ABSTRACTS ARE IN ALPHABETICAL ORDER (PI)

Adenwalla,S, To investigate the interaction between ferroelectric copolymers of thin films, the ferroelectric-to-paraelectric phase transition temperature of alternate multi-layered Langmuir-Blodgett (LB) thin films of 80% vinylidene-fluoride and 20% trifluoroethylene copolymer(P(VDF-TrFE 80:20)) and 50% vinylidene-fluoride and 50% trifluoroethylene copolymer (P(VDF-TrFE 50:50)) have been studied with x-ray diffraction and capacitance vs. temperature measurement. We investigated the following samples: $(1:1)_{10}$, $(5/5)_2$ and $(10/10)_1$ multilayers, where the numbers in the brackets indicate the number of layers of P(VDF-TrFE 80:20) and P(VDF-TrFE 50:50) and the subscript denotes the number of repeats . All samples have the same total thickness of 20 monolayers. The 50:50 and 80:20 copolymers have widely separated phase transition temperatures, an advantage in these systems where the phase transition is very broad. The use of synchrotron x-ray diffraction allowed us to probe the samples as they are going through the phase transition and to quantify the amount of material in the ferroelectric and paraelectric phase. We have observed the existence of an interaction between P (VDF-TrFE 80:20) and P (VDF-TrFE 50:50). The phase transition temperatures of multi-layered samples are the intermediate of the phase transition temperatures of the two copolymers for the (5/5) and (1/1) samples. The closer the thickness of alternating layers of the two copolymers is to the calculated coherence length of 4nm, the closer the behavior of the multi-layered sample to a composite material. We have also observed two separate phase transitions of the two copolymers on the $(10/10)_1$ multi-layered sample, an indication of the lack of interaction between the two copolymers. The study of interaction between different ferroelectric copolymer layers shows good agreement with the calculated coherence length of interaction. These results could be a cornerstone of the study of inter-chain dipole vs. intra-chain coupling in ferroelectric copolymers.

Andres, Robert, University of North Dakota The primary goal of this three-year project is to make estimates of carbon dioxide emissions from fossil fuel combustion with a focus on decreasing the temporal resolution of these national estimates from annual to seasonal (approximately 38% of the project lifetime has passed and nine of the 21 countries selected for examination have been completed at the monthly time scale, other countries are in various states of completion). Since, oftentimes, the increased temporal resolution data is compiled on sub-country spatial scales, a secondary goal of this project is to refine the spatial variability of these emissions for some countries (three countries have been completed). The tertiary goal of this project is to calculate the 13C signature of these emissions at both increased temporal and spatial resolutions. These data will improve our understanding of the global carbon cycle, thus better enabling the broader community to predict and respond to global environmental changes currently observed and anticipated. This project will also directly support the North American Carbon Program, a component of the United States Interagency Carbon Cycle Science Program. Finally, the Carbon Dioxide Information Analysis Center (CDIAC) at Oak Ridge National Laboratory will archive and distribute the data generated by this project.

April, Gary, University of Alabama A multidisciplinary research cluster of scientists and engineers at the University of Alabama and Alabama A&M University is developing

new supported catalysts for hydrogen generation, purification, storage, and use in fuel cells. The US government's FreedomCAR and Hydrogen Fuel Initiatives call for technologies that are highly dependent on chemical reactions catalyzed by supported platinum group metals. The team will improve these catalysts dramatically by using a combination of new experimental and theoretical techniques. It will develop and refine methods to control the composition, size, and shape of the catalytic metal nanoparticles and to manipulate the interaction of the particles with their supports — including novel supports designed specifically for fuel cell applications. This directly supports DOE's Office of Hydrogen, Fuel Cells and Infrastructure Technologies and the Alabama DOE EPSCoR plan to increase the ability of universities to compete for energy-related funding; improve the human resource base; increase awareness of the need for science and engineering education; and attract new industry to Alabama. Program Coordination will be through the statewide EPSCoR structure that links EPSCoR institutions with DOE laboratories (e.g., ANL, ORNL), and other governmental agencies. Human resource development activities are integrated throughout the project and include formation of complimentary research partnerships between the participants and DOE laboratories and industrial affiliates. As an additional improvement to research infrastructure, new principal investigators have been added to the project and major equipment will be purchased.

Bass, Henry E, University Of Mississippi In this program the powerful technique of Resonant Ultrasound Spectroscopy will be brought to bear on highly correlated complex transition metal oxides. In these materials the spin, lattice, and charge degrees of freedom are strongly coupled. The elastic properties of a material provide information as to how the material responds to strain. Especially near a phase transition, the temperature dependence of the elastic moduli provides information about the coupling of the order parameter to strains of different symmetries. This information will be crucial in understanding some of the more exotic forms of order in TMOs, especially those involving orbital degrees of freedom that are highly directional.

Bellaiche, Laurent, University of Arkansas: State-of-the-art experimental and computational tools will be combined (and further developed) to investigate structural, piezoelectric and dielectric properties of ferroelectric nanostructures --- i.e., thin films, superlattices, nanotubes, quantum wires and colloidal quantum dots. The funding of this proposal will lead to a new fundamental knowledge since the properties of ferroelectric nanostructures are poorly understood and/or mainly unknown while being very sensitive to their associated degrees of freedom (e.g., shape, size, surface termination, electrical and mechanical boundary conditions, etc…). This knowledge, as well as the inverse-method numerical approach, will be used to guide the discovery of nanosystems with optimum properties and to design new energy-related devices. The collaboration between the University of Arkansas and Argonne National Laboratory will also be of large benefits to graduate and postdoctoral students. The broad expertise resulting from the assembling of the proposed team further enhances the chance of success of the present proposal.

Bolton, Tim, Kansas State University KASP seeks to develop and implement advanced semiconductor detectors for high energy physics. The two major projects underway are the Layer 0 upgrade for the D-Zero experiment at Fermilab and R&D on hybrid silicon-scintillator calorimeter technology for a future linear collider. The D-Zero upgrade will enhance the experiment's ability to detect and "tag" b-type quarks and in doing so significantly improve measurements of properties of the top quark, Nature's heaviest fundamental particle. It will also improve the chances for the first observation of the Higgs boson, supersymmetry, and other "new physics" at the Tevatron. KASP scientists Bean and Sidwell hold key management positions in this project. Expertise acquired in silicon detectors at Fermilab has already let the two KASP groups contribute productively to CMS, a next generation hadron collider experiment under construction at CERN, Geneva, Switzerland. A high energy electron-positron linear collider is the highest priority intermediate term new science project for the Dept. of Energy. KASP R&D focuses on maintaining the superior spatial resolution inherent in silicon devices while reducing overall detector cost. DOE EPSCoR has allowed both KASP universities to acquire critical semiconductor instrumentation and infrastructure that has allowed them to play leading roles in the large international scientific collaborations pursuing Tevatron and Linear Collider physics. Equally important, it has permitted Kansas to recruit outstanding new faculty members to the state, and to provide dozens of local undergraduates and high school teachers the opportunity to experience cutting edge high energy physics research. DOE support for KASP has been matched by generous contributions from the Kansas Technology Enterprise Corporation (KTEC).

Bromemshank, Jerry, University of Montana The program builds on basic research in electron transfer science for the creation and investigation of new materials for electron transfer properties, with an emphasis on their use in optical, electro-optic, and photonic devices. The ongoing program already has contributed to the formation of four new technology-based businesses and as well as a commercialization center in Montana. The project brings together 12 faculty-level investigators from three campuses, including biochemists, chemical engineers, physicists, inorganic and organic chemists, and computational modelers in support of the chemical/physical research. Electron transfer is the most fundamental chemical reaction and can bring about important changes in material properties when it occurs. It is the fundamental mechanism behind the functional properties of many photonic materials. Materials to be investigated include: 1) protein systems that have potential to lead to biological sensors; 2) organic donor-acceptor pairs which form the molecular equivalent of a diode and have potential for use in photovoltaics (solar cells) and light emitting diodes (LEDs) which may enable flexible, plastic displays; 3) solvatochromic materials that change color when exposed to certain chemical vapors and may find use in sensors; 4) photochromics and electrochromics (exhibit a color change when exposed to light or an electrical field, respectively) which have applications in self-darkening windows, mirrors, and eye protection; 5) two-photon absorbers which have special light absorption properties; and 6) platinum nanowires which are being explored for a proprietary control system application with Wavelength Electronics. The human resource development component of the project has been closely coupled with the research cluster, emphasizes participation by Native Americans and women, and uses the DOE Access Grid communications system for interactions across

the internet, including person to person and distributed meetings, collaborative work sessions, lectures, tutorials, seminars, and training. Ultimately, the project should lead to new contributions to science as well as successful commercialization of several technologies and materials. In three years, it has already resulted in more than 216 publications and presentations. The key investigators also have successfully competed for additional grants from DOE, NSF, DoD, DEPSCoR, NIH, and NASA. This program will also provide training and jobs in high technology fields, and lead to further growth of Montana's existing electro-optics, electro-electronics, and electrochromics industries, lead to the development of unique capabilities in the areas of photostrictive ceramics and, possibly, of biological macromolecules (as ET conduits), and more.

Burns, Teresa, Coastal Carolina University, The focus of the grant is to combine thermodynamic and structural measurements at Coastal Carolina University and at Oak Ridge National Laboratory to study ordering of polar molecules adsorbed on surfaces. Adsorption measurements of methyl bromide on MgO at University of Tennessee were done, demonstrating layering behavior that depends on temperature (see below). The work was presented at the American Physical Society March Meeting in Montreal and is in preparation for publication. Work will continue this summer with measurements on other adsorption systems. Structural measurements will follow as beamtime becomes available.

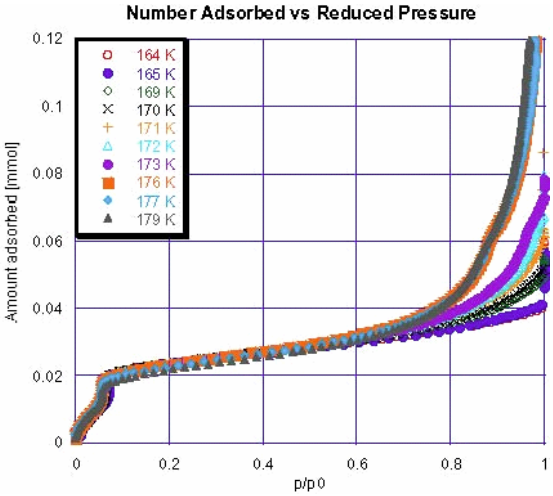
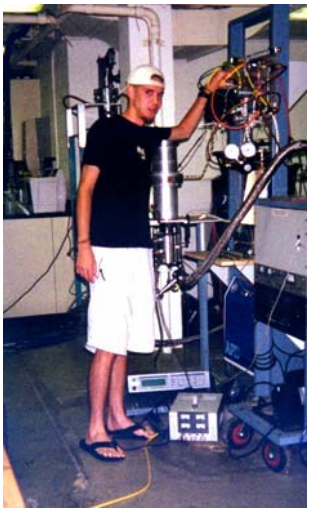
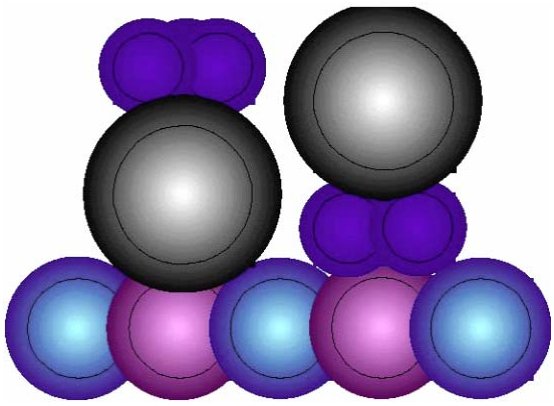


Figure 1: Methyl Bromide on MgO isotherms measured at set-point temperatures of 164 K to 179 K. Actual temperatures are determined using the saturated vapor pressure for MeBr at the set-point temperature.



Undergraduate TJ Harper makes adsorption measurements; shown is the gas handling system, the helium cryostat, and vacuum system. Work was completed in Dr. John Larese's lab at the University of Tennesee.

Undergraduate student Katherine Cilwa used UV-VIS spectroscopy, and IR spectroscopy to characterize the adsorption of benzene from solution, to develop materials and methods for such studies.This work was completed for her senior Honors Thesis, and was presented at Honors Seminar at Coastal Carolina University. Katie is now in graduate school at the Ohio State University.



Schematic diagram of dipole adsorption. The positive metal ions are pink; the halogen is gray, the hydrogen is blue, the carbon is black, and the dipoles are shown adsorbed in opposition.

Carlson Eric, University of Alabama The anisotropic diffusion equation is important to a variety of modeling applications. These applications include, among many others, diffusion through biological tissues, heat and mass transfer in microelectronics, and contaminant transport in ground water systems. Despite its importance and relative simplicity, only limited, proprietary capabilities exist for the numerical solution of this equation in heterogeneous systems. The project team is developing a set of modules and perfecting novel gridding techniques that promote efficient numerical solutions to the anisotropic diffusion equation. The new modules rely on the ACTS Toolkit, a set of high performance modules available to the public. The team is also developing tools that may be applied to composite (multiple region) systems of arbitrary shape through the use of an embedded domain framework, which means that regions are immersed in structured grids without requiring contortion of the grids to accommodate the shapes. Members of the project have developed unique tools that, when used in conjunction with advanced medical images, can be used to predict communication pathways in the brain. The project team has established a collaborative relationship with the Alzheimer's Disease Research Center (ADRC) at the University of Kentucky to investigate differences between these pathways in people with and without Alzheimer's Disease. The ADRC will provide data to this project to help tune the new tools.

Chen, Donna, University of South Carolina Although the reactivity of metals on oxides is important for heterogeneous catalysis applications, little is known about metal-on-oxide chemistry at the atomic level, and the influence of surface morphology on chemical activity is still not fully understood. The goal of this project is to understand how the surface chemistry of oxide-supported metal nanoparticles is affected by particle size and structure, metal-oxide interactions and metal-metal interactions in bimetallic nanoparticles. We have examined the growth and surface chemistry of catalytically active metals such as Cu, and Ni on a single-crystal TiO_2(110) surface under ultrahigh vacuum conditions. The sizes and size distributions of these particles have been characterized by scanning tunneling microscopy. We have demonstrated that the diffusion/flux ratio during deposition is the key to preparing particles with uniform size distributions; in general the smallest diffusion/flux ratio results in the narrowest size distribution. Furthermore, particles of different sizes can be prepared by room temperature deposition followed by annealing to elevated temperature, while maintaining the uniform size distributions. The rate limiting step in the sintering of Cu and Ni particles has been found to be atom detachment rather than atom diffusion. Thus, the slower sintering of the Ni compared to Cu particles can be explained by the stronger metal-metal bonds in the case of Ni. Methanol oxidation chemistry was studied on Cu particles of different sizes. Although the Cu particles and films were more reactive toward methanol chemistry than single-crystal Cu surfaces, methanol reactivity was identical on oxygen-covered Cu particles of different sizes (30 Å diameter-100 Å in diameter). In contrast, the hydrodesulphurization of methanethiol was different on Ni particles of different sizes. Both small (35 Å diameter, 8 Å height) and large (80 Å diameter, 20 Å height) Ni particles produced hydrogen and methane as the major gaseous products from the decomposition of methanethiol, but reaction on the small particles occurred at lower temperature. The methanethiol studies were conducted in collaboration with Jan Hrbek's group at Brookhaven National Laboratory since the facilities at the

National Synchrotron Light Source were used for the high resolution photoemission experiments.

Chevillle, Alan, Oklahoma State University We have undertaken development and adaptation of time domain THz measurement techniques to investigate the electronic properties of complex matter in the terahertz frequency region from 25 GHz to beyond 5 THz (<1 ? >165 cm-1). We have pursued three parallel track in adapting THz Time Domain Spectroscopy (THz-TDS) to measurement of complex matter. The first key need to a reliable way to characterize the complex dielectric constant of thin films with high accuracy when the wavelength of the THz radiation is much longer than the thickness of the film. We have pursued two techniques for measurement of thin films. These are waveguide spectroscopy and THz interferometry. Additionally in consultation with LANL we are working on a technique to reliably characterize complex matter across a broad spectral bandwidth extending to relatively low frequencies- 5-25 GHz, where the wavelengths are comparable to, or larger than the sample to be measured. We have been working on near field sources for these measurements. We have made fundamental progress in development of THz waveguides for spectroscopic measurements. The efficient coupling of broadband THz pulses into waveguides of different configurations is achieved by quasi-optics, which incorporates hyper-spherical or plano-cylindrical silicon lenses. Single-mode and low-loss propagation was demonstrated in a plastic ribbon waveguide with pulse broadening due to group velocity dispersion, and in a parallel metal plate waveguide with non-dispersive TEM mode propagation. Planar dielectric waveguides have extensive fringing fields of the propagating THz waves outside the waveguide enabling THz-TDS studies of surface-specific molecular adsorption layers. We also have developed low-loss parallel plate metallic waveguides with extremely low loss and negligible dispersion. These studies have made possible new applications of THz radiation. One of these applications is waveguide THz time-domain spectroscopy (THz-TDS), which can be used to measure the absorption and dielectric constant of a thin nm layer in the waveguide. To enable THz spectroscopy, which compares a sample pulse to a reference pulse, we have focused on in-place layer fabrication and removal techniques for the parallel plate waveguides. For the case of a metal waveguide with a thin layer of the substance to be detected, the total loss comes from both the metal walls and the substance layer. By comparing the signal from the empty guide with that from the waveguide containing the layer of material to be detected, the amplitude and phase change caused by the layer can be extracted. Since THz-TDS is a phase sensitive measurement technique, the absorption and index of refraction of the layer material can then be obtained. The sensitivity of this measurement is proportional to the ratio between the length and the plate separation of the waveguide, so that when properly configured, this method can be used to characterize extremely thin layers of low-loss materials. We have been able to detect a layer of adsorbed water with a thickness of 25 nm, equivalent to approximately 80 molecular layers. From these measurements we could extract an index of refraction and absorption similar to that of bulk water. An alternative technique to measure thin films is THz interferometry which splits the THz pulse train into two equal parts, providing a near ð, frequency independent phase shift to one of the parts. In this case destructive interference occurs, eliminating the background signal, drift, and some noise sources. The THz interferometer acts as a phase coherent white light

interferometer with film thickness resolution less than the Sparrow criterion, which states that two pulses are resolvable if there is a minima between their peaks. The time resolution of 1 fs or the ability to detect films of thickness on the order of 100 nm. We have used interferometry for characterization of high resistivity, >10 k?-cm silicon. Index changes of < 10-4 can be measured, corresponding to a change in optical path length of 342 nm. At 0.7 THz, the peak of the THz amplitude spectrum, this is an optical path length change of ë/1250. Extrapolating the results to a unity signal to noise ratio, the measurement limit of the system is 32 nm or ë/13,500. An additional goal of our project was development of human resources to provide the highly trained personnel both of which LANL depends on. To date we have two former students employed at LANL, one former undergraduate and one Ph.D.

Choobineh, Fred University of Nebraska The Nebraska DOE-EPSCoR Implementation grant supports an interdisciplinary research team of faculty, postdoctoral researchers, and students from six departments from the University of Nebraska to investigate the carbon sequestration potential of key rainfed and irrigated agricultural ecosystems in the north-central USA. Funding from DOE-EPSCoR has helped establish a state-of-the-art field research facility at the University of Nebraska Agricultural Research and Development Center (near Ithaca, NE) that addresses a priority research area identified in the Nebraska EPSCoR Strategic Plan, and focuses on improving basic understanding of biophysical constraints to increased soil C storage in a region where crop production is the predominant land use. The research facility is unique for three reasons: (i) it allows year-round measurement of CO_2 fluxes at the landscape level, coupled with detailed process-level soil-plant studies in production-scale cropping systems that are representative of the region; (ii) it utilizes state-of-the-art farming practices, typical of progressive farmers, which support substantial improvements in input use efficiency, grain and biomass yields compared to today's average farmer; and (iii) it monitors the use of all inputs, energy, and greenhouse gas (GHG) emissions to permit a holistic systems approach for full-cost accounting of C inputs and outputs and net effects on global warming potential. Our overall research program is focused on: (a) quantifying the interannual variability in amounts of C sequestered at the landscape-level employing eddy covariance flux systems through multiple 2-year crop rotation cycles as influenced by crop and soil management and climate variability; (b) explaining this variation in relation to relevant controlling factors, based on detailed studies of key soil and plant processes; (c) developing improved analytical techniques for estimating canopy biophysical properties based on remotely-sensed data; and, (d) concurrently measuring the release and consumption of nitrous oxide and methane and quantifying the intrinsic "C costs" of mechanical field operations, nitrogen (N) fertilizer, irrigation, and grain drying to establish full-cost accounting of global warming potential associated with these cropping systems. Funding obtained through DOE-EPSCoR has been leveraged with other funds to extend the EPSCoR studies in several key areas. The results from our research program will greatly increase our knowledge of seminal process controls on C sequestration and, based on this insight, allow improvements in ecosystem models to more accurately simulate C cycling in major agroecosystems of the north-central USA.

Davari, Asad, West Virginia University The proposed research will seek methodologies and algorithms for the real-time on-line modeling and intelligent control of large-scale nonlinear systems and to apply them to the circulating fluidized bed (CFB). The goal is to obtain an optimal convergence rate and an optimal learning rate of neural networks (NN) for real-time modeling and on-line control of the CFB. In collaboration research with the National Energy Technology Lab (NETL), off-line models and adaptive NN controllers have been developed for the stand pipe section of the CFB. One of the major obstacles in this approach has been the requirement for very low training times, as large training times would cripple the model and would not be effective to be implemented in real-time. We are proposing to make use of the results obtained and to extend these to fundamental and basic research on real-time, on-line modeling and control of the standpipe. We would then apply these results to the entire CFB. In order to develop the most suitable model, we plan to investigate multiplayer perceptrons applications and several other NN-based techniques such as the cerebellar model articulation controller (CMAC) and wavelet networks. NETL currently uses CFB modeling and control to address the basic issues of design and operation to increase efficiency and lower emissions. The advanced control strategy we propose would continually monitor the various operating parameters for the system and would be a major advance in intelligent control.

Daw, Murray, Clemson University We are investigating the motion of screw dislocations in BCC metals at the fundamental atomistic scale, calculating the electronic states by first-principles. We have done the calculations for molybdenum and iron. The Mo results confirm calculations reported previously by other groups. We believe that this is the first time such calculations have been done for iron.

Djalali, Chaden, University of South Carolina The main goal of this proposal is the design of the best suited frozen spin polarized target for the HALL B detector of the Thomas Jefferson National Accelerator Facility (JLab). The current project has made substantial progress and is right on track to not only achieve its goals but to exceed them. The PIs Chaden Djalali and Dave Tedeschi with the senior research associate, Dr. Oleksandr Dzyubak and graduate student Nicolas Recalde have been involved in the design, simulation and prototype testing of the holding magnets for the polarized target. The main polarizing magnet is being tested at Jlab. Our current involvement with the polarized target has strengthened USC's role in the JLab collaboration and allows us to make important contribution to both the detector development and the scientific program. Three top-rated approved experiments will be using the polarized target that will be built by the end of this project.

Dutrow, Barbara, Louisiana of State University Fluids interacting with the crust are critical to the production of geothermal energy, migration of hydrocarbons, sequestration of carbon, deposition of ores and transportation or containment of contaminants. It is increasingly important to develop tools to understand the nature and movement of fluids with respect to their environment so that their former presence in the rock record can be accurately deciphered and their behavior predicted. This research addresses these issues through an integration of field, analytical and computational modeling studies of fluid-

rock interactions in crustal environments. The thermal, chemical and mechanical processes that drive fluid flow and fluid-rock interactions are often coupled e.g. the output of one process affects the input of another. This feedback has the potential to dramatically modify fluid-rock interactions, interpretations of crustal processes and their signature in the rock record. It is commonly held that rock heterogeneities (e.g. permeability) play a prominent role in dynamics of open fluid-rock systems. Our initial work established that initial heterogeneities were NOT required to develop complicated flow and transport when coupling occurred amongst the processes. This research focuses on computational modeling of coupled processes inherent in fluid-rock systems to advance our knowledge of these fundamental processes. Integration of detailed mineral chemical analyses and textures of fluid-infiltrated rocks elucidates the signatures left by coupled processes in the rock record (e.g. their rates, scales, temporal sequence) associated with fluid-rock interactions during crustal evolution. This work partners a petrologist from LSU with an applied mathematician and a geophysicist from Los Alamos National Lab to take advantage of a unique cross-disciplinary approach and opportunity.

Edgar, J.H., Kansas State University Boron compounds with boron icosahedra ($B_{12}C_2$, $B_{12}P_2$, and $B_{12}As_2$) have the unusual property of self-healing radiation damage. Electron irradiating a series of compounds with different structures, Carrard et al[1] observed no defects in boron compounds containing icosahedra, regardless of the electron energy or flux (calculated to be sufficient to displace all boron atoms up to seven times). This surprising characteristic was attributed to the strong Coulomb attraction between positively charged boron interstitial ions and highly negatively charged regions formed by degraded boron icosahedra. Self-healing occurred without any thermal activation. In this study, the process to deposit $B_{12}As_2$ (E_g = 3.47 eV) thin films on 6H-SiC substrates using hydride reactants is advanced.[2] The crystal symmetry, lattice constants, and thermal stability make 6H-SiC a much better substrates for these films that silicon, previously most studied substrate. The $B_{12}As_2$ thin films were prepared from diborane and arsine in a hydrogen carrier gas at a growth rate of 4 μm/h at 1400 °C and 100 torr. The best electrical properties[3] achieved included a hole mobility and concentration of 80 $cm^2/V{\cdot}s$ and 3.4 x 10^{18} cm^{-3} respectively in undoped thin films. Four challenges were identified for the heteroepitaxy of $B_{12}As_2$ on 6H-SiC. While the [111] axis in $B_{12}As_2$ always aligns with the c-axis of the 6H-SiC, there are two in-plane orientations possible, thus rotational twinning in the films frequently occurs. Because the in-plane lattice constant of the boride semiconductor is twice that of SiC, defects due to translational variants are also possible. Thus, boron-rich boundaries may occur between intersecting domains that nucleate on the substrate with fractional lattice constant distances. The silicon carbide substrate undergoes some thermal and chemical decomposition as deposition is initiated, incorporating silicon and carbon into the thin film. The incorporation of these elements into the epitaxial film complicates efforts to controllably dope the samples. Lastly, difference in the coefficients of thermal expansion cause films thicker than approximately 1.5 microns to crack. Strategies for overcoming these problems are being addressed.

Famouri, Parviz, West of Virginia University This proposed work focuses on the investigation of sophisticated control algorithms, used widely in the electronics and

instrumentation fields, to the control of a circulating fluidized bed (CFB). Preliminary work has shown that Extended Kalman Filtering is effective in estimating the state vector of the standpipe portion of the solids flow loop. This work is being extended in conjunction with improving the model for the circulating fluidized bed. The accurate modeling of the transient behavior of the key elements of the entire circulating fluidized bed process has been undertaken. These elements include the standpipe, riser, regulating valves, gas injection ports, and solids collection and separation equipment. The object of these models is to capture the dynamics of the sub-processes comprising the system, in order to accurately reproduce the transient response of the circulating bed process to variations in operating parameters. The model is both fast and robust. Since the model has been established and tested the control algorithms will be tuned to control optimally the CFB.

Fink, Mark, Tulane University The collaboration between Mark Fink (Tulane University) and R. Morris Bullock (Brookhaven National Laboratory) is an effort to understand some of the fundamental processes involved in catalytic bond activations with low coordinate palladium species. The project involves the generation of reactive low-valent palladium species as transients using laser flash photolysis and the subsequent investigation of their reactions with chloroarenes and hydrosilanes. The information obtained from these studies will help elucidate fundamental reaction steps involved in many important catalytic reactions.

Greenwood, Zeno, Louisiana Tech University We propose to collaborate on two tasks in support of the D0 Experiment: the establishment and operation of a remote cluster of Linux PC's to be used as a Monte Carlo farm and remote data analysis center; and the creation and maintenance of a facility for the testing and understanding of new Silicon devices for the D0 Layer Zero effort.

Gudkov, Vladimir, University of South Carolina The project provides theoretical support for the experimental program in fundamental neutron physics at the SNS. This includes the study of neutron properties, neutron beta-decay, parity violation effects and time reversal violation effects. The main purpose of the proposed research is to work on theoretical problems related to experiments which have got the high priority at the SNS. Therefore, we will make a complete analysis of beta-decay process including calculations of radiative corrections and recoil corrections for angular correlations for polarized neutron decay, with an accuracy better that is supposed to be achieved in the planning experiments. Based on the results of the calculations we will provide analysis of sensitivity of angular correlations to be able to search for the possible extensions of the Standard model. Also we will help to plan other experiments to address significant problems of modern physics and will work on their theoretical support.

Headrick, Randall, University of Vermont Amorphous multilayers have many potential uses, such as for optics in applications such as soft-x-ray imaging, micro-tomography, and extended-UV lithography. Although physical deposition techniques (sputter deposition, etc.) are widely used, the effect of energetic physical deposition on the interface roughness of amorphous thin films is only beginning to be appreciated. In

this proposal, we describe a project to study and optimize thin film growth kinetics in amorphous multilayers of non-reacting materials such as Mo-B4C and Co-C. Our investigations will be of two types: (1) In-situ synchrotron experiments aimed at determining the fundamental mechanisms of surface relaxation of amorphous thin films. We wish to study the effect of energetic species in promoting the relaxation of surface roughness during the formation of interfaces. (2) Developing optimized multilayer deposition techniques. We will carry out these investigations by depositing multilayers using either pulsed laser deposition or magnetron sputtering, and then determining interface roughness.

Hoffman, Mark, University of North Dakota New methods of electronic structure theory will be developed and implemented computationally that will enable more accurate descriptions of chemical reactions of larger molecular systems than possible by current approaches. The methods will be developed in the framework of quasidegenerate perturbation theory (QDPT), and will be as applicable to excited electronic states as to the ground state. The GVVPT2 variant of QDPT, originated in this laboratory, has been shown to be among the most promising new general approaches, and is the focus of the proposed developments. Algorithm design and computational realization will emphasize usage of parallel architecture. Applications of the methods will emphasize chemical reactions that have significant regions of radical-radical interactions. Reactions of interest to combustion chemistry, as exemplified by the CN+O2 reaction, and to organic photochemistry, as exemplified by tetramethylethane diradical, will be studied to assess the accuracies and efficiencies of the developed methods.

Hohn, K.L., Kansas State University This project studies the structural, electronic, and catalytic differences between microcrystalline and nanocrystalline vanadium compounds. Three vanadium-containing nanocrystals are being prepared using a modified sol-gel procedure: V/MgO, V/SiO_2, and VPO. These represent active oxidation catalysts for a number of industrially relevant reactions. These catalysts are characterized by x-ray diffraction, infrared spectroscopy, temperature programmed reduction, Raman spectroscopy, and x-ray absorption spectroscopy. These materials are then tested in model reactions, including oxidative dehydrogenation of alkanes (V/MgO), oxidation of methanol to formaldehyde (V/SiO_2), and butane partial oxidation to maleic anhydride (VPO). The end result of this research will be a better fundamental understanding for how crystal size affects the local environment of vanadium in mixed metal oxides that will have broad applicability in designing selective oxidation catalysts.

House, Edwin, Idaho State University One of the goals of the Idaho EPSCoR Committee is the development of a strong program in nanotechnology. In this cluster, the interaction between seven research groups in the Chemistry and Physics Departments at the University of Idaho (UI), Boise State University (BSU) and Idaho State University (ISU), all of whom are working on some aspect of wide-band-gap semiconductors, will be coordinated. The end goal of the cluster is the development of novel optoelectronic devices. Nanoparticles of several known wide-band-gap semiconductors, including doped ZnO and TiO2, will be fabricated and tested as to their potential for use of more efficient solar photovoltaic cells, blue light emitting and laser diodes, high-speed field effect

transistors, high-temperature electronic devices, transparent conductors, and other photoelectronic devices.The project involves a collaboration between Chemistry and Physics faculty at UI, BSU and ISU, and has the support of both industry and personnel at the Pacific Northwest National Laboratory (PNNL) and the Idaho Engineering and Environmental Laboratory (INEEL).

Kang, Bruce S, West Virginia University The objective of this project is to develop and evaluate behavior of molybdenum silicide alloys for land-based power plant turbines able to withstand temperature exceeding 1000ºC. In addition to relevant experimental work, we have conducted computational modeling studies of ternary system of Molybdenum, Silicon and Boron over a wide range of temperature. Our current research effort is on ductilizing the Mo phase by dispersing $MgAl_2O_4$ spinel particles. Mo alloys with different volume fractions of spinel particles are processed at ORNL, and fracture and mechanical properties as well as the related atomistic modeling simulations are then investigated at WVU. The structural and physical properties of spinel has gained resurgent interest due to the recent experimental discovery of significant ductility enhancement of Mo-based structural materials by spinel dispersions. It is commonly believed that spinel particles will capture or precipitate embrittling impurities such as nitrogen and oxygen ions in the Mo phase, thereby strengthening the structural toughness. However, the exact mechanism is still yet to be found. Through our modeling and simulation of spinel, we proposed the new idea of electrostatic surface potential induced impurity precipitation/segregation along the spinel-Mo boundary to explain the ductility enhancement and decreased oxidation or pest reaction at the Mo grain boundaries (see Figure. 1). Our TB techniques are used to calculate the surface/interface potential, and predict the composition of spinel that renders optimal ductility enhancement.

Kao, Chung, University of Oklahoma We propose to investigate physics of fundamental importance: the mechanism by which particles acquire mass, the reasons why the top quark is so heavy while the neutrinos are so light, the supersymmetry between bosons and fermions, unification of fundamental forces, the sources of CP violation, and the possibility of extra dimensions. A major focus will be detecting Higgs bosons and new particles and measuring their properties, as well as searching for new phenomena and higher symmetries beyond the Standard Model. We plan to make predictions for the production rates of signals and backgrounds at hadron colliders. Furthermore, we will analyze experimental data for the Fermilab Tevatron Run II as well as develop techniques and computer software to search for both direct and indirect signatures of new physics at the Fermilab Tevatron and the CERN Large Hadron Collider.

Katiyar, R.S University of Puerto Rico The main goal of our research program is to focus on understanding the science of Li intercalated ionic/polymer materials for their uses in developing the technology for the fabrication of solid state ionic devices especially rechargeable Li ion batteries. Although numerous class of insertion-deinsertion type electrode materials for the battery applications were synthesized over the last two decades, little improvement in the capacity as well as making it all solid state has been

achieved. Our research effort is aimed at finding the best performing combination of economical anode-electrolyte-cathode system that yields appreciable gain in the rate capability with high cycleability. An approach based on Ab-initio quantum-mechanical molecular dynamic simulations has been adopted to predict theoretically novel-type intercalation compounds and simulate the Li^+ intercalation process in these materials. These calculations will provide a feedback to our material preparation effort to optimize the above technologically important properties. A soft solution approach has been adopted to synthesize these electrodes in nano-crystalline form to increase the electrode-electrolyte interfacial area and shorter Li^+ diffusion distance, which in turn is expected to yield improved electrochemical performance. Studies on polymer based solid electrolytes, in lieu of commonly used liquid electrolytes, have recently achieved significant attention in Li ion rechargeable batteries. We have initiated our research on polymer-nano-ceramic composite electrolytes to increase their Li^+ ion conductivity at room temperature. Since the chemical stability of electrodes and the control of electrode-electrolyte interface are important, fundamental issues of charge transport in such nano-composites and the study of its interface with cathode and anode need to be addressed, and our research is focused on the experimental investigation of the interface defects and charge transport phenomena in polymer-ceramic based solid electrolytes. A multi-disciplinary research team has been formed to accomplish the research tasks described above that includes theoreticians for ab-initio calculations to predict new materials and their electrochemical behavior, material scientists and solid state chemists for nano-synthesis of materials for electrodes and electrolyte (utilizing sol-gel, PLD, RF/DC magnetron sputtering, CVD techniques), and physicists for understanding the kinetics for Li^+ diffusion and the structure-property behavior (utilizing cyclic voltammetry, charge-discharge probe, XRD, DSC/DTA, SEM, XPS, TEM, micro-Raman, FTIR, ellipsometry, AFM/STM, impedance spectroscopy, and synchrotron studies using advanced photon source). The development of human resources in the frontier of Science and Technology is the key factor in this multi-disciplinary collaborative project. UPR students will have an opportunity to get training on the state-of-the-art technology at UPR as well as at the collaborating universities and the National Laboratories, thus strengthening the master and doctoral programs offered by UPR. The skilled manpower training in the project will also meet the demand for the high-tech job market for the energy related industries that will in turn contribute to the economic developments of the Nation.

Kellar, Jon, South Dakota School of Mines and Technology The goal of this research is to develop the science underlying the formation and effects of transcrystalline regions ion carbon fiber reinforced thermoplastic matrix composite systems and to identify and exploit this understanding to allow controlles tailoring of the interphase transcrystallinity for specific applications. Possible applications of tailored thermoplastic matrix composites abound in the next generation vehicle programs in which weight savings of 40% are required with essentially no increase in vehicle cost. This goal will be achieved by measuring the adhesion, both thermodynamic and practical, of carbon fibers by thermoplastic polymers. In addition to adhesion measurements, component material properties will be determined and the extent of transcrystalline interphases generated under various processing conditions measured by atomic force microscopy. With this

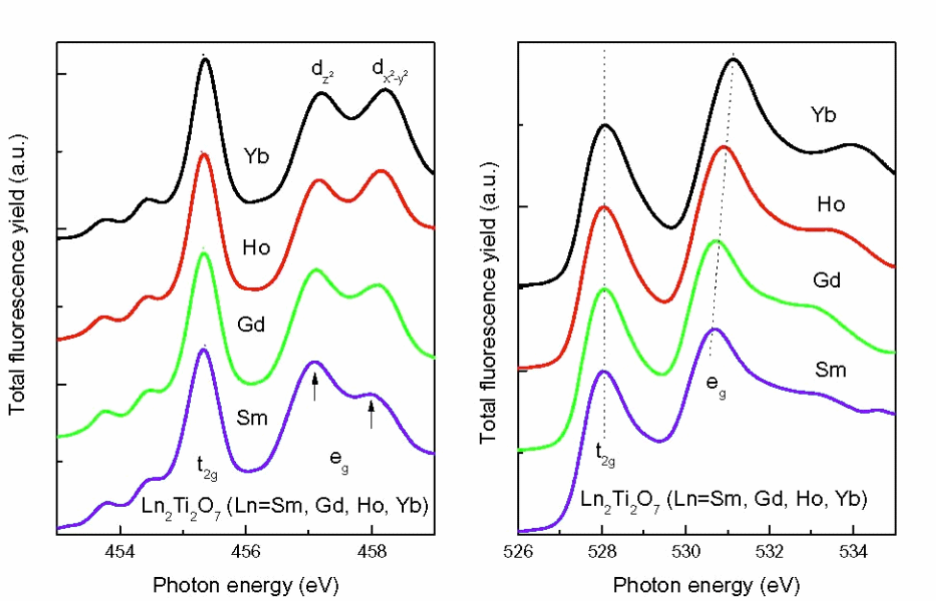
knowledge, thermoplastic matrix composites with tailored interphases will be manufactured using two new processing methods and usage related mechanical behavior evaluated.

Khonsari, Michael, Louisiana State University The mission of this research cluster is to establish Louisiana as a national center for the development of grid computing technology with applications in oil/gas exploration and production. The overall research goal is to design, deploy, and evaluate a large-scale ubiquitous computing and monitoring system (UCoMS) for exploration and management of energy resources in the Gulf of Mexico. UCoMS will support computationally intensive fine-grained simulations, enabling real-time processing and storage of massive amounts of data. Developing a proof-of-concept UCoMS prototype will facilitate the integration of research into practical implementation in the field. This information, for example, will provide for enhanced safety monitoring on offshore well platforms. The project addresses five key research issues at the algorithmic and software levels: (1) Development of efficient task migration and task farming schemes to support long execution tasks such as reservoir simulation; (2) Further development of the Grid Application ToolKit (GAT) supporting grid computing; (3) Design and implementation of an efficient real-time job-scheduling algorithm that guarantees real-time responses with Quality of Service requirements for specific jobs, such as real-time drilling control; (4) Design and development of more efficient protocols for reliable wireless communication networks to support ubiquitous access to the computational grid; and (5) Development and evaluation of application tools for computationally intensive seismic analyses and reservoir characterization using the UCoMS computational grid. Participating Institutions: University of Louisiana at Lafayette; Louisiana State University A&M College; Southern University; and Louisiana Board of Regents.

Lee, Byung, University of Vermont The project aims at predicting the cost of executing a computer program function, and finds immediate applications in database query optimization, parallel or distributed resource scheduling, mobile agent price negotiation, etc. We have been pursuing three different approaches to date. The first one is a static approach by which a cost data set is generated through a run of function executions and modeled using regression. Both parametric and nonparametric regression techniques have been used for different characteristics of the program functions. The second one is a dynamic approach. Particularly, it is a "self-tuning" approach by which cost data are automatically modeled as they are generated during run-time, and is designed to work well in an environment with limited resources (e.g., memory, computation time). This approach builds a cost model incrementally as the functions are executed and, when memory runs out, compresses the model at the minimum expense of the model precision. The third one is the hybrid of a static approach and a dynamic approach. Particularly, it is a predictive approach by which the patterns of the function executions are identified and used to predict the functions to be executed in a given future time interval. This approach is effective in using the limited resources more efficiently.

Lindle, Dennis, University of Nevada-Las Vegas Pyrochlore materials are promising for technological applications such as catalysis, microelectronic devices, fuel cells, sensors for high-radiation environments, and host matrices for nuclear wastes resulting

from their unique properties. The structural and electronic properties of $Ln_2Ti_2O_7$ (Ln=Sm, Gd, Ho and Yb) have been characterized using Ti 2p and O 1s near-edge x-ray absorption fine structure (NEXAFS). The NEXAFS spectra provide information on the chemical bonding, which show that the decrease of ionic radius of Ln (from Sm to Yb) leading to a stronger crystal field strength (10Dq) of the TiO_6 octahedron.



Ti 2p (left) and O 1s (right) NEXAFS spectra from $Ln_2Ti_2O_7$(100) (Ln=Sm, Gd, Ho and Yb) single crystals.

Liu, Keh-Fei, University of Kentucky This is a project to undertake an ambitious lattice Quantum Chromodynamics calculation of the fundamental quantities such as the quark mass, the chiral behavior of hadron masses and pion decay constants, and exotic mesons using a recently formulated overlap fermion action which has the correct chiral symmetry and nice scaling behavior. We will also calculate baryon spectroscopy including the excited nucleon (N*), Lambda, and pentaquarks which are under intense experimental study at DOE's Jefferson Lab. Our calculation will lend theoretical support for these experimental efforts. We will also calculate nucleon form factors, such as the flavor-singlet axial coupling constant, the strangeness content, and the strangeness magnetic and electric form factors in order to access the systematic errors associated with chiral extrapolation, the finite volume, and continuum extrapolation. These quantities are also being measured experimentally at Jefferson Lab as other high energy labs.

Loye, Hanno zur, University of South Carolina The work described in this proposal will be a collaborative effort between Prof. Hanno zur Loye at the University of South Carolina and Dr. Tom Vogt at Brookhaven National Laboratory. The collaborative research will focus on the synthesis and the structural characterization of perovskites and perovskite related oxides and will target new oxide systems where we have demonstrated expertise in synthesis, yet lack the experimental capabilities to answer important

structural issues. Synthetically, we will focus on two subgroups of perovskite structures, the double and triple perovskites, and the 2H-perovskite related oxides belonging to the A3n+3mA'nB3m+nO9m+6n family. In the first part of the proposal, our goal of synthesizing and structurally characterizing new ruthenium, iridium, rhodium and ruthenium containing double and triple perovskites, with the emphasis on exercising control over the oxidation state(s) of the metals, is described. These oxides will be of interest for their electronic and magnetic properties that will be investigated as well. In the second part of the proposal, a detailed investigation is described to elucidate the "mechanism" of the structural transformation from commensurate to incommensurate, that is often observed for 2H-perovskite related oxides, and is believed to be caused by an uptake (or loss) of "extra" oxygen with a concomitant change in the ratio of octahedra to trigonal prisms in the structure. In both cases, access to the synchrotron is central to these investigations, as it will provide us with the capabilities to determine accurately the structures and, more importantly, to investigate in-situ the effects of pressure and temperature (part one) and oxygen partial pressure and temperature (part two) on the oxide materials of interest. The structural characterization will be carried out at BNL beamline X7A of the National Synchrotron Light Source (NSLS), while the magnetic studies and TEM measurements of the oxides will be performed both at BNL and in South Carolina.

Mankey, Gary, University of Alabama The proposed work is a collaborative project between the research groups of Dr. J.L. Robertson at Oak Ridge National Laboratory (ORNL) and Dr. G.J. Mankey at the University of Alabama (UA). The main thrust is developing neutron optical devices for the study of magnetic thin films and interfaces. The project is particularly timely, since facility upgrades are currently underway at the High Flux Isotope Reactor (HFIR). New neutron optical devices will be designed and built to take maximum advantage of the increased flux that the upgraded beamlines at HFIR will provide. The proposed devices will make possible detailed studies of the magnetic structure of thin films, multilayers, and interfaces that are not feasible at present. In particular, the new devices will enable us to study much thinner films, determine magnetic structures at interfaces and probe spin wave dynamics of thin films. The project builds on experience gained since the collaboration was formed a few years ago. To date, the collaboration has proved fruitful, generating a recent publication in Physical Review B1. An ongoing collaboration with IBM in this research area highlights the technological relevance of the research. The results obtained to date suggest a set of new experiments that will elucidate the microscopic origin of the exchange bias effect. Performing these new experiments will reveal the origin of this and other microscopic magnetic effects and enable the partners to become world leaders in this important research area.

Mann, Michael, University of North Dakota: The long-term goal is to merge wind energy, hydrogen production, and fuel cells to bring emission-free and reliable stationary power to commercial viability. The approach is to expand system models as a tool to investigate integration and control issues; to examine the long-term effects of wind-electrolysis performance; and to design, integrate, and quantify system improvement by implementing a single power electronics package. The project team is working with NREL to expand the versatility of RPMSim by developing new/upgraded electrolysis,

fuel cell, and hydrogen storage modules. The model will be used to examine the viability of various power system control schemes. Using knowledge gained during his eight-month exchange visit at NREL, a doctoral student is designing a test facility to investigate electrolysis issues including gas purity and production rates under the variable input supplied from a wind turbine. The group is also working with Basin Electric Cooperative in addressing dynamic scheduling of an electrolysis system planned for installation on Basin's 1.3 MW wind turbine.

Marinescu, Catalina, Clemson University The creation of a reduced dimensionality electronic device whose functioning is based not on the flow of positive and negative charges under the effect of an electric potential, but on the magnetically induced motion of up and down spins might announce a new era in technology. It is highly anticipated that spin-based quantum electronic devices will be the fundamental entities in information technology and computing. This proposal is focused on the interesting physics that lies behind spin-dependent transport phenomena and their possible practical applications. Starting from the spin-dependent interaction between two electrons confined in a two dimensional magnetic semiconductor heterostructure, we propose to investigate problems related to spin and charge relaxation processes, magnetotransport, tunneling phenomena, and magnetic instabilities. The aim of our research is to give a comprehensive picture of the physics involved that will explain the existing data and will provide insight for future experimental work.

McCall, Katherine, University of Nevada, Reno The aim of this work is to use neutron scattering techniques to explore the dynamics and structure of water in rock samples. The dynamics of water in rock at low (residual) saturation are directly related to the transport properties of fluids within the host rock. The structure of water in rock may be related to the elastic behavior of the rock, which in many cases is nonlinear and hysteretic. Neutron scattering techniques allow us to study water in intact rock samples at both the molecular and microstructural scales. Our samples are Berea sandstone, Calico Hills and Prow Pass tuffs from Yucca Mountain, NV, and pure samples of the tuff constituents, specifically mordenite and clinoptilolite. We have chosen Berea sandstone because its macroscopic elastic behavior is known to be highly unusual, and the microscopic mechanisms producing this behavior are not understood. We have chosen Yucca Mountain tuff, because Yucca Mountain, Nevada is the proposed location of a high level nuclear waste repository. Neutron scattering methods have a number of properties that are extremely useful for the study of earth materials. In contrast to X-rays, neutrons have very low absorption cross-sections for most elements so that entire bulk samples of considerable size can be "illuminated" by the neutron beam. Similarly, samples that are optically opaque can be readily investigated by inelastic neutron scattering techniques. Neutrons are sensitive to both light and heavy atoms, and can, for example, readily distinguish between Al and Si, neighboring atoms in the periodic table that are difficult to tell apart by X-ray diffraction. Finally, neutrons are particularly sensitive to hydrogen and thus can be used to study the motions, both vibrational and diffusive, of H-containing molecules in rocks, most notably of course, water. Our studies are primarily studies of guest molecules (in our case, water) in a host material (rock). To date, we have used three neutron scattering techniques: quasielastic neutron scattering

(QNS), inelastic neutron scattering (INS), and neutron powder diffraction (NPD). We use QNS to measure the translational and rotational diffusional motion of water in rock; INS vibrational spectra allow us to determine the nature of residual water in a sample (disassociated, chemisorbed, or physisorbed); and NPD measurements allow us to determine the locations of residual water molecules (and the associated dynamic disorder), and thereby understand the binding of water molecules in our samples. In all cases, the signature of the water is clearly evident, and the data are of high quality. Analysis of the data is ongoing.

McNeider, Richard, University of Alabama-Huntsville: The reduction of the diurnal temperature range (DTR) is the most significant signal in the recent climate record, yet its cause is not clear. UAH will collaborate with DOE scientists at BNL and PNL to examine the increase in downwelling radiation due to condensational growth of hygroscopic aerosols in the nocturnal boundary layer. Previous high-resolution boundary layer modeling studies showed that this effect can increase downwelling radiation by 13-20 W m-2. Thus, regional and global changes in aerosol burdens might make this effect a significant climate forcing factor in explaining DTR damping. This study will conduct modeling and observational studies to quantify this effect. Huntsville, Alabama is an ideal site for the program, because it routinely experiences high relative humidity, in conjunction with some of the highest regional average aerosol loading in the U.S; and because it exploits unique, new, and comprehensive observational and modeling capabilities at UAH.

Murray, M, University of Kansas, Lawrence The purpose of Relativistic Heavy Ion Collidor, RHIC, is to map the phase structure of the strong nuclear force, QCD. A great deal of evidence supporting the creation of partonic matter in AuAu collisions has been accumulated in the first three years of RHIC running. However QCD is a rich theory that probably has many phases. It has been suggested that when viewed by a fast probe a heavy nucleus may resemble a sheet of highly correlated gluons called the Color Glass Condensate. After a AuAu collision the fields generated by the color charges on the two sheets of gluons would break up into a dense system of partons which one would expect to approach chemical and kinetic equilibrium while rapidly expanding in both the longitudinal and transverse directions. Eventually the partons must hadronize and after further rescattering the hadrons freeze-out. Recent d-Au results from BRAHMS lend some support to the color glass hypothesis. We have just started our EPSCoR contract and re currently in the process of hiring a new post-doc to join KU effort in investigating the production of high momentum particles from both d-Au and AuAu collisiions. We hope to leverage these efforts with local expertise in flow measurements. This will give an extra dimension to our analysis by allowing us to study particle production as a function of the orientation of the colliding nuclei.

Naseem, Hameed, University of Arkansas The heart of the project is in the investigation of various mechanisms involved in the nucleation and growth of silicon crystals during metal induced low temperature solid phase crystallization. Several models have been proposed over the years to explain metal induced crystallization (MIC). Yet, no comprehensive model has emerged that can explain such drastic reductions in

crystallization temperature. We aim to investigate the basic science underlying this potentially enabling technology through the use of both sputtered and plasma deposited hydrogenated and unhydrogenated amorphous silicon thin films. The mechanisms learned in this investigation can be used to engineer new materials with desired optimum characteristics for various large impact consumer markets. The significance of the work related to its application in solar cells and Thin Film Transistors (TFTs) on flex are far reaching. The initial results obtained thus far are very exciting. Low-power laser beams ($50\text{-}120\ W/cm^2$) are being used to enhance the MIC process. This laser power is three orders of magnitude less than what is commonly used in the conventional CW laser crystallization. This outcome has a great potential for TFT fabrication in low cost large area flat panel display technology. On the other hand, thermal annealing as an excitation source has also produced interesting effects. We have been able to produce grain sizes of 15 to 20 μm in 300 nm thick crystallized films by introducing a thin oxide barrier layer between aluminum and silicon. A patent application has been filed with the U. S. Patent Office. This ability to grow polycrystalline silicon films having extremely large grain size at low temperatures brings the goal of fabricating high efficiency solar cells and TFT a step closer to reality. Furthermore, new insights have been obtained in the understanding of the basic mechanisms involved. The Multi-chamber Cluster Tool has been upgraded to deposit sputtered films of varying hydrogen content and a correlation has been found between the hydrogen content and the crystallization onset temperature. The high end material characterization necessary for the investigation are being made in collaboration with national laboratories such as National Renewable Energy Laboratory (NREL), National Center for Electron Microscopy (NCEM) and Oak Ridge National Laboratory (ORNL). One-on-one relationship with scientists at NREL has been established since last year. Analytical results are being discussed over the phone and through emails. Visits to ORNL and NECM are scheduled this summer (2004.) These visits will expand the opportunities for the University of Arkansas to write proposals and carry out competitive research through collaborations with scientists at these DOE facilities.

Pandey, R, University of Alabama Magnetic semiconductors are expected to play an important role in spintronics. Currently favored transition metal-doped magnetic semiconductors suffer from two major drawbacks. They are: the unalterable nature of doping and weak exchange interaction leading to magnetic transitions below room temperature. The oxide semiconductors ilmenite-hematite (IH) and anatase TiO_2 (ATO) have been processed reproducibly by us (IH at UA and ATO in PNNL) showing attractive semiconducting and magnetic properties at and above room temperature. We propose a close collaboration between UA, PNNL and ORNL for an in-depth study of these materials to understand the fundamental physical mechanisms involved that give rise to their unique properties. Only then a viable spintronics technology can evolve based on an oxide system. Our objectives and research goals outlined in the proposal are realistic to attain given the competence, experience and the synergy that already exist at the DOE labs (PNNL and ORNL) and UA.

Pierre, John W, University of Wyoming Accurate knowledge of power system dynamic characteristics is vital to controlling and operating a power system near its

reliability limits. Good supplements to simulation model-based approaches are needed. Today, with extensive real-time data available from power systems, methods of extracting system dynamic characteristics from measured data have significant potential. This research involves investigators in three EPSCoR states, each having vital interest in the energy industry. The team of researchers is working closely with collaborators at PNNL to investigate this topic. The long-term goal is to provide real-time system information from measurements, allowing operators to achieve reliable operation and control of power systems. This project is investigating the development and application of advanced measurement-based techniques for estimating power system dynamic characteristics and to assess the performance of those techniques. These methods are based both on measurements of ambient conditions with no known driving input and on measurements where a known probing signal is employed. Both block processing and adaptive methods are being explored. At this point, ambient techniques have been developed to not only estimate the major modes of the system but also to place confidence interval on those estimates. Probing experiments were carried out in the summer and fall of 2003 in cooperation with Bonneville Power Administration, and initial analysis results have been obtained using newer signal processing techniques. A 19 machine model is also being modified to allow for both ambient noise conditions and for the injection of probing signals.

Putkaradze, Vakhtang, University of New Mexico Flows in expanding/contracting channels are ubiquitous in a vast variety of engineering applications. Exact solutions of Navier-Stokes equations describing flows in expanding/contracting channels were first found by Jeffery and Hamel in the beginning of last century. Despite the fundamental character of this type of flow and its tremendous practical importance, many questions regarding it remain unanswered. We are the first to construct an experimental apparatus for investigation of these flows based on Particle Image Velocimetry (PIV) technique which surpasses in accuracy and control any Jeffery-Hamel experiment done before us. For each value of the aperture angle ˜??we observe the symmetry-breaking bifurcation at some value of the flow rate which is substantially below the value predicted by the Jeffery-Hamel theory. The bifurcation is hysteretic, and the structure of the hysteresis differs greatly from that predicted by both previous theoretical work and numerical simulations using the DOE SALSA code. To explain this apparent discrepancy, we use a triple-prong approach combining analytical, numerical and experimental methods. The academic value of this project lies in the achievement of complete understanding of the bifurcation structure in Jeffery-Hamel flows. One of the practical applications will be optimization of an injector design for a given flow rate. In addition, as the Jeffery-Hamel flow problem has a relatively simple geometry but nevertheless presents a highly non-trivial series of bifurcations, it is ideally suited for validation of the advanced DOE numerical codes.

Rankin, Stephen E., University of Kentucky In collaboration with scientists from Sandia National Laboratories in Albuquerque, New Mexico, we are conducting a joint computational and experimental investigation the synthesis of nanostructured ceramics, by using evaporation to drive molecular assembly. In the process under investigation, simple ingredients are used: a ceramic precursor, ethanol, water, a small amount of

catalyst, and a surfactant. Weak interactions between the surfactant and growing ceramic species drive the formation of an ordered co-assembled thin film during dip coating. Extracting or decomposing the surfactant leads to an ordered array of pores. We use a combination of theoretical approaches to understand competing aspects of the process. On one hand, we use a quantitatively realistic dynamic Monte Carlo simulation of silica polymerization with continuum calculations of processing flows. We currently are refining this approach to allow more accurate predictions of the process dynamics and structure development. One the other hand, we use coarse-grained lattice Monte Carlo simulations of surfactant solutions to examine the effects on nanoscale pore ordering of such process variables as surface chemistry, surface texture and composition potential gradients. We are currently confirming one of the predictions of these Monte Carlo simulations experimentally. The simulations suggest that if a glass surface is partially treated with silanes so that it is equally interactive with polar or non-polar species, it should align cylindrical pores normal to the surface of the substrate. This would be a very attractive configuration because it makes the pores accessible to the fluid phase in contact with the film, and would allow the films to be used in separation processes such as membranes or as filters/concentrators for sensors. We have used the surfactant Brij-56 to create films with close-packed arrays of cylindrical pores. When they are coated onto ordinary glass slides, the pores are aligned parallel to the slide, so that many of the pores are inaccessible. However, when the pores are partially methyl-treated, we have observed x-ray and TEM evidence (consistent with the simulations) that the pores orient perpendicular to the glass slides. In addition to this experimental validation of the predictions of the simulations, we are in the process of refining the lattice Monte Carlo simulation by using a finer lattice and incorporating more realistic dynamics. We are moving closer to the overarching of goal of creating a theoretical framework to relate macroscopic control parameters (such as surface chemistry) and nanostructure in surfactant-templated porous ceramic thin films.

Roddick, Dean, University of Wyoming: Our proposal describes the development of a new class of ruthenium-based ionic and “super-ionic” hydrogenation catalysts and their application to the ongoing challenging problems of aromatic and heteroaromatic hydrogenation as well as remediation (hydrodesulfurization (HDS) and hydrodenitrogenation (HDN)) of coal and petroleum feedstocks. An extension of ionic hydrogenation catalysis to fluoroalkenes introduces a new synthetic method for the synthesis of hydrofluorocarbons (HFC’s), which are essential components of modern refrigerants, blowing agents, and anesthetics. The project involves a collaboration between Dean Roddick (University of Wyoming) and Morris Bullock (Brookhaven National Laboratory). University of Wyoming graduate students will be involved in the synthesis of catalyst precursors and surveying of catalyst activity. A postdoctoral researcher will split time between Brookhaven and the University of Wyoming carrying out systematic studies of catalyst mechanism and applications, exploiting the complementary chemical expertise of the Roddick and Bullock organometallic research programs.

Scime, Earl, West Virginia University The project proposed here is collaborative effort between the Plasma Physics group (P-24) at Los Alamos National Laboratory (LANL) and the West Virginia University (WVU) helicon source group to measure extremely short wavelength fluctuations in high-density plasmas. With such a diagnostic, it will be possible to test theoretical models of helicon source physics (important for both basic science and plasma processing applications) as well as investigate the role of small-scale fluctuations during magnetic reconnection (required to understand how small scale fluctuations modify the plasma conductivity during reconnection). In addition to these fundamental plasma science objectives, students in the plasma physics program at West Virginia University (WVU) will become familiar with microwave scattering techniques now employed at major magnetic fusion research facilities in a hands-on, table-top sized, experimental environment.

Seger, Janet, Creighton University: Ultra-peripheral collisions of relativistic heavy ions (UPCs) allow the study of coherent long-range interactions. This project, a partnership between Creighton University and Lawrence Berkeley National Laboratory, will focus on analysis of UPC data collected with the Solenoidal Tracker at RHIC (STAR). One goal for the next three years is to expand STAR's vector meson spectroscopy measurements to heavier mesons such as the ö and J/Ø, well as more exotic mesons. A second goal is to look for evidence of gluon shadowing in the J/Ø and heavy quark cross sections. In addition, we plan to work on the development of enhanced triggering algorithms for ultra-peripheral collisions at STAR. Since Creighton has recently joined the ALICE collaboration, we propose to simultaneously lay the groundwork for studying UPCs with the ALICE detector at the Large Hadron Collider (LHC) by studying the capabilities of ALICE to trigger on UPC events.

Shannon, Curtis, Auburn University The overall goal of this project is to develop and characterize new materials for improved performance in solar and thermoelectric energy conversion devices. In materials synthesis, both solid state and electrochemical routes to new materials and composites are actively being pursued. Although a wide range of surface and bulk characterization techniques exists, a technological barrier to the complete characterization of thin film thermoelectric materials is the measurement of their thermal conductivities. To overcome this barrier, an apparatus for the measurement of thin film thermal conductivities using the 3-˜ method is being developed. The current status of these research thrusts is summarized below. Growth of ZnO by Vapor Phase Epitaxy (VPE) and Electrodeposition ZnO is a wide band gap semiconductor with applications in solar energy conversion devices. Low cost, environmentally benign syntheses of this material have been developed based on VPE and electrochemistry. Both of these synthetic routes avoid the use of potentially toxic metal-organic precursor compounds as sources for Zn. Physical property measurements are being carried out on these materials. Low-Dimensional Materials for Thermoelectric Applications. Calculations and preliminary experimental data suggest that low dimensional materials may have enhanced thermoelectric efficiencies compared to their bulk phase counterparts. Inexpensive and massively parallel routes to these materials are the desired outcome of this research thrust. Electrochemical atomic layer epitaxy is a growth method characterized by atomic level control of film thickness. This method is being used to

grow multilayer superlattices of PbTe-based materials that are confined in one dimension. Electrodeposition of these phases into nanoporous aluminum oxide templates yields nanowire structures and, in some instances, nanotubes. Low-temperature solid state synthesis can allow the formation of one- and two- dimensional reduced dimension solids with large unit cell dimensions. A wide range of telluride and selenide phases have been prepared. For example, CeNiSb3 samples have been synthesized and characterized. Although not promising as a thermoelectric, this material was shown to be a heavy fermion conductor. Measurement of Thin Film Thermal Conductivity Using the 3-˜ Technique. The efficiency of a thermoelectric material is related to the ratio of the thermopower to the thermal conductivity. While thermopower measurements can be made trivially, it is experimentally difficult to measure the thermal conductivity of an ultrathin film in contact with a bulk substrate. An apparatus that allows for the measurement of thin film thermal conductivity values has been built and is currently in the preliminary testing phase.

Smith, David Y, University of Vermont, We are engaged in a study of the optical and magnetooptical properties of matter at short wavelengths in collaboration with researchers at Argonne and Brookhaven National Laboratories. Emphasis is on general linear-response methods of optical data analysis and the integration of theory with experiments using synchrotron photon sources. Our goal is to relate uv and x-ray optical properties of matter directly to electronic and magnetic structures. Most recently, we have developed a new method of analyzing uv and soft-x-ray reflectance measurements on bulk materials with absorptions so high that direct transmission measurements are impossible. This has allowed us to obtain, for the first time, the absorption spectra of representative silicate glasses in the uv and xuv. A new formulation of dispersion theory, combined with these absorption spectra, shows that the refractive index of glasses in the visible is dominated by the polarization (a virtual process) associated with the uv and xuv absorptions (real processes). Specifically, the visible index is, to an excellent approximation, a power series in photon energy with coefficients that are spectral moments of the uv-xuv absorption. The newly available absorption spectra also provide insights into the structure and bonding of glass modifiers to the surrounding matrix of glass former. Preliminary electronic-energy-level calculations using quantum-chemical techniques suggest that, in the alkali-silicate glasses, prominent uv absorptions can be associated with non-bridging oxygen orbitals involving glass-former ions. In principal, these results indicate a path to the development of a predictive technological model of optical materials. Our moments methods are also applicable to magnetooptics. Preliminary results show that the off-resonance Faraday effect, and hence the frequency-dependendent Verdet constant, can be expressed as a power series in photon energy with coefficients that are moments of the magnetic circular dichroism (MCD). A comparison of theory with experiment will be undertaken shortly. If successful, this approach provides a method of estimating magnetic splittings at strong resonances (where the MCD cannot be measured) from measurements of the Verdet constant at energies for which the magnetic material is transparent.

Stencel, John M, University of Kentucky, The Kentucky DOE EPSCoR Program encompasses two cooperative Research Clusters at the University of Kentucky,

University of Louisville and Northern Kentucky University that interact with DOE National Laboratories.The Materials Research cluster focuses on theoretical and experimental investigations for understanding new nanoscale materials and MEMS techniques for creating novel microdevices and integrated microsensors. The theoretical studies examine the structural, electronic, magnetic and optical properties of single-walled carbon naontubes, and Si and Si-Ge nanoclusters. The experimental MEMS research addresses advanced techniques for micro-milling/drilling, micro-embossing, micro-molding, electroplating, micro-stamping, micro-lamination, SAM's, wafer-level bonding, etchstop diffusion, and carbon nanotube growth. The Theoretical Subatomic Physics Research Cluster focuses on understanding the nature of fundamental interactions of and between particles and fields. They include strong and weak interactions, as well as quantum gravity and other phenomena beyond the reach of existing experiments. The Cluster includes three research areas: phenomenological tests of the Standard Model (such as CP violation in heavy meson systems) which may point to new physics; theoretical extensions of the Standard Model, including supersymmetry and string theory; and tests of these extensions (such as predictions about the production of microscopic black holes).

Tritt, Terry, Clemson University This proposal revolves around the investigations of the thermal and electrical transport properties of new and novel solid-state systems, with the specific goal of achieving higher efficiency solid-state power generation materials. This program will build a very strong collaborative research effort between researchers at Oak Ridge National Laboratory (ONRL) and Clemson University. The project's objective is to take the state of SC's capacity for research, development, design, and implementation of the next generation advanced thermoelectric (TE) materials to a world-class level. The magnitude of the funds involved in this program will be able to build a nationally recognized research center of excellence in the focused area of the next generation TE materials for power conversion and/or refrigeration technologies. World-class facilities and infrastructure to synthesize and characterize new classes of thermoelectric materials will be put into place. Young faculty will be hired and given sufficient start-up packages to develop state-of-the-art programs in materials synthesis (Phase I) and neutron diffraction (Phase II). All of this should poise this group for competition for major non-EPSCoR funded programs such as an NSF-Materials Research Center and major non-EPSCoR DOE and DOD funding. A close association and interaction with scientists at Oak Ridge National Laboratory has already been established and that relationship will be greatly expanded in this program. Several classes of materials will be investigated with potential for thermoelectric (TE) applications. In addition, each of these classes of materials poses several interesting scientific questions, which we wish to also address in this investigation. Graduate and undergraduate students will be extensively involved in this project, thus gaining significant training and educational opportunities through the interaction with the broad expertise and facilities of a national laboratory such as ORNL. A number of minority and under-represented (female) students will be involved in the project and there is a component involving a subcontract and research collaboration with a SC HBCU (SC State University).

Turner, Joseph, University of Nebraska-Lincoln The proposed research is a collaborative effort focused on the fundamentals of ultrasound propagation through materials with evolving microstructure due to recrystallization and sintering. A combined theoretical, numerical, and experimental research project is proposed. Theoretical models of elastic wave propagation through these complex materials will be developed using stochastic wave field techniques. The numerical simulations will be focused on finite element wave propagation solutions. The experimental efforts will be used to corroborate the models developed and to develop new experimental techniques. The ultrasonic experiments will provide information about the microstructure as it changes during high temperature processing. Processes such as annealing and sintering can significantly alter the macroscopic mechanical properties. These changes are complex functions of the processing parameters including time, temperature, pressure, and atmosphere, among others. It is anticipated that the proposed research will improve the understanding of the underlying materials mechanisms that occur as the microstructure evolves.

Wallace, Susan S, University of Vermont The DOE EPSCoR Initiative in Structural and Computational Biology/Bioinformatics Phase II continues to support infrastructure in these areas in the State of Vermont. The structural biology group works on determination of the exact structure of important biological molecules using a variety of sophisticated techniques such as x-ray diffraction, nuclear magnetic resonance spectroscopy and cryo-electron microscopy. Research of this nature is essential for the understanding of biological processes and allows, for example, for rational design of new drugs. The DOE EPSCoR grant has contributed to the purchase of the necessary instrumentation and upgrade, supported technical staff and funded specific research projects in structural biology. The resources of the program have also been effectively utilized to support graduate students, undergraduate summer interns and to recruit talented new faculty in the structural biology area to Vermont. The computational group is a true multidisciplinary effort directed at bringing the tools of modern computational science to solve biological problems. With the explosion of knowledge areas such as structural biology and the analysis of the human genome, biological scientists are faced with massive amounts of data. In order to extract useful information from the data, sophisticated mathematic and computational tools are required. The Vermont DOE EPSCoR computational biology group is composed of faculty in the biological sciences and in computer science. The program has contributed to the recruitment of new faculty members, funded pilot projects in computer science and was an important component in the development of a Ph.D. program in computer science at UVM with an identified track in computational biology. The program has also been involved in building structural/computational biology computing resources including servers, a secure network and a class room and the program supports computing clusters, web servers, visualization stations and the UVM biodesktop for handling and presenting biological data models. The DOE EPSCoR program also has a broad impact encompassing education and outreach in addition to research and physical infrastructure development. The educational activities include an external seminar speaker series in structural biology and workshops in bioinformatics and evolutionary computing. An annual retreat is

ongoing. DOE EPSCoR Phase II is continuing to develop our evolving state resources in structural and computational biology.

Wood, Scott, University of Idaho In this project, ternary surface-complexation models for the sorption of Nd^{3+}, Gd^{3+} and UO_2^{2+} onto nontronite and goethite in the presence of oxalate, citrate, EDTA and humic acid will be developed. These models will permit quantitative assessment of the degree to which Gd (added as a neutron absorber) and U (present in spent nuclear fuel) might become separated should buried nuclear waste come in contact with and be corroded by groundwater in the presence of natural and/or anthropogenic organic ligands. Because trivalent lanthanides (Nd, Gd) and hexavalent U are reasonable analogues of trivalent (Am^{3+}, Cm^{3+}, Pu^{3+}) and hexavalent (Pu^{6+}) actinides, respectively, our data will also provide insight into the behavior of radionuclides in sites contaminated by mixed nuclear-organic waste. The surface-complexation models will be constrained by potentiometric surface titrations, batch sorption measurements, and surface-sensitive spectroscopic techniques (XAS, XPS, FTIR, AFM, TEM). To date, we have carried out sorption experiments on binary systems involving sorption of Nd, Gd or U on goethite or nontronite. In systems where CO_2 is excluded, the sorption curves vs. pH for each of the metals show near-zero adsorption at acid pH, a rapid increase to nearly 100% adsorption over the pH range 5-6 (sorption edges), and 100% sorption at higher pH. The sorption curves are independent of ionic strength, suggesting that inner-sphere surface complexes are formed by these metals on goethite. In contrast, the low-pH portion of the sorption curves for Nd and Gd onto nontronite are sensitive to ionic strength, suggesting an ion exchange mechanism. At 0.1 M ionic strength, sorption of REE onto nontronite ranges from 70 to 90% over the pH range 3 to 5, then rises to 100% over the pH range 5-6, and remains at 100% to the highest pH measured, pH = 11. At 0.01 M ionic strength, sorption of Gd onto nontronite is nearly 100% over the entire pH range. On both nontronite and goethite, adsorption is not reversible, the amount adsorbed being higher upon back titration (from basic to acidic pH). Addition of CO_2 to the system results in the shifting of the sorption edge for Gd onto goethite to lower pH, the amount of shift being proportional to the partial pressure of CO_2. This implies the formation of ternary surface complexes involving Gd, carbonate and goethite. Experiments involving CO_2 and U are in progress. Binary experiments involving sorption of oxalate and fulvic acid onto goethite are also in progress, in preparation for ternary experiments.

Zappi, Mark, Mississippi State University The Mississippi University Research Consortium for the Utilization of Biomass was formed in 2000 based on funding obtained from the US Department of Energy (via its ESPCoR Program) and the State of Mississippi. Total funding is $7.2 Million over a six year period. Members include Mississippi State University (lead university), Jackson State University, University of Mississippi, and University of Southern Mississippi. The mission of the Consortium is to development technologies that are capable of producing valuable products from Mississippi-grown biomass resources, development of additional research capabilities within Mississippi, and the education of future engineers and scientists within Mississippi with expertise in the production of chemicals from biomass feeds. Currently,

the major emphasis among Consortium members is directed toward development of industrial processes for the production of ethanol from lignocellulosic materials. The ethanol produced from these processes will be used as a renewable source of transportation fuel. The processes under development include fermentation of syngas produced from gasification of biomass, acid hydrolysis conversion of cellulose and hemicellulose followed by fermentation of the resulting hydrolyzate, and enzymatic conversion of lignocellulosic materials into fermentable products. Additional efforts are underway for the production of novel chemicals from lignin using innovative enzymes, production of acetic acid from syngas fermentation, production of ethanol using reformed natural gas as a feedstock via fermentation, optimization of biogas production from waste feedstocks, and production of biodiesel using novel processing techniques. It is noteworthy to mention that most of these efforts are being performed with close interaction with industrial developmental partners with hopes of establishing viable new industries within the State of Mississippi. The activities of the Consortium are being leveraged with Mississippi industries with hopes of ultimately positioning Mississippi as a leader in bioprocessing for production of a wide variety of chemicals ranging from energetic fuels, such as biodiesel and ethanol, to nutraceuticals, such as omega-3 fatty acids. Given the vast biomass production capabilities of Mississippi, it is strongly believe that processing of Mississippi primary production-based biomass into secondary production materials will yield numerous in-state industries within Mississippi.