers of kaons and pions decay into muons (and undetected neutrinos). Earlier work has shown parent pions and kaons whose decays are detected within a TPC may be distinguished uniquely from each other in a two-dimensional plot of muon-emission angle versus momentum difference (between each parent meson and its decay muon). Since pions and kaons have zero spin, each muon decay-product emerges isotropically in its parent meson's rest frame. Identification of particle type provides the parent meson's rest mass and, thus, its total energy. This means the measurement of each decay event is kinematically complete. Thus, Lorentz Transformations may be used to transform each component of the decaying muon's laboratory four-momentum into the "rest frame" of its parent meson, where the muon decay is isotropic. An aggregated plot of muon directions from many "parent rest frames" will be isotropic in each (selected) sub-volume of the TPC unless there is a problem within the TPC, in its tracking algorithms, etc. Thus, a continuous monitoring of the performance of STAR's Main TPC is possible using this subset of charged particles, as detected within the TPC.

20. Coal Surface Charging Property Characterization by Petrographic Analysis, UV Photoelectron Spectroscopy, Fluorescent Microsphere Imaging Technique, and Electrostatic Force Microscopy

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Cleaning coal is probably one of the most significant steps in environmentally safe conversion of coal to energy; it is especially important in the reduction of acid rain. In about 50% of plants in the United States, physical cleaning of coal prior to burning is more cost effective than flue-gas desulfurization for removing inorganic sulfur. Therefore, in 1989 the Department of Energy specified the following primary goals of physical benefication: 80% energy recovery, 70% pyritic sulfur rejection, and ash content of less than 3%. Our three-year EPSCoR program goal is to perform microstructural surface characterization of the charging process, thus enabling us to optimize dry-coal cleaning by electrostatic separation. Our specific research objectives are to: (1) correlate electrostatic charging characteristics of coal particles with such surface properties as mineral inclusions in the different classes of mackerel matrix, the effective work function distribution, and the physisorption and chemisorption of gases; (2) perform qualitative measurement of charge transfer, charge distribution, and charge decay on a microscopic scale to understand charging processes of different classes of mackerels and inorganic substances; (3) map the electrostatic charge distribution on the surface of individual coal particles and polished coal surfaces to correlate charging and separation; and (4) improve charging and separation processes in the electrostatic beneficiation of coal. The surface charge characterization methods to be developed in the EPSCoR program can be applied to: (1) other mineral cleaning processes applicable to many materials, from diamonds to zirconia, (2) electrophotographic development with toner, and (3) electrostatic spray painting with polymer powders.

STATE OF IDAHO

A. Projects Supported by EPSCoR

21. Laboratory and In Situ Evaluation of Enzyme Activity-Dependent Fluorescent Probes Specific for Chlorinated Solvent Degrading Bacteria

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This project represents a scientific collaboration between Idaho State University and the Idaho National Engineering and Environmental Laboratory (INEEL). We will investigate the efficacy of joining two new technologies, enzyme activity-dependent fluorescent probes and nutrient diffusing substrate devices, in order to assess the capacity of microorganisms to degrade trichloroethylene (TCE) in laboratory experiments and within a chlorinated solvent plume at the INEEL. The probes to be addressed in this work are chemical substrates, which are transformed by bacterial enzymes directly involved in TCE degradation. Researchers at the INEEL have received a patent describing nutrient-diffusing substrate (NDS) devices that can be lowered into monitoring wells and are readily colonized by subsurface bacteria. We will modify these devices to deliver enzyme activity-specific probes. Initial experiments will be conducted in the laboratory with groundwater and microbial isolates from the INEEL Test Area North (TAN) site. After sufficient laboratory assessment of the combined probe-NDS approach, we will conduct field experiments at the TAN site. We will use NDS devices to deliver specific probe compounds into the contaminated aquifer via monitoring wells at various locations within the TCE contaminant plume. After appropriate in situ incubation periods, the NDS devices will be collected, and probe response will be assessed via fluorometric and epifluorescent microscopic techniques. Conditions within the monitoring wells, such as nutrient and oxygen levels, will be manipulated experimentally in conjunction with probe assessment to generate information regarding the metabolic status of TCE degrading bacteria and the efficacy of biostimulation as a bioremediation strategy.

22. Exploring the Chemistry of ans-Chromocene Complexes, Their Fundamental Reactivity and Potential Application as Homogeneous Catalysts

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A reliable, high-yielding synthetic route to ansa-metallocene complexes of chromium(II) and chromium(III) has been developed which will allow the reaction chemistry of bent-sandwich chromocene to finally be explored. A variety of ansa-chromocene derivatives have been targeted in order to investigate the reactivity and possible catalytic applications of these complexes. The electrochemistry of various ansa-chromocene species will also be examined in order to determine the accessibility of the uncommon Cr(IV) oxidation state. Modifications to the basic ansa-metallocene ligand framework are also proposed, including permethylation of the cyclopentadienyl rings and replacement of the cyclopentadienyl rings with indenyl ligands. High-pressure NMR, IR, and ESR technology developed by scientists at Pacific Northwest National Laboratories (PNNL) will be used to examine the behavior of the ansa-chromocene complexes, as well as the unbridged species, in situ, under high pressures (hundreds of bars) of gaseous reagents such as H_2, ethylene, CO, N_2, CO_2, and CH_4. The detection of novel Lewis base adducts and oxidative addition products of bridged and unbridged chromocenes is expected, along with unprecedented reactivity resulting from h5–h3 ring slippage promoted by high pressures of substrate.

B. Projects Supported by Office of Science

23. Science Team Leader: Biotransformation and Biodegradation

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Summary not available.

24. Biodegradation and Biotransformation of Mixed Wastes Containing Metals and Chlorinated Xenobiotic Compounds by Microbial Consortia Enriched Under Different Conditions

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The overall objective of this application is to determine whether anaerobic consortia enriched under various conditions can be used to remediate trichloroethylene (TCE)-containing wastes which are also contaminated with a heavy metal (this will be expanded to include other chlorinated compounds and other metals according to the wishes of DOE). The more interesting aspect is the planned work with cores from DOE sites; these efforts will examine community development when these cores are exposed to water containing defined mixtures of chlorinated compounds and metals. Enrichments, the source of the consortia, will be developed under aerobic, fermentative, methanogenic, syntrophic, and sulfate reducing conditions in the presence of TCE and cadmium (Cd). The bacterial make-up of effective consortia will be determined. Consortia will be tested for their ability to degrade TCE and at least two other xenobiotics and to simultaneously immobilize Cd under conditions similar to those used in generating them. Successful treatments will be optimized. The studies will be done successively in batch systems, simulated flowing aquifers, and in situ in a polluted aquifer. The application stresses biodegradation of xenobiotics in the presence of toxic metals more than it does simultaneous biotransformation of the toxic metals.

25. Microbially Induced Reduction of Toxic Metals and Radionuclides: Competing Geochemical and Enzymatic Processes

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This research is part of the Biogeochemical Dynamics Scientific Program Element, DOE/OBER Natural and Accelerated Bioremediation Research Program (NABIR). Focus will be on the influence of direct microbial reduction versus metabolite-induced reduction of Cr and Co-EDTA. Specifically, the research will: (1) define under what conditions microbiological or chemical mechanisms dominate the reduction of Co(III)EDTA and Cr(VI), (2) quantify the reduction rates and mechanisms controlling the mobility of Cr and Co, and (3) identify reaction products both in solution and solid phase.

** Formerly with the University of Idaho.*

STATE OF KANSAS

A. Projects Supported by EPSCoR

26. Molecular Simulations of Complex Fluids in Confined Geometries

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The PIs group at Kansas State University and Dr. Heffelfinger's group at the Sandia National Laboratories have ongoing research program in the area of molecular modeling. Sandia has developed, not only state-of-the-art materials modeling methods, but also companion parallel algorithms for several of these methods. The capabilities of these codes, however, to treat complex molecular and charged systems are incomplete and the accuracy of simulations is also limited due to the interaction potentials employed. This proposed work is aimed at addressing these deficiencies in the Sandia's capabilities. In collaboration with Dr. Heffelfinger's group, the PI and his students will (1) develop accurate force fields from ab initio quantum chemical calculations and incorporate the force fields into the dual-control volume grand canonical ensemble molecular dynamics (DCV-GCMD) code developed at Sandia to treat complex molecular systems with high accuracy, and (2) implement the Cell Multipole Method in the existing codes, making simulations of a large-scale charged system practical with the aid of parallel computing and allowing one to rigorously treat aqueous systems and charged surfaces. The development of the molecular modeling capabilities as proposed will impact technology development for many problems of interest to Sandia and other DOE laboratories. One example important to several types of environmental clean-up problems is the surface conduction of ions in porous materials. Furthermore, the processing of high-level radioactive waste, such as found in the Hanford Tanks, may be feasible via the development of tailored ceramic membrane separations technology. In addition, DOE/EPSCoR funding will foster the career development of the PI, provide educational opportunities for undergraduate and graduate students, and enhance research and technology capabilities at Kansas.

27. Molecular Dynamics Simulations of the Effects of Salts on the Aggregation Properties of Benzene

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The removal of hazardous organic pollutants from the environment is a major DOE undertaking which requires the development of new or improved separation techniques. Many of the common pollutants are small nonpolar organic molecules which are only sparingly soluble in water. This solubility can be increased or decreased by the addition of different salts. The proposed research is aimed at understanding the interactions between benzene (a model nonpolar organic molecule) and both water and salt ions at the atomic level. This information will in turn lead to improved theories of salt effects and the possibility of designing solutions with specific salting in/out properties. Molecular dynamics simulations using both serial and parallel computers will be performed to obtain the atomic-level detail necessary for a complete understanding of these interactions and how they affect the aggregation properties, and hence, the solubility of nonpolar molecules in solution. Our initial studies will focus on benzene in (1) water, (2) 2.0 *M* sodium sulfate (strong salting out salt), (3) 2.0 *M* sodium bromide (weak/neutral salting out salt) and (4) 2.0 *M* tetramethylammonium bromide (salting in salt).

28. Atomistic Studies of Nanotribology

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In the collaborative research proposed with Dr. Salmeron's group at Lawrence Berkeley National Laboratory, the goal is to understand atomistic processes responsible for phenomena like friction, adhesion, contact formation, lubrication, and wear, which present themselves when microscopically sized objects come in contact with each other. Theoretical investigations working in tandem with experimental probes will span several stages of increasing complexity. The first step involves characterization of the temperature-dependent properties of the tip and of the tip/substrate interface, as a function of the tip size, elemental composition, and relative orientation and commensurability with respect to the substrate. These calculations of the structural, vibrational and thermodynamical properties will be based on many-body, semi-empirical interaction potentials. At a later stage, first-principles electronic structure calculations will be performed for selected systems. Our goal is to trace the changes in force fields, relaxation effects, and in the nature of localized vibrational excitations at the tip/substrate interface to the strength of adhesive and frictional forces as atoms are moved or manipulated on a surface. Next, we will examine the emergence of plasticity in these systems by calculating the effect of high applied forces on wear processes, leading to the rupture of atomic bonds and the creation of dislocations. Finally, to achieve our long-term objective of developing an understanding of atomic-level adhesion, friction and wear in terms of the nature of the chemical bond, we will extend the above procedure to several combinations of metals (tip and substrate), and to directionally bonded materials like diamond and SiC to serve as tips on Si surfaces.

B. Projects Supported by Office of Science

29. Optical and Electrical Properties of III–V Nitride Wide Bandgap Semiconductors

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Optical and electrical properties of GaN and $Al_xGa_{1-x}N$ will be studied, including alloys, epitaxial layers, and quantum well structures. The recombination rates for all possible mechanisms will be studied by time-resolved picosecond laser spectroscopy. These will be characterized as a function of temperature, alloy composition, applied electric and magnetic fields, and parameters of the exciting photons. Nonlinear properties will also be measured. Electrical property measurements will focus on the effects of *p*-type dopants and native defects at temperatures up to 600°C.

30. Structure, Dynamics and Thermodynamics of Metal Surfaces

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The theoretical study will investigate the temperature-dependent microscopic structure, dynamics, and thermodynamical properties of stepped transition metal surfaces. Many body potentials will be used to study a set of vicinal surfaces including the metals, Al, Cu, Ag, and Pt. The effect of atomic vibrations will also be included.

31. Atomic Physics with Highly Charged Ions

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The primary goal of the project is to understand, at the most basic level, binary collisions involving highly charged ions and individual targets and to provide conceptual frameworks and descriptions useful in understanding interactions of highly charged ions with matter in more complex situations. The facilities used include: (1) a cryogenic electron beam ion source (CRYEBIS) capable of delivering highly charged ions up to bare argon and Xe46+ at velocities between 0.1 and 2.0 a.u., (2) a tandem-LINAC accelerator delivering fast beams with specific energies up to 4 MeV/u in charge states up to, for example, hydrogen-like chlorine, and (3) an ion-ion collision facility. The targets used include neutral gases, ions, Rydberg atoms, clusters, and solid surfaces. The nine main areas of research are electron production in ion-atom collisions, quasi-free electron-ion processes in ion-atom collisions, single- and double-electronic transitions in ion-atom collisions, collisions with and production of Rydberg atoms and ions, ion-ion collisions, ion-molecule collisions, ion-surface and ion-^{60}C interactions, synchrotron radiation studies of atoms using cold-target recoil momentum spectroscopy (COLTRIMS) and ion-atom collision theory. Two areas of emerging research are: (1) the discovery of new symmetries in low-energy ionization of atoms by slow projectiles performed with COLTRIMS coupled with electron momentum imaging; (2) the discovery of narrow electron jets in the forward and backward directions of electron spectra from swift ion-solid collisions. These jets of electrons with a 2.50 half-angle divergence are interpreted in terms of the channeling of electrons in the plasma-like wake of the projectile tracks in carbon foils. Color images of the data demonstrating these effects can be viewed on the J R Macdonald Laboratory home page at www.phys.ksu.edu/area/jrm/ under Emerging Research.

32. Atomic Physics of Strongly Correlated Systems

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This research program focuses on the physics of strongly correlated atomic systems. The hyperspherical method is being developed for studing three-electron atomic systems, with the main emphasis on doubly and triply excited states. New numerical schemes are being developed such that the adiabatic potential curves for any symmetry can be calculated for any three-electron systems. The first goal is to show that there are no bound states or resonances for doubly negatively charged atomic hydrogen. For doubly excited states the goal is to develop hyperspherical close-coupling method to obtain accurate positions and widths and photoabsorption cross sections. For triply excited states the goal is to analyze the correlation patterns of these states in order to find new classification schemes. The method will also be developed for three-valence electron systems such that optical spectra and low-lying resonances can be analyzed. In ion-atom collisions the close-coupling method using two-center atomic orbitals will be used to perform calculations for collision systems—the area of interest of experimentalists. The focus will be on the detailed partial cross sections to individual final states, as well as differential cross sections. The collision system of protons with helium will be examined further with a larger extended basis set following the scheme developed last year.

33. Homogeneous Models of Ammoxidation Catalysis

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The hexamolybdate cluster, $[Mo_6 O_{19}]2-$, displays an MoO_6 coordination environment conspicuously similar to that within the ammoxidation catalyst component MoO_3. Our attention continues to focus on the preparation and study of organoimido derivatives of the hexamolybdate as structural and reactivity models for key nitrogenous surface species which have been proposed as intermediates in industrial ammoxidation chemistry. By applying a combination of electrochemical, structural and multinuclear NMR spectroscopic methods, we have established that substitution of organoimido groups for oxo ligands within the hexamolybdate causes a progressive buildup of electron density which accumulates at the remaining terminal and bridging oxo sites in these derivatives. This finding provides important insights for understanding the hydrogen abstraction chemistry which accompanies the redox events in ammoxidation. We are initiating theoretical investigations parallel to our chemical studies, and are now engaged in the synthesis of organoimido derivatives of other polyoxometalate clusters in which enhanced oxidation ability can be expected.

34. Heavy Quark and Neutrino Physics

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A high-energy group formerly at Ohio State University transferred to Kansas State University in the summer of 1993. Since then, startup, DOE, NSF EPSCoR and City of Manhattan funds averaging over $1 million per year have been used to build an effective program. Facilities have been developed for large-scale construction, clean-room testing of silicon microstrip detectors and electronic design. The KSU group consists of three faculty, one research faculty, four grad students and a small number of support personnel. A cosmology theorist also was added and has applied for DOE funding. This year we plan to add an assistant professor and an additional grad student. The group's research over the past 6 years has been devoted to Fermilab fixed-target experiments E653, E791 and COSMOS, as well as the D0 collider effort. E653 measured beauty-particle cross sections and lifetimes, as well as studying charm semileptonic decays. E791 was a high-statistics study of charm production in which KSU again concentrated on semileptonic decays, for example providing the best current limit against D0 mixing. E791 was the largest high-energy analysis effort of the early 1990s, and KSU did 40% of the work. COSMOS was a major extension of previous work done by the group at OSU which until 1997 provided the best limit against muon-to-tau neutrino mixing. The experiment was terminated just prior to construction when Japanese collaborators comprising half the work force resigned. The KSU group then joined DO and presently serve as co-leader of the silicon microstrip upgrade, as well as several associated subsystems. Physics interests include serving for charged and neutral Higgs, particularly with techniques involving vertex or impact-parameter tags.

35. Research in Theoretical Particle Physics

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This research spans space and time domains from cosmological to sub-nuclear. Calculations of event rates of hits of neutrinos of astrophysical origin in a radio cherenkov detection array in Antarctica, RICE, have been made and are being refined. Neutrino tomography of the earth using the same array and sources has been proposed using a novel, essentially model-independent technique. Further research in neutrino physics includes the expansion of the analysis of accelerator and astrophysical neutrino data to include the effects of new types of neutrino interactions, along with the effects of finite neutrino masses in a unified scheme. One application is to novel theories that include not only modified neutrino properties but also exotic, heavy quarks. Research is ongoing to propose collider searches for these particles, expanding on our earlier work that set lower limits on their masses. On another topic in large-scale effects, new statistical techniques have been developed to analyze polarization data from distant galaxies. A strong correlation has been found, and more sources of data are being tapped to further probe the effect. In the realm of the theory of strong interactions of known quarks and gluons, namely quantum chromodynamics, new predictions of the production of pions and nucleons from electron-nucleus collisions have been made. More generally, further tests of the so-called "color-filtering" effect, pioneered under previous support of the group, are being exhaustively expanded.

36. Strong External Field Effects in Decay and Photodetachment of Negative Ions

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We propose to study the decay and photodetachment of alkali-metal negative ions in the presence of strong external static electric and magnetic fields. Placing atoms and ions in combinations of laser and static fields allows one to manipulate the detachment rate and to observe basic quantum-mechanical effects such as two-path and multi-path interference. Reflection of the detached electron wave from the potential barrier created by a static external field may lead to rescattering, which, if observed, would yield important information about the electron-atom scattering amplitude with the laser resolution. Photodetachment cross sections for the low-lying resonance states of alkali negative ions are of particular interest and parallel current experimental work. While for light targets, such as lithium and sodium, calculations can be based on the non-relativistic Schrödinger equation, such an approach becomes increasingly questionable for the heavier elements: rubidium, cesium, and francium. For these heavier atoms, relativistic effects are apparent in the electronic structure of the neutral atoms through large fine-structure splittings, and have a counterpart in fine-structure split multiplets of resonances of the akali-metal negative-ions. In the proposed work previous accurate relativistic calculations on low-energy electron scattering from neutral cesium atoms will be extended in two ways. First, electron scattering and photodetachment from several heavy targets will be studied in order to establish trends for relativistic interactions as the nuclear charge is increased. Second, electron-atom scattering and photodetachment processes that include the influence of static external electric fields will be considered. The proposed work will lead to a new set of computer programs to investigate photoprocesses of stable or resonant systems with two active electrons in an external electric field. The provided basic atomic data are relevant for applications in the fields of chemistry, physics and electrical engineering.

37. Research in Heavy-Ion Nuclear Physics

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Our group of two faculty members and from two to three graduate students has a program of detector development and nuclear reaction studies. One goal of this research at lower energies is to explore the behavior of nuclei under extreme conditions of temperature and spin. Such studies can lead to a better understanding of interplay of forces within the nucleus and the manner in which the balance of forces can result in highly deformed, quasi-stable nuclear shapes. At Kansas we are building large-acceptance counters for these experiments to identify nuclear reaction products. We are also studying the role of projectile breakup on the fusion reaction mechanism. Understanding the influence of projectile breakup is important as we start to consider the use of radioactive nuclear beams to produce new isotopes far from the region of nuclear stability. As a separate project, which has become our principal focus, we are collaborating with researchers from a large number of different institutions to develop a detector system, called BRAHMS, that will explore collisions between two relativistic heavy ions. Such collisions are expected to create a novel state of matter called the "quark-gluon plasma." We are developing the detector subsystem of BRAHMS that will tell whether the heavy-ions hit head-on, or experience a more grazing collision.

38. Processes Affecting Carbon Fluxes of Grassland Ecosystems Under Elevated Atmospheric CO_2

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The long-term study is being completed. The objective remains the same: to determine the extent to which a C_4-dominated grassland will sequester carbon in residual plant and soil components of the system. There are four components to the field study: at both ambient and elevated CO_2 levels, (1) measure biomass accumulation of above- and below-ground plant material, differentiated into C_3 and C_4 components; (2) measure changes of soil microbial activity, soil C and soil N (including fractionations of both C and N); (3) experiments on carbon fixation in relation to water stress; and (4) mesoscale modeling.

STATE OF KENTUCKY

A. Projects Supported by EPSCoR

39. Kentucky DOE/EPSCoR Program

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The Kentucky DOE/EPSCoR Program includes four research clusters and one education or human resource development cluster. The interdisciplinary research clusters are: Fossil Energy; Environmental Sciences; High-Energy and Nuclear Physics; and Materials Research. They are to be performed at seven Kentucky universities: Berea College, Eastern Kentucky University, Kentucky State University, Murray State University, the University of Kentucky, University of Louisville and Western Kentucky University. The research is collaborative, involving personnel at seven DOE National Laboratories and nine U.S. industries. The education cluster includes work at six universities within Kentucky, including Murray State University, Northern Kentucky University, Pikeville College, University of Kentucky, University of Louisville and Western Kentucky University. They cooperatively participate in this education effort. All projects strive (1) to improve the content of science and engineering educational opportunities throughout the Commonwealth, and (2) to affect students in middle and high school, pre-service science teachers, high school teachers in science and math, science and engineering graduate students, and faculty at four-year Appalachian and historically black colleges and universities.

40. Research Cluster 1. Fossil Energy—Characterization and On-line Measurement of Critical Elements in Coal and Coal Combustion

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This research cluster is developing commercially useful instrumentation and software for increasing the efficiency by which coal is used as an energy source and is defining coal properties that will impact future energy utilization scenarios. Research in one of the projects at the University of Kentucky concentrates on trace elements in coal—their speciation, quantitative measurement and removal. Analytical techniques, including EXAFS and neutron activation, are used to quantify trace-element concentrations. Another analytical project at the University of Kentucky is defining the techniques and protocol to produce quantitative signatures of ultrafine particulate that can serve as fingerprints for airborne $PM_{2.5}$. This project also is assessing the mode of occurrence of S, Cl and HAP's in these particulates. The two commercialization projects include one at the Western Kentucky University. It has developed the instrumentation, algorithms, and is now finalizing developmental work on prototype equipment for their patented pulsed fast, thermal neutron analysis (PFTNA) methods to measure elements and the BTU contents of coals. The prototype equipment is to be used to demonstrate the ability to measure these characteristics in an on-line mode of operation. The other commercialization project is housed at the University of Kentucky and concentrates on developing advanced computer models and algorithms for controlling fuel and mineral blending.

41. Research Cluster 2: Environmental Sciences—Organic Carbon in Large Reservoir Systems and Reservoir-Watershed Linkages in Hydroelectric Reservoirs

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This cluster consists of two projects located at Murray State University. It concentrates on reservoir biology, organic carbon/nitrogen accumulation, and biochemical transformations in two of the largest reservoirs in the United States, and complements research at the Center for Reservoir Research at Murray State University. Direct interaction with personnel at Oak Ridge National Laboratory, the University of Kentucky and the University of Louisville are integral to the cluster research. Besides establishing the link between reservoir biology and organic carbon/nitrogen accumulation in Kentucky and Barkeley Lakes in western Kentucky, the cluster examines the effects of water-level management on hydrology and water quality in two hydroelectric reservoirs. It has initiated hydrology research that complements ongoing and planned biogeochemistry and microbial ecology studies and will define the effects of hydro-power management on fresh-water lakes. Both of these projects take advantage of an on-going Distinguished Lecture Series in Water Science that was established at Murray under DOE/EPSCoR funding.

42. Research Cluster 3: High-Energy and Nuclear Physics—Experimental Nuclear Physics at TJNAF and High-Energy Physics Research

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This cluster consists of three projects: two involve experimental work at the Thomas Jefferson National Accelerator Facility (TJNAF); the other is a high-energy computational project. At the TJNAF, a Möller polarimeter, designed, constructed and installed by University of Kentucky scientists is being used in Hall A collaboration. Currently, a ^{3}He polarized target has been designed and is under construction for work at the TJNAF. Studies of hadronic structure and interactions are also planned, including work on the fundamental properties of neutrons, electric form factors and transverse spin structure functions. The high-energy project is a theoretical effort in cooperation with the Fermi Laboratory and entails fundamental lattice-gauge calculations. These calculations have been facilitated by the development of advanced computing platforms and algorithms at the university. By using specially designed simulations, the research will continue to study nucleon form factors and hadron properties.

43. Research Cluster 4: Materials Research—Thermal Barrier, Alloys, Sensor and Microelectromechanical Materials

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This cluster consists of four projects, one of which was initiated at the beginning of the Implementation Grant in 1994. It has investigated and developed synthesis and characterization techniques for zirconia materials as wear and thermal barriers. Comparisons between samples prepared by plasma spray techniques and by industrial collaborators have shown the important advantages to the developed sol-gel preparation methods being used by the project investigators. Microstructural and life-cycle tests are scheduled, with some information being provided through cooperation with Argonne National Laboratory and Sandia National Laboratories. Three other projects are to begin during 1999 and are designed (1) to help strengthen budding research efforts at three universities and (2) to establish initiating data, contacts and instrumentation. These projects are on the development of microelectromechanical systems (MEMS), the enhancement of low-field magnetostriction in thin, multilayer films for device and sensor applications, and the optimization of heat treatment of Al-Si-Mg alloys. These projects are located at Kentucky State University, University of Kentucky, University of Louisville and Western Kentucky University.

44. Human Resource Development Cluster: The Kentucky HRD Alliance

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A Chemistry for Pre-Service Elementary Teachers project has successfully developed a course and laboratory that has become an accredited course for Department of Education majors. A Science Alliance project establishes links to science teachers throughout the state and offers retraining and advanced teaching resources for classroom instruction. The urban-based student project, called INSPIRE (INcreasing Student Preparedness and Interest in the Requisites for Engineering), presents summer activities and instruction for high school minorities and women in engineering, while a project entitled Incorporating Nuclear and Radiochemistry in Undergraduate Chemistry and Secondary Science from the UK concentrates on nuclear and radiochemistry instruction to "educate the educators" from HBCUs and Appalachian-based colleges. Another project, the Students Weatherization/ Audit Training (SWAT), trains high school students and teachers in energy conservation and assessment. A High School Energy Internships recruits high school students to become involved in a two-week summer research and analytical experimentation program at an energy research laboratory. The Science Works - Physics Proficiency in Elementary and Middle Grades project is designed to provide physics content understanding and classroom materials for teachers throughout the Commonwealth. Finally, KY DOE/EPSCoR initiated and supports the ongoing Entrepreneurship and Enterprise Development which teaches faculty and students in four principles of business, including Evaluating Ideas, Proprietary Protection, Capital, and Business Planning.

45. Fundamental Studies of Interfacial Strain in Composite Materials using Advanced Diffraction Techniques

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Composite materials are prone to interfacial residual stresses because of compatibility constraints at the interface and the different physical responses (e.g., thermal expansion, elasticity, etc.) of the two constituent materials. Because internal stresses can have profound effects on the macroscopic physical properties of the composite system, it is important to understand the origins of the stresses and their implications for the interfacial properties. This research program aims to shed light on this important interfacial phenomenon by:
(1) developing an experimental protocol for measuring strain and stress distributions in composite materials arising from interface compatibility constraints and (2) elucidating fundamental relationships between the atomic structure and chemistry of an interface and the magnitude, extent and symmetry of the interfacial stress tensor. Because interfacial stress is a complex, multilength-scale phenomenon, we employ model composite systems that facilitate quantitative experimental investigations from the atomic to macroscopic levels. A variety of electron, X-ray and neutron-diffraction techniques are used to rigorously study both the atomic structure of the interfaces

and the interfacial strain distributions. Collaborations between the University of Kentucky and Oak Ridge National Laboratory are an integral and necessary component of the program. Ultimately, this research should lead to a better understanding of the intimate connection between interface structure and interfacial stresses.

B. Projects Supported by Office of Science

46. Dynamic Flux Line Response in Layered Superconductors with Tailored Defect Structures

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Electron beam lithography is to be used to provide controlled columnar defects in high-quality Pb/Ge and WGe/Ge multilayer materials. These will be studied using vibrating reed and torque magnetometry and ac susceptibility. These artificial structures are models for layered superconductors, such as the high-T_c cuprates, with columnar defects. Because of the extensive capability to control nearly all parameters in these model systems, they provide unique opportunities to test both fundamental many-body theories and quantitative models of magnetic flux line dynamics in irradiated high-T_c materials.

47. Solid-State Electronic Structure and Properties of Neutral Carbon-Based Radicals

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This research is directed towards the synthesis of organic solids derived from neutral radicals which are derivatives of the phenalenyl system. Many compounds in this series should be solid-state organic conductors. Some may be metallic and may possibly be superconductors. The solid-state properties of these systems in the context of their electron transport and magnetic properties are main issues. The virtue of these systems is that they are overall neutral and can be sublimed and transferred into films. A long-term thrust of this work is to understand the relationship between solid-state properties and molecular structure.

48. Coherent Excitation of Autoionizing Resonances

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Atomic ionization by electron impact is being investigated by (e,2e) spectroscopy. Experiments with a cadmium target have observed interference effects between partial waves of differing multipolarity. Pairs of (e,2e) energy spectra are measured at three carefully chosen ejected-electron directions in the energy range dominated by autoionization via Cd 4d95s25p. Interference effects are enhanced by taking the sum and difference of the spectral pairs. A comprehensive set of spectra have been obtained for an incident electron beam energy of 150eV and scattering angles between 2 and 18, which covers the range of momentum transfer 0.2 to 1 au. The experimental results have been compared with a plane wave Born approximation calculation. It is found that the calculated monopole and quadrupole phases (relative to the dipole) are incorrect by ±4 at small momentum transfer; in fact a simple constant correction to these phases appears to be valid over the entire momentum transfer range investigated. The relative Born magnitudes are extremely good for the spectral pair taken along the momentum-transfer axis, but are extremely bad for the other two chosen directions. With increasing scattering angle a reduction in the 4d95s25p 3P1/1P1 intensity ratio in the sum spectra is observed, probably due to an increase in exchange scattering. At the largest momentum transfer, previously unobserved 4d95s25p J = 3 autoionizing levels are seen. A second (e,2e) spectrometer has been configured for similar interference experiments on helium autoionizing levels.

49. The Dynamics of Weakly Bound States in Collisions and Fields

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The dynamics of atomic Rydberg states in time-dependent external fields and in ion-atom collisions are investigated using theory. Dynamical processes involving Rydberg atoms are central problems of plasma physics, but are difficult to predict quantitatively due to the large numbers of states coupled by any external field. A theory describing the mixing of nearly degenerate Rydberg states in ion-atom collisions is now complete and in good agreement with absolute experimental measurements; this theory is fully quantum mechanical and based on a Floquet analysis of the collision process. Classical studies of charge transfer reactions involving Rydberg targets are fueling new experimental investigations into the dynamics of electron capture. A study of multiphoton microwave spectroscopy of Rydberg states has resulted in a new formulation and understanding of Floquet theory, complementing decades of experimental work in the field. A conclusive demonstration of the utility of Floquet theory for the description of dynamics in half-cycle electromagnetic pulses is emerging from an analysis of recent experiments in which Rydberg atoms pass through a cavity containing a circularly polarized microwave field. Finally, new theoretical models of the experimental technique of selective field ionization are now in qualitative agreement with observations.

50. Metallocarboxylate Chemistry

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Our goal is to provide a base of information that may assist in the development of catalyst systems which can convert CO_2 to useful C_1 or C_2 products. The special focus of this project is on the transition metal organometallic chemistry of carbon dioxide. The studies include the development of synthetic strategies leading to a variety of CO_2 complexes, spectral and structural characterizations of them, and explorations of their chemical reactions. During the past year, we have used transmetalation reactions of a CO_2-bridged rhenium-tin complex to generate new CO_2-bridged complexes having unusual structural types (including one with two bridging carbon dioxide ligands). Also, work has been initiated on a broad spectrum of ruthenium(II) polypyridyl complexes with carboxylate (–COOH, –COOR, and CO_2) ligands; such compounds are little known but often proposed as intermediates in catalytic reductions of CO_2. New complexes with bipyridyl, phenan- throline and terpyridyl ligands, including some with mixed polypyridyl ligands, have been prepared, and several have been structurally characterized.

51. Hydrogen Atom and Molecule Collisions

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Collisions of excited atomic hydrogen with other atoms and ions are studied by emission spectroscopy in the infrared, visible, and vacuum ultraviolet, by laser-induced fluorescence, and by theoretical work on atomic spectral line broadening. In addition to H2, H2+, and H3+, the atom-atom systems which are considered are those with H in combination with C, N, and O, leading to the radicals CH, NH, and OH, with applications to combustion, astrophysics, plasma processes, and the basic physics of spectral line broadening. Work is in progress now on observations and theory of the shape of the Lyman-line of atomic hydrogen with the development of a laser-produced plasma in the jet from a pulsed valve to permit observations in the windowless vacuum ultraviolet. Other experiments on a laser-produced plasma in a static cell are being used to study collisions of more than two hydrogen atoms, in order to understand the effects of many-body collisions on spectral line formation. The addition of O in very small quantities yields the OH+ ion. Its reactions to produce OH, and the subsequent radiative dissociation into atomic O and H, are followed with spectroscopic diagnostics.

52. Acetyl-CoA Cleavage and Synthesis in Methanogens: Mechanistic, Enzymological, and Metabolic Studies

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We are employing biochemical methods to study the acetyl-CoA decarbonylase/ synthase complex found in methanogenic Archaea. The results of our experiments will allow us to elucidate the complicated biochemical mechanism used by the enzyme complex to catalyze the following reaction: CO_2 + $2Fd_{red}(Fe^{2+})$ + $2H^+$ + CH_3- H_4SPt + CoA ⇌ acetyl-CoA + H_4SPt + $2Fd_{ox}(Fe^{3+})$ + H_2O, where H_4SPt and CH_3-H_4SPt are tetrahydrosarcinapterin and N^5-methyl-tetrahydrosarcinapterin, respectively, and $Fd_{red}(Fe^{2+})$ and $Fd_{ox}(Fe^{3+})$ are the reduced and oxidized forms of the redox protein ferredoxin. Additionally, we will use the biochemical knowledge gained to better understand how the oxidation-reduction potential of the environment regulates methanogen physiology.

53. Mechanism and Significance of Post-Translational Modifications in the Large Subunit of Ribulose-Bisphosphate Carboxylase/Oxygenase

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The methylation of Lys-14 in the large subunit (LS) of ribulose-1,5-bisphosphate carboxylase/oxygenase (Rubisco) by Rubisco LS N-methyltransferase (Rubisco LSMT) occurs by an ordered bi-bireaction mechanism. Kinetic and binding analyses of the initial interaction between Rubisco LSMT and des(methyl) forms of Rubisco, revealed a tight (KD 0.1 n*M*) and specific interaction which was identified as a consequence of a relatively slow kass (7,368 M^{-1} s^{-1}) and kdiss (8×10^{-7} s^{-1}). The molecular determinants of this tight and specific interaction were investigated by ELISA analyses of binding between truncated forms of Rubisco LSMT expressed in *E. coli* and immobilized Rubisco. The results demonstrated that among 19 different carboxy- and amino-terminal truncations, representing the removal of 4 to 380 amino acids out of a total of 489, all showed positive signals for binding to Rubisco. While some of the truncated Rubisco LSMT constructs showed noticeably weaker binding to Rubisco than full-length Rubisco LSMT, all maintained a high specificity for Rubisco. Thus, the interaction between Rubisco LSMT and Rubisco appears to be a consequence of multiple binding domains spread over a large portion of the Rubisco LSMT protein. Related studies determined the location of a cross-link between the LS of Rubisco and Rubisco LSMT catalyzed by a homobifunctional sulfhydryl-specific cross-linking reagent (BMH). Cross-linking between Rubisco LSMT and the LS of Rubisco generated a 106-kDa product which was a result of cross-linking between Cys-459 in the LS of Rubisco and Cys-119 or Cys-188 in Rubisco LSMT.

54. Studies of a Novel Pathway for Biosynthesis of Straight and Branched, Odd and Even Length, Medium-Chain Fatty Acids in Plants

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Fatty acids (FA) of various chain lengths are key components of plant membranes, waxes, reserve oils, and certain compounds volatilized by plants. These natural products are exploited commercially as food components, lubricants, emulsifiers, etc., and are being researched for their use as renewable, biodegradable polymers, biofuels, stimulants for biodegradation of pollutants, etc. We have described a new pathway (termed α-keto acid elongation, α-KAE) that utilizes enzymes of branched chain amino acid (BCAA) metabolism to synthesize straight-chain, iso- and anteiso-branched, short- and medium-chain length FA in trichome glands of certain plants. Results of a completed survey indicate that α-KAE appears to be restricted to trichome glands of petunia and Nicotiana species. Branched and straight medium chain FA of seeds, acid components of epicuticular wax esters and at least one petal-volatilized, anteiso-branched alcohol are elongated by fatty acid synthase and not α-KAE. But, iso and anteiso primers for branched species are provided by BCAA metabolism. A direct assay was established to monitor isopropylmalate synthase (key enzyme of BCAA metabolism) that is 4 times more sensitive than conventional assays. This assay has revealed new properties of this enzyme. Efforts to isolate genes involved in BCAA metabolism and α-KAE are in progress.

55. Contribution Studies of CP Violation and Other Physics Topics with Babar Collaboration

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Dr. David Brown at the University of Louisville has been active with the BaBar collaboration. He is the coordinator for the Graphics Area of BaBar Software, overseeing development of code for offline, online, systems-specific, and analysis-related displays. He and his students are active in production and quality assurance of simulated data, and development of Particle Identification tools. Further, the group is developing analyses in B to baryon decays as part of a study of the Kobayashi-Maskawa Matrix elements. Dr. Brown is working in the BaBar Soft QCD group on analyses of gluon fragmentation and two-photon baryoproduction.

56. Research in Theoretical Nuclear Physics

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A program to study nucleon and hadron structure and spectroscopy is funded. We study nucleon structure with lattice-gauge Monte Carlo calculations. This includes the orbital angular momentum of the quarks and the gluon spin in the nucleon, the sea contributions to strange electromagnetic, axial and pseudoscalar form factors and the moments of the structure function. We are also undertaking the calculation of glueball masses and their transition matrix elements with the improved action to help discern the glueball candidates in various experiments. We also study heavy-quark effective theories on the lattice by using a general variational approach in the static, fixed-velocity and non-relativistic approximations to extract ground and excited state properties of heavy-light mesons, and to probe directly the nonperturbative dynamics of quarks and gluons. We will calculate the renormalized Isgur-Wise function directly on the lattice and will study the matrix elements of four-fermion operators for hadrons containing a static quark.

57. Studies of Hadronic Structure Using Electromagnetic Probes

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Using the electron accelerator facilities at the University of Maine, MIT-Bates, DESY, and the Thomas Jefferson National Accelerator Facility (TJNAF), we are performing experimental studies of the electric form factor of the neutron, the strangeness content and spin structure of the nucleon, the fundamental pion-photon vertex, and electromagnetic interactions in few body systems. The principal investigators (PIs) are each leading efforts to develop major scientific equipment in support of this program, and are each spokespersons for physics proposals involving this instrumentation. One of the PIs, along with collaborators from the Kharkov Institute of Physics and Technology and TJNAF, is working on a Moller polarimeter as part of the development of the spin physics program for Hall A at TJNAF. The PI is co-spokesperson for the development and construction of the polarimeter and participates actively in the spin physics program. The unique small-angle capabilities of this device will enable one to access new physics at small momentum transfers. A program is under way to study the gamma-gamma-pi-zero interaction vertex via the real and virtual Primakoff effect. Such studies are expected to provide fundamental information about the pion's electromagnetic interactions. One experiment was conditionally approved by TJNAF PAC12, with one of the PIs as spokesperson. A related experiment to perform a precision measurement of the pi-zero lifetime in Hall B of TJNAF has also been approved, with one of the PIs as a spokesperson. Three years ago a new collaboration was formed to develop a dense polarized helium-3 target for Hall A which can be used to study fundamental properties of the neutron. One PI has major responsibilities in the target development and installation. He is co-spokesperson of two approved experiments that will measure the (1) electric form factor of the neutron very precisely at high four-momentum transfers and (2) search for higher twist effects in the spin structure function g2n(x,Q^2). So far there are six fully approved experiments using a polarized helium-3 target. Further, one of the PIs is continuing participation in the SAMPLE and HERMES experiments. SAMPLE is an ongoing experiment at the MIT-Bates accelerator which tries to extract the contribution of the strange quarks to the proton's magnetic moment. The HERMES experiment is installed in the HERA electron ring at DESY. This experiment applies the novel technique of internal polarized targets to deep inelastic scattering. HERMES has the unique capability of performing high-precision semi-inclusive measurements to disentangle the contributions of the different quark flavors to the nucleon's spin. Studies of the He(e,e'p) reaction are also being performed at the University of Maine over a range of kinematics with the aim of examining non-nucleonic effects, such as meson-exchange currents and isobar configurations as well as short-range correlations.

58. Tests of Fundamental Symmetries

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This research program concerns tests of discrete symmetries in hadronic processes, with the end of discerning and computing the hadronic ambiguities which could hamper the diagnosis of physics beyond the Standard Model. For example, the discrete symmetry CP is known to be violated in nature; in the Standard Model its violation is realized as a single phase in the Cabbibo-Kobayashi-Maskawa (CKM) matrix, which relates the quark weak-interaction eigenstates to those of mass. Despite the observation of CP violation in the neutral kaon system in 1964, the Standard Model picture has had little testing. Indeed, the mission of the future B factories is to elucidate the mechanism of CP violation, to search for the presence of physics beyond the Standard Model. Our focus is not on models of "new" physics, nor is it on how particular "new" models may be probed; rather, we scrutinize hadronic processes which can obfuscate the clarity of certain tests of the Standard Model. Particularly, we consider the role of isospin violation, and our especial interest is in tests of the unitarity of the CKM matrix, as probed in hadronic B-decays, in polarized neutron β-decay, and in superallowed Fermi transitions in nuclei. In this manner we hope to resolve the hadronic ambiguities which may bedevil the search for physics beyond the Standard Model.

STATE OF LOUISIANA

A. Projects Supported by EPSCoR

59. Louisiana DOE/EPSCoR Program

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The challenge of the Louisiana DOE/EPSCoR Program is to enhance research and training capabilities in areas that are not only highly relevant to DOE, but also have immediate potential for impacting Louisiana's economy. Louisiana made significant commitment to infrastructure improvement by establishing the constitutionally dedicated Board of Regents Support Fund in 1987. Since then, $494.5 million has been targeted at improving Louisiana's research and training infrastructure. Louisiana' energy-related goals in this EPSCoR program are to develop (1) new materials science technologies relevant to future economic development, (2) a comprehensive understanding of how waste generated by oil and gas production and by petrochemical manufacture impact Louisiana's commercially important environments, and (3) a comprehensive approach to establishing education, training, and mentoring programs that recruit students and faculty into following careers in energy-related areas. The DOE's interest in materials science and environmental restoration and waste management closely parallels Louisiana's strategic opportunities for economic growth. The Louisiana DOE/EPSCoR

Program has realized significant progress in these areas.

60. Human Resource Development Component

Developing the human capital of the state is an important and systemic goal of stimulating research and economic development infrastructure in Louisiana. The Human Resource Development Component programs are tied to EPSCoR research cluster activity and leverage other state systemic programs in planned collaborative interactions through the following activities: (1) administering a Precollege Research Internship for teachers with DOE/EPSCoR Cluster Researchers, (2) disseminating 500+ science manuals with specific energy-related content developed by reform-minded high school science teachers through regular distribution at conferences and via the Internet, (3) administering an energy-related research and mentoring program for twenty high-potential undergraduate students, and (4) strengthening the overall pipeline through formalized collaborations to move toward sustainability of the DOE/EPSCoR Program. These highly focused programs address each phase of the human resource development infrastructure, thus maximizing the potential to make concrete and lasting advances in Louisiana's precollege and college human resource development. These programs provide both new technology and personnel for helping Louisiana expand its industrial base and best utilize its unique environmental resources. Of particular importance: Louisiana's major research universities work in partnership with regional universities, particularly HBCUs, to educate workers capable of carrying out the DOE's priorities for the next century.

61. Inorganic Synthesis and Lase-Induced Photochemistry Relevant to the Fabrication of Electronic Materials

This materials science research group is composed of investigators from four universities within the State of Louisiana: Tulane, Xavier, LSU, and Loyola. While the individual programs of these investigators are rooted in basic research involving chemistry and physics, they have a significant component directed toward materials research, primarily electronic materials. The fundamental and practical ramifications of the proposed research will have an impact on major DOE interest areas, ranging from understanding chemical bond cleavage to producing solar cells. Major projects involve the synthesis of novel materials precursors, the application of unique thin-film deposition strategies, and the utilization of innovative photochemical techniques. This cluster reflects the growing awareness and national importance of materials research in energy-related disciplines such as chemistry. Additionally, industrial ties are being established, an active outreach program is in place, and "tech-transfer" opportunities are being fostered. The breadth and quality of student participation, representing both graduate and undergraduate students, is impressive as well as the true research collaborations that have been established across participating universities. The progress made during the first five years of this grant has been remarkable. Over seventy papers have been written, and additional external support in excess of $2 million has been received.

62. Enhancing Corrosion Inhibition and Adhesion of Thermal Sprayed Tungsten-Carbide on Steel

This research cluster studies the causes of corrosion and mechanical failures in thermally sprayed tungsten-carbide (WC) coatings on steel by studying the materials and processes themselves. This approach has yielded real solutions in the commercial sector while attaining the goals of the EPSCoR program. New methodologies have already been made available to industry, including a test procedure to measure shear bond strength of coatings, better methods to measure oxide-layer formation during processing, and methods to provide quantitative correlation between surface morphology and corrosion rate. Current objectives include characteristic comparisons of identical coatings, a systematic study of process control parameters and continued investigation of basic science and engineering with regard to oxide layers. Additional objectives include evaluation of contaminant effect on corrosion and adhesion, the study of bonding/corrosion resistant underlayers, the correlation of corrosion characteristics with coating porosity, hardness and microstructure and ion implantation. The five Louisiana universities, including two HBCUs, of this cluster have made significant progress in Human Resource Development by involving both undergraduate and graduate students in the project. Additionally, high school teachers have participated in summer research programs, and seven master theses have been completed or are in progress. Two students are working on Ph.D. programs.

63. Louisiana Environmental Toxicology Program

The central theme of the EPSCoR Grant is the assessment of human and ecological toxicological risks associated with energy source development (e.g., oil/gas production), energy production (e.g., power plants), and associated wastes (e.g., produced waters, refinery effluents). The primary focus of the research is on the determination of toxicological consequences of exposure to energy-related materials and wastes at several levels of biological organization, including ecosystems, populations, organisms, specific tissues and the molecular level. Special emphasis will be placed upon genetic and reproductive risks and on trophic relationships. The study will examine effects of energy-related contaminants (1) on organisms at the base of the food web, including small invertebrates; (2) on organisms by examining changes in growth of fishes, amphibians and macroinvertebrates; and (3) on mammalian laboratory and feral species. The effects on the genetic diversity and fitness of fish populations will be assessed along contaminant gradients using model experimental systems. The effects of toxicants to which humans may be exposed directly through inhalation or indirectly through accumulation in food webs will be examined in rodent models. Assessments of the impacts of exposure to contaminants on metabolic functions of liver, gill, lung and central nervous systems will be performed using several endpoints.

64. New and Novel Large-Scale Synthesis of Buckybowls

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The possibility that the recently uncovered class of carbon cage compounds, known as the fullerenes, may lead to the development of new and technologically important materials has launched a rapidly growing and highly competitive research effort worldwide. The proposed research focuses on polynuclear aromatic hydrocarbons (PAHs) with carbon frameworks that can be identified on the buckminsterfullerene ("buckyball") C_{60} surface. These novel hydrocarbons, referred to as "buckybowls," are expected to have properties that are quite different from typical PAHs due to their curved surfaces, and the potential modification of their aromatic properties. However, a limitation to the investigation of these compounds—as well as a limitation to any potential commercial applications—lies with the current methods of synthesis. In most all of the cases so far, these buckybowls have been prepared with a flash vacuum pyrolysis as the last step in the synthesis, and this technique generally affords only milligram quantities. This proposed collaboration between LSU and

Oak Ridge National Laboratory will investigate new and novel approaches to making these new hydrocarbons in amounts that will allow for adequate investigation of their properties, and exploitation of their potential in new applications. The proposed approach will be to replace the gas-phase thermal processes with solid- or liquid-phase reactions, wherein the buckybowl precursors are "isolated" to prevent intermolecular reactions by attachment to solid supports or by microwave activation in a matrix.

65. Synthetic and Thermodynamic Investigations of Ancillary Ligand Influence on Catalytic Organometallic Systems

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This research project is a collaboration with two researchers at Los Alamos National Laboratory in the area of homogeneous catalysis. In a first instance we have synthesized partially fluorinated phosphine ligands for use in homogeneous catalysis in an effort to examine catalysis in nontraditional media using these ligands. The ligands do not display significant partitioning in biphasic fluorous-phase catalysis due to the low level of fluorination on the ligand. This same characteristic offers stereoelectronic control and fine-tuning capabilities when the catalysis is conducted in supercritical carbon dioxide ($ScCO_2$). The Tumas group at LANL is presently testing the reactivity of transition metal complexes bearing these ligands in catalytic transformations. Preliminary results indicate the ligand families to be able to support catalysis in such a medium. In a second arena, we have applied our expertise in solution calorimetry to the oxidative addition of boranes to transition metal centers in order to carry out thermochemical studies of borane reactivity with transition-metal complexes. This important activation reaction is a key step in catalytic hydroboration of olefins. Solution calorimetry are now coming online and will be communicated shortly. The thermochemistry of a number of relevant organometallic systems is being examined by solution calorimetry.

66. Alloy Thin-films and Surfaces for New Materials

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The unique properties of alloy thin-films and surfaces present the technological world with attractive new candidates for the development of (1) stronger high-temperature materials, (2) faster and more reliable microelectronic devices, and (3) better specialized bimetallic catalysts. To this end, this research program is focused on preparing, characterizing, and understanding the interconnecting physical and chemical properties of a variety of alloy surfaces and thin-films. We are employing a number of unique experimental probes in order to elucidate the correlation between atomic structure/ composition, electronic structure, and catalytic/chemisorption properties of these unique material systems. The research is centered on three parallel areas: (1) surface atomic and electronic structure of clean and modified intermetallic alloys (study of low-index faces of NiAl, FeAl and corresponding epitaxially grown metal alloy thin-films on these surfaces); (2) surface atomic and electronic structure of heteroepitaxially grown bulk-immiscible alloys (study of surface and thin-film alloy formation on low-index face substrates: Ag/Ni, Ag/Cu, Ni/Au, Pt/Au, Cu/Ni); and (3) surface chemistry of bimetallic thin-film alloys (study of CO, H_2, and H_2O chemisorption properties on the above-mentioned alloy thin-films and surfaces). In each of these areas, a battery of cutting-edge experimental techniques are being employed (e.g., synchrotron-based angle-resolved photoemission and core-level spectroscopy, surface X-ray diffraction and reflectivity, low-energy electron diffraction, and variable temperature scanning tunneling microscopy/spectroscopy). The goal of this project is not the isolated study of a single system, but rather the study of many related systems in order to extract general trends regarding the novel physical and chemical properties of alloy thin-films and surfaces.

B. Projects Supported by Office of Science

67. Molecular Dynamics Simulations of Nanostructured Materials on Parallel Computers

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Large-scale molecular dynamics simulations of ceramic and semiconductor systems are carried out at the microscopic level. Mechanical properties of environmentally benign substance, such as aerogel silica, will be studied, along with thermal properties of ceramic silicon nitrides and the crack propagation and fracture of thin films of these materials. In addition, new algorithms for parallel, distributed memory computing will be implemented.

68. Magnetic Properties and Spectroscopic Studies of Selected Rare-Earth-Transition Metal Intermetallic Alloys

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Hard magnetic alloys of the type $(NdDy)_2(Fe_{14-x-y}Co_xT_z)B_{1-n}C_n$ or $R_2(Fe_{17-x-y-z}Co_xCu_yT_z)C_n$ or $R(Fe,Co,T)_{12}C_n$ will be synthesized and characterized as to their microstructural and magnetic properties. The structural details and crystal field effects will be related to the magnetic properties as a function of various compositions and heat treatments.

69. Novel Micellar and Calixarene Derivatives for Selective Luminescence Measurements

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Research for this funding period has focused on continued studies of calixarenes as host molecules for analytical measurements. As reported in last year's report, several novel chiral calixarenes have been synthesized by use of a novel synthetic scheme developed on this program. Some of these calixarenes are being used as pseudophases in capillary electrophoresis to achieve selective chiral separations. These chiral calix(4)arene derivatives, when combined with electrokinetic capillary chromatography, have produced enantioseparation of three binaphthyl derivatives at pH values below 7. The structures of the calixarene derivatives and the buffer pH were found to be important factors in the chiral separations. Even more selective chiral separations are achieved when these chiral pseudophases are used in combination with achiral micellar media such as sodium dodecyl sulphate. Currently the general utility of these new chiral selectors is being examined for other chiral separations in capillary electrophoresis.

70. Polynuclear Aromatic Hydrocarbons with Curved Surfaces: Models and Precursors for Fullerenes

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The discovery of the fullerenes has provoked considerable interest in potential applications including batteries, conductivity, catalysis, and hydrogen storage, among others. This program deals with the synthesis and chemistry of polynuclear aromatic hydrocarbons possessing carbon frameworks represented on the buckminsterfullerene [C_{60}] surface. These so-called "buckybowls" serve as fullerene-models. The simplest example is corannulene, $C_{20}H_{10}$, the polar cap of buckminsterfullerene. However, corannulene undergoes rapid bowl-to-bowl inversion that lessens its utility as a fullerene model, and this program has sought "locked" bowl-shaped hydrocarbons: over 20 carbons and more than one five-membered ring (five-membered rings provide curvature). Goals include (1) the synthesis of new "fullerene-fragments"; (2) examination of the properties of these novel hydrocarbons, especially how large they must become before their properties become less PAH-like and more fullerene-like; and (3) the combination of fullerene-fragments to produce carbon cages. This program produced the first "locked" buckybowl (cyclopentacorannulene) and the first synthesis of a "semibuckminsterfullerene" ($C_{30}H_{12}$ corresponding to one-half of buckminsterfullerene). To date, two such hydrocarbons have been prepared. The synthesis of a $C_{32}H_{12}$ fragment was recently accomplished, and progress has been made toward the synthesis of $C_{46}H_{16}$. The latter hydrocarbon will represent the largest fullerene-fragment produced yet (by ten carbons), if successful.

71. Identification and Temporal Behavior of Radical Intermediates Formed during the Combustion and Pyrolysis of Gaseous Fuel

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We have extended our complementary shock tube studies of the thermal decompositions of the azines to include, in addition to pyrazine, pyrimidine and pyridine. The pyrolyses were investigated using laser schlieren densitometric measurements performed by Professor John Kiefer and his group at the University of Illinois, Chicago, and time-of-flight mass spectrometric determinations of the dynamic concentration profiles of reactants, products, and intermediates detected during the available observation times of 1 ms. The complementary experiments covered the temperature and total pressure ranges of 1600–2300 K and 150–350 torr, respectively. A free-radical chain reaction with initiation by ring C-H fission for all three azines is proposed. The measured C-H fission rates are compared and analyzed by RRKM theory. Barriers of 103 kcal/mol for pyrazine, 98 for pyrimidine and 105 for pyridine were calculated, supporting values lower than the barrier for C-H fission in benzene, 112 kcal/mol. The lower barriers for the azines are explained by the additional contributions of azyl radical resonance structures due to the neighboring N-C interactions which serve to further stabilize the azyl radicals. These results are related to the formation of various NO_x species produced during the combustion of heavy oils and coal.

72. The Preparation and Catalytic Applications of Silica, Alumina and Zirconia Supported Thermally Resistant Mono and Bimetallic Catalysts

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A new generation of thermally resistant supported metal catalysts prepared by the sol-gel method is currently under development. These catalysts derive their superior thermal properties by minimizing sintering processes which occur by surface diffusion. Because surface diffusion is substantially decreased when metal particle size is matched to the average pore diameter of the support, synthetic procedures aimed at attaining this match are under study. The resultant materials are being tested in the combustion of propane and methane, the dehydrogenation of *n*-butane , and the hydroisomerization of *n*-butane by superacid solid catalysts. Catalyst deactivation studies are being performed using a wide variety of in-situ spectroscopic techniques. The synthesis of catalytic ceramic membrane reactors to study dehydrogenation reactions is under study. It is anticipated that the separation and dehydrogenation properties of platinum and palladium can synergistically be used to improve olefin yields by shifting the position of equilibrium. The catalytic membrane reactor devices will be prepared using the slip casting method.

73. Dynamics of Multielectron Systems Interacting with Matter and Light

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The general theme of this project in atomic collisions is interdependency of electrons in atomic systems. Specifically, the dynamics of electron correlation are studied by examining reactions in which electron correlation is dominant. These phenomena occur in few electron transitions in fast collisions of photons and charged projectiles with atoms and molecules. Using synchrotron radiation one may observe both single and double ionization of simple atomic systems. Calculations are done using configuration interactions that specify the nature of electron correlation in terms of initial and final state correlation. Two and few electron transitions are also studied in interactions of atoms and simple molecules with charged projectiles. Two-center correlation is studied in systems in which projectile electrons interact with target electrons. Using first-order perturbation theory it was possible to relate cross sections for charged-particle impact to Compton scattering by photons. These relations are now being tested experimentally and are providing an emerging picture of mechanisms for the dynamics of electron correlation. A more complete description of these and other methods is included in *Electron Correlation Dynamics in Atomic Collisions*, published by Cambridge University Press in 1997.

74. Photoinduced Energy and Electron Transfer Reactions in Light Harvesting Arrays of Transition Metal Complex Chromophores

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Ruthenium(II) diimine complexes have been shown to be particularly effective sensitizers for dye-sensitized photoelectrochemical cells having nanocrystalline TiO_2 as a high-surface-area adsorbate for the dye. Our efforts have focused on (1) devising new light harvesting arrays capable of absorbing a higher fraction of incident photons per adsorbed molecule and (2) understanding and controlling excitation energy migration in multimetallic Ru(II) diimine complexes. Through systematic investigations of intramolecular energy transfer in bimetallic complexes, bridging diimine ligands (linked bis-2,2'-bipyridyl ligands) have been found which are capable of mediating energy migration between adjacent metal centers with 100% efficiency. In addition, simple synthetic strategies have been developed for preparing the most effective of these ligands. Using these ligands, arrays of chromophores can be prepared at interfaces via sequential reaction of complementary components in which coordinate covalent bonds are formed. Methods have been developed for synthesis of multimetallic arrays in which intact chromophoric centers are linked, thus avoiding problems associated with synthesizing sensitizers at the semiconductor-solution interface. This is achieved by preparing diimine complexes having phosphonic acid substituents and taking advantage of the exceedingly low solubility of various metal phosphonates. Light-absorbing complexes can then be deposited in a stepwise fashion on a metal oxide semiconductor surface. It has been demonstrated that films of these complexes are electroactive and that films having at least three layers of complex are uniform and pinhole free on SnO_2.

75. Photochemical Studies of Two-Component Organic Systems within the Restricted Spaces of Zeolites

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In this project we propose to establish that by confining reactants to a particularly shaped space, zeolites can direct reactions to specific products. Reactions to be investigated are initiated by light, where possible, by visible light. This strategy will have an impact on how fine chemicals are synthesized in the laboratory and in industry. One of the reactions investigated is the oxidation of olefins. Unprecedented selectivity has been observed when the reaction is carried out within the restricted spaces of a zeolite. The main reagent used in this reaction are abundantly available "air" and "sunlight." The products are synthetically most useful alcohols. This reaction will be studied in great detail so that it can be developed into a "clean" method to activate (functionalize) hydrocarbons. Another aspect of the research deals with generating and stabilizing highly reactive intermediates within zeolites. Intermediates, such as carbocations, cation radicals, and carbenes, are highly energy-rich. They are considered to be very reactive and are established to live for less than a few microseconds in solution. It has been shown that radicals can be generated readily within zeolites and that they have a considerably long lifetime when encapsulated within the confined spaces of a zeolite. Future studies will be directed towards restraining the reactivity of energy-rich reactive species.

76. Identification of Chloride-Binding Domains in Photosystem II

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This project describes research which will elucidate the interaction of chloride with the oxygen-evolving site of Photosystem II (PS II). These interactions will be studied using a combination of physiological, biochemical and molecular tools. First, site-specific protein-labeling reagents will be used to differentially modify various PS II preparations in the presence and absence of chloride. Differentially modified domains will be identified by the use of “Cleveland Mapping,” mass spectrometry and N-terminal protein sequencing. Individually modified amino acid residues will be identified using a mass spectrometer equipped with a reflectron, allowing the analysis of metastable fragments by the use of post-source decay methods. These experiments will identify regions and individual amino acids on the intrinsic components which interact differentially with the cofactor. Second, a comprehensive analysis of several CP 47 mutants, including R448S and K321G, which exhibit alterations in their chloride requirement for oxygen evolution will be performed. Of particular interest is the examination of the phenotypes exhibited by these mutants during in vivo chloride depletion and reconstitution experiments. Oxygen evolution capacity, analysis of fluorescence yield parameters and an analysis of their flash oxygen yield properties are proposed. Third, suppressor analysis will be performed on spontaneous and chemically induced revertants of the CP 47 mutants R448S and K321G. Intergenic suppressors will be identified, mapped and sequenced to determine the identity of proteins interacting with these locations (^{321}K and ^{448}R) which modulate the chloride requirement for oxygen evolution in the CP 47 protein.

77. Molecular Characterization of Bacterial Respiration on Minerals

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Aerobic respiration on reduced iron is a principal metabolic activity exhibited by certain chemolithotrophic bacteria that inhabit ore-bearing geological formations exposed to the atmosphere. Each phylogenetically distinct group of iron-oxidizing bacteria expresses one or more unique acid-stable, redox-active biomolecules in conspicuous quantities during aerobic respiration on iron. Structural and functional studies continue on two such novel biomolecules that have been purified to electrophoretic homogeneity: rusticyanin from *Thiobacillus ferrooxidans* and cytochrome$_{579}$ from *Leptospirillum ferrooxidans*. The aim of these studies is to determine the role of each protein in the iron respiratory chain of its respective organism. Other redox-active components present in cell-free extracts of iron-oxidizing organisms continue to be sought, isolated, and investigated with regard to their roles in the same respiratory chains. Another aim is to investigate the mechanisms, consequences, and principal features of bacterial adhesion to insoluble minerals. The specific, selective adhesion of *T. ferrooxidans* to pyrite was recently shown to be mediated by aporusticyanin located on the outer surface of the bacterial cell. Efforts are in progress to identify, isolate, and characterize other mineral-specific receptors expressed in different genera of the chemolithotrophic bacteria that respire on insoluble minerals. It is anticipated that this project will provide useful information toward manipulating *T. ferrooxidans* and related organisms for commercial use.

78. Biochemistry of Dissimilatory Sulfur Oxidation

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Dissimilatory sulfur-oxidizing bacteria obtain all of their energy for metabolism from the aerobic oxidation of reduced inorganic sulfur compounds. Despite the environmental and economic importance of these organisms, there is still much uncertainty regarding the actual metabolic pathways and the stoichiometries of these bacterial oxidation reactions. This project has two major experimental goals: (1) to quantify the adherence of sulfur-oxidizing bacteria to their insoluble elemental substrate; and (2) to define the substrate oxidation pathways, the electron transport mechanisms, and the modes of energy conservation employed by various species of the thiobacilli. Studies on the interaction between bacteria and insoluble sulfur exploit field flow fractionation, laser Doppler velocimetry, electrical impedance, static and dynamic light scattering, surface tension, contact angle, and other measurements commonly employed to characterize colloidal particles. Studies on the latter goal currently focus on the enzymology of polythionate degradation in those thiobacilli that accumulate polythionates in the culture medium. Efforts to isolate and characterize trithionate hydrolase, thiosulfate dehydrogenase, and tetrationate hydrolase from cell-free extracts of both neutrophilic and acidophilic thiobacilli are in progress. It is anticipated that this information will be of value in the eventual manipulation of the thiobacilli and related organisms to benefit both the environment and the mining industry.

79. Numerical Simulations of Plasma Turbulance in the Tokamak Scrape Off Layer and Near the Divertor

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The purpose of this project is to study mechanisms of turbulence in the tokamak edge by means of nonlinear fluid simulations. The instabilities that have been studied are the parallel velocity shear instability in a sheared magnetic field, the radiative condensation mode in noncoronal equilibrium, and interchange modes driven by the existence of neutral particles. By means of the simulations and analytical work, we have not just predicted the behavior of these instabilities in an edge plasma, but because we have taken a fundamental plasma science approach, have developed some insight in identifying the mechanisms controlling the nonlinear behavior of these modes. We have recently begun work on another instability of importance to the edge, the sheath-driven electron temperature gradient mode. We are in the process of improving the fluid model by including nonlinear kinetic effects in the fluid equations in order to observe what quantitative effect this may have on our previous results that were based solely upon fluid equations. Unlike most university research projects in fusion science that typically involve graduate students and postdoctoral scientists, this project involves undergraduate students who work directly with the faculty member on the research. Much of the work has been performed in collaboration with physicists from the Plasma Science and Fusion Center at MIT.

80. Information Systems Technology for Energy and Environmental Applications

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The Internet is fast becoming the source to which individuals turn for information in many areas. This distributed collection of information resources and services has the potential to be enormously helpful in performing information-intensive tasks, such as those found in environmental and energy applications. But these information sources are extremely varied in content and format. Accessing available resources is further compounded by the problem of variability in client/server protocols. Furthermore, there is practically no evaluation of the usefulness or reliability of the data available on the Internet. The objective of this project is to develop an Energy and Environmental Information Resources Center. The Center will develop software tools based on the enabling technologies of digital library and data mining. These software tools can be considered as information agents since they meet user needs by providing the relevant information and by suggesting analysis tools, depending on the nature of the requests and search results. The Center will also develop a repository of information, especially that pertaining to the Gulf Coast region, which is important for energy and environmental operations. The Center will cater to clients from private and public sectors and support activities of individuals involved in scientific research, business and economic development, government policy, and education. Research will be conducted in multimedia indexing, data mining, parallel and distributed computing, and graphics and visualization. The development of information technology methods to manage energy and environmental issues is vital to the nation's interests. Energy demand from oil and gas is expected to remain at high levels well into the future. The Gulf of Mexico region is the source of almost 85% of the nation's oil and natural gas (including imports). It is a region rich in natural resources, but it is also an environmentally fragile area. Prudent development of public and private energy and natural resources depends on having information and technologies to understand, quantify, and assess the risks and consequences of oil and gas development and transportation. Timely and ready access to relevant information, especially by the energy industries, is critical for environmentally and economically sound utilization of this ecological system. This project supports DOE's mission for both energy security and environmental quality. Furthermore, the project's digital library development work is being conducted in collaboration with the information science professionals at the DOE Office of Scientific and Technical Information.

81. Reducing Energy Consumption and Pollution in Plastic-Manufacturing Processes: Phase Behavior Roots of Fouling Phenomena that Cause Energy and Product Waste

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The overall goal of this project is to understand the phase behavior of ethylene copolymers in compressible fluid streams, such as copolymer solutions in supercritical and near-critical fluids. Such understanding is needed to develop new plastic-manufacturing processes that are less energy-intensive, and produce less pollution and less waste products. Specifically, such understanding is needed to be able to control undesirable phase transitions and, hence, eliminate the root cause of fouling phenomena in pipelines, reactors and separators. This is in contrast to mitigating the fouling consequences using specially treated surfaces and additives. The approach is a synthesis of experiment and thermodynamic modeling. The experiments will be aimed at accurate phase-transition data for well-characterized model polyolefin systems. The thermodynamic modeling will focus on predicting such phase transitions. The basis for this approach is a series of preliminary but promising experimental and computational results with an equation of state, referred to as the copolymer statistical associating fluid theory (SAFT). The copolymer SAFT should explicitly account for the effects of microstructure on the thermodynamic properties of copolymers. This has never been done before and will impact the way we characterize very large, structured molecules. The objectives proposed for this project will concern a specific system of ethylene copolymers and small olefins. The focus will be on the effect of branchiness (hence crystallinity) and molecular weight on the phase transitions that induce undesirable fouling phenomena.

82. Combining Steam-Methane Reforming, Water-Gas Shift, and CO_2 Removal in a Single-Step Process for Hydrogen Production

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The objective of this project is to investigate a number of options for improving the steam-methane reforming process for hydrogen production. It has been recognized for several decades that an improved process is theoretically possible if some of the processing steps, now conducted separately, are combined. However, the identification of a practical approach to implementation of the improved process has proved to be elusive. This proposal identifies a catalyst and processing conditions that may allow the reforming and shift reactions to be conducted in the presence of a carbon dioxide acceptor (lime). If successful it will identify a practical approach for realizing the benefits of the combined process.

83. Monte-Carlo Simulation of Surface Growth

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In this project we plan to carry out systematic, large-scale Monte-Carlo simulation of surface growth in both the submonolayer regime and in the large-scale, late time-scaling regime. In the submonolayer regime, we are interested in simulating the coarsening of the island-size distributions at fixed coverages as a function of time after the incident flux of atoms has been turned off. We want to study the temperature dependence of coarsening in surface growth at different temperatures, up to and beyond the critical-phase separation temperature. In the scaling regime, different growth mechanisms led to different universality classes, characterized by independent exponents. Different macroscopic growth equations describe these growth processes. However, it is difficult to distinguish between these equations by measurement or calculation of the exponents alone. We want to study the local slope through calculation of the height-height correlation function. This quantity is a unique feature that can be used to distinguish the linear diffusion processes from the nonlinear ones. We expect that our computational approaches and our results will be applicable to a broad range of related materials and processes.

84. Research in Elementary Particle Physics and Cosmic Ray Physics

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The Louisiana State University high-energy physics group-theory task is studying lattice-gauge theories. The experimental task is studying electron-positron collisions above the Z at the L3 experiment at CERN, atmospheric and solar neutrinos at the Super Kamiokanda experiment in Japan and neutrino physics, especially evidence for neutrino oscillations, at the LSND experiment at Los Alamos and the BooNE experiment at FERMILAB. Recently, LSU has joined the Auger experiment, which will search for the origins of the highest-energy cosmic rays.

85. Research in Particle Physics

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The Liquid Scintillator Neutrino Detector (LSND) and Oak Ridge Large Neutrino Detector (ORLaND) are being funded at Southern University, Baton Rouge, by the High-Energy Physics Division of the Department of Energy. LSND is a neutrino experiment at the Los Alamos National Laboratory, New Mexico. There are 12 collaborating institutions including Southern University. We are involved in all phases of this experiment, which included construction and commissioning of the detector, data taking, data analyzing and software development. Based on LSND data, Southern University student Tony Cochran completed his M.S. thesis in the summer of 1998. A new graduate student, Rodica Samodi, is expected to analyze LSND data for her M.S. thesis. She is currently finishing her course work, and will start her thesis very soon. Also, we are currently analyzing LSND data for a publication to be published in a refereed physics journal. A postdoc, two students and one faculty member are currently working on this experiment. The ORLaND is a proposed neutrino experiment which is expected to begin at Oak Ridge National Laboratory. Southern University has a leading part in this experiment, with Dr. Fazely as the deputy spokesperson. The proposal has already been completed, and a physics panel of leading physicists in the country will review it very soon. Southern contributions to this experiment were to provide support for detector simulation and to prepare the proposal for the final manuscript. Southern is currently preparing an electronics data acquisition system needed for various physics tests by these nuclear and particle physics experiments.

86. Weak Interactions in Nuclear Physics and Nuclear Astrophysics, using Many-body Theory

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The weak nuclear interaction is key to understanding astrophysical processes, from controlling the gravitational collapse of massive stars to allowing neutrino observatories to peer inside our sun. We are developing new mathematical and computational techniques to describe the nuclear reactions relevant to weak interactions, including extensions of the "traditional" matrix-diagonalization approach to the nuclear shell model, as well as alternative

Monte Carlo and statistical methods. The techniques we are developing include (1) random matrix models of nuclear level densities, needed for neutron capture in r-process nucleosynthesis; (2) statistical methods for strength function distributions, needed for electron capture on iron group nuclides in pre-supernova cores, which in turn governs the critical lepton fraction in gravitational collapse; and (3) new base sets for the nuclear shell model that will incorporate both single-particle and collective degrees of freedom. These techniques are then applied to nucleosynthesis, neutrino transport in supernova, and the neutrino capture cross-sections for terrestrial detection of neutrinos from the sun and type-II supernovae.

87. The Structure of Nuclei Far From Stability

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Atomic nuclei are fundamental to our studies of everything from quarks to cosmology. Nuclei are the laboratories in which we study the smallest constituents of matter and the fundamental symmetries of nature. Nuclear reactions powered the stars and forged the elements during the Big Bang and supernova explosions. The excitement of modern nuclear physics is its interdisciplinary nature and its use of a wide range of techniques and tools. Although a number of national facilities are utilized, the major part of the program focuses on the Holifield Radioactive Beam Facility at Oak Ridge National Laboratory. This facility is providing a new frontier in nuclear-structure physics. The research will also provide additional insight into nuclear astrophysics through the study of reactions and decays which bear on our understanding of nucleosynthesis. The principal foci of the experimental program is the study of nuclei far from stability, using radioactive ion beams and a "state-of-the-art" recoil mass spectrometer.

88. Field-Portable Immunoassay Instruments and Reagents to Measure Chelators and Mobile Forms of Uranium

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The Holy Grail of bioremediation assessment is the ability to measure contaminants faster, cheaper, and better. This proposed research promises to do just that. They propose to develop a hand-held detector that is inexpensive (about $5,000) to buy, inexpensive to operate (less than $100 per sample), rapid (less than one hour per test) and can be operated by minimally trained personnel. They propose using immunoassays, which are used for example in home pregnancy tests, that will provide information on a metal's oxidation state and speciation.

STATE OF MAINE

A. Projects Supported by EPSCoR

89. Maine DOE EPSCoR Implementation Award

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This renewal application builds upon progress made to date to strengthen the state's and the nation's energy-related research and development infrastructure as initiated under Maine's 1993 DOE/EPSCoR Implementation Cooperative Agreement and as continued under DOE/EPSCoR Round 2. The purpose of this section is to document the management and coordination infrastructure used to implement Maine's DOE/EPSCoR Program and its progress in meeting program milestones and schedules. The Maine DOE/EPSCoR Program offers to: (1) continue support of a Human Genome Research Cluster to its next logical growth stage; (2) continue support of a University of Maine Materials Science Research Cluster in Tribology; (3) strengthen and expand a University of Southern Maine/Maine Geological Survey/University of Maine Research Project in geophysics and geochemistry; (4) continue and enhance the Maine Research Internships for Teachers and Students (MERITS), a K-12 program that includes a new technical development component; (5) support two research projects: one in intelligent systems research and education at the University of Maine and the other in molecular biology infrastructure building at the University of Southern Maine; (6) continue support for energy conservation technology and hazardous materials management training programs at Kennebec Valley Technical College; (7) link K-12 schools and libraries throughout the state to EPSCoR-supported research clusters through communications networks, such as the Internet, to promote interaction between cluster researchers and the state's science and mathematics instruction; (8) coordinate a series of R&D commercialization workshops, partnering with Kentucky's DOE/EPSCoR; (9) link DOE labs with research and development opportunities in Maine; and (10) strive for continuous management and coordination improvements.

Research Clusters Initiatives

90. Hierarchical Chromosome Organization in Mice (The Jackson Laboratory, Eastern Maine Medical Center, Maine Medical Center Research Institute and the University of Maine)

The basic research aspect of this cluster concerns the development of methodologies for structural and functional mapping of mammalian chromosomes. The proposal requests funding for continued implementation of a comprehensive strategy to establish a nationally competitive human genome research program in the State of Maine. This plan builds upon the major achievements of Round 1, strengthening the successful research components and expanding opportunities for scientists around the State. The elements of the plan are (1) provide funding for innovative investigators to pursue projects in genome research with the goal of achieving national competitiveness; (2) train Maine researchers from diverse institutions in contemporary genetic techniques; (3) assist scientists in the planning and preparation of competitive national grant applications; (4) support an outreach program to expose secondary students and undergraduates to genome research; (5) attract young scientists to train in the state, and (6) create access to existing and emerging technologies around the world. The research goals fall within the Human Genome Program of the DOE's Office of Health and Environmental Research. The nation's Human Genome Project is a national endeavor originated by the DOE. Five major projects address genome organization and function using new and cutting-edge technologies. Together, they exploit the special advantages of mice as an experimental system for human genome analysis. The approaches span the hierarchy of chromosome structure: (1) automated karyotype analysis using artificial neural networks; (2) developing techniques for purifying specific mouse chromosomes to study their architecture; (3) constructing a physical map of the mouse Y chromosome—the most technically challenging chromosome in the genome; (4) deducing structure/function relationships by comparative analysis of human and mouse Y chromosomes; and (5) systematically identifying gene functions by generating deletion complexes of specific chromosomal regions. The human genome cluster encompasses scientists from university, basic research, and clinical institutions. Inter-institutional collaborations established during the initial award period will be reinforced, and new relationships formed. An Investigator Enhancement Program will aggressively encourage interactions and stimulate new projects. A major emphasis is placed on the practical training of inexperienced scientists to prepare strong grant applications. Interactions established with three national laboratories during the first year of funding (Lawrence Livermore, Los Alamos, and Oak Ridge) will be continued and strengthened, and an outreach program is proposed to expose young Mainers to science research. Considering the impressive progress made to date, the expanded scope of this cluster is certain to make great strides towards Maine's national competitiveness and achievement in the Human Genome Project.

91. Physical Mechanisms in Tribology (University of Maine)

This proposal, from the Laboratory of Surface Science and Technology at the University of Maine, is a direct outgrowth of a former DOE/EPSCoR HRD project known as the "Micromechanical and Thermochemical Properties of Composite Materials." This group is establishing a research cluster for Micro-Tribology, with emphasis on the friction and wear of advanced materials. Tribology is the study of interacting interfaces between materials that are in relative motion and includes the study of friction, adhesion, lubrication and wear. Tribology is important in nearly all areas of technology and is a major factor in determining the energy efficiency and lifetime of equipment. In spite of this importance, the basic physical and chemical processes that determine tribological properties are not well understood particularly at sub-micrometer dimensions. For example, contact between two solid materials is not continuous but occurs through small asperities. Theories of friction and wear assume that the properties of these asperities can be described by parameters measured for macroscopic materials even though this is known to be incorrect in many cases. The primary goal of the cluster is to establish a competitive tribology research program at the University of Maine. This program will emphasize quantitative study of friction-and-wear mechanisms at the nanometer-to-micrometer-length scale for polymers, ceramics, semiconductors and their interfaces with other materials. The applicants emphasize these materials, rather than metals, because of their increasing use in technical applications and because they allow the applicants a wide range of physical parameters. A linking feature of all of the projects is a concentration on determining the properties of single, sub-micrometer asperities in sliding contact with various substrates. Metal, ceramic and polymer asperities will be used. During the first three years, the cluster will experimentally explore the limits to current continuum theories of friction and wear and establish a database for the development of new theories. They will expand their research to include the effects of lubricant films. An important aspect of their initial research is to develop new experimental apparatus and techniques to carry out the research. Infrastructure improvements include establishing a tribology research laboratory. The cluster is replacing an obsolete atomic force microscope, purchasing a pin-on-disk tribometer, and constructing a nano-tribometer specifically designed for dynamic studies of friction and wear involving point contacts. This group of instruments will allow the cluster to study tribological processes from molecular to macroscopic scales and will be available to other research groups at the University of Maine and in-State industries. Human resource improvements will include technical training of postdoctoral scientists, graduate students and undergraduate students. One University of Maine faculty member will obtain a Ph.D. An atomic-force microscope will be introduced into the graduate and undergraduate laboratory courses in physics. The cluster will work with the University's Department of Industrial Cooperation and Paper Surface Science Program to focus on materials relevant to Maine industries. The cluster will also work with the Maine Physics Teachers Association and the DOE/ESPCoR MERITS to establish a summer internship for high school science students.

Human Resources Development Initiatives

92. Maine Research Internships for Teachers and Students (MERITS)

This program is targeted for expansion in 1996 and 1997 with other sources of funds, including DOE/EPSCoR. Maine EPSCoR will continue to support the MERITS program with DOE/EPSCoR funds at the same level of support provided in Round 2. DOE/EPSCoR funds will provide support for K-12 teachers, high school student-teacher teams, and undergraduate student research in energy-related areas. Special emphasis is placed on involving equal numbers of young women and young men as part of the selection process. Linkages have been formed between the human genome and materials science clusters and several other HRDs for the following year. Incorporated into this expanded program is a technical college component, called "Tech Prep," which integrates students into a technical college education beginning in their junior year of high school, leading them through a rigorous curriculum which finishes with an associate degree or a certificate in a technical field. MERITS has received State EPSCoR, NSF/EPSCoR, and DOE/EPSCoR support and has provided research opportunities for 47 high school students, 41 teachers, and 27 under-graduate students since its creation in 1992 by Maine EPSCoR and Maine Mathematics and Science Alliance (MMSA). MMSA is a non-profit 501(c)(3) organization created to administer the state's 5-year, $10-million National Science Foundation award to reform K-12 science and mathematics education.

93. Energy Conservation Training Program (Kennebec Valley Technical College)

Maine EPSCoR will continue to support the lab and classes at Kennebec Valley Technical College begun in mid-1994 with state funds from the 1993 DOE/EPSCoR Implementation Grant. This program is currently finishing its hands-on training lab and offering classes to current and future electrical/electronic technicians in "cutting edge" energy conservation technology. This program will become completely self-sufficient in 1998 after the program has grown in enrollment and KVTC takes over full financial support.

94. Hazardous Materials Management Training (Kennebec Valley Technical College)

Maine EPSCoR will continue to support the hazardous materials management training classes at Kennebec Valley Technical College begun in mid-1994 with funds from the 1993 DOE/EPSCoR Implementation Grant. These training sessions currently train Maine's Emergency Medical Service Technicians in areas such as nuclear materials handling, radiation effects, and hazardous materials response. No other program like this exists in Maine. This program will become completely self-sufficient in 1998 after the program has grown in enrollment and KVTC takes over full financial support.

95. Collaborative Groundwater Resource Group (University of Southern Maine, University of Maine, Maine Geological Survey)

Maine EPSCoR will continue to support the University of Southern Maine (USM)'s Geoscience Department and the Maine Geological Survey (MGS) for their effort to address important groundwater issues in the state. This project is expanding in its third year by collaborating more significantly with the University of Maine (UMaine) at Orono's Geoscience Department and the Sawyer

Environmental Institute. UMaine is in the process of hiring a new faculty member with expertise in hydrogeochemistry. This new staff member will collaborate with the recently hired geophysicist at USM to offer more diverse classes and seminars on both campuses, train undergraduate and graduate students, provide student internships at the MGS and federal DOE labs, and add appropriate equipment to each teaching lab. This reformulated group is actively addressing the need for technology transfer to industry and public sector geologists in the state with an emphasis on geophysical applications to Maine groundwater problems.

96. Technology Transfer: Industry/Faculty Collaborations (Center for Innovation in Biomedical Technology and the Center for Technology Transfer)

Maine EPSCoR will continue to support industry/faculty collaborations through the Center for Innovation for Biomedical Technology (CIBT) and the Center for Technology Transfer (CTT) to foster the transfer of human genome, materials and sensor technologies to the private sector. CIBT and CTT are two of three industry-led 501(c)(3) industry outreach centers supported by Maine EPSCoR and MSTF. CIBT supports human genome investigators through a competitive grant program, "Cooperative Development Grant Program," and effectively links human genome investigators with investigators working in for-profit biotechnology industry. CTT accomplishes the same task in sensor technology and composite materials research. Investigators involved with this center, supported by a competitive grant program, "Challenge Grant Program," are linked with specific industry needs within the state, such as hazardous waste detection in the metals product manufacturing industry, the detection of transmission line sap for the electric power industry, and sea pen security for the aquaculture industry. Board members who oversee these centers include individuals from the specific industries served by them, as well as from labor, technical colleges, universities, non-profit research and health care institutions, and state government.

97. Development of Intelligent Systems Expertise in Maine (University of Maine)

This project is a first of its kind in the state and perhaps in the nation. The PIs will focus their efforts on the application of intelligent systems technology to promote energy-efficiency and enhanced productivity in the pulp and paper, electric power, and a targeted number of smaller industries within the state of Maine. The work of the PIs will bring the University, industry, and local education together to enhance the state's S&T infrastructure and prepare it to meet the global challenges of the future. Without lowering its standard of living, Maine industry cannot compete in a world economy using manual labor or mechanized processes using low levels of automation. The future of Maine industry lies in the ability to sense, gather, and process information to utilize energy in the most efficient manner. Maine industry will be forced to incorporate advanced sensor applications, computer automation, adaptive/robotics control, distributed processing, networking, and database management at levels heretofore unseen to handle large amounts of energy and compete in a world economy. Increasingly, information will be processed nearer its source using inexpensive microprocessors incorporating neural networks, fuzzy logic, artificial intelligence, or other advanced methods of data processing. The coordinated application of all these technologies form the basis of the term, "intelligent systems," as used in this proposal. The University of Maine's Department of Electrical and Computer Engineering consists of a highly diverse group of educators with expertise spanning the spectrum of intelligent systems technology. Supported by key faculty in the Department of Chemical Engineering and the University of Southern Maine, the applicants propose to transfer understanding of intelligent systems in an unprecedented industry outreach program designed to bring industry and educators together in an organized effort to increase the energy efficiency, productivity, and economic security of large portions of the pulp and paper, electric power, and selected, smaller industries within Maine. The applicants also wish to heighten the general public's awareness of the need to apply advanced engineering methods to promote energy efficiency. To this end, they propose an innovative educational effort aimed primarily at high school students and teachers in local industry towns. The program, conducted by graduate and undergraduate students under our guidance, will involve local high school students in the process of solving engineering problems from inception to resolution. The goal is to give high school students and teachers a better understanding of engineering methods, a familiarity with technology used in their own local industry, and the need for seeking higher education to solve energy-related engineering problems. The University of Maine is committed to enhancing energy education in the State of Maine. The applicants have budgeted a new faculty position to further strengthen the project team in the application of intelligent systems technology to electric power systems. The College of Engineering has agreed to convert this project-funded position to a full-time tenure-track faculty position at the project conclusion.

98. Molecular Biology Infrastructure Capacity Building (University of Southern Maine)

The first objective of these human resources development activities is to provide modern biology education for undergraduate and graduate students, and continuing education for employees of commercial and nonprofit organizations. The second objective, which follows from the first, is to increase the research capabilities at the University of Southern Maine and, by extension, of the Maine biotechnology community. These objectives will be achieved by: (1) recruiting and providing support for two faculty positions at the University of Southern Maine, (2) creating scholarships designated for students enrolled in a modern biology curriculum at the University of Southern Maine, (3) creating an internship program through which undergraduate students can obtain modern biology experience in company and research organization laboratories, (4) providing graduate student fellowships for students in the Applied Immunology Program, (5) providing continuing education for employees of biotechnology companies and nonprofit organizations, and (6) creating an advisory board with company and nonprofit organization representation. At USM students can focus on cell biology and biochemistry within the biological sciences program or complete an interdisciplinary program in biotechnology. A graduate program in applied immunology is closely affiliated with the undergraduate programs. An articulation arrangement enables motivated and forward-thinking students to complete a bachelor's and master's program in five years. The graduate program is also aligned with various nonprofit research organizations, as well as with area biotechnology companies, the Foundation for Blood Research (FBR), and the Maine Medical Center Research Institute (MMCRI).Other nonprofits include the Jackson Laboratory and the Bigelow Laboratory for Ocean Sciences, as well as colleges and universities. There are already close collaborations with nonprofit research organizations such as the Foundation for Blood Research (FBR) and the Maine Medical Center Research Institute (MMCRI), and with several biotechnology companies in Maine. USM, FBR, and MMCRI, and a number of companies have some expertise in molecular biology but there is not yet a "critical mass" of individuals who have such expertise. Additionally, involvement through one of their researcher grant programs or with the human genome research cluster located at the Jackson Laboratory in Bar Harbor will provide for additional training and educational opportunities as well as for research collaboration.

99. K-12: Maine Internet Education Consortium

The Maine Internet Education Consortium (MIEC) was formed as a public/private partnership in the summer of 1995 under the direction of MSTF. Bringing together educators, university researchers, administrators, and librarians from across the state, the MSTF envisioned a model training program at three sites to begin to address the technology training needs of teachers and students in the state. This last fall, the Maine Public Utilities Commission (PUC) required NYNEX, our local New England phone company, over the next five years to repay its ratepayers over $20 million of money they were overcharged. Innovatively though, they offered NYNEX the opportunity to repay the money by hooking up every school and public library in the state to a 56 Kbps, dedicated, digital line. In the next five years, the state's schools and libraries will be fully networked with access to the Internet and the World Wide Web. Serendipitously, the MIEC training program was advanced enough to answer the training component needs of the NYNEX PUC ruling. MIEC's training program, built around a train-the-trainer model, will now serve the entire state, rather than a small portion. A program director plus appropriate staff will be hired and will operate out of MSTF. Each community in the state will be expected to submit a "technology plan" and to make their technology training needs known to the MIEC and its staff who will then set up a training program tailored to the community's technology education requirements. Schools and libraries, along with their communities, will be expected to sustain and enhance their individual programs. MSTF has sought and received additional funding from the UNUM Foundation ($48,000 thus far) to help support the MIEC. Other funding sources are being contacted as the project moves forward. The NYNEX funds for the training will total approximately $500,000 over the next year (see budget page, Sect. 3.8). The original $50,000 in DOE/EPSCoR Round 2 funds has leveraged over $548,000 from private sources in this year alone with more to come in the outlying years. The benefits of such a program in the state cannot be overstated. It would increase access to S&T information; increase teachers' capacity to teach by incorporating new methods of instruction with greater access to information; increase the understanding and application of S&T for all Maine teachers and students, with special emphasis on underrepresented women, minorities, and individuals with disabilities; increase the link between schools and research institutions to facilitate the transfer of knowledge; and use technology to improve information management by teachers and students.

B. Projects Supported by Office of Science

100. Synthesis, Characterization and Mechanical Behavior of Binary and Ternary Oxide Films

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Research focuses on the (1) fundamental properties of metal/oxide and oxide/oxide heterogeneous interfaces with emphasis on effects of interfacial defects, impurities, carbon layers, and amorphous phases on interfacial morphology, adhesion, electronic structure, and high-temperature stability; (2) deposition of ultra-thin metal and oxide films (viz, Al, Ti, Cu, Mg0, Y_2O_3, and SiO_2) on single-crystal Al_2O_3 substrates; and (3) determination of film epitaxy and interface morphology by in-situ RHEED analysis and Atomic Force Microscopy, with determination of composition, chemical bonding, interdiffusion, segregation and electronic structure information by X-ray and ultraviolet photoemission, Auger spectroscopy, and EELS.

101. Organic Carbon Burial in the Cape Hatteras Ocean Margin: Relationship with Mineral Surfaces

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This research assesses the role of mineral surface areas in controlling organic carbon burial and determines the control(s) on replacement of terrigenous carbon by marine carbon in the coastal zone.

102. Database Management Research for the Human Genome Project

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Summary not available.

103. Flexible Greenhouse Gas Emission Banking Systems

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Permit trading systems are more efficient than alternative regulations in a variety of circumstances. Most research has been on same-period trading between industries or regions. However, banking systems allow owners of permits to put aside current allowances for use in later years, essentially permitting reallocation of resources to the highest value without time constraints. Intertemporal systems allow the additional time flexibility so that firms can manage pollutant flows according to some internally determined optimal time path. There is growing literature on the properties of these intertemporal permit trading systems. The current literature on intertemporal systems is focused on pollutants that are short lived, hence termed "flow" pollutants. However, this research proposes to investigate theoretical and numerical characteristics of systems that are designed for "stock" (long-lived) pollutants. The application is to carbon dioxide; however, most of the results should apply to other long-lived pollutants, such as radionuclides from DOE legacy programs.

STATE OF MISSISSIPPI

A. Projects Supported by EPSCoR

104. Impact of Random Numbers on Parallel Monte Carlo Applications

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The Department of Energy (DOE) mission has always included scientific areas where Monte Carlo computation is fundamental. In fact, at any given time, a substantial fraction of high-performance computing cycles at DOE facilities are devoted to Monte Carlo methods. This situation has persisted for as long as the DOE has been involved in computational methods. Loosely, a Monte Carlo method is any numerical technique that uses randomness in some way. Randomness is computationally embodied in a deterministic random number generator (RNG) that is used to simulate randomness in a computationally desirable context. It is fair to say, then, that a Monte Carlo algorithm can be viewed as a computational "black box," where random numbers are the input, and the quantities of interest are the output. Clearly, the fidelity of the output is highly dependent on properties of the input. Thus, it is equally clear that for high-end DOE Monte Carlo applications to succeed, these applications must rely on high-quality RNGs. Over the past three years, the PI has been developing a Scalable Parallel Random Number Generators (SPRNG) library under a DARPA contract in collaboration with the National Center for Supercomputing Applications (NCSA) in Urbana, Illinois. SPRNG (http://www.ncsa.uiuc.edu/Apps/SPRNG) was designed in a close collaboration between mathematicians, computer scientists, and computational scientists to produce a comprehensive random number generation tool for parallel Monte Carlo applications. The goal of this project will be to design a comprehensive random number generation tool for high-end DOE Monte Carlo applications. In particular, the new tool will include:

- incorporation of new RNGs that have DOE-appropriate speed/memory tuning,
- study and incorporation of different parallelizations of current RNGs,
- new testing routines physically based on DOE Monte Carlo applications, and
- development of new capabilities within DOE Monte Carlo applications.

B. Projects Supported by Office of Science

105. Enabling Technology for Building High-Performance Distributed Information Storage and Retrieval System

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The goal of this research is to develop a novel method of managing large-scale inverted files as a core enabling technology for building High-Performance Distributed Information Storage and Retrieval Systems (DIRSs). By using the Distributed-Parallel Storage System (DPSS), developed at Lawrence Berkeley National Laboratory, as a high-performance storage server, our method naturally inherits the advantages of the DPSS over other storage systems, including high data rates, cost effectiveness and scalability. Through the development and evaluation of a high-performance inverted file system in distributed storage environments, we will investigate several theoretical and technological research issues, including inverted file block allocation and layout strategies, asynchronous application-controlled cache management, dynamic incremental updates of inverted files, and hierarchical and dynamic evolution of reliability schemes. Our research investigation in this direction will not only contribute to the development of high-performance DIRS but will also contribute to enhancing the functionality of the DPSS.

106. Experimental Study of Electroweak and Heavy-Flavor Physics

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The Experimental High-Energy-Physics Group at the University of Mississippi consists of four tenured faculty, three postdoctoral associates, and several graduate students. Additional support is provided by the Physics Department machine shop, an electronics technician, a computer system manager and a draftsman. The group is active primarily in studies in heavy-flavor physics, coupled with extensive detector R&D and fabrication. Our current experiments involving data analysis are Fermilab E791 "The

Hadroproduction of Charm" and SLD. E791 and previous experiments have produced over 50 publications on charm production and decays. The UMiss group has recently worked on topics in charmed baryon decays and lifetimes, production and decay of charmed mesons, production correlations between D-mesons and fragmenting pions, rare and forbidden decays of the D-meson, and SUSY production. We have provided considerable infrastructure to this program through support of data aquisition systems, muon and cerenkov particle identification systems, particle tracking systems, assembly and support of a UNIX farm and distributive software to reconstruct over 20TB of data, and finally leadership of numerous other analyses. In SLD the UMiss group will continue to concentrate on the commissioning of the SLD 45-degree drift chambers—a subsystem of the Warm Iron Calorimeter which performs SLD's muon tracking, and the analysis for electroweak lepton asymmetry parameters. With these experiments approaching completion, we have assumed a major role in the BaBar experiment at SLAC and have initiated a limited involvement in CMS at CERN. In the BaBar program—which will be our primary physics program for the next several years—we have provided tooling over the past three years for the construction of the calorimeter, designed and fabricated the equipment and provided oversight for the mechanical quality control of the approximately 6000 CsI(Tl) crystals, and established the database for the this effort. With the completion of the detector we have expanded our work in software development, concentrating on calibration of the calorimeter with radiative bhabhas. In addition, we shall continue studies of long-term radiation damage of selected CsI(Tl) crystals. Initially, we shall contribute to the physics analyses for the CP-violation program but, as the data set grows, we shall devote increasing efforts to studies in charm physics. In the US CMS HCAL program we are designing and fabricating optical readout boxes for the HE and HOB calorimeters and designing and fabricating fiber splicers. In addition, in the US CMS tracking program R&D studies are being carried out on cooling arrangements for the pixel detector. Silicon pixel detectors, which can survive near the interaction region of the LHC (where radiation levels and track densities are enormous), are being designed to give tracking information, allowing for the detection of charm, bottom, and top mesons. Finally, muon collider R&D work has recently been initiated with the fabrication of prototype RF cavities in our shop.

107. Experimental Nuclear Structure Study

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We study nuclear structure at high angular momentum and far from stability. The experiments are carried out using heavy-ion nuclear accelerators at various national and university laboratories. Large detector arrays, such as the Gammasphere, are required for most of our experiments. Recently, we performed several experiments for the light dysprosium isotopes (153–156Dy) to study their high-spin band termination property, the phase transition at higher temperature, and the superdeformation (SD). We searched for SD in a new mass region (A~170). Using the ultra-cold fusion from symmetric reactions, we successfully populated and identified a triaxial superdeformed rotational band in 168Hf. Further experiment has been approved to measure the lifetime of these new transitions at Argonne National Laboratory. We are interested in neutron-deficient mercury and gold isotopes because of the very rich nuclear structure information exhibited in this region, such as the shape-coexistence phenomenon. In addition, we have been working on neutron-rich medium-mass nuclei from the spontaneous fission of 252Cf and 242Pu, and neutron-rich P, S, Cl isotopes through the measurements of beta-delayed gamma rays from the projectile fragmentation beams. The research group includes graduate students, a postdoctoral research associate, a visiting scholar, and several undergraduate students. As the education/outreach activity, we have been involving students from local high schools for their senior-year research projects.

108. Nuclear Structure Studies of Exotic Nuclei

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The study of low-energy nuclear structure at Mississippi State University is concentrated on research in two regions. The first involves the structure of nuclei in the Z = 14 to 20 and N = 20 to 28 regions which is being studied at the National Superconducting Cyclotron Laboratory at Michigan State University. This study has focused on the structure of the heavier sulphur isotopes which exhibit some moderate deformation. For our studies, radioactive nuclei are produced by fragmentation, separated, and stopped on a moveable wheel. Once stopped, the decay of the nuclei is observed with beta and gamma detectors. Decay-level schemes have been established for eleven nuclei. The purpose of this research is to understand the strength of shell closures in the region and to determine the primary driving force for this deformation. The results of the decay experiments tend to support a conclusion of less deformation than has been indicated by B(E2) measurements using Coulomb excitation. The second area of research involves the study of nuclei near the N = Z line just below 100Sn. These nuclei, which are of interest in understanding the rp-process of nucleosynthesis, are being studied at the Holifield Radioactive Ion Beam Facility at Oak Ridge National Laboratory. This research is in its early stages and will be greatly enhanced by the planned development of a 56Ni radioactive ion beam.

STATE OF MONTANA

A. Projects Supported by EPSCoR

109. The Montana Organization for Research in Energy (MORE) Collaborative Research and Human Resources Development Program

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MORE administers Montana's Implementation Award, which is in its sixth year. MORE is a consortium of educational, governmental, and industrial partners. Research partners include the region's major power, oil, and gas industries. MORE's research clusters are closely linked with DOE's Fossil Fuels programs, the Renewable Energy Resources programs at Sandia National Laboratories, and the National Renewable Energy Laboratory (NREL). The Human Resources Outreach Program (MORE-HRD) is a national model for technology and information transfer. This program emphasizes statewide awareness and training in energy resources, brings scientists into K-12 schools and tribal community colleges, provides on-site training to rural schools, and is emerging as a Connected Learning Community, featuring electronic communications and a mobile multi-media training laboratory. The Wind Energy Research Cluster focuses on (1) improving the structural performance of turbine blades, and (2) assisting in the commercial development of regional wind energy resources. The Petroleum Research Cluster centers on (1) identifying efficient methods for characterization and extraction of known petroleum reserves, and (2) emphasizes the integration of a variety of disciplines and the use of advanced tools such as visualization graphics and artificial neural networks. Both Research Clusters are well on their way to establishing National Centers for Energy Research and Education.

110. MORE Petroleum Reservoir Characterization Research Cluster

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This program is funded by MT DOE/EPSCoR program in collaboration with Burlington Resources, Marathon Oil, JN Oil and Gas and Ballard Petroleum. The objective of the research is to develop three-dimensional models of oil/gas fields for the most economic development of the resource. The project has specific application to lengthening the producing life of some of Montana's older oil fields. A unique aspect of the research is the degree of integration of inter-campus researchers from various disciplines including reservoir simulation, applied mathematics, computer visualization, geology, and geophysics. Advanced computing tools, such as visualization graphics and artificial neural networks, are used to correlate data sets of widely varying types and physical scale. Current activities are focused on development of Self Organizing Feature Maps (SOFM) for the interpretation of seismic data and well-log analysis techniques, petrographic image analysis using computer algorithms to automatically classify pore spaces by type and roughness, geologic models that are currently being used by JN Oil and Gas and Beartooth Oil, inversion techniques for reservoir parameter estimation, and 3-D seismic surveys from several of the region's oil fields covering most of the field types being studied under DOE CLASS program.

111. MORE Wind Energy Research Cluster

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This program is funded by MT DOE/EPSCoR in collaboration with Montana Power, Headwaters Composites, Glacier Electric, Atlantic Orient Corporation (AOC), and other U.S. wind turbine companies. The research objectives include: (1) to develop wind turbine blades with improved strength, resistance to fatigue, buckling, and structural dynamics; and (2) to assist in the development of the substantial wind resources in Montana and the region. Research thrusts include improved blade structural design and manufacturing technology, modeling and testing of blade substructure elements including stiffeners, ply drops, and the development of improved reinforcing fabrics; measuring strains in the root section where the blade connects to the turbine, validation of nonlinear buckling prediction technology, and a power quality study. A major avian study, funded by NREL, has been completed. Three wind-turbine demonstration projects are being conducted in Montana: a small stand-alone hybrid wind/photovoltaic installation at Red Bluff, a weak radial enhancement distributed generation project using a 50-kW turbine at Madison Valley, and a 100-kW utility-grade turbine on the Blackfeet Reservation. The Blackfeet project serves as a catalyst for further development of the huge wind resource in the area and as a focus for education and technology programs at the Blackfeet Community College.

112. MORE Human Resources Development Program

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This program was initially funded by Montana DOE/EPSCoR. Since its inception, it has grown to include the Department of Education, the Environmental Protection Agency, National Science Foundation, Federal Emergency and Management Agency, and private companies. It also has emerged nationally as a model program for technology and information transfer. MORE-HRD emphasizes one-on-one training and follow-up activities in schools that effectively use computers and electronic communications. Teachers and students from middle schools, high schools, and tribal colleges are involved in ongoing wind energy, petroleum, and environmental characterization research. Highlights of the program include sustained contact with teachers and students in rural schools, an annual summer Energy Camp, a Connected Learning Community, a Mobile Multi-Media-Training Laboratory, and a new Minority Engineering Program (MEP) at Montana Tech. In addition, MORE-HRD provides a means of researching the effectiveness of inquiry-based approaches to education in K-12 and college-level classrooms, improved assessment methods, and the involvement of students in hands-on research, both via participation with the research clusters and via the conduct of real-time research over the Internet.

113. MORE Management and Coordination

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MORE's Directors maintain their own research programs. Dr. Scmidt has a NSF study of nonlinear glassy and relaxer behavior in ferroelectrics, a DEFSCoR investigation of large amplitude electromechanical response and fatigue of PMN-PT and PZN-PT crystals, a NASA inquiry of advanced materials for active noise and position control, and a NSF REU to support summer research for undergraduates. Dr. Bromenshenk directs a U.S. Army Center for Environmental Health Research (USA CEHR) contract to develop novel methods for monitoring air quality and the terrestrial environment and a Defense Advanced Research Projects Agency (DARPA) contract for bioreporting and seeking agents of harm. This latter contract supports more than 25 senior scientists from two universities (The University of Montana and the Ohio State University), chemical analysis and instrumentation, microelectronics, and microbial bioengineering research groups at DOE's Oak Ridge National Laboratory (ORNL), an explosives research group at Sandia National Laboratories (Sandia), a radio-frequency electronics group at Battelle Pacific Northwest National Laboratory, immunoassay specialists from the Environmental Protection Agency's Human Exposure Research Branch in Las Vegas, a disease vector specialist at the Navy Disease Ecology Center, and microbiological specialists at the Monmouth Microbial Aerosol Laboratory in Oregon.

114. Optical Sensors for Accelerator Diagnostics

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This proposal addresses an urgent current need for novel diagnostic sensors and systems to enable improved operation of the electron beam accelerator and imaging system known as DARHT currently being developed at the DOE's Los Alamos National Laboratory. DARHT is a key component of the DOE's Stockpile Stewardship Program. DARHT system operation with increased pulsed duration is desired, creating the need for new sensor designs, as compared with devices currently used in the existing short-pulse accelerator. This proposal will investigate the development of new optical sensors and apply them to this particularly demanding need. Optical sensors based on Faraday rotation in optical crystalline or glassy materials are proposed to measure magnetic field magnitude and direction at high frequencies with sufficient signal-to-noise ratio for use in beam diagnostics. Similarly, optical sensors using the Pockels effect in crystalline materials will be used to monitor electric field distributions associated with beam propagation. Optical sensors provide a series of benefits over existing sensor alternatives. The most immediate advantages include complete galvanic isolation between sensor head and control room electronics, intrinsically high-bandwidth cabling with no EMI issues, high-sensitivity sensor elements at reasonable cost, low-cost interface electronics compared with existing sensor systems, and a potential for multiplexing a multitude of sensors along one or a few sensor cables. The principal investigator will have a close collaborative effort with Dr. M. Brubaker at LANL during the course of this project. Both individuals have had extensive previous experience developing optical sensors for the utility industry.

B. Projects Supported by Office of Science

115. Theory of Turbulent Heat and Particle Fluxes in ExB Shear Flow and Computational Modeling of the Stability of Novel Stellarators

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In this project we are investigating two separate topics of theoretical and computational research concerning stability and transport in plasmas relevant to magnetic fusion energy research. First, the effect of ExB shear flow on turbulent heat and particle fluxes is being studied. Recent work has shown that ExB shear flow can affect the cross phase between electrostatic potential and pressure fluctuations, as well as fluctuation levels, thus affecting the particle fluxes. Here, we are exploring the connection between the cross phase and Reynolds stress-flow generation. This is a feedback loop between the generation of the flow and modification of the transport cross phase. Understanding the effect of shear flow on heat and particle fluxes will help understanding of enhanced confinement regimes. Second, stability of novel stellarator designs is being investigated. Low-aspect ratio stellarators are being developed which have improved single-particle confinement properties by modifying the flux surfaces to align with constant J*-surfaces. These are called quasi-omnigeneic stellarators (QOS). For a good representation of the equilibrium, a large number of Boozer harmonics are required (>1000). To enhance the computational speed, a parallel version of VMEC is being developed using high-performance fortran. While the initial designs of QOS have many promising features, the stability of ballooning modes in these devices is one of the primary outstanding issues. A fast-ballooning stability algorithm has been developed and is being incorporated into an optimization code.

116. Comparative Analyses of Subsurface Bacterial Community Structure

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To refine and apply laboratory methods for extraction of DNA from field samples and to use profile analysis of DNA variability to investigate and differentiate bacterial communities without lengthy and often inconclusive culturing and isolating individual species.

117. Microbially Promoted Solubilization of Steel Corrosion Products and Fate of Associated Actinides

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Summary not available.

STATE OF NEBRASKA

A. Projects Supported by EPSCoR

None

B. Projects Supported by Office of Science

118. Fundamental Magnetic-Hardening Studies of Nanocrystalline and Nanocomposite Magnets

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This research is directed towards the synthesis of organic solids derived from neutral radicals, which are derivatives of the phenalenyl system. Many compounds in this series should be solid-state organic conductors. Some may be metallic and may possibly be superconductors. The solid-state properties of these systems in the context of their electron transport and magnetic properties are main issues. The virtue of these systems is that they are overall neutral and can be sublimed and transferred into films. A long-term thrust of this work is to understand the relationship between solid-state properties and molecular structure.

119. Dynamics of Few-Body Atomic Processes

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This project is concerned with elucidating the dynamics of few-body atomic processes. Single and multiphoton detachment studies are conducted of negative ions, particularly the negative alkali metal ions, using eigenchannel R-matrix methods. A major goal is to determine the role of high, doubly excited, two-electron states below high excitation thresholds on such processes. This role will be determined by detailed analyses of resonance energies, two-electron state density plots, resonant and nonresonant cross-section components, etc. Contrasts and similarities between negative ion spectra will also be determined and compared to that of the prototypical 3-body Coulomb system, H-. Long-range interactions between alkali metal atoms that are relevant to experimental studies of such atoms in traps are also being studied.

120. Enzymology of Aceticlastic Methanogenesis

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An understanding of the mechanism of methane formation is critical since methane is an important fuel and a significant greenhouse gas whose concentration is rising at a rate of 1% per year. We are studying the mechanism of methanogenesis from acetate, which is the major substrate for methanogens in nature. We are focusing on three important steps in aceticlastic methanogenesis: (1) the initial step of acetyl-CoA disassembly by the molecular aggregate that contains CO dehydrogenase/acetyl-CoA synthase (CODH/ACS) and a corrinoid/iron-sulfur protein (C/Fe-SP); (2) the methyl-CoM reductase (MCR) catalyzed reaction that generates methane and a heterodisulfide (CoB-S-S-CoM) from methyl-Coenzyme M (methyl-CoM) and Coenzyme B (CoB); and (3) the heterodisulfide reductase (HDR) reaction that reduces CoB-S-S-CoM to the free thiols, CoB-SH and CoM-SH, for the next round of methanogenesis. We are using a combination of kinetics, electrochemistry, and spectroscopy to establish the reaction mechanisms of these enzymes. In the last year, a protocol to generate highly active MCR has been developed and the HDR has been characterized as a heme/iron-sulfur protein. The studies are expected to lead to important insights into how natural gas is formed in nature and into the structure and function of metals in biology.

121. Tomato Bushy Stunt Virus And DI RNAs as a Model for Studying Mechanisms of RNA Virus Replication, Pathogenicity, and Recombination

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Our research on tomato bushy stunt virus (TBSV) has focused on determinants affecting replication, pathogenicity and recombination. TBSV is a small isometric virus that contains a single-stranded RNA genome with five major genes. We analyzed the importance of an additional small gene designated pX, at the 3′ end of the genome. Bioassays showed that mutations of the translational initiation codon designed to disrupt translation of the pX-encoded protein were unable to accumulate to detectable levels in cucumber protoplasts. Although these results suggested a role for the putative pX protein, introduction of a premature stop-codon to truncate expression of the pX protein were unable to replicate. In contrast, a comparable pX mutation that affected the same nucleotides without changing the predicted amino-acid sequence greatly reduced RNA accumulation. Therefore, the pX RNA sequences, rather than the predicted pX protein, influence genome replication. The requirement for pX also appears to be host dependent because comparisons revealed that subtle pX gene mutations that interfere with accumulation of TBSV RNA in cucumber or *Nicotiana benthamiana*, did not affect replication in *Chenopodium quinoaprotoplasts* or plants. Irrespective of the host, the *cis*-acting pX gene sequences were not required for replication of defective interfering RNAs that require helper TBSV for replication in trans. These experiments thus suggest that the pX *cis*-acting element interacts with one or more host components whose composition differ slightly between different plants.

122. Role of the Rubisco Small Subunit

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Ribulose-1,5-bisphosphate carboxylase/oxygenase (Rubisco) catalyzes the rate-limiting step of photosynthetic CO_2 fixation. Because of its low carboxylation efficiency and competitive inhibition by O_2, Rubisco has been viewed as a potential target for engineering-enhanced crop-plant productivity. The Rubisco holoenzyme is comprised of two subunits, each present in eight copies. Much is known about the structure-function relationships of the chloroplast-encoded large subunit. It contains the active site. Much less is known about the role of the nuclear-encoded small subunit. There is a family of small-subunit genes in crop plants, making it difficult to substitute engineered small subunits into the holoenzyme. A photosynthesis-deficient mutant of the green alga *Chlamydomonas reinhardtii* has recently been recovered that lacks both members of the small-subunit gene family. Because this mutant can be rescued via transformation with a single small-subunit gene, it is now possible to answer questions about small-subunit function. Alanine-scanning mutagenesis is being used to elucidate the significance of small-subunit structural regions that are unique to the Rubisco of eukaryotes. Most substitutions do not eliminate enzyme function, indicating that these regions are not essential for holoenzyme assembly or catalysis. In contrast, random mutagenesis is being used to define those regions of the small subunit that are essential. Because Rubisco enzymes from different species display differences in CO_2/O_2 specificity, heterologous small-subunits will also be introduced into *Chlamydomonas* to assess the contribution of small subunits to catalytic efficiency.

123. Fabrication and Characterization of Micron-Scale Ferromagnetic Features

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This project focuses on the study of micro-scale features of ferromagnetic nickel, cobalt, cobalt-palladium alloys and cobalt-palladium heterostructures fabricated by "direct writing" (i.e., by selective area deposition from organometallic compounds). There are two goals for this research program. First, by making magnetic features smaller and smaller, in a variety of different shapes, the project will elucidate the influence of defects on magnetization reversal and coercivity. Second, the project will determine if there is any coupling between small ferromagnetic features (approx. 1 micron), possibly substrate-mediated, on the length scale of 1000 angstroms smaller. This research project is based upon conventional methods for imaging magnetic domains. Polarized-light microscopy permits not only imaging micron-scale features but also determines the magnetic orientation and coercivity with some spatial resolution. A microscope will be used to make polar Kerr rotation measurements and obtain spatially selective magnetic information. A unique capability for probing the electronic structure of our magnetic features at resonance: spin polarized inverse photoemission, with both longitudinal and transverse spin polarization, will also be used. Essential to this project is a new technique for fabricating micro-scale ferromagnetic features. Organometallic chemical vapor deposition techniques, sufficient to deposit pure metal features with excellent spacial resolution, have been developed at this laboratory. These techniques allow selective deposition of large uniform arrays of nickel, cobalt, cobalt-palladium alloys and cobalt-palladium heterostructures in features as small as 0.2 microns, and as thin as a few monolayers or as thick as 10 microns. Multilayers can be made by the successive deposition of different metals or alloys by the sequential photolysis of different organometallic source compounds. While unconventional in many respects, this project utilizes a technology that is compatible with the fabrication of metal features 100 angstroms across in one scanning-tunneling microscopy run. The approach is superior to techniques employing ion beams or conventional lithography and is inexpensive and compatible with the fabrication of the next generation of optical and magnetic recording media.

124. A Study of Ultra-Relativistic Heavy Ion Collisions

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This project contributes to the investigation of the behavior of hadronic matter under extreme conditions. Its focus is the search for indications of a phase transition from hadronic to quark matter. It is believed that the conditions necessary for the formation of a quark-gluon plasma include large energy densities over extended volumes as can be obtained at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory. The measurement of enhanced strangeness production may prove to be an effective tool in verifying the existence of a quark-gluon plasma. Concurrent studies of two-photon and photonuclear processes provide additional opportunities for physics contributions. This project supports the development of software and hardware interfaces to be used to carry out research using the Solenoidal Tracker At RHIC (STAR). Creighton University is responsible for the slow controls system required for the STAR experiment. This system will monitor over 25,000 detector parameters. The work also involves the analysis of data from detector tests. The tools developed for this work will be applied to the study of strangeness enhancement and peripheral collision physics using the STAR detector. An integral part of this endeavor is to provide research opportunities for undergraduate students.

125. Genetically Engineered Multivalent Single-Chain Antibody Constructs for Cancer Therapy

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The overall objective of this project is to generate, characterize, increase production and affinity of multivalent antibody constructs reactive with the tumor-associated Sialyl-Tn antigen and to determine the utility of these specific antibodies for the diagnosis and treatment of cancer. The first specific goal is to develop and characterize expression systems for high-level production of covalently linked multivalent forms of MAb CC49 single-chain constructs in both yeast and Sp2/0 cell line in addition to *E. coli* cells. The second specific goal is to determine the relative biodistribution and therapeutic efficacy of multivalent scFv constructs in athymic murine xenograft models, comparing different scFv forms and radionuclide conjugates. The third specific goal is to engineer the scFv molecule for the development of humanized CC49 scFv constructs using the CDR grafted humanized variable region genes for the heavy- and light-chain of MAb CC49. The fourth specific goal is to generate and characterize human monoclonal antibodies specific to the Sialyl-Tn epitope of tumor cell mucins from antibody variable region genes from the peripheral lymphocytes of Sialyl-Tn immunized patients.

STATE OF NEVADA

A. Projects Supported by EPSCoR

126. Nevada DOE/EPSCoR Program

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The goals of the Nevada DOE/EPSCoR Program are to stimulate high-quality energy-related research in Nevada and to develop the manpower and infrastructure in science, mathematics and engineering to meet future needs. A priority is to increase the cooperation and collaboration between university personnel from the two campuses of the University of Nevada and the Desert Research Institute with DOE, its contractors and national laboratories, the Nevada Test Site, and energy-related industries and agencies. The state-wide program has three major components. The Human Resources cluster stimulates leveraged research, broader educational opportunities and industrial partnerships to supply talent to meet Nevada's future energy needs. The Chemical Physics cluster engages scientists in research projects in laser and ion physics, synchrotron radiation and nanostructures. Major thrusts are the development of centers for High-Pressure Science and Engineering in Las Vegas and for High-Energy-Density Science and Technology in Reno as part of DOE's Science-Based Stockpile Stewardship Program. The Plant Responses to CO_2 cluster engages scientists in studies of the responses of desert ecosystems to elevated levels of atmospheric carbon dioxide. A free-air carbon-dioxide enrichment (FACE) facility has been developed at the Nevada Test Site to provide a national center for such studies.

127. Nevada DOE/EPSCoR Human Resources Development Cluster

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This cluster supports activities within the University and Community College System of Nevada to stimulate research, build collaborations to support state high-technology needs, and to develop the required human resources. More than 900 industry, academic and government scientists and engineers have participated in these programs, yielding $4.7 million in new competitive research funding, an 18:1 return on investment. Annual Nevada Science and Technology Symposia highlight research and development opportunities and encourage proposals for competitive research. University scientists and engineers join with representatives from industry and government to identify research opportunities and partnerships. Co-sponsors in these symposia include the DOE Nevada Operations Office and the Nevada Commission on Economic Development. The cluster also assists other events that support state high-technology industry, including the Global Energy Exchange Forum, the Nevada Governor's Economic Development Conferences, and the Nevada Legislative Forum for Renewable Energy. Assistance includes program planning, logistics and preparation of proceedings. The DOE EPSCoR Young Scholars Program is a summer research experience program for Nevada undergraduates interested in pursuing science and engineering careers. This program is fully integrated into the summer research programs at each campus. To date, 45 students have participated, of which

44% are women and 31% are from under-represented groups.

128. Nevada DOE/EPSCoR Chemical Physics Cluster

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This cluster supports the development of research facilities and collaborative programs to probe the properties and behavior of matter at extreme temperatures, pressures and densities, employing lasers and synchrotron radiation, and supported by theoretical efforts. Active collaborations include 18 universities and research laboratories, including Lawrence Livermore, Los Alamos, Lawrence Berkeley, and Sandia National Laboratories. Nevada researchers have led the development of two user beamlines at the Advance Light Source in Berkeley. Using synchrotron radiation, they have recently demonstrated the inadequacy of the widely applied dipole approximation for the photoelectric effect, which affects data tabulations used in many fields. Absolute cross sections have been measured for single- and double-electron-impact ionization of multiply charged atomic ions, demonstrating the importance of indirect pathways to ionization. In addition, two major research facilities are being developed under the DOE Science-Based Stockpile Stewardship Program: the Nevada Terawatt Facility, centered around a 2-terawatt z-pinch plasma device in Reno, the highest power electrical discharge at any U.S. university for plasma physics research; and the High-Pressure Science and Engineering Center in Las Vegas, which performs static and dynamic high-pressure studies of matter to validate and improve computational models over a largely unexplored range of pressures and temperatures.

129. The Nevada Desert FACE Facility

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DOE EPSCoR has supported the construction and operation of the Nevada Desert FACE (Free Air CO_2 Enrichment) Facility (NDFF), one of only seven operational FACE sites in the world. The NDFF will allow a decades-long study of the response of a native desert ecosystem to a level of atmospheric CO_2 that will occur by the mid-twenty-first century. It is the only facility in both an arid region and a natural, unmanaged ecosystem. Since deserts have been predicted to be the most sensitive of any terrestrial ecosystem to global change, the NDFF offers a unique opportunity for scientists to conduct studies of global change biology, from the level of gene expression to ecosystem structure and function, that have the potential to reveal the biological consequences of rising atmospheric CO_2. Nevada scientists have attracted several million dollars in highly competitive federal funding to support research at the NDFF. After only two years of NDFF operations, several peer-reviewed publications have indicated not only the substantial and unique utility of this facility for global change research, but also that predictions of the impact of rising atmospheric CO_2 on this dominant terrestrial ecosystem are correct in some areas and in need of significant revision in others.

130. Experimental Benchmarking of Fire Modeling Simulations

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A three-year research program is proposed to design, conduct and analyze a set of experiments that simulate a large nuclear waste transport cask engulfed in a 10-CFR.71 regulatory pool fire. These experiments will be conducted at the Sandia National Laboratories (SNL). Recent experimental observation and computer simulations show that the thermal conditions within these fires are significantly altered by the presence of a large-sized, thermally massive object. As a result, simple σT_{Fire}^4 thermal boundary conditions are not adequate for predicting the heat flux to casks in a pool fire. These predictions are frequently required for cask design studies. The data gathered by the proposed experiments will be used to benchmark and adjust the Cask Analysis Fire Environment (CAFE) computer code that is currently under development at SNL. This code models the conditions within these large-scale fire environments and can be run on standard computer workstations. CAFE will be a very useful cask design tool once its fire models are verified. These results will be of interest to any organization that requires packages to move nuclear materials, including DOE/DP, DOE/EM, and DOE/RW.

131. Probing of Rotational Orientation and Helical Trajectories by Ion Imaging

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Experiments are in progress studying preferred molecular trajectories produced in the photodissociation of related, but structurally distinct, nitrosoalkanes. The experiments measure the correlation between the angular momentum and velocity vectors of products in the frame of the energized parent nitrosoalkane parent molecule, in addition to scalar populations distributions among product quantum states. The angular momentum distribution of the nitric oxide (NO) product is probed by polarized resonance-enhanced multiphoton ionization laser spectroscopy. Two-dimensional ion imaging methods are used to measure velocities and spatial anisotropies in correlation with angular momentum polarization. The experiments are performed in low-temperature molecular beams. The new experiments build on previous experimental results from the laboratory of the PI that demonstrate that it is possible to measure nonstatistical dynamics and vector properties even when the available energy shows a nearly statistical distribution. The studies explore two new effects not previously examined in detailed vector correlation experiments: (1) the effect of molecular rigidity and conformations on product trajectories and (2) preferential helical product trajectories produced in the photodissociation of chiral molecules. In our experiments we are especially interested in producing a dynamical picture of mechanisms for regio- and stereo-selective chemical reactions and for the generation of net preferential directional forces that can lead to the extraction of macroscopic amounts of work from molecule sized systems such as biological motors and hypothetical nanotechnology devices.

B. Projects Supported by Office of Science

132. System Carbon Fluxes and Sequestration in Ponderosa Pine at Varied Nitrogen and Water Availabilities: A Long-Term Field Experiment at Elevated CO_2

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This research is designed to determine in a forest system the extent to which soil nitrogen availability interacts with elevated CO_2 to influence patterns and processes of ecosystem carbon sequestration.

133. Collaboration: Effects of Elevated CO_2 on Root Dynamics and Root Function in a Mojave Desert Ecosystem

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The goal of this research is to determine the effects of elevated atmospheric CO_2 on belowground fine-root productivity, fine-root turnover, and root function in an intact desert ecosystem.

134. Mexico City Particulate IMADA-AVER Study

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Summary not available.

135. A New Treatment of Cirrus Radiative Properties: Testing with Field and Laboratory Measurements

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This research focuses on the improvement of the treatment of the microphysical and radiative properties of cirrus clouds in cloud-resolving models

136. Automated DNA Laboratory

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Summary not available.

137. Enhanced Detection of Fungal Contaminants Using Polymerase Chain Reaction

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Summary not available.

138. Partial Support Meteorological Coordinating Council

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The Department of Energy's (DOE) Meteorological Coordinating Council (DMCC) provides coordination of meteorological support and operations in order to address the DOE's objectives related to environment, safety and health. The DMCC goals are to enhance awareness of atmospheric science applications throughout the DOE complex, promote cost-effective support of meteorological site operations, alleviate the use of common methods, procedures and standards, and plan for future needs, requirements and missions. The MCC will support the Office of Biological and Environmental Research (OBER), Environmental Sciences Division (ESD) through their participation in various activities of the Office of the Federal Coordinator for Meteorology (OFCM). This support will utilize coordination resources of the DMCC in order to provide Departmental input to the annual Federal Plan for Meteorological Services and Supporting Research, and other relevant activities.

139. Transient Responses in Ecosystem Free-Air CO_2 Enrichment (FACE) Experiments

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The objective of this research is to determine how results from short-term FACE experiments, where ecological responses to abrupt perturbation are measured, can best be used to understand and predict long-term responses to the anticipated very gradual CO_2 change in the natural world.

140. Long-Ranged Polymer Dynamic Behavior and Conductivity in Battery Polymer Electrolytes: Poly(ethylene oxide)/Salt Systems

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In this project, light scattering— principally the noninvasive dynamic light-scattering technique known as photon correlation spectroscopy—is being used to study relaxations of poly(ethylene oxide)(PEO)in the melt, both with and without lithium perchlorate. The purpose of this work is to reveal how relaxations, particularly long-ranged PEO relaxations in PEO solid polymer electrolytes are related to lithium ion conductivity in these electrolyte systems. Following the project plan outlined in the FY 1995 project summary, the first phase study of the effects of lithium ions on PEO global behavior in methanol solutions has been

completed and the results reported in the literature (P. A. Banka et al., Macromolecules, vol. 29, pp. 3956–3959). The study of the effect of lithium ions on PEO coil internal motions is also progressing, but completion of this portion of the project awaits delivery of a satisfactory high-molecular-weight, narrow molecular weight distribution PEO sample. Significant progress has also been made on the second phase of the project dealing with melt PEO samples. We have now observed a well-defined more-or-less monomodal relatively fast relaxation in highly entangled melts which is accompanied by a very slow relaxation associated with a visibly "grainy" structure in incompletely annealed samples. For melts of low-molecular-weight unentangled PEO we observe a single, relatively faster relaxation with no graininess or associated slow relaxation. To better understand the nature of conductivity in SPEs, we are investigating the effects of lithium perchlorate on these relaxations and will compare the results both with those for poly(propylene oxide) melts and with conductivity data.

141. Screening Resonances in Plasmas

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The interaction potential between atomic ions and electrons in plasmas has consistently been modified to include short-range order and dynamical screening effects introduced by neighboring ions and fast electrons. These modifications determine one-electron properties (e.g., spectral lines which serve as key quantities in plasma diagnostics) as well as multiple-electron properties (e.g., dielectronic recombination rates which account for plasma losses). So far, the applications have been restricted to the usual Debye-Hückel theory, which has been used to extend standard and nonstandard atomic structure programs. Furthermore, the approach to screening has been generalized to encompass dynamic screening effects in order to account for ion motions. The approach allows the simultaneous evaluation of level broadening and continuum threshold lowering. Basic features of line broadening have been incorporated into the theory, while line splitting (due to deviations of the immediate ion environment from sphericity) is presently being programmed. Calculations for the important case of a hydrogen plasma exhibit an unexpectedly high abundance of negative hydrogen ions in a variety of plasma conditions and even the possibility of excited states of this ion. The main focus of this study, the occurrence and stability of the negative hydrogen ion in plasmas, has so far been of interest for astrophysical plasmas, this ion being the main contributor to the opacity of white dwarf stars and one of the main contributors to the opacity of the solar chromosphere. The present findings indicate, however, that the opacity of a broader range of plasmas may be affected also (e.g., laboratory plasmas and, possibly, even fusion plasmas).

142. Thermochemistry of Hydrocarbon Radicals: Guided Ion-Beam Studies

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Gas-phase negative-ion chemistry methods are used to measure enthalpies of formation of small organic radicals important in combustion processes. Using guided ion-beam mass spectrometry, we measure threshold energies of endoergic proton transfer and hydrogen atom transfer reactions of hydrocarbon molecules with negative reagent ions. The measured threshold energies yield the RH bond dissociation energy of the corresponding neutral molecule, or equivalently, the enthalpy of formation of the R• organic radical. Using guided ion-beam techniques to study endoergic reactions allows accurate determinations of RH bond dissociation energies for species that are not easily investigated by thermal ion and neutral kinetics techniques. Examples include extremely weak gas-phase acids, such as saturated alkanes, polyacetylenes, and the differential RH bond dissociation energies at various positions in substituted aromatic and conjugated compounds. Systems to be investigated are radicals important in combustion processes, including, for example, acetylenic and aromatic hydrocarbon radicals that lead to formation of polycyclic aromatic hydrocarbons and soot.

143. Energetic Photon and Electron Interactions with Positive Ions

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This project involves complementary experimental investigations of inner-shell excitation and ionization of multiply charged positive ions by energetic beams of electrons and photons. Absolute electron-impact ionization cross-section measurements are being carried out at the multicharged ion research facility at the University of Nevada, Reno, using a new crossed-beams apparatus based on the "animated-beams" technique. Ion beams are produced by a 14.4-GHz electron-cyclotron-resonance (ECR) ion source. A high-efficiency electron spectrometer is being developed to detect and energy-analyze ejected electrons for the first time from such collisions. The photoionization measurements will be conducted at the Advanced Light Source, for which an experimental end-station is being designed and constructed for the new undulator beamline 10.0. This collinear-beams apparatus will facilitate absolute photoionization cross-section measurements for both negative and positive ions, including multiply charged ions to be produced by a permanent-magnet ECR ion source. A common objective of these synergistic electron and photon impact experiments is a deeper understanding of the complex multielectron interactions that govern charge-changing processes involving ions in high-temperature environments, such as those occurring in stellar, X-ray-laser and thermonuclear fusion plasmas.

144. The Nevada Terawatt Facility/ Stabilization and Confinement of Hot, Dense, High-Beta Plasma

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A high-repetition-rate, 2-trillion-watt z-pinch (HDZP-II from Los Alamos National Lab: 2 MV, 1 MA, 100 ns, 200 kJ, 1.9 ohm; generating twice the electrical power of the entire U.S.) has been reassembled at the Nevada Terawatt Facility (NTF) at UNR. This extremely powerful and general research tool will produce high-power electrical pulses, hot, dense plasma (ionized matter), and high-intensity beams of ions, electrons, and X rays. Its uses range from investigating fundamental questions in plasma and atomic physics, to advancing the techniques of radiography, to developing practical applications in the medical, materials, and environmental sciences. Plans for the next year include investigating the physics of wire-array z-pinches (the early-time evolution of a current-driven wire, the plasma turbulence around and between wires, the acceleration of a plasma current sheet by a magnetic field, and the suppression or reduction of instabilities) and developing a bright, micron-sized X-ray source for point-projection microscopy. The heating, expansion, and dynamics of wires driven by current prepulses similar to those at the Sandia

National Laboratories' Z facility (100 kV, 2 kA, 50 ns) are currently being examined. Time-resolved laser-absorption and interferometric images (10-micron, 0.1-ns resolution) are obtained with a streak camera and an Nd:glass laser (30-ns, 1064- or 532-nm). Time-resolved X-ray imaging and backlighting, imaging spectroscopy, and additional laser diagnostics are under development. Optical, laser, and radiographic measurements will be compared with computer modeling.

145. Multicomponent Convection in Porous Media and Fractures

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The objectives of this research are to understand the physical and chemical processes controlling multicomponent convection in natural porous and fractured media and to develop quantitative relationships between system parameters (solute concentrations, permeability and system geometry) and convective transport. From these experimentally and numerically derived relationships, estimates of the magnitude of convective mass transport will be developed to determine the role of multicomponent convection in contaminant transport and groundwater remediation.

146. Growth of Faults, Scaling of Fault Structure, and Hydrologic Implications

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Our main objectives are to develop a physical model of the three-dimensional hydrogeologic structure of fault zones based on field mapping, mechanical modeling, and probabilistic modeling. Based on this model we will develop inverse techniques for evaluating fault zone hydrology from well test data.

STATE OF NORTH DAKOTA

A. Projects Supported by EPSCoR

147. Removal of Organic Contaminants From Water Via Spray Processes

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A collaborative research project is proposed between the Department of Chemistry at the University of North Dakota and Los Alamos National Laboratory to study the separation of organic molecules from aqueous matrices using spray processes. We will study the completeness of removal and the speed with which compounds are separated from aqueous matrices. Many studies focusing on this goal will be pursued, including investigations of the behavior of solute molecules under the many variable conditions that can occur in spray processes. These include common parameters such as pressure and temperature, and also the effect of different methods of forming a spray, including pneumatic nebulization, thermally enhanced nebulization, and ultrasonically enhanced nebulization. Also, we will study the dependence of solute behavior with the chemistry of the aqueous matrix (ionic strength, use of organic modifiers) and with the chemistry of the matrix into which the solutes are being extracted (noble gases, organic gases, supercritical fluids). The effect of aqueous matrix surface area on transport rate of solutes will be studied, comparing static systems with sprays of different droplet sizes. Experimentally, all of these investigations will be accomplished using small-scale spray chambers directly monitored by on-line detectors.

B. Projects Supported by Office of Science

148. Analysis of In Situ Cloud Microphysical Measurements from the ARM Remote Cloud Sensing IOP

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Summary not available.

STATE OF OKLAHOMA

A. Projects Supported by EPSCoR

149. Electronic Transport in Disordered Two-Dimensional Electron Systems

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This proposal requests support for theoretical studies of electronic transport in disordered two-dimensional (2-D) electron systems. We propose to study four problems involving metal-insulator transitions (MIT): (1) disordered 2-D systems where electron-electron interaction is important; (2) disordered 2-D systems with perpendicular magnetic field; (3) double-quantum wells with an in-plane magnetic field; (4) possible giant magneto-resistance in nonmagnetic granular films. The first problem is aimed at understanding the recently reported MIT in 2-D systems. We believe that there is a new liquid phase in the 2-D electron system at low enough electron densities, and the recently observed MIT results from the percolation transition of the liquid phase through the disorder landscape. We propose to carry out various model calculations to substantialize this idea. In the second problem, we study the localization problem with a perpendicular magnetic field. The goal here is to understand the evolution of the extended states as the magnetic field approaches zero, where eventually all the states are localized. The third problem addresses the MIT with an in-plane magnetic field in coupled double quantum wells. There are some numerical evidences to support a possible KT-type MIT in such a system. We plan to understand on a solid ground the physical nature of the transition and to explore experimental conditions for observing such a transition. In the last problem, we propose a novel type of giant magneto-resistance (GMR) in nonmagnetic granular materials with hopping conduction. The advantage of the novel GMR is the nonexistence of hysteresis in resistance because of the absence of magnetic elements.

150. Novel Catalyst Development and Process Optimization for CO_2 Reforming of CH_4

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The objective of the proposal is to develop a process suitable for commercialization in which synthesis gas, a mixture of hydrogen and carbon monoxide, is produced from carbon dioxide and natural gas. Synthesis gas is a feedstock for producing high-quality, liquid transportation fuels, petrochemicals and oxygenated compounds. Recent studies have shown that synthesis gas can be produced by carbon dioxide reforming of methane over various catalysts. However, a catalyst capable of operating under conditions required for commercialization, high temperatures, high methane:carbon dioxide ratios, and high pressures has not been found. It is our goal to synthesize, characterize, and test catalytic materials to determine the properties and surface structure of the materials. In parallel, we will design a flow sheet for the process, which will include the catalyst parameters in the optimization. We plan to determine the optimum conditions for the process (i.e., temperature, pressure, conversion, etc.) as well as the optimum catalyst parameters (i.e., metal loading, support, promoter loading, etc.) for operation under these conditions. The FETC has the laboratory-scale equipment and expertise for performing experiments under synthesis production conditions. Collaboration with the FETC will also provide the opportunity for the graduate students to spend a summer or academic term at the DOE facility, providing an excellent educational forum. The result of this research will be a fundamental understanding of catalyst development and process design, which may lead to the successful development of a commercial process for carbon dioxide reforming of methane.

B. Projects Supported by Office of Science

151. Novel Superconductivity in Two-Dimensional Electron System

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Summary not available.

152. Quinone Binding and Reduction in the Photosynthetic Reaction Center

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A vast amount of experimental data makes photosynthetic reaction centers (RCs) the paradigm for biological energy transduction. Furthermore, an enormous number of synthetic structures modeling biological electron transfer (ET) incorporate components of the RC, but most models lack the exquisite selectivity and control of ET exhibited by RC proteins. Our work combines quantum chemical and molecular dynamics computations of quinone and semiquinone anion binding to bacterial photosynthetic RCs. Goals are to determine (1) the effect of RC protein modulation upon binding and electrochemistry of quinone electron aceptors; (2) the inhibition of ET through unfavorable thermodynamics and/or kinetics by protein-induced effects on quinones; and (3) the thermodynamic and kinetic effects on ET through variance of quinone substituents or amino acid side chains. Insight gained here will pave the way for studies of subsequent quinone reduction steps in photosynthesis and quinone oxidation-reduction chemistry in other energy storage systems modeled upon the photosynthetic RC.

153. Transition Metal-Mediated Thermal and Photochemical Carbon Dioxide Activation

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The overall goals of this project are to elucidate the patterns of reactivity, both thermal and photochemical, of coordinated CO_2 and to develop catalytic processes based on these patterns. Our activities during the past year have been concentrated in three areas:
(1) investigation of the Pd-catalyzed carboxylation of organotin compounds;
(2) study of potential metal-mediated carboxylation of cyclopropanes; and (3) study of group 16 (O,S,Se,Te) atom additions of $Cp_2TaH(CO)$. Regarding (1), we have discovered that Pd(0) complexes catalyze the efficient carboxylation of allylstannanes by CO_2, producing allylcarboxylate-Sn esters. This reaction, whose scope and mechanism are under investigation, constitutes the first example of transition metal activation of main group M-C bonds towards carboxylation. For project (2), a potential means for inserting CO_2 into reactive C-C bonds, a number of cyclopropanes have been screened for reactivity with Pd(0) and Ni(0) complexes in the presence of CO_2. Since carboxylation products (e.g., lactones) have not yet been observed, more reactive complexes and cyclopropanes are now under investigation. Study (3), which seeks to model heterogenous CO sulfurization and oxidation, has led to the generation of labile X-atom transfer intermediates, tentatively assigned as $Cp_2TaH(CO)X$ and $Cp_2TaH(COX)$.

154. The Structure of Pectins from Cotton Suspension Culture Cell Walls

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In work over the last eleven years on pectins from cotton suspension culture cell walls, we have concluded that pectins are based on only two backbone structures. One is a (1-4)-linked galacturonan and the other is a repeated disaccharide of galacturonic acid and rhamnose (rhamnogalacturonan). The homogalacturonan-based pectin regions fall into three common types: (1) true homogalacturonans with varying degrees of methyl esterification;
(2) Rhamnogalacturonan II, a homogalacturonan section with complex sidechains clustered such that it can be isolated as an ~5,000 Dalton fragment after endopolygalacturonase digestion of cell walls; and (3) xylogalacturonan, a homogalacturonan backbone with frequent single xylose substituents linked to the galacturonic acid residues. The goal of the project is to learn more about the structure, and if possible, function of the various pectic regions and to determine which regions are covalently attached to each other. We also want to determine how they are linked to each other by isolating and characterizing junction zones between them. To help achieve these goals we

are developing highly sensitive methods for carbohydrate analysis and sequencing using capillary electrophoresis, enzyme and chemical digestions, and spectroscopic methods. In addition, we are comparing the pectins of cotton cotyledons to those of the tissue cultures in case culturing induces major modifications in the structures.

155. Energetics and Kinetics of Syntrophic Aromatic Degradation

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The anaerobic bacterium *Syntrophus acidotrophicus* strain SB in coculture with the methanogen, *Methanospirillum hungatei*, degraded benzoate to a minimum threshold concentration at which no further benzoate degradation occurred, even with extended incubation. The addition of sodium acetate, but not sodium chloride, affected the threshold value; increased acetate concentrations resulted in increased benzoate threshold concentrations. Cocultures that initially contained 2.5 m*M* benzoate with either 0 or 10 m*M* acetate degraded benzoate to very low threshold concentrations, less than 500 n*M*. In contrast, cocultures with 30 or 60 m*M* acetate added, degraded benzoate to threshold concentrations of 4.4 u*M* and 1.5 m*M*, respectively. The final partial pressure of hydrogen in the methanogenic cocultures ranged from 1.5 to 3.0 Pa. At threshold, the Gibb's free-energy change under physiological conditions was still favorable, ranging from -14 to -21 kJ/mol. These data show that substrate degradation thresholds do occur under methanogenic conditions and that the threshold values can be substantial under conditions where hydrogen is low if acetate is allowed to accumulate to high concentrations. Similar free-energy values obtained under sulfate-reducing and methanogenic conditions when the threshold is reached support the hypothesis that substrate thresholds are thermodynamically controlled and that substrate degradation may be precluded even though the free-energy change is still favorable.

156. Theoretical Research in Weak, Electromagnetic, and Strong Interactions

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This project covers a wide area of current research in High-Energy Theoretical Physics, such as TeV-scale superstring and collider phenomenology of large extra dimensions, models of neutrino masses and mixings, extra Z bosons, and supersymmetry signals at the present and future colliders. In the TeV-scale superstring, a scenario is proposed in which not only the graviton, but also the gauge bosons, propagate into the large extra dimensions when the collider energy exceeds the energy threshold of these extra dimensions. In addition to modifying gravitational interaction at the millimeter scale, this scenario also give rise to the interesting modification to the QCD dijet cross sections at the high-energy colliders. We also proposed the effects on the Higgs boson mass, and on its decay modes, as well as supersymmetry effects in theories with large extra compact dimensions. In the neutrino masses and mixings project, we proposed models of neutrino masses with an extra, light sterile neutrino, involving four or five parameters. These models satisfy all the present experimental results, and makes several interesting predictions which can be tested in the upcoming experiments. We also proposed how to get specific textures for the neutrino mass matrices from theories with large extra compact dimensions. In the extra Z boson, we plan to investigate the mass bounds, and the collider signals for an extra Z boson coupling only to the right-handed fermions. In the supersymmetry project, we plan to investigate the supersymmetric tau and non-tau lepton signals at the Tevatron RUN 2.

157. Experimental Physics Investigations Using Colliding Beam Detectors at Fermilab, Cornell (Tasks A and C) and Nonperturbative Quantum Field Theory (Task B)

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The University of Oklahoma High-Energy Physics group (OU-HEP) consists of four experimental and one theoretical faculty, four postdoctoral physicists and four graduate students in the process of writing their Ph.D. theses. Experimental tasks continue the development and testing of silicon microstrip and pixel detectors for Fermilab's DO and Cornell's CLEO-III programs and the future detector ATLAS at the LHC in Europe. Data analysis regarding QCD, top-quark, W-mass, search for new particles (charged Higgs, etc.), inclusive kaon yields and others are being carried out for both DO and CLEO. A search for possible magnetic monopoles is being conducted here at OU (Fermilab experiment E-882). The theory task is involved in the monopole search, as well as carrying out its own program developing nonperturbative methods in quantum field theory, theoretical work on magnetic monopole binding to nuclei and vacuum energy phenomena (i.e., Casimir and Chern-Simmons effects). The CLEO effort is longstanding and will phase down, while DO will remain strong and lead into the future physics of the LHC. The collaboration with the two additional experimental faculty at Langston University, funded previously via subcontracts from OU, is as of now directly funded separately by DOE.

158. Intrinsic Bioremediation of Gas Condensate Hydrocarbons: Development of a Scientific Basis to Support Regulatory Decisions at Hydrocarbon Contaminated Sites

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Our goal is to determine whether, and at what rate, intrinsic bioremediation of hydrocarbons by indigenous microorganisms occurs by conducting laboratory and field studies of anaerobic biodegradation of benzene, toluene, ethylbenzene, and xylene (BTEX) and of other gas-condensate hydrocarbons.

159. The Immobilization of Radionuclides and Metals in the Subsurface by Sulfate-Reducing Bacteria

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Our proposed goals are to develop and evaluate biotechnological approaches for the remediation of subsurface environments contaminated with radionuclides and heavy metals. We know that sulfate-reducing microbial communities have the ability to immobilize radionuclides such as Co and U, as well as other metals that are present at DOE sites. This can occur by reaction with biologically produced sulfide as well as through the use of these metals as terminal electron acceptors for these organisms. To understand the ability of these organisms to catalyze desirable metal transformations requires knowledge of how they exist in their natural state. Specific objectives are listed below:

1. An examination of the factors that accelerate microbial radionuclide and metal immobilization process. We have attempted to answer how we can best immobilize the radionuclides of interest in the subsurface. Our approach employs the extrapolation of information from pure cultures to environmental samples. 2. A determination of the spatial heterogeneity associated with sulfate-reducing microbial communities in the subsurface. We have hypothesized that the activity of sulfate reducing microbial communities is not uniform through the subsurface but exists predominantly in discreet "hot spots." These hot spots are where sulfate reduction and hence contaminant immobilization will occur most readily. By understanding the factors that control the location of these hot spots, we will have considerable insight on how to stimulate sulfate reduction in other subterranean locales. 3. A determination of the potential for reoxidation and consequent remobilization of radionuclides in the subsurface. Immobilization of metals mitigates their environmental threat, however; the stability of immobilized complexes must be evaluated in order to determine the longevity of the remediation effort. We will attempt to chemically characterize the immobilized complexes and evaluate their susceptibility to remobilization under various redox conditions.

160. The Physics of Two-Phase Immiscible Fluid Flow in Single Fractures and Fractured Rock

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The objective is to develop a quantitative understanding of the critical processes controlling two-phase flow and transport in fractures based on detailed physical experiments and high-resolution numerical simulations. This understanding may subsequently be abstracted for use in conceptual models applied on a large scale to applied programs in petroleum extraction and the isolation of hazardous or radioactive waste.

161. Development and Application of a Paleomagnetic/Geochemical Method for Contraining the Timing of Fluid Migration and Other Diagentic Events

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The goal of this project is to develop paleomagnetic methods for dating diagenetic events in sedimentary rocks. Specific objectives include testing the hypotheses that fluid flow (e.g., basinal fluids, hydrocarbons), clay diagenesis and organic matter maturation are viable mechanisms for the occurrence of pervasive chemical remanent magnetizations (CRMs) that are commonly observed in sedimentary systems.

COMMONWEALTH OF PUERTO RICO

A. Projects Supported by EPSCoR

162. Particles, Processes and Materials for Modern Energy Needs: Development of a DOE EPSCoR Project in Puerto Rico

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The Puerto Rico Department of Energy Experimental Program to Stimulate Competitive Research (PR-DOE/EPSCoR) was initiated on September 30, 1994, for a two-year period, and renewed for a third year in July 1996. At this point (4.3 years into the project), the program is operating extremely well, and is on-track to meet the majority of its goals and objectives. Three research clusters (High-Energy Particle Physics, Novel Thin-Film Materials for Optoelectronic Applications, and Catalytic Processes for Energy Sources and Environmental Detoxification) have been established, with a total of 28 faculty researchers. The research clusters are currently working towards innovative solutions to problems of national Department of Energy priorities, as well as those of local needs. The program has stimulated a strong student research participation, with nine (9) postdoctorals, forty-four (44) graduate students and twenty-two (22) undergraduates currently funded in the project, and still more working on related projects through other funding. This participation is helping to supply Puerto Rico with the human resources in the future for dealing with energy-related issues. The establishment of the research clusters, together with the active student participation, has already led to significant scientific and technical accomplishments. A total of 228 publications in refereed journals and 447 presentations in national and international forums have resulted directly from PR-DOE/EPSCoR researchers since the inception of the project. Furthermore, researchers and students have been interfaced with ongoing research at the DOE national laboratories. Over sixty (60) students, both undergraduate and graduate, have participated in extended stays at different national laboratory facilities since the project began. The combination of these efforts have already served to strengthen research opportunities at all levels in the higher education institutions in Puerto Rico, and we will continue to build on this development. PR-DOE/EPSCoR has developed an active Human Resources component geared towards the promotion of scientific literacy and motivation towards scientific careers at the K-12 level, in addition to the graduate and undergraduate education opportunities described above. A collaborative program with the Puerto Rico Department of Education has researchers going to junior high and high school classrooms to explain their research and their role as scientists within the community. The program to date has been highly successful, and a vigorous agenda is planned for the remainder of the project. Curriculum development has also been an important approach towards stimulating more students into careers as scientists. PR-DOE/EPSCoR has worked side-by-side with the Puerto Rico Statewide Strategic Initiative (PR-SSI) in this area. A multi-use teacher training laboratory, funded under this grant, has been constructed on the Arecibo campus of the University of Puerto Rico, and is having a significant impact on curriculum development by allowing teachers to develop (with guidance) their own instruction materials.

163. Human Resources Development

The long-lasting effects of the DOE-EPSCoR Program will come from the changes it is able to make the people it touches. Puerto Rico has a wealth of human resources that it has barely begun to tap for scientific endeavors. Science and engineering put to society's service is the key to the solution of the energy-related problems in Puerto Rico, a heavily industrialized, foreign-oil dependent, densely populated island, where potential environmental impacts of energy utilization must be carefully assessed. The Human Resources Development component of Puerto Rico's DOE-EPSCoR project has carried out a series of activities since 1994 aimed at increasing the number of junior and senior local scientists and engineers involved in energy-related research. These activities touch all the levels of the educational and research structure from pre-college to senior researcher. The emphasis is on the development of our youngest minds through several activities aimed at the pre-college level: a teacher training laboratory, visits by researchers, Saturday academies for teachers and students. Other activities, such as the Summer Internships for undergraduate students, complement the human resource development that occurs naturally within the research clusters where junior researchers, postgraduate assistants, graduate and undergraduate students develop through their immersion in leading-edge projects and their collaborative interaction with senior researchers.

164. Cluster I—High-Energy Physics

The DOE-EPSCoR grant has allowed the High-Energy Physics Cluster to greatly increase its participation in experiments at the Fermi National Accelerator Laboratory. During the last two years, the cluster continued to make significant contributions to the acquisition and analysis of data from E831. The data run was highly successful, surpassing the goals in amount and quality. E831's data set (26000 Gb) will be the basis for measurements of charm quark physics of unprecedented precision. The cluster completed projects in the analysis of data from its detectors and continues to participate in the general analysis and data reduction. The latter projects will be completed shortly, and the emphasis will then be on detailed analysis and simulation which constitute the major part of the proposed research. Another major project is the use of modern statistical methods in high-energy physics. During the last year Dr. Wolfgang Rolke has concentrated on the development of a new method for the estimation of parameters of interest in high-energy physics. In the last two years there have been two important developments impacting on the cluster's long-term future. One is the commitment the cluster has made to the effort to carry out a B physics experiment (BTEV) at the Fermilab collider. The other is the addition of Dr. Will Johns to our group. BTEV proposes to study the decay of particles containing b (and c) quarks in the forward region and has the ambitious goal of measuring CP violation in the B sector. Such an experiment was a long-range goal of our original EPSCoR proposal contemplated at that time for the SSC. Plans for its implementation at Fermilab are gathering momentum. Fermilab has approved a BTEV R&D project and has built an experimental hall at a new collider intersection region. Both Dr. Lopez and Dr. Johns are members of the BTEV muon group which is designing and will be building that detector. A recently hired Assistant Professor, Dr. Johns has many years of experience in charm physics, specifically in E831 and its predecessor, E687. He has also made a commitment to BTEV. With an expanded group and a solid proposal for the long term, the cluster is well prepared for the future.

165. Cluster II—Novel Thin-Film Materials for Optoelectronics Applications

This cluster focuses its efforts in ongoing investigations on thin films of novel optoelectronics, especially ferroelectric (FE) thin films and display materials in which our scientific understanding will be enhanced, leading to the fabrication of prototype devices of DOE relevance, such as waveguides, FE film-based high-voltage performance capacitors and memories; and display devices. Two closely interacting research activities, materials preparation and materials characterization, form the basis for this cluster. Film growth is carried out using pulsed laser deposition (PLD), molecular beam epitaxy (MBE), radio frequency sputtering (RFS), and sol-gel techniques. Our materials preparation efforts include the growth of oxide thin films of doped and undoped SBN, KTN , SBT, PLT, and $CaTiO_3$ using PLD, RFS, and sol-gel techniques. Undoped and doped epitaxial films of the $BaMgF_4$ family onto group-III nitride epilayer substrates are grown using MBE. We are evaluating the effect of post-growth thermal treatments on the grown films as a possible tool to improve the quality of the films. The prepared materials are investigated by nonlinear optical studies, including degenerate four-wave-mixing (DFWM) techniques using CW and pulsed laser sources; laser Raman scattering, luminescence, infrared, static light scattering and photon correlation spectroscopies. In addition to this the dielectric, hysteresis, piezoelectric, pyroelectric, electro-optic, and differential thermal measurements on films are carried out to quantify some of their opto-electronic and physical properties. Laser spectroscopy and photo dynamics of the doped materials, including up conversion, energy transfer, quantum confinement and phonon-electron interaction are also investigated. These studies help us understand how growth conditions affect the film structure (strain, grain size, and inhomogeneity), thereby affecting the dielectric, optical and electronic properties relevant to their future application in optoelectronic devices. The studies also shed light on the thickness versus FE behavior, the spectrum of relaxation times, FE fluctuations and phase transitions, the stability of the ferroelectric phase, and order-disorder behavior in FE relaxors and its relation to the phase transition dynamics.

166. Cluster III—Catalytic Processes in Energy Sources and Environmental Detoxification

The principal objective of the cluster research is to develop broad-based new energy research initiatives in Puerto Rico. This goal is addressed by this cluster in its broad focus, which spans the spectrum of basic to applied research. The Cluster III research is embodied in the title, Catalytic Processes in Energy Sources and Environmental Detoxification, and in its two projects: (1) Energy Sources, both traditional and new, and (2) Environmental Detoxification, focusing on the invention and implementation of new technologies. The cluster assembles a critical mass of productive, dedicated research groups, establishing the basis for an integrated energy-related research program throughout Puerto Rico. With the goal of increasing the degree of research overlap, new collaborative initiatives have been established both within the cluster and with personnel in national laboratories, local government agencies, industry and other universities. The senior investigators (12) have been brought together from the two major universities on the Island to contribute energy-related research in both chemistry and chemical engineering. The Cluster provides the core around which participants are stimulated and encouraged to take their research to reach out to first, their students, second, other cluster participants and third, to other researchers in national laboratories, universities and industries throughout the world. Our technical mission includes both basic and applied research. In this way, invention and discovery, relevance and reality are constantly experienced by each of the participants. It is with a broader vision of research, namely moving forward mindful of the consequences of our work, that these two cluster subgroups are brought together. Comprised of six (6) senior researchers, the Energy Sources project provides contributions to the understanding of combustion and its by-products in the environment, while also examining potential new catalysts and materials, designed to enhance energy conversion and storage for future technologies. The Environmental Detoxification project, with six (6) senior personnel, provides the mechanism for the invention of new technology for cleaning up environmental contaminants as well as improving upon existing methods. Progress has been made on both fronts, and the proposal outlines new research to make further advances, both in chemical and solar catalytic processes. The activities of the cluster have been both extensive and far-reaching, considering its short time of existence. The cooperation and collaborations resulting from these projects have further enhanced the development of energy-related research in Puerto Rico beyond the technical achievements. The DOE-EPSCoR initiative has also provided us with an opportunity to link energy-related research to student development, and this impact has been significant. Cluster personnel have spent summers at several national laboratories and associated research facilities [i.e., ORNL, SNL, LANL, PETC, LBL(UCB), NREL].

167. Investigations of Charged Interfaces for Electric Vehicle Applications

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This project addresses the development of ultracapacitors and related systems to serve in electric vehicles. We will address issues of interest in the development of electric vehicle applications: The voltammogram shows features which are attributed to structures at the surface. These structure of these phases will be investigated by X rays by the Argonne group of Z. Nagy and H. Yoo. Theoretical models to explain the structural transformations and the charge transfer process will be formulated by our group in Puerto Rico. Some of the work using tight binding, embedded atom and equivalent crystal metods, has been done. To derive proper molecular parameters to be used in the semiempirical method a program of density functional (DFT)/pseudopotential calculations is being started in collaboration with Andy Rappe of the University of Pennsylvania. I will be spending at least a month this summer at Argonne working on the recent surface diffraction measurements on RuO: the mechanism of electron transfer and charge distribution in electrodes. We have recently published two works that clearly show that the electron transfer in the Cu/Au(111) case occurs with jumps. The realistic theory of the diffuse and inner layer capacitances depends on a reliable equation and on a realistic model of water potential. Significant progress in both directions has been achieved: An analytical model of tetrahedral water has been solved. The theory of ionic solutions in this “water” is being written up. A systematic series of analytical approximation based on the Multiyukawa closure of the Ornstein Zernike equation is being published in *Molecular Physics* this year. This will be used in conjunction with the DFT for a comprehensive, yet tractable theory of the interface.

B. Projects Supported by the Office of Science

168. Charm Decays and High-Energy Photoproduction

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This project involves continued participation by the Physics Department at the Mayaguez Campus of the University of Puerto Rico (UPR) in high-energy physics experiments carried out at Fermilab. The UPR is a member of the E831 collaboration (FOCUS) which includes Fermilab and leading U.S., Italian, Brazilian, and Korean universities. E831 is an upgrade to the E687 spectrometer, with the goal of a tenfold increase in the statistics for the study of the photoproduction and decay of charmed particles. E687 completed its last data run in January 1992. Approximately 100,000 charm events were fully reconstructed from this data, and results of the analysis have appeared in over 35 publications. The UPR has been participating in E687 and E831 since 1985. For E831 it undertook responsibility for four major detectors which were ready on time for the start of the run in July 1996. The UPR also developed the software for the analysis of the data and the simulation of the inner muon detector. E831's run ended in September 1997, and the primary data analysis in September 1998. The UPR group is presently carrying out a significant portion of the subdivision of the huge E831 data set (24,000 GB). It has also developed software for the analysis of closed charm states and semileptonic decays, which will constitute its main focus of analysis in the near future. This past year the group has started to work on the design for a future experiment to study CP violation in B decays in the Fermilab collider (BTEV). Activity has started in the preliminary simulation of the BTEV muon detector and the design of the front-end electronics for this detector's readout.

STATE OF SOUTH CAROLINA

A. Projects Supported by EPSCoR

169. South Carolina DOE/EPSCoR Research Implementation Agreement

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170. Cluster: Electrochemical Power Sources

It is proposed herein to continue building a research cluster that is focused on electrochemical power sources (fuel cells, batteries, and supercapacitors). This research cluster is of interest to Department of Energy personnel in the Office of Transportation Technology (OTT) and in the Office of Basic Energy Sciences (BES). It is also of interest to personnel at other government agencies, such as the Army Office of Research, national laboratories, and companies. The primary reason for continuing to build this research cluster is that it brings together experts and junior faculty in complementary areas of research to foster collaboration in the area of electrochemical power sources. This research cluster will continue to consist of faculty teams working together on several projects. These teams will include experts (mentors) and junior (target) faculty. There will be six mentor faculty members working with 15 target faculty members on six projects related to electrochemical power sources. The purpose of this research cluster is to develop expertise, designs and methodologies that can be used to develop improved proton-exchange membrane (PEM) fuel cells, production methods for pure hydrogen for use in PEM fuel cells, lithium ion and polymer batteries, nickel/metal hydride batteries, and supercapacitors. The goals of the projects in this research cluster include the development of design tools for PEM fuel cells by mathematical modeling, production of hydrogen from gasoline or diesel fuel, new separators for PEM fuel cells and lithium-based batteries, new chemical sensors for use in electrochemical power sources, and new electrodes for lithium-based batteries and supercapacitors. Collaborative efforts are currently underway with Argonne National Laboratory (PEM fuel cells), Los Alamos National Laboratory (PEM fuel cells), Energy Partners (PEM fuel cells), W. L. Gore and Associates (PEM fuel cell separators), Motorola (PEM fuel cells), 3M (PEM fuel cells), Mine Safety Appliances (lithium batteries), Westvaco (lithium ion batteries and supercapacitors), Celgard (lithium ion batteries), Westinghouse Savannah River Company (metal hydrides and PEM fuel cells), and others. This research cluster is also of interest to other companies such as H-Power (PEM fuel cells) and Yardney (lithium batteries). These companies may establish collaborative research programs in the future. During these last two years of the project, we plan to build infrastructure in the Department of Chemical Engineering by hiring a tenure-track faculty member with experience with spectroscopy of catalytic surfaces. This expertise is required to understand the effect of CO poisoning in fuel cells and to aid in the understanding and characterization of novel, albeit commercially available, binary and tertiary catalysts for CO tolerant catalysts for fuel cell electrodes. This expertise will allow studies of the interaction of these catalysts with PEM fuel cell operating conditions. These studies have the potential for significant breakthroughs. This expertise will also foster interaction with Dr. Angel and Dr. Murphy in Chemistry (spectroscopy) with Dr. Amiridis (Project 2) for hydrogen production catalyst. Start-up funds are requested for surface-enhanced Raman equipment to study the membrane/electrode/reformate interface during CO poisoning. With this addition the research cluster will be assured of containing all of the necessary individuals for studying PEM fuel cell catalysts and membranes exposed to reformed hydrogen fuel. The project will be self-sustaining after the completion of the six-year award period because the team will include modelers, macroscopic or performance experimenters, microscopic catalysts researchers, and fabrication and sensor researchers from Projects 4 and 5. The value added by the previous awards include the acquisition of fuel-cell test-bed facilities, the development of system and single-cell models, the development of parameter estimation tools specifically for PEM fuel cells, and the development of a database for commercial membrane performance and test protocol. The value added by the renewal award for the 5th and 6th years include the acquisition of spectroscopic equipment and a tenure-track faculty member to aid in the fundamental understanding of CO-tolerant catalysts.

171. Project 1: Mathematical Modeling of Proton Exchange Membrane Fuel Cells and Stacks

This project will be a continuation of the work started in October 1995. The objective of this project is to address some of the primary issues associated with Proton Exchange Member (PEM) fuel cells and PEM fuel cell stack design. For this renewal period, the objectives of this project are to address the primary issues associated with reformate use in PEM fuel cells, PEM fuel cell stacks, and system designs that use PEM stacks. These objectives will be achieved through mathematical modeling and experimental work with single cells, stacks, and systems. We have developed a modular stack model that uses simple models for flow fields, single cells, and flow in stacks. We have also developed a system model for an industrial vehicle (John Deere's PEM fuel cell powered Gator, with fuel cell built by Energy Partners). We are planning to extend this model to handle transient conditions. We have modified a computational fluid dynamic package (FLUENT) to study the local current density distribution in two dimensions on a gas diffusion layer-membrane electrode assembly (MEA), resulting from the prediction of three-dimensional flow distributions of humid hydrogen and air streams. We have determined experimentally the effect that compressing the gas diffusion layer has on the optimal humidity conditions for GORE SELECT composite membranes. We have measured the dynamics of CO poisoning for GORE PRIMEA MEAs. We plan to extend the CFD model to account for the transient response of the MEA to changes in the humidity and increased transient levels of CO. We plan to improve the predictions of the system model through relaxation of present assumptions and validation through instrumentation and experimentation of an industrial vehicle. This project is of interest to OTT, BES, and ONR. It will also be of interest to fuel cell assemblers and membrane producers and to fuel cell research groups in national laboratories (for example, Los Alamos National Laboratory). We are currently working with W. L. Gore to study the performance at ambient pressure of their ultra thin membranes. This will expand the commercially available database. We are currently working with Analytic Power Corporation to develop a mathematical model to describe water distribution in fuel cells. We intend to hire a chemical engineering tenure-track faculty member that can study the membrane/electrode/reformate interface using spectroscopic techniques such as surface enhanced Raman. This addition will allow us to complete the transition of studies from microscopic catalytic behavior through macroscopic single-cell membrane and electrode behavior, through stack design and, finally, to system design.

172. Project 2: Hydrogen Production via the Direct Cracking of Hydrocarbons

The objective of this project is the development of a new method for the production of hydrogen via the direct catalytic cracking of methane. The hydrogen that will be produced by this process will be suitable for subsequent use in proton-exchange membrane (PEM) fuel cells for generation of electricity. The proposed research will employ new synthetic strategies, kinetic analyses and various characterization techniques to achieve this objective. It is expected that this project will lead to an understanding of (1) the fundamental chemistry involved in several steps of the process—including the synthesis of new catalysts, the cracking of methane, the accumulation of filamentous carbon, and the gasification of carbon (during catalyst regeneration), and (2) the electrochemical properties of the filamentous carbon that extends beyond the current state of knowledge in the field.

173. Project 3: Novel Fluorinated Electrolytes for Batteries and Fuel Cells

The objectives of this project are to develop novel fluorinated polymer electrolytes with improved properties for applications in PEM cells as the separator membrane and in the fabrication of membrane and electrode assemblies (MEAs). Preparation, thermal analysis and materials fabrication of novel polymer materials (DesMarteau), structural characterization by luminescent spectroscopy and TEM (Sun), X-ray scattering (Pennington) and electrochemical characterization of materials and fuel cell testing (Creager) have been carried out at Clemson University. These efforts provide input for development of molecular-level models (Ploehn) at USC to relate molecular level nanostructures in polymers to the polymer's molecular topological architecture and chemical composition. The ultimate goal is a fundamental knowledge of structure-property-performance relationships of fluorinated ionomers in conjunction with the development of superior polymer electrolytes.

174. Project 4: Fiber-Optic Chemical Sensors for In-Situ Battery Diagnostics

The objective of the chemical sensor research is to provide unique chemical information to those groups responsible for modeling and improving existing batteries and energy storage devices. This will be accomplished by developing in-situ fiber-optic spectroscopic probes that are designed specifically for use in electrochemical devices. This work requires miniaturizing spectroscopic probes that already exist and developing new ones for selected chemical measurements, such as pH and water. Specific tasks proposed here include: use of the imaging fiber-optic sensors to make diffusion and transport measurements in polyelectrolyte (PE) membranes under potential, as close as possible to device conditions; further improvement of imaging sensors by measuring fluorescence lifetimes for determining the spatial distribution of analyte concentrations as a function of time; completing development of a pH sensor and transfer of measurement capabilities to collaborators in chemical engineering; development of a fiber-optic Li+ sensor for measuring Li+ concentrations in a cell and the use for measurement of Li+ during cell operation; and continued development of mathematical techniques to determine species concentrations from imaging sensor data.

175. Project 5: New Materials, Modeling and Design Tools for In-Situ Battery Diagnostics

This materials-oriented project will continue to carry out research in three complementary areas, with the overall objective being to develop the expertise that will be used to fabricate novel electrode materials for both electrochemical capacitors and lithium ion batteries. Innovative sol-gel techniques will continue to be explored, along with new electroless deposition and electrochemical synthesis techniques. Also, both macroscopic and microscopic models will continue to be developed to enhance both the practical and fundamental aspects associated with the design and development of improved electrode materials that exhibit both increased power and storage densities relative to existing capacitors and lithium ion batteries. These objectives will be accomplished by carrying out extensive experimental and theoretical studies in three interrelated areas with the following descriptive titles: (1) New Materials and Models for the Development of Improved Electrochemical Capacitors and Lithium Ion Batteries; (2) New Materials and Models for the Development of Electrochemically Precipitated Metal-Oxide Films for use in Capacitors and Batteries; and (3) New Molecular Modeling Tools for Characterizing the Nanostructure of Porous Electrode Materials. The electrode fabrication technology being developed in this project may also be used for the fabrication of membrane and electrode assemblies used in PEM fuel cells.

176. Flow and Infiltration Through Structured Fibrous Media

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The project's objective is to computationally investigate the mechanisms of fluid flow and infiltration through Structured Fibrous Porous Media. In the context of this research, Ameso-scale@ is associated with the diameter of the fibers comprising the porous medium (typically below 10µ). The term Astructured@ is used to characterize media whose internal topology is (1) decisively inhomogeneous and (2) has a detrimental influence on flow patterns and the resultant effective properties. The meso-scale structure of SFPM is explicitly considered in the simulations, which are carried out on geometries containing many discrete fibers. We will deal primarily with fully saturated flows, in which we will quantify the effect of structuring in general and of fiber clustering in particular on flow patterns and on hydraulic permeability. Such predictions will be compared with experimental MRI measurements and will be correlated to morphological parameters which quantify the structure of these media. In collaboration with researchers at LANL, we will also investigate unsaturated flows, in particular the deformation and mobilization of air pockets trapped within fiber tows, as well as the propagation of free surfaces through and around fiber bundles. We will consider viscous fluids, as well as cases where fluid inertia is not negligible. One application of this research is in the area of liquid molding used in the manufacturing of high-performance structural composites. However, these results will be equally applicable to any process characterized by flow across structured fiber arrays, such as in nuclear technology, filtration and membrane separations, drying of paper wood and textiles, physiological flow, reaction engineering and biotechnology.

B. Projects Supported by the Office of Science

177. Characterization and Thermophysical Properties of Bi-Based Ceramic Superconductors: Part B

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Summary not available.

178. Properties of Doped Bi-Based High-Tc Superconductors

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This research involves a systematic substitution of Cu in CuO layers of the 2212 and 2223 phases of high-temperature superconductors by transition metals (Fe, Co, Ni, Zn). The issue of whether the superconducting pairing state of the cuprates has *d*-wave or *s*-wave orbital symmetry can be addressed by studying the physical properties such as susceptibility, specific heat and transport.

179. Theoretical Studies of Energy and Momentum Exchange in Atomic and Molecular Scattering from Surfaces

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Summary not available.

180. Mechanism of Pitting Corrosion Prevention by Nitrite for Carbon Steel Exposed to Dilute Salt Solutions

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Summary not available.

181. Studies of the Transformations of Sulfur Containing Heterocycles by Transition Metal Cluster Compounds

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Recent studies have focused on the activation of three- and four-membered strained ring heterocycles containing sulfur and selenium by polynuclear metal carbonyl complexes. The principal objective is to develop catalysts for the formation of polythio- and polyselenoether macrocycles by ring-opening cyclooligmerization reactions of these precursors. Goals include synthesis of new macrocycles and the development of more efficient routes to known ones and then investigating their potential to serve as ligands for transition metals. Studies include determination of the mechanisms of the cyclooligomerization reactions. The ligand behavior of the macrocycles is being investigated by X-ray crystallographic characterizations of the metal complexes.

182. Synthesis, Characterization, and Testing of Novel Anode and Cathode Materials for Li-Ion Batteries

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This year several new cathode materials were synthesized: LiMn2-yCoyO4, LiMn2-yCryO4, CrOx, and LiCr3Ox. The effect of Co and Cr on the capacity fade of LiMn2O4 and LiMn2O4 was investigated. Cobalt and chromium doping in LiMn2O4 improved the cycling performance of the cathode due to the stabilization of the oxide spinel structure. This was observed for small quantities of doped Co or Cr. The optimum Co concentration in LixCoyMn2-yO4 was found to be y = 1/6, and the optimum concentration of Cr in LiCryMn2-yO4was found to be y = 0.1. These mixed-oxide cathodes provided an overall capacity of 110 Ah/kg with very-small-capacity fade with cycling. New CrOx cathode material has been also synthesized with a capacity of 245 Ah/kg and a discharge voltage of 3.0 V. Also, Pd-graphite, Sn-graphite and Ag-graphite composite anodes were synthesized. These anodes provided larger capacity than graphite alone. Electrochemical Impedance Spectroscopy (EIS) was used to determine the diffusion coefficient of Li ions in these anode materials.

183. The Magnesium Chelation Step in Chlorophyll Biosynthesis

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In photosynthetic organisms, the synthesis of new energy-generating membranes requires the coordinate synthesis of proteins, their associated cofactors, and various lipids. The important cofactors, chlorophyll and heme, share a common biosynthetic pathway, diverging at the point of metal ion insertion. Mg-chelatase catalyzes the insertion of magnesium into protoporphyrin-IX, the first step unique to chlorophyll synthesis. Our work is focused on the mechanism and regulation of this enzyme as it is a key to understanding how plants produce the proper proportion of chlorophyll and heme from a common pathway. We have shown by fractionation of chloroplast extracts and by cloning of the chlD gene that the enzyme in higher plants consists of three subunits (two other genes, chlI and H, have already been identified). Sequencing of the chlD gene suggests that it encodes a protein of 82.9 kDa (including a putative chloroplast transit peptide). The protein has a nucleotide binding motif and an unusual stretch of prolines followed by a stretch of polyglutamate. It is 58% homologous to the cyanobacterial protein. We have expressed the C-terminal third of the protein in *E. coli*. Although the expressed protein cannot substitute for a fraction containing the authentic pea D subunit in a reconstitution assay, it stimulates (20–25%) activity when added to a soluble extract that contains all three components. Work is continuing on the expression of a full-length D subunit for subsequent analysis of the role of this protein in the reaction.

184. Molecular Mechanisms Controlling Proton Pumping by Bacteriorhodopsin

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Bacteriorhodopsin (bR) is the simplest biological system for the transduction of light energy. This single, small-membrane protein converts light energy directly to transmembrane proton gradient. The extraordinary stability of bR makes it an outstanding subject for bioenergetic studies. The focus of our studies is the determination of the key mechanisms of light-induced proton transfer during light-energy transduction in bR. Site-directed mutagenesis, spectroscopic methods and chemical modification techniques are being developed and applied. The most important accomplishments are: (1) discovery of the complex titration of the primary proton acceptor, Asp85; (2) development of the concept of coupling of the primary proton acceptor Asp85 with the proton release group; (3) discovery of the role of transient protonation of Asp85 in the catalysis of thermal isomerization of the chromophore; and (4) development of methodology to routinely map the technically challenging bR by mass spectroscopy. These findings comprise a new approach for the investigation and interpretation of the properties of the pigment in the initial (ground state) and the photolyzed intermediate states. These properties are particularly important for understanding of early and late light-induced proton release in bR and its mutants. The insights gained from these results are fundamental to the understanding of proton transport through membrane proteins and hence, the conversion of light into energy.

185. Regulatory Role of ANT in Organ Initiation and Growth

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Genetic and molecular experiments in *Arabidopsis thaliana* have contributed much to our understanding of the specification of organ identity in flowers. However, many other processes in the development of a flower, including the determination of organ number and position, the development of particular cell types, and the acquisition of the final appearance (shape and size) of floral organs, remain poorly understood. One gene that affects both the number and the appearance of floral organs is ANT. ANT mutants possess a reduced number of sepals, petals, and stamens, narrow floral organs, and ovules without integuments. Thus, ANT is required for proper organ growth and, in some cases, organ initiation. The common bond between these different processes is cellular proliferation, and we propose that ANT is a critical factor controlling the number of cell divisions in floral organ primordia. In addition, ANT may also influence the plane of cell division. This is suggested by the effects of ant mutations on the shape of floral organs. ANT is thought to function as a transcription factor due to the presence of two AP2-domains, which have been shown to bind DNA in related proteins. In addition, ANT contains several putative activation domains and a potential nuclear localization signal. We will examine the proposed ability of ANT to regulate cell division by characterizing transgenic plants containing high levels of ANT expression. These transgenic plants produce larger flowers than wild-type plants, providing strong evidence that ANT is a key regulator of cell division in flowers. In order to understand how ANT acts in this process, we will identify and characterize functional domains of the protein. This will include investigating the function of the putative DNA-binding and transcriptional activation domains. Knowledge of the DNA binding site and activation properties of ANT will be important in future studies to identity target genes. The proposed experiments will be extremely useful in understanding the regulatory mechanisms used by ANT in the control of plant growth and organ initiation.

186. Experimental Particle Physics

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The High-Energy Physics group at South Carolina is engaged in accelerator-based research. The main directions of research are neutrino physics and heavy quark physics. The neutrino personnel are searching for the tau neutrino and for neutrino mass at experiments at Fermilab (DONUT), at Oak Ridge National Lab (proposed ORLaND experiment) and elsewhere. The heavy quark personnel are studying CP violation and semileptonic decays of charm quarks at Fermilab (FOCUS experiment) and at the Stanford Linear Accelerator Center (BaBar experiment).

187. Relationship Between the Adhesive Properties of Bacteria and Their Transport and Colonization in the Subsurface Environment

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Dr. Fletcher's research has the following objectives: (1) to determine the environmental transport of subsurface bacterial strains and their adhesion mutants and, (2) to determine the cell surfaces properties that control attachment and the influence of attachment on transport of bacteria through porous media. Dr. Fletcher hypothesizes that bacterial attachment and retention will occur primarily at the interfaces with permeability-change; to date, her research has focused on column studies. At present, and to complete experiments at the intermediate scale, the investigator is working closely with Dr. Steve Silliman/Notre Dame who has expertise in using flow cells with controlled physical heterogeneities. Dr. Silliman adds skills of modeling flow dynamics and chemical transport through porous media to Dr. Fletcher's expertise in bacterial attachment; together they will exploit Dr. Silliman's flow cells which incorporate different "permeabilities" derived from statistically packed, well-characterized mixtures of sediments. Thus, very controlled experiments can be completed to track microbiota with various attachment properties through a system of known hydraulics. Such strong, interdisciplinary research teaming will provide new field-relevant understanding of bacterial transport to meet goals in the NABIR Program Scientific Management Strategy Plan.

188. Radiation Leukemogenesis: Applying Basic Science to Epidemiological Estimates of Low-Dose Risks and Dose-Rate Effects

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The goal of this research is to investigate and develop mathematical models that link data from the basic sciences to epidemiological data to estimate risks of chronic myeloid leukemia from low-dose, low-dose-rate exposures to radiation.

STATE OF SOUTH DAKOTA

A. Projects Supported by EPSCoR

189. Investigation of the Interphase Region in Polymer Matrix - Glass Fiber Reinforced Composites Using the Interfacial Force Microscope

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The objectives of the research are twofold. First, the research will provide a critical vehicle to enhance South Dakota researchers' participation in nationally important energy-related research while building and strengthening partnerships between the South Dakota School of Mines and Technology (SDSM&T) and Sandia National Laboratories (SNL), Albuquerque, NM. Second, the critical relationships between interphase chemistry, mechanical properties and adhesion will be investigated in polymer matrix glass fiber reinforced composites. The interphase chemistry will be characterized using Fourier transform infrared evanescent wave spectroscopy. The nanomechanical properties of the chemically characterized interphases will then be investigated by employing the Interfacial Force Microscope (IFM), invented by Dr. J. E. Houston at SNL. This is possible because of the unique sensor the IFM utilizes. For the Department of Energy, this research has a large range of applications. For example, the development of the new generation of vehicles could substantially benefit from the ability to "engineer" advanced light-weight polymer matrix composite materials. In addition, techniques developed during the research program may be applied to investigate the aging of polymer matrix fiber composites, an important consideration in the long-term storage of our Nation's armament.

STATE OF VERMONT

A. Projects Supported by EPSCoR

190. Structure/Function Analysis of DNA-Glycosylases that Repair Oxidized Purines and Pyrimidines and the Influence of Surrounding DNA Sequence on Their Interactions

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The overall goal of this project is to elucidate the structure/function relationships between oxidized DNA bases and the DNA repair enzymes that recognize and remove them. The bacterium *Escherichia* coli contains two DNA glycosylases/AP lyases that share sequence homology with each other on their *N*-terminal and *C*-terminal ends: formamidopyrimidine DNA glycosylase (Fpg), which recognizes oxidized purines; and endonuclease VIII, which recognizes oxidized pyrimidines. Both proteins are highly hydrophobic, and Fpg has been refractory to structural determination by X-ray crystallography. The NMR solution structures of both of these proteins will be determined in this collaboration, using a 750-MHZ spectrometer. Our laboratory has previously demonstrated, using four randomized nucleotides on either side of the 8-oxoG lesion, that specific sequence contexts affect recognition and cleavage of 8-oxoG-containing substrates by Fpg protein. One particular sequence context also facilitated misinsertion of A during translesion synthesis, and this sequence was overrepresented surrounding G→T transversions in the lac I, Factor IX and p53 databases. The fact that this sequence was overrepresented in human genomes as well as bacterial suggested that the DNA itself exhibited specific structural features that facilitated cleavage by Fpg and misinsertion of A by DNA polymerase. To test this hypotheses that NMR solution structures of decamers containing 8-oxoG in the well-cleaved and poorly cleaved sequences will be determined. The ultimate objective is to understand the fundamental mechanisms that underpin base excision repair processing of oxidative DNA lesions at the atomic level. We expect results from these studies to aid in understanding the biological effects and consequences of DNA damages produced by toxic agents in the many DOE waste sites so that cleanup can be accomplished in a safe, effective and timely manner.

B. Projects Supported by Office of Science

191. Collaborative Project: Research on Strongly Coupled Plasmas

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A DOE-supported collaborative project of theoretical/computational research on strongly coupled plasmas is being carried out by the University of Vermont (Dr. Kenneth I. Golden, Principal Investigator) and Boston College (Dr. Gabor Kalman, Principal Investigator). Strong Coulomb interactions are featured by a variety of physical systems. Of primary interest are bilayer and superlattice plasmas, laboratory dusty plasmas, and charged particles confined in traps and storage rings. The joint UVM/BC research project focuses on these systems. The main objective is to understand the static and dynamical properties of the strongly correlated liquid phase. The part of the program directed at the static properties will address the determination of the equilibrium correlation and static structure functions, equation of state, phase boundaries, etc. The part directed at the dynamical properties will address the frequency-dependent dynamical structure functions and dielectric response tensors, and dispersion and damping of the collective modes. The approach to be followed for the generation of the pair correlation and static structure function data is the hypernetted chain (HNC)approximation adapted to the various plasma configurations. The dynamical calculations will be based on the quasilocalized charge approximation (QLCA) and velocity-average approximation (VAA) formulated by the principal investigators some time ago and applied to the strongly coupled one-component plasma in three and two dimensions, to correlated multilayer plasmas, and to laboratory dusty plasmas. The joint UVM/BC collaborative project is expected to provide fundamental new information about the equations of state, phase transitions, and collective mode structures for a variety of laboratory systems exhibiting strongly coupled plasma behavior.

192. An Immunological Approach to the Study of DNA Damage and Repair

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Summary not available.

193. The Role of Fracture Intersections in the Flow and Transport Properties of Rock

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Fluid flow in fractured rock is an important phenomenon to understand in connection with energy production and containment or disposal of toxic wastes. Both discrete fracture and effective continum approaches to the modeling of flow and transport in fracture networks need to be based on a sound understanding of flow in single fractures, how flow is transferred across intersections, and how multiple fractures form a network. We suggest that due to surface roughness and the consequent channeling in single fractures, volume flow and solute mixing behavior at fracture intersections will be considerably different from that expected based on simple assumptions and experiments with smooth-walled fractures. The objective of this project, therefore, is to gain a more complete understanding of flow channeling by physically modeling and analyzing several configurations of flow and transport through fracture intersections.

We are addressing several problems concerning flow and transport through fracture intersections using a combination of numerical modeling, quantitative measurements, and visual observation of processes in real rough-walled fractures. Our observations include: channeling in single fractures, channeling within and through single fracture intersections, and channeling through fracture networks. These studies consider bulk flow, transport of solutes, and transport of multiple immiscible phases. These observations will ultimately be used to develop quantitative models describing the channeling and mixing behavior in 3-D intersections of rough-walled fractures.

This work makes use of our abilities to (1) quantify surface roughness through profilometry, (2) construct high-quality replicas of actual fractured rock in transparent plastics, (3) simulate surface roughness with the computer, (4) construct bench-scale fracture systems, (5) observe actual flow and transport with quantitative visualization techniques, and (6) conduct detailed numerical simulations of flow and transport in heterogeneous media. For this work we use a combination of quantitative measurements, visual and magnetic resonance imaging (MRI) observations of flow through real rough-walled fractures, and numerical modeling via lattice Boltzmann (BGK) methods.

STATE OF WEST VIRGINIA

A. Projects Supported by EPSCoR

194. Correlation of Point Defects in CdZnTe with Charge Transport: Application to Room-Temperature X-Ray and Gamma-Ray Detectors

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Applications requiring room-temperature X-ray and gamma-ray detectors are increasing rapidly and now include nuclear medicine, space sciences, national security, environmental remediation, nonproliferation inspections, etc. To meet these needs, a new generation of detectors based on single crystals of cadmium zinc telluride (CdZnTe) is being developed. This DOE EPSCoR project supports a collaboration between Sandia National Labs and West Virginia University. The project goal is to apply experimental techniques including electron paramagnetic resonance (EPR), photo-induced EPR, and photoluminescence (PL) in order to gain a better understanding of the role of point defects in CdZnTe. Despite the tremendous promise of this material, there is a need to further lower the leakage currents in detector-grade material and also to increase the efficiency of charge collection. Thus, the study and characterization of point defects are an important part of the overall thrust to develop detectors based on CdZnTe. In general, all aspects of carrier trapping in this material must be understood and minimized. Samples are provided by Sandia National Labs for the experimental investigations at WVU. The project provides support for one graduate student to spend part-time at Sandia.

195. Numerical Modeling of Reactive Multiphase Flow for FCC and Hot-Gas Desulfurization Circulating Fluidized Beds

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The objective of this proposal is to simulate Circulating Fluidized Beds in cooperation with the numerical modeling group at the Federal Energy Technology Center (FETC) in Morgantown. Specifically, we are modeling Fluid Catalytic Cracking (FCC) Units that are utilized in refineries, and Desulfurization units that are integral parts of the Advanced Coal Fired Power Systems Projects that are currently under development at FETC. Two students began work in January and will work for the next three years developing and improving the three-dimensional Navier-Stokes-based model for circulating fluidized beds. One of the students is designing fluid catalytic cracking units and the other is designing desulfurization units. For optimal design of commercial-scale equipment, we need to be able to predict the behavior of large units from experimental data obtained from smaller units. Unfortunately, little exists in the way of a unifying multiphase flow theory. This is due primarily to a lack of understanding of hydrodynamics. The material inside the reactor can be viewed as two interpenetrating phases: a solid-particulate phase, which as a mixture flows like a fluid and thus has aggregate properties such as viscosity, local solid-phase density, granular temperature, velocity, etc.; and a continuous-gas phase. The equations that govern the hydrodynamics of these phases are coupled with the heat equation and mole balance of the various chemical species. These equations must be solved simultaneously to theoretically predict the performance of the reactor. Fundamental research/theory development such as that being developed by this project needs to be done to quantitatively design these units from first principles.

B. Projects Supported by Office of Science

196. Modeling of Diffusion of Plutonium in Other Metals and of Gaseous Species in Plutonium-Based Systems

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No summary available.

197. Experimental Investigation of Collisionless Electron-Electron Microinstabilities

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The proposed research program focuses on issues of fundamental plasma physics in a plasma parameter regime relatively unexplored by laboratory experiments. The results of the research will have direct applications for our understanding of space plasma phenomena and may provide insight into phenomena that may occur in next generation of high-temperature, moderate-density, high-beta, fusion experiments.

198. Homeostatic Adjustment of Loblolly Pine to CO_2 Enrichment in a Forest Ecosystem

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STATE OF WYOMING

A. Projects Supported by EPSCoR

199. Wyoming DOE/EPSCoR Implementation Award

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With the importance of energy and environmental issues to Wyoming, the DOE/EPSCoR program originally articulated and continues to emphasize three goals:
(1) establish Wyoming as the nation's leader in research associated with fossil fuel utilization and associated environmental technologies;
(2) make Wyoming coal, oil and natural gas more available and more competitive sources of energy while enhancing the utilization of Wyoming's renewable energy resources, including wind and solar generation; and
(3) develop capabilities in Wyoming to support energy-related industry in environmental monitoring, assessment, mitigation and remediation as well as in renewable energy and its impact on the nation's electric power infrastructure. While these goals emphasize the needs of Wyoming, they coincide with those of the nation and specifically with the DOE. Although ambitious, Wyoming's governmental leaders, research institutions and industries are committed to attaining these goals. The Wyoming DOE/EPSCoR program supports three research clusters:

1. Fossil Energy Cluster—emphasizes coal beneficiation and the chemistry of novel catalysts useful in refining and environmental industries.

2. Electrical Energy Cluster—studies the impacts of efficient control of motors and the economical use of solar generation in power distribution systems.

3. Environmental Cluster—develops electrokinetic and biological remediation as well as methods to reduce the VOC emissions from important industries.

200. Fossil-Energy Research Cluster

The research conducted by the Fossil Energy Cluster consists of four projects which address issues of fundamental and applied research in developing value-added products from fossil fuel feedstocks and in reducing the potential for harmful emissions in the use of fossil fuels in industrial environments. The first project is aimed at developing a novel process using CO_2 for producing a stable, higher-calorific value coal from the wet low-sulfur sub-bituminous coal abundantly available in Wyoming. The second project seeks fundamental characterization of the critical role of air in enhancing the strength of form coke briquettes manufactured from Wyoming coals. The third project addresses the need for developing new catalysts which will permit highly selective reforming of fossil-fuel based feedstock. The fourth project is aimed at developing new catalysts that will promote efficient and economic removal of nitrogen oxides from flue gases generated by fossil-fuel combustion sources. These projects, selected by the Wyoming EPSCoR Coordinating Committee, reflect the strong interest of the State and the University of Wyoming in developing research programs with an emphasis on the environmentally benign use of the natural resources available within the state.

201. Efficient Utilization of Electrical Energy Research Cluster

The focus of this cluster is to address three topics in the area of efficient electrical energy utilization. The first two projects examine technologies associated with efficient electric motors: advanced techniques for optimal energy control of electric motors, and evaluation of electromagnetic radiation effects of energy-efficient motor control methods. The final project examines the technical and economic issues involved in the power system interface for using photovoltaic technologies on the power grid. There are three common threads between these topics: (1) each is concerned with efficiency improvement, (2) each contains elements leading to a better understanding of the adverse effects resulting from some efficiency improvement methodologies, and (3) each is carefully selected so that the expertise and facilities currently available are maximally leveraged during the EPSCoR funding period to produce highly competitive and self-sustaining research programs. One example of the common thread between the three projects is the on-going research regarding both conducted and radiated radio frequency emissions measurement. The instrumentation acquired for Project 2 is being used to identify and measure emissions from the motor controllers designed and built in Project 1. In addition, the power inverters interfacing the solar photovoltaic output in Project 3 are also under study regarding RFI emissions.

202. Environmental Remediation and Waste-Reduction Research Cluster

The goal of this cluster is to develop science and technology needed to remediate polluted sites, or to prevent pollution. Rather than merely study environmental problems, this cluster seeks means to solve problems. To do this, a compatible group of faculty and students from a diverse set of disciplines, including microbiology and soil science, as well as chemical, civil, electrical, mechanical and petroleum engineering was assembled. Three projects are directed toward remediation technology. The first project conducts research in the basic genetics and regulation of microbial dechlorination of pentachlorophenol, a common soil contaminant. The second investigates the role of fungi in phytoremediation of metal contaminated soils. The third project studies electrokinetic methods of removing residual hydrocarbons, such as gasoline, from soil. Three other projects emphasize pollution prevention and waste disposal. The first project involves finding methods of drying natural gas that will reduce or eliminate the release of toluene and other contaminants to the atmosphere. Another project is developing a process for using supercritical carbon dioxide instead of volatile organic compounds in spray coating processes widely used in industry. The final project is part of a larger effort to develop an environmentally benign process for the disposal of high explosives.

203. Supercritical Solubility of Binders Used in Explosive Formulations

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The subject of this project is to measure the supercritical fluid solubility of polymers and other components used in binder formulations for plastic-bonded explosives. Currently, these explosives are formulated using a lacquer process. This process is largely unchanged since it was first developed in the early 1950s, and it generates large quantities of contaminated water. Several alternative formulation methods, based on supercritical fluids, have been proposed. These fluids could be used as solvents, replacing the lacquer solvent, or as antisolvents, causing the binder to precipitate from the lacquer. These new formulation techniques would eliminate the wastewater stream, and they may yield formulated explosives with improved properties due to a more even distribution of the binder. Supercritical solvents may also be used for the recovery of materials from obsolete explosives. All of these new processes would require data on the supercritical solubility of the binders. Initially, we are examining the carbon dioxide solubility of binders that are currently used in DOE formulations. Our experimental apparatus is limited to about 6,000 psig. Based on similar investigations reported in the literature, we do not expect significant solubilization at these pressures. This research is being carried out with assistance from Los Alamos National Laboratory, where binder solubilities are being investigated at higher pressures. We plan to investigate the use of cosolvents with carbon dioxide, and also the use of alternative supercritical solvents, such as dimethyl ether. Later, we may try alternative polymers that may be more soluble in supercritical solvents.

APPENDIX A

FUNDING AWARDS FOR FY 1999

Table A.1. Number of Projects and Funding Level for Designated EPSCoR States
(Funded by the Office of Science)

State	Number of Projects	Funding Level ($K)
Alabama	18	2,485
Arkansas	2	100
Idaho	5	832
Kansas	13	3,903
Kentucky	20	1,975
Louisiana	30	5,364
Maine	15	1,240
Mississippi	5	643
Montana	10	309
Nebraska	8	939
Nevada	20	1,879
North Dakota	2	97
Oklahoma	13	1,861
Puerto Rico*	7	836
South Carolina	20	1,742
South Dakota	1	50
Vermont	4	567
West Virginia	5	350
Wyoming	5	794
Total	**203**	**25,966**

*Commonwealth of Puerto Rico.

Table A.2. Number of Projects and Funding Level for Designated EPSCoR States
(Funded by the DOE EPSCoR Program)

State	Number of Projects	Funding Level ($K)
Alabama	5	825
Arkansas	2	100
Idaho	2	100
Kansas	3	139
Kentucky	7	831
Louisiana	7	150
Maine	11	750
Mississippi	1	50
Montana	7	75
Nebraska	0	0
Nevada	6	855
North Dakota	1	47
Oklahoma	2	100
Puerto Rico*	6	800
South Carolina	8	800
South Dakota	1	50
Vermont	1	25
West Virginia	2	100
Wyoming	5	794
Total	**77**	**6,591**

*Commonwealth of Puerto Rico.

Table A.3. Number of Projects and Funding Level for Designated EPSCoR States
(Funded by the Various Program Offices)

Funding Office	Number of Projects	Funding Level ($K)
OASCR	6	3,326
OBER	29	3,874
OBES*	57	6,538
DOE EPSCoR**	77	6,591
OFES	12	1,152
OHENP	22	4,485
Total	**203**	**25,966**

*Does not include DOE EPSCoR.
**Funded by OBES.

Table A.4. Number of Projects and Funding Level for Designated EPSCoR States
(Funded by the Office of Advanced Scientific Computing Research)

State	Number of Projects	Funding Level ($K)
Alabama	1	90
Arkansas	0	0
Idaho	0	0
Kansas	0	0
Kentucky	0	0
Louisiana	3	3,236
Maine	0	0
Mississippi	1	0
Montana	0	0
Nebraska	1	0
Nevada	0	0
North Dakota	0	0
Oklahoma	0	0
Puerto Rico*	0	0
South Carolina	0	0
South Dakota	0	0
Vermont	0	0
West Virginia	0	0
Wyoming	0	0
Total	**6**	**3,326**

*Commonwealth of Puerto Rico.

Table A.5. Number of Projects and Funding Level for Designated EPSCoR States
(Funded by the Office of Biological and Environmental Research)

State	Number of Projects	Funding Level ($K)
Alabama	3	500
Arkansas	0	0
Idaho	3	731
Kansas	1	166
Kentucky	0	0
Louisiana	1	247
Maine	3	490
Mississippi	0	0
Montana	2	130
Nebraska	1	325
Nevada	8	537
North Dakota	1	50
Oklahoma	2	395
Puerto Rico*	0	0
South Carolina	2	108
South Dakota	0	0
Vermont	1	95
West Virginia	1	100
Wyoming	0	0
Total	**29**	**3,874**

*Commonwealth of Puerto Rico.

Table A.6. Number of Projects and Funding Level for Designated EPSCoR States
(Funded by the Office of Basic Energy Sciences)**

State	Number of Projects	Funding Level ($K)
Alabama	1	135
Arkansas	0	0
Idaho	0	0
Kansas	5	2,673
Kentucky	9	769
Louisiana	13	725
Maine	1	0
Mississippi	0	0
Montana	0	24
Nebraska	5	424
Nevada	5	337
North Dakota	0	0
Oklahoma	7	629
Puerto Rico*	0	0
South Carolina	9	425
South Dakota	0	0
Vermont	1	397
West Virginia	1	0
Wyoming	0	0
Total	**57**	**6,538**

*Commonwealth of Puerto Rico.
**Excludes DOE EPSCoR Program.

Table A.7. Number of Projects and Funding Level for Designated EPSCoR States
(Funded by the Office of Fusion Energy Sciences)

State	Number of Projects	Funding Level ($K)
Alabama	6	621
Arkansas	0	0
Idaho	0	0
Kansas	1	70
Kentucky	0	0
Louisiana	1	30
Maine	0	0
Mississippi	0	0
Montana	1	81
Nebraska	0	0
Nevada	1	150
North Dakota	0	0
Oklahoma	0	0
Puerto Rico*	0	0
South Carolina	0	0
South Dakota	0	0
Vermont	1	50
West Virginia	1	150
Wyoming	0	0
Total	**12**	**1,152**

*Commonwealth of Puerto Rico.

Table A.8. Number of Projects and Funding Level for Designated EPSCoR States
(Funded by the Office of High-Energy and Nuclear Physics)

State	Number of Projects	Funding Level ($K)
Alabama	3	314
Arkansas	0	0
Idaho	0	0
Kansas	3	855
Kentucky	4	375
Louisiana	4	976
Maine	0	0
Mississippi	3	593
Montana	0	0
Nebraska	1	190
Nevada	0	0
North Dakota	0	0
Oklahoma	2	737
Puerto Rico*	1	36
South Carolina	1	409
South Dakota	0	0
Vermont	0	0
West Virginia	0	0
Wyoming	0	0
Total	**22**	**4,485**

*Commonwealth of Puerto Rico.

APPENDIX B

PROGRAM INFORMATION

B.1 DEPARTMENT OF ENERGY PROGRAM AREAS

The research activities within the Department of Energy (DOE) are performed within the following program areas: Civilian and Radioactive Waste Management; Defense; Energy Efficiency and Renewable Energy; Environmental Management; Fissile Materials Disposition; Fossil Energy; Nonproliferation and National Security; Nuclear Energy, Science, and Technology; and Science.

Each program has its own mission and research objectives. The following summaries describe briefly each office and how it responds to the challenges of DOE: *to ensure that our nation continues to be a leader in science and technology whose research supports our Nation's energy security, national security, environmental quality, and contributes to a better quality of life for all Americans.*

Following are the DOE program areas and a description of their respective missions.

CIVILIAN AND RADIOACTIVE WASTE MANAGEMENT PROGRAM

The Nuclear Waste Policy Act of 1982 established the Office of Civilian Radioactive Waste Management (OCRWM) within DOE. The main goal was to develop and manage a Federal system for disposing of all spent nuclear fuel from commercial nuclear reactors and high-level radioactive waste (HLW) resulting from atomic energy defense activities.

The statute outlines detailed direction for the scientific, technical, and institutional development of the system. The statute also requires that waste management facilities be licensed by the U.S. Nuclear Regulatory Commission (NRC).

The long-term goal of the OCRWM program is to safely dispose of HLW and spent fuel in a geologic repository. With this goal in mind, the Yucca Mountain Characterization Project is evaluating the suitability of Yucca Mountain (located about 100 miles northwest of Las Vegas, Nevada) as a potential site for development. The preparation of an environmental impact statement, along with other information to satisfy the Nuclear Waste Policy Act, is under way. If Yucca Mountain is determined to be suitable, a license application for repository construction will be forwarded to the NRC.

To be a fully viable option, DOE must demonstrate that Yucca Mountain would protect public health and safety and the environment for thousands of years. Uncertainties still exist about key natural processes, the basic design, and how the site and design would interact. DOE is completing critical testing and analyses to address these issues. When these issues are resolved, a decision will be made by the Secretary of Energy on whether to recommend the Yucca Mountain site to the President.

DEFENSE PROGRAMS

The mission of Defense Programs is to ensure the safety, reliability, and performance of nuclear weapons without underground nuclear testing. The Office of Defense provides an infrastructure and the intellectual ability to maintain the nuclear weapons stockpile, which includes replacing limited life components and ensuring an adequate supply of tritium. Defense also provides the ability to reconstitute underground nuclear testing and nuclear weapons production capabilities as required to meet future national security requirements.

Office of Emergency Response

The world's leading scientists, engineers, and technicians from over 50 years of managing the nation's nuclear weapons are a vital part of the DOE Defense Program. When the need arises, DOE is prepared to respond immediately to any type of radiological accident or incident anywhere in the world.

Seven radiological energy response areas compose the Office of Emergency Response: the Aerial Measuring System (AMS), the Atmospheric Release Advisory Capability (ARAC), the Accident Response Group (ARG), the Federal Radiological Monitoring and Assessment Center (FRMAC), the Nuclear Emergency Search Team (NEST), and the Radiological Assistance Program (RAP), and the Radiation Emergency Assistance Center/Training Site(REAC/TS).

AMS detects, measures and tracks radioactive material in an emergency situation to determine contamination levels. ARAC uses sophisticated computer models to develop predictive plots. ARG is deployed to manage or support the successful resolution of a U.S. nuclear weapons accident anywhere in the world. FRMAC coordinates radiological monitoring and assessment activities with those of state and local agencies. NEST provides the U.S. specialized technical expertise to the Federal response in resolving nuclear/radiological terrorist incidents. RAP is typically the first to respond to an emergency, because it is responsible for assessing the emergency situation and deciding on the steps needed to minimize the hazards. REAC/FS provides the treatment and medical consultation for injuries resulting from radiation exposure and contamination. In addition, it serves as a training facility.

ENERGY EFFICIENCY AND RENEWABLE ENERGY PROGRAM

The Office of Energy Efficiency and Renewable Energy (EERE) is responsible for developing and deploying efficient and clean energy technologies that meet our Nation's energy needs, enhance our environment, and strengthen our national competitiveness. The results of the EERE programs are significant – a more efficient U.S. industrial base, a developing clean energy technology industry, and tremendous energy savings in homes, offices, and government buildings. Future predictions include a car of the next decade with triple-the-fuel economy of our present sedans.

EERE's program activities are conducted in partnership with the private sector, state and local governments, DOE national laboratories, and universities. EERE is organized around five energy sections – industry, transportation, buildings, power, and Federal agencies. This orientation toward energy technology users has aided the EERE programs to focus on addressing the needs of the Nation through the marketplace.

ENVIRONMENTAL MANAGEMENT PROGRAM

The Environmental Management (EM) Program centers around four major areas: waste management, environmental restoration, science and technology, and nuclear material and facility stabilization.

Office of Waste Management

The Office of Waste Management (WM) responds to the public's increasing concern about protecting human health and preserving the quality of the environment. Thus DOE has made waste cleanup and environmental restoration a top priority. The WM program directs the treatment in preparation for storage and disposal, and disposal of waste generated by DOE's activities. DOE must safely store the waste generated by it current operations, as well as a significant backlog of waste generated in the past. The final step in the waste management process is waste disposal – the permanent isolation of the waste.

Office of Environmental Restoration

The Office of Environmental Restoration was created in 1989 within the newly established Office of Environmental Management to consolidate, centralize, and promote the cleanup of contaminated waste sites and surplus facilities with the DOE Complex.

Environmental restoration is the process by which contaminated sites are identified, characterized, and existing contamination is contained or recovered and disposed to allow beneficial reuse of the property.

The DOE Environmental Restoration Program is also involved in assessment and cleanup activities at 132 sites throughout the United States and Puerto Rico.

Office of Science and Technology

The Office of Science and Technology (OST) provides the full range of S&T resources and capabilities, from basic research to development, and from demonstration to deployment of technical assistance. OST delivers and supports fully developed, deployable scientific and technological solutions to EM cleanup and long-term environmental stewardship problems.

Office of Nuclear Material and Facility Stabilization

The Office of Nuclear Material and Facility Stabilization stabilizes nuclear materials and spent nuclear fuel and prepares them for eventual disposal using procedures that protect people and the environment. This office oversees the deactivation of excess contaminated facilities in a timely manner to reduce the risk associated with maintaining aged facilities and reduced outyear mortgages. This office also has coordination responsibilities for Savannah River and Rocky Flats, and additional responsibility for the K-Basins and the Plutonium Finishing Plant at Richland, Washington.

The Spent Nuclear Fuel Program (SFP) develops and implements policies, strategies, and programs to safely, effectively, and efficiently manage the present and future inventory of DOE-owned nuclear and foreign research reactor spent nuclear fuel. The National Spent Nuclear Fuel Program (NSNF) project (1) identifies and integrates SNF requirements to ensure safe existing storage and the resolution of vulnerabilities; (2) manages and coordinates foreign research reactor SNF acceptance program activities within the Department of State, foreign research reactor operations and foreign government officials, DOE Field Offices, and the agencies required to plan and negotiate contracts; (3) manages implementation of the Interagency Agreement between DOE and NRC regarding oversight of shipments of foreign research reactor SNF into the United States; and (4) manages many other SNF program activities requiring interfacing with NRC staff, EM, RW, and other Federal agencies to ensure that they are properly translated into long-term disposal requirements for spent nuclear fuel.

FISSILE MATERIALS DISPOSITION PROGRAM

The Office of Fissile Materials Disposition is responsible for the Department's technical and management activities to provide for the safe, secure, environmentally sound, and inspectable future storage of surplus weapons-usable fissile materials and the disposition of materials declared surplus to our national defense needs.

This office works with Russia to conduct joint small-scale tests and demonstrations of plutonium disposition technologies and provides technical and engineering support to the U.S. Government Interagency Working Group on Plutonium Disposition. It also strives to eliminate surplus weapons-usable fissile materials in a manner that encourages reciprocal action abroad.

The Office of Fissile Materials Disposition Program has successfully prepared two Environmental Impact Statements:

1. a 1996 decision that called for elimination of the proliferation threat of stockpiles of surplus, highly enriched uranium (where practical) by blending down the material for sale as low-enriched uranium ((LEU) and use in commercial nuclear reactor fuel to recover its economic value;

2. a 1997 decision that instructed the Department to reduce the number of sites where plutonium is stored and to develop a hybrid disposition strategy for surplus plutonium disposition strategy for immobilization of plutonium with HLW and the burning of some of the surplus plutonium as mixed-oxide (MOX) fuel in existing, domestic, commercial reactors.

Both methods would convert the surplus plutonium to spent fuel or other forms – both unsuitable for use in nuclear weapons.

FOSSIL ENERGY PROGRAM

The mission of the Fossil Energy Program is to enhance U.S. economic and energy security by doing the following: (1) managing and performing energy-related research that promotes the efficient and environmentally sound production and use of fossil fuels; (2) partnering with industry and others to advance clean and efficient fossil energy technologies toward commercialization in the United States and foreign markets; (3) managing the Strategic Petroleum Reserve to reduce vulnerability to economic, national security, and consequences of foreign policy problems that could interrupt our supply; and (4) encouraging the development of information and policies that benefit the public and ensure access to adequate levels of affordable and clean energy.

The availability of affordable energy will be essential to our Nation's economic strength in the coming decades. Major energy forecasts concur that fossil fuels will be the dominant energy source for the foreseeable future. Even though Americans want to continue to enjoy the economic benefits of lower-cost energy, they also want reliable energy supplies that do not harm the environment. Advances in fossil fuel technology, coupled with the continued readiness of the Strategic Petroleum Reserve (the emergency stockpile), are key to achieving this goal.

The Federal research, development and demonstration (RD&D) area has evolved in response to several strategic elements: power generation from natural gas; coal; renewable sources; nuclear fission and fusion; liquid and gaseous fuels from conventional and alternative sources; and end-use efficiency.

NONPROLIFERATION AND NATIONAL SECURITY PROGRAM

The Department of Energy has long been deeply involved in preventing the proliferation of nuclear weapons technology and the protection of nuclear material and facilities. In the post-Cold War Era, the Department and its system of national laboratories have conducted a vigorous program of nonproliferation research and development aimed at countering the threat of proliferation.

This office oversees a core program of nuclear nonproliferation activities concurrent with an efficient use of the unique technical capability of supporting and developing advanced technologies that aid in the detection and countering of emerging proliferation threats.

This wide spectrum of services for a broad range of domestic constituencies and nonproliferation regimes is carried out by five main offices—each with its own mission and responsibility for some of the Department's top national and international security programs: Office of Research and Development, Office of International Nuclear Safety, Office of Arms Control and Nonproliferation, Office of Safeguards And Security, and Office of Emergency Operation.

The nonproliferation of nuclear weapons is one of the Nation's highest priorities. The nonproliferation focus centers around five major objectives:

1. to secure nuclear materials in the former Soviet Union;

2. to ensure safe, secure long-term storage and disposition of surplus fissile materials;

3. to establish transparent and irreversible nuclear reductions;

4. to strengthen the nuclear nonproliferation regime; and

5. to control exports of nuclear technology and materials.

The Department of Energy is responsible for the U.S. government's research and development functions for monitoring nuclear explosions in the context of a Comprehensive Test Ban Treaty (CTBT). The research and development focuses on detecting, locating, identifying, and characterizing nuclear explosions in all environments worldwide.

NUCLEAR ENERGY, SCIENCE, AND TECHNOLOGY PROGRAM

The Office of Nuclear Energy, Science, and Technology supports five areas of research: Isotopes Programs, Nuclear Energy Research Initiative (NERI), Depleted Uranium Hexafluoride Management, Space and Defense Programs, and Nuclear Facilities Management.

Isotope Programs

The Department of Energy's Isotope Programs produce and sell hundreds of stable and radioactive isotopes that are widely used by domestic and international customers for medicine, industry, and research.

Isotopes are produced when there is no U.S. private sector capability, or other production capacity is insufficient to meet U.S. needs. The Isotope Program has requested funds for FY 2000 for two major initiatives: (1) continuation of the construction of the Los Alamos Target Irradiation Station in New Mexico, and (2) the implementation of the Advanced Nuclear Medicine Initiative.

The Department of Energy, through this office, will sponsor the Advanced Nuclear Medicine Initiative. The initiative will support peer-reviewed research to further advance nuclear medicine technology in the United States. Three major elements define the Advanced Nuclear Medicine Initiative:

1. Sponsor nuclear medical science using a peer-review selection process. Support will be in two forms: direct research grants and making isotopes available for research at prices researchers can afford.

2. Encourage the training of individuals in nuclear medicine by establishing scholarships and fellowships for nuclear medicine specialists and by sponsoring summer internships at appropriate institutions.

3. Initiate a focuses program to apply alpha-emitting isotopes available in the United States from the Department to fight a wide range of malignant diseases, including most common cancers and infectious diseases (e.g., meningitis and AIDS). Nonmalignant applications may include the treatment of other immune disorders and rheumatoid and degenerating joint disease.

Isotope Programs is the Nation's primary provider of a diverse range of short-lived isotopes needed for medical application and other important research. These isotopes are purchased in small quantities for use by researchers at universities and hospitals.

An important facility that produces these research isotopes is the Los Alamos Neutron Science Center Accelerator. Because of facility modifications related to the primary laboratory mission, the center will not produce isotopes for research after FY 1999 unless a new Los Alamos Production Facility is built. Construction of the new facility will allow continued and enhanced medical isotope production into the future.

Nuclear Energy Research Initiative

Early in 1997, the President requested his Committee of Advisors on Science and Technology (PCAST) to evaluate the current national energy R&D portfolio and provide a strategy to ensure that the United States has a program to address the Nation's energy and environmental needs for the twenty-first century.

The PCAST group on Energy R&D determined that establishing nuclear energy as a viable and expandable option was important and that a well-focused R&D effort to address the potential barriers with a Nuclear Energy Research Initiative (NERI) was needed. This new initiative should fund research based on competitive selection of proposals from the national laboratories, universities, and industry.

The Department endorsed the PCAST recommendation and received FY 1999 appropriations for NERI to address the key issues affecting the future of nuclear energy and to preserve our Nation's nuclear science and technology leadership. To achieve this long-range goal, the following objectives have been established:

1. Develop new reactor and fuel cycle concepts and seek scientific and technology breakthrough in nuclear energy to enhance the performance, efficiency, reliability, proliferation resistance, and economics of nuclear power.

2. Advance U.S. nuclear technology to maintain the Nation's international leadership in issues related to nuclear technology.

3. Promote and maintain a nuclear science and technology infrastructure to meet future technical challenges.

NERI will fund innovative scientific and inquiring research and development in the following areas:

1. Proliferation-resistant reactors or fuel cycles.

2. New reactor designs with higher efficiency, lower-cost, and improved safety to compete in the global market; lower-output reactors for use where large reactors are not feasible.

3. Advanced nuclear fuels.

4. New technologies for management of nuclear waste.

5. Fundamental nuclear science.

The NERI program has a competitive, peer-reviewed R&D selection process to find researcher-initiated R&D proposals from universities, national laboratories, and industry.

Depleted Uranium Hexafluoride Management Program

The U.S. Department of Energy has a program for long-term management and use of depleted uranium hexafluoride (UF_6) – a product of the uranium enrichment process. As part of this effort, DOE has prepared a Programmatic Environmental Impact Statement (PEIS) for the Depleted UF_6 Management Program.

Uranium is a radioactive element that occurs naturally in the earth's surface. It is used as fuel for nuclear reactors. Uranium-bearing ores are mined, and the uranium is processed as a reactor fuel.

In nature, uranium atoms exist in several forms called isotopes, primarily uranium-238 or uranium-235. Most of the mass (99.3%) will be composed of atoms of U-238, and a very small amount will consist of U-235.

Using uranium as a fuel in the types of nuclear reactors usually found in the United States requires that the uranium be enriched so that the percentage is increased, typically by 3 to 5%. To enrich uranium, a process called gaseous diffusion was developed by the United States in the 1940s. The gaseous diffusion process creates two products: enriched UF_6 and depleted UF_6.

Enriched uranium is used for defense needs by the United States and in making fuel for commercial light-water reactors. Highly enriched uraniun-235, typically used for military purposes, has not been produced since 1992.

Depleted UF_6 has had only limited uses. Thus large quantifies of depleted UF_6 have accumulated at the gaseous diffusion plants where it was created. Long-term management of this depleted UF_6 is being investigated under the DOE Depleted Management Program.

The Cylinder Management Program manages the depleted UF_6 cylinders at Paducah, Kentucky; Oak Ridge, Tennessee; and Portsmouth, Ohio. Management activities include inspecting, monitoring, and taking all actions necessary to ensure that the containers retain their integrity.

Space and Defense Power Systems Program

The Space and Defense Radioisotope Thermoelectric Generator (RTG) Program provides support for radioisotope power source development, demonstrating, testing, and delivery. Radioisotope power sources are the enabling technology for space applications requiring proven, reliable, and maintenance-free power supplies capable of producing up to several kW of power and the ability to operate under severe environmental conditions for many years. Many previous space missions have used radioisotope power sources.

The program will develop new, state-of-the-art power supplies required to support the National Aeronautics and Space Administration (NASA) space missions. Without these power supplies, NASA missions to explore deep space and the surfaces of planets could not occur. In keeping with policies made with our customer agencies, NASA will provide funds to DOE to support mission-specific development and hardware fabrication.

DOE and its predecessor agencies have provided nuclear power systems for use in space applications for over 35 years. These systems are safe, proven, reliable, maintenance-free, and capable of producing either heat or electricity for decades under remote harsh environments such as in deep-space exploration.

Nuclear Facilities Management Program

The goals of the Nuclear Facilities Management Program are to ensure cost-effective, environmentally compliant operation of sites and facilities managed by the Office of Nuclear Energy, Science, and Technology in support of Departmental missions; to place excess facilities into an industrially and radiologically safe shutdown condition; and to maintain the physical and technical infrastructure necessary to achieve the DOE mission.

The primary areas of activity under this program are the shutdown of the Experimental Breeder Reactor-II (at Argonne National Laboratory-West, Idaho Falls, Idaho), the maintenance of the Fast Flux Test Facility in a safe, standby condition, and the demonstration of electrometallurgical spent fuel treatment technology.

SCIENCE PROGRAMS

The Office of Science funds basic research to advance the scientific knowledge required to provide new and improved energy technologies, to understand the health and environmental implications of energy production and use, and to maintain U.S. leadership in discovering the fundamental nature of energy and matter.

The mission of the Office of Science is to advance basic research and the instruments of service that are foundations for DOE's applied goals, a base for U.S. technology innovation, and a source of remarkable insights into the physical and biological world and the nature of matter and energy.

As part of its mission, the Office of Science plans, conducts, and operates major scientific user facilities to serve researchers at universities and national laboratories. The Office sponsors thousands of research projects at hundreds of scientific institutions, both public and private, in the United States. Investments are made in graduate research and education to ensure the next generation of highly capable scientists and engineers. Selections are made from broad geographical regions and from a diversity of backgrounds and cultural settings.

Five divisions compose the Office of Science: Office of Advanced Scientific Computing Research, Office of Biological and Environmental Research, Office of Basic Energy Sciences, Office of Fusion Energy Sciences, and Office of High-Energy and Nuclear Physics. Each has its own mission that supports the specific goals of the Office of Science.

Office of Advanced Scientific and Computing Research

The mission of the Office of Advanced Scientific and Computing Research (OASCR) is to perform computational, networking, technology, and advanced energy projects research in support of the goals of the Office of Science strategic plan and the mission of the Department of Energy.

The Office serves as a link between science programs and laboratories and national economic competitiveness by conducting long-term, high-risk industry-relevant research and development projects in critical technology areas. Major involvement in activities include the High-Performance Computing and Communications (EPCC), the National Information Infrastructure (NIT), the American Textiles Consortium (ANUMXO, the Advanced Computation Technology Initiative (ACTI), and the Environmental Technology Partnerships (ETP). The Office leads and manages the Technical Information Management Program for the Department, providing direction and coordination for the dissemination of scientific and technical information resulting from the research and development and environmental programs.

OASCR is composed of three divisions. Each division has its own specific mission, as outlined below.

Mathematical, Information, and Computational Sciences Division (MICS)

MICS fosters and supports fundamental research in advanced computing (applied mathematics, computer science, and networking), and operates supercomputer networking and related facilities to enable the analysis, modeling, simulation, and prediction of complex phenomena important to the Department.

Advanced Energy Projects and Technology Research Division (AEPTR)

AEPTR supports high-risk, energy-related research to advance science toward innovative applications that could significantly impact the Nation's energy economy. AEPTR carries out its mission through a range of funding and partnership mechanisms. Formal research collaborations are established between the Office of Science multiprogram laboratories and industry. Awards are given for research contracted at DOE laboratories by single investigators and research grants.

Office of Scientific and Technical Information (OSTI)

OSTI is the office responsible for leading the Department's Technical Information Management Program (TINV) and for providing direction and coordination for the dissemination of scientific and technical information (STI) resulting from the Department's research and development (R&D) environmental programs. In efforts to disseminate STI, OSTI has produced the DOE Information Bridge, which allows access to full-text STI and Energy Files: Virtual Library of Energy Science and Technology, which provides a vast array of information and resources pertaining to energy science and technology.

OSTI also coordinates the Department-wide Scientific and Technical Information Program (STIP) – a complex-wide collaboration to lead the Department in the Information Age.

Biological and Environmental Research Program

The Office of Biological and Environmental Research (OBER) manages DOE's Biological and Environmental Research (BER) program and includes these primary areas: Life Sciences, Medical Sciences, and Environmental Sciences.

The mission of the BER program is to develop the knowledge needed to identify, understand, and anticipate the long-term health and environmental consequences of energy production, development and use. These goals are carried out through the program's support of peer-reviewed research at the DOE National Laboratories, universities, and institutions. The vision of BER is to bring revolutionary solutions to energy-related biomedical and environmental challenges.

Life Sciences Division

The Life Sciences Division manages a diverse portfolio of research to develop basic biological information and to advance technology in support of DOE missions in biology, medicine, and the environment. Specific research areas are the following:

- Human Genome research – to create and apply new technologies and research mapping, sequencing, and information management for characterizing the molecular nature of the human genome.

- ELSI research – to anticipate and address ethical, legal, and social implications arising from genome research.

- Structural biology user facilities – to develop and support the Department's national facilities for use in fundamental structural biology.

- Structural biology research - to develop novel technologies for the determination of protein structure and function.

- Microbial genome research – to characterize and exploit the genomes and diversity of microbes with potential relevance for energy, bioremediation, and climate.

- Low-dose radiation research – to understand and characterize the risks to health from exposures to low levels of radiation.

Within the Department of Energy, all research conducted at DOE, supported by DOE funds, or performed by DOE employees must comply with Federal regulations and DOE Orders to protect humans. The Life Sciences Division manages the DOE Human Subject Program.

Medical Sciences Division

The Medical Sciences Division (MSD) supports research in several distinct areas of science and technology that address a broad range of basic and applied research application in the fields of medicine and biophysics. The Medical Applications program fosters research to develop the beneficial applications of nuclear and other energy-related technologies for medical diagnosis and treatment. The infrastructure promotes many viable partnerships among the major research areas of molecular nuclear medicine, radiopharmaceutical development, medical imaging, boran neutron capture therapy, and the application of laser in medicine.

The technology developed under this program provides for the noninvasive detection and localization of biochemical dysfunction associated with disease and disorders, lesions in the body, the quantitative measurement of dynamic organ function, and the selective treatment of cancer with molecular radiation therapy.

The Biophysical Research Program elements have a common theme of research, development, and application of new technologies. The Measurement Science Program supports research in analytical chemistry directed at meeting the needs for new measurement technology for selected environmental and life sciences. The Structural Biology Program supports access to the national user facilities (e.g., the synchrotron light and neutron beam sources) by scientists in industry, universities, and government laboratories. It also funds research into new technologies for more effective use of these facilities. The Computational Biology Program focuses on understanding inverse protein folding. The work of the Genome Instrumentation Program centers on the development of advanced sequencing technologies and the automation of all stages of chromosome mapping and sequencing.

Environmental Sciences Division

The Environmental Sciences Division supports research in two basic program areas: Global Change Research and Environmental Remediation Research.

Global Change Research activities include the process research and modeling efforts needed to (1) improve understanding of factors affecting the Earth's radiant-energy balance; (2) predict accurately any global and regional climate change induced by increasing atmospheric concentrations of greenhouse gases; (3) quantify sources and sinks of energy-related greenhouse gases (especially carbon dioxide); and (4) improve the scientific basis for assessing the potential consequences of climatic changes, including the potential ecological, social, and economic implications of human-induced climatic changes caused by increases in greenhouse gases in the atmosphere and the cost and benefits of alternative response options.

Research is focused on understanding the basic biological, chemical, and physical processes of the Earth's atmosphere, land, and oceans. Research determines how these processes may be affected by energy production and use (e.g., the emission of carbon dioxide from fossil fuel combustion). A significant portion of the research is designed to provide the data that will enable an objective evaluation of the potential for (and consequences of) global warning.

Environmental Remediation Research is focused on developing an understanding of the fundamental physical, chemical, geological and biological processes that must be marshaled for the development and advancement of new, effective, and efficient processes for the remediation and restoration of the Nation's nuclear weapons production sites. A basic effort is a comprehensive research program in bioremediation that integrates the full range of fundamental scientific disciplines required to advance this emerging technology into a sustained cost-effective technology.

Basic Energy Sciences Program

The mission of the Basic Energy Sciences (BES) program is to foster and support fundamental research in the natural sciences and engineering to provide a basis for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use. As part of its mission, BES plans, constructs and operates major scientific user facilities to serve researchers at universities, national laboratories, and industrial laboratories. The program supports more than 2,400 scientists at 200 U.S. research institutions.

Materials Sciences Division

The Division of Materials Sciences supports basic research in condensed matter physics, metals and ceramics sciences, and materials chemistry. The basic research seeks to understand the atomistic basis of materials properties and behavior and how to make materials perform better at acceptable cost through new methods of synthesis and processing. Basic research is supported in corrosion, metals, ceramics, alloys, semiconductor superconductors, polymers, metallic glasses, ceramic matrix composites, nondestructive evaluation, magnetic materials, surface science, neutron and X-ray scattering, chemical and physical properties, and new instrumentation. The research leads ultimately to the development of materials that improve the efficiency, economy, environmental acceptability, and safety in energy generation, conversion, transmission, and use. These studies of materials affect developments in numerous areas, such as solar energy conversion, transportation, electric power production, and petroleum refining.

Chemical Sciences Division

The Division of Chemical Sciences has two major components. The disciplinary areas within each component are connected to and address needs of the principal DOE mission goals and objectives. One major component is comprised of atomic, molecular and optical (AMO) physics; chemical physics; photochemistry; and radiation chemistry. This research provides a foundation for understanding the fundamental interactions of atoms, molecules, and ions with protons and electrons. This work also increases our fundamental understanding of chemical reactivity, which in turn, enables the production of more efficient combustion systems with reduced emissions of pollutants. It also increases the knowledge of solar photo conversion processes resulting in new, improved systems and production methods. The other major component of the research program is comprised of inorganic chemistry, organic chemistry, analytical chemistry, separations science, heavy-element chemistry, and aspects of chemical engineering sciences. The research supported in this Division provides a better molecular-level understanding of homogeneous and heterogeneous reactions occurring at surfaces, interfaces, and in bulk media. This knowledge has resulted in improvements to known homogeneous and heterogeneous catalytic systems and to new catalysts for the production of fuels and chemicals; better analytical methods in a wide variety of applications in energy processes and environmental sciences; new knowledge of actinide elements and separations important for environmental remediation and waste management; and better methods of describing turbulent combustion and predicting thermophysical properties of multicomponent systems.

Energy Biosciences Division

The Division of Energy Biosciences supports research to provide a basic understanding of the biological phenomena associated with the capture, transformation storage and utilization of energy. The research on plants and nonmedical microorganisms focuses on a range of biological processes, including photosynthesis, bioenergetics, primary and secondary metabolism, the synthesis and degradation of biopolymers such as lignin and cellulose, anaerobic fermentations, genetic regulation of growth and development, thermophily (e.g., bacterial) growth under high temperatures), and other phenomena with the potential to impact biological energy production and conversion. The research supported is fundamental and is selected to support in a broad fashion the Department’s goals and objectives in energy production, environmental management and energy conservation.

Engineering and Geosciences Division

The Division of Engineering and Geosciences conducts research in two disciplinary areas – Engineering and Geosciences. In Engineering Research the goals are to extend the body of knowledge underlying current engineering practice to create new options for improving energy efficiency and to broaden the technical and conceptual knowledge base for solving the engineering problems of energy technologies. In Geosciences Research, the goal is on fundamental knowledge of the processes that transport, concentrate, emplace, and modify the energy and mineral resources and by-products of energy production. The research supports existing energy technologies and strengthens the foundation for the development of future energy technologies. Ultimately, the research impacts control of industrial processes to improve efficiency and reduce pollution, to increase energy supplies, and to lower cost and increase the effectiveness of environmental remediation of polluted sites.

Fusion Energy Sciences Program

The mission of the U.S. Fusion Energy Sciences Program is to acquire the knowledge base needed for an economically and environmentally attractive fusion energy source. The process of nuclear fusion (evident in stars, including the Sun) releases great quantities of energy. Fusion occurs when the nuclei of lighter elements (e.g., hydrogen) are fused together at extremely high temperatures and pressures to form heavier elements (such as helium). Intensive work began in the late 1970s to develop practical methods for harnessing reactions with the hope of realizing the potential of this energy source. Achieving the benefits of power from fusion has proved to be a difficult long-term challenge.

Fusion energy is an important but long-range goal of the Nation’s energy strategy because of its many potential advantages as an energy resource. The successful application of practical fusion energy technologies some time in the twenty-first century could help to enhance the Nation’s energy, provide an environmentally acceptable alternative to fossil-fuel combustion, and help ensure continued economic growth through a reliable electricity supply.

Fusion power plants would not produce air pollutants that contribute to acid rain and that may contribute to global climate change. They could minimize the environmental risks associated with the burning of fossil fuels and could substantially decrease the demand for premium hydrocarbon fuels.

High-Energy and Nuclear Physics Program

The Office of High-Energy and Nuclear Physics is a $1-billion-per-year basic research program that provides new insights into the nature of energy and matter and operates large world-class scientific facilities for the Nation. High-energy and nuclear physics research is conducted by over 3,000 researchers and over 1,000 graduate students from over 100 universities and the National Laboratories.

Most high-energy and nuclear physics is conducted using accelerators that produce beams of subatomic particles (e.g., protons and electrons) or nuclei moving essentially at the speed of light. When a beam collides with another beam or a fixed target, new particles are created from the kinetic energy in the beam.

High-Energy Physics Program

High-energy physics is the quest to uncover the nature of matter at its most fundamental level. With this knowledge, we strive to understand why the universe is the way it is. Experiments over the past thirty years have conclusively determined that the elementary particles and their interactions are described by the Standard Model of particle physics. According to the Standard Model, the fundamental constituents of matter consist of three families of quarks and leptons. T'he quarks and leptons interact through the electroweak force; quarks alone, however, feel the strong force. The strong force, quantum thermodynamics (QCD), governs the binding of quarks into protons and neutrons and ultimately into nuclei. The electroweak force has two aspects. One results in electromagnetic interactions and gives rise to electromagnetic waves, such as radio, light X rays; the other results in the weak interactions that govern radioactive decay and make possible the generation of energy in stars. Research in high-energy physics is conducted at several facilities in the United States, including the following:

- Fermilab – located near Chicago - is the world's highest-energy accelerator and the only facility capable of producing the top quark. Beams of protons and antiprotons are collided with energies of 900 billion electron volts (GeV) per beam. The $250 million Main Injector Project is under construction and, when completed in 1999, is expected to increase the data output by 500%.

- The Stanford Linear Accelerator Center (SLAC) at Stanford University, in California, collides beams of electron and antielectrons with energies of 50 GeV per beam. The $300 million B-Factory is under construction and, when completed in 1999, will collide 9 GeV electrons with 3 GeV antielectrons to produce B mesons (containing bottom quarks) to study why matter dominated over antimatter in the early moments of the "Big Bang."

- The Alternating Gradient Synchrotron at Brookhaven National Laboratory on Long Island provides the world's most intense kaon beams for studies of the strange quark.

Nuclear Physics Program

The mission of the Nuclear Physics program is to promote nuclear physics research through the development and support of basic research scientists and facilities. Nuclear physics research seeks to understand the fundamental forces and particles of nature as manifested in nuclear matter. As an essential component of that objective, the Nuclear Physics program educates young scientists, provides intellectual and technical support for other nuclear-based technologies, provides access to our facilities for other disciplines, and creates a flow of technical innovations for use outside the program. About 100 students receive their Ph.D.s with support from the Nuclear Physics program each year, more than half meet the high demand by nuclear-related industries for those with nuclear training. As part of its base program, Nuclear Physics manages the Nuclear Data Program, which measures, evaluates, computes, and disseminates basic information for fusion and fission energy programs and industries, for nuclear medicine and waste remediation programs, and for national security. Many other agencies (NASA, NCI, NIST) use nuclear physics facilities for their own research. Notable is the use by semiconductor manufacturers to develop and test radiation-hardened components for earth satellites to be able to withstand the cosmic ray bombardment. Nuclear physics research in the United States is supported mainly by two agencies, the Department of Energy and the National Science Foundation. DOE provides about 85 percent of the funding, much of which is directed toward the development, construction and operation of large state-of-the art accelerator facilities and detectors at national laboratories. These facilities are used extensively by researchers supported by DOE, NSF and other agencies. A primary scientific objective of nuclear physics is to study the location, motion, and interactions of quarks within nuclear matter. To accomplish this, a new facility was constructed (the Thomas Jefferson National Accelerator Facility in Newport News, Virginia) to provide high-quality continuous beams of electrons. Construction of TJNAF required close interaction with industry to acquaint them with the new technology and fabrication techniques of superconducting RF cavities. Industrial firms have shown an eagerness to demonstrate feasibility of superconducting technology to develop free electron lasers for a variety of commercial applications. Similar, close partnerships are being formed with universities to maximize the scientific payback from the new facility.

In an entirely different scientific direction, the Relativistic Heavy Ion Collider (RHIC) is being constructed at Brookhaven National Laboratory to investigate the characteristics of hot dense nuclear matter formed by collisions of gold beams at energies which will lead to a transition to a quark-gluon plasma. This plasma, in which quarks are deconfined from their nuclear constraints to roam freely within nuclear matter, reproduces the condition of the universe about one millionth of a second after the "Big Bang." Based on superconducting magnet technology pioneered by High-Energy Physics Program, the RHIC project has successfully transferred to U.S. industry the capability of supplying superconducting pulsed dipoles and quadrupoles for the accelerator; this is the first time such magnets have been commercially produced in the United States. The Holifield Radioactive Ion Beam Facility (RIB) is being built at Oak Ridge National Laboratory to investigate exotic nuclear structure and nuclear reactions that occur in solar burning and supernovas. These measurements are of crucial importance for understanding astrophysical processes and cannot be obtained in any other way. At Argonne National Laboratory, Gammasphere is using 110 new germanium/BGO detectors that were developed in partnership with industry to investigate nuclei with superdeformed shapes. The scientific/manufacturer team developed a novel technique of doubling the resolution of these detectors without substantially changing their complexity or cost. The Sudbury Neutrino Observatory (SNO) is about to begin operation of a detector that is intended to resolve the intriguing puzzle of missing solar neutrinos. Ongoing measurements of the solar neutrino flux with gallium-based detectors have shown that the measured flux is a factor of 2 or 3 below predictions of the standard solar model, indicating either that there is a serious misunderstanding of the basic solar burning process, or that exciting new properties of the neutrino itself are required to explain the flux loss. This experiment is composed of a broad international cooperative effort between U.S., Canadian, and British scientists, the INCO Corporation, which is providing a large deep cavern in its nickel mine in Sudbury, Ontario, and the Atomic Energy Commission of Canada that is providing 1000 tons of extra-pure heavy water. Connecting all these areas of research are the theory workshops conducted by the Institute of Nuclear Theory at the University of Washington.

B.2 DOE RESEARCH PROGRAM WEB SITES

The DOE /EPSCoR Research Implementation Awards are open to the entire range of energy-related disciplines supported by the Department of Energy. Valuable information on the DOE Research Programs is available at the following web sites:

- Department of Energy (General Information): http://www.doe.gov
- Office of Science (formerly Energy Research): http://www.er.doe.gov
- Basic Energy Sciences: http://www.er.doe.gov/production/bes/bes.html
- Biological and Environmental Research: http://www.er.doe.gov/production/ober/ober_top.html
- Advanced Scientific Computing Research (formerly Computational and Technology Research): http://www.er.doe.gov/octr/index.html
- Fusion Energy Sciences: http://www.ofe.er.doe.gov
- High-Energy and Nuclear Physics: http://www.er.doe.gov/production/henp/henp.html
- Office of Defense Programs: http://www.dp.doe.gov/Public/default.htm
- Office of Energy Efficiency and Renewable Energy: http://www.eren.doe.gov
- Office of Fossil Energy: http://www.fe.doe.gov
- Office of Environmental Management: http://www.em.doe.gov
- Office of Civilian Radioactive Waste Management: http://www.rw.doe.gov
- Office of Nuclear Energy: http://www.ne.doe.gov
- Office of Fissile Materials Disposition: http://twilight.saic.com/md/mdmain.asp
- Office of Nonproliferation and National Security: http://www.nn.doe.gov/nn home.htm

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