Making Wind Work for Alaska: Supporting the Development of Sustainable, Resilient, Cost-Effective Wind-Diesel Systems for Isolated Communities- EPSCoR Implementation Award

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Students:	4 Postdoctoral Fellow(s), 4 Graduate(s), 3 Undergraduate(s)
Funding:	$2,901,363 (Three years)

This project will expand existing capacity at the University of Alaska in the niche market technology of hybrid wind-diesel systems. Our central project theme is delivering low-cost, reliable, and sustainable energy from a wind-diesel platform that is designed to address a critical research need for rural Alaska. While many parts of the state have excellent wind resource, most communities in rural Alaska are more similar to less-developed countries than to places in the continental U.S. Small populations, isolated off-grid systems, difficult environmental conditions, dependence on imported fuels, lack of roads and infrastructure, and slim, mixed cash-subsistence economies all combine to produce the highest energy costs in the country, with electric power approaching $1 per kWhr, and gasoline prices as high as $10 per gallon.

With abundant wind resources across many rural regions of the state, Alaska is already considered a world leader in wind-diesel technologies, but many installed systems are not performing as designed. The work plan will first focus on improving understanding of the performance of existing wind-diesel systems. To accomplish this, the PIs will work with the Alaska Energy Authority to develop a comprehensive database of wind system experience, including underlying climatic and socioeconomic characteristics, actual operating data, projected vs. actual capital and O&M costs, and a catalogue of catastrophic anomalies. This database will form the foundation for the rest of the research program, with the overarching goal of delivering low-cost, reliable, and sustainable energy from a wind-diesel platform. Specifically, we propose to address:

1) High Penetration: Technical issues related to higher penetration of wind, such as power stability, long term energy storage, and advanced control technologies including the use of excess wind power to supplement residential and commercial space heating and transportation.

2) Cold Climate: Issues related to operation of turbines and ancillary equipment in cold climates and remote locations, such as production loss due to rime ice buildup, remote monitoring, and foundation design in areas with geo-technical problems.

3) Socioeconomics: Social, economic, and political barriers to the development of wind, including local capacity to develop and support sustainable systems.

The focal point for development of our collaborative research plan is the Wind Diesel Applications Center (WiDAC), based at the University of Alaska. WiDAC was formed in 2008 as a consortium of university, national laboratory, and over 50 industry partners with the goal of supporting deployment of cost-effective wind-diesel technologies. The program outlined in this proposal was developed through a series of discussions with our WiDAC partners, and will significantly increase the University of Alaska's ability to carry out the Center's mission through key new faculty hires, graduate student fellowships, faculty and staff training opportunities at national labs, and acquisition of needed equipment. Because WiDAC is a strong partnership among manufacturers, the research community, and the technology end-users, it will serve as a practical and effective mechanism to ensure the goals laid out in this proposal can not only be successfully met, but that the overall program will be sustainable beyond the timeframe of this project.

Fundamental Investigations of Mechanical and Chemical Degradation Mechanisms in Lithium Ion Battery Materials - EPSCoR Implementation Award

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Students:	7 Postdoctoral Fellow(s), 9 Graduate(s), 8Undergraduate(s)
Funding:	$6,174,882 (Three years)

Despite the rapid advances in lithium ion battery (LIB) technology in recent years, major obstacles remain for vehicular applications of LIBs. It is widely recognized that further critical breakthroughs in the science and technology of lithium ion battery materials are necessary to develop the next generation of low-cost, long-life, higher energy density batteries for extended range electric vehicles. The objective of the proposed effort under the DOE EPSCoR Implementation grant is to establish a comprehensive and internationally recognized research program, at Brown University and University of Rhode Island, to understand degradation and improve the cycle and calendar life of lithium ion battery materials.

We propose a series of fundamental investigations on mechanical and chemical degradation mechanisms in lithium ion battery materials, which will help enable new higher capacity and higher energy-density electrode materials to meet the USABC (United State Automotive Battery Consortium) goals of 5,000 cycles and 15 years. The proposed work encompasses critical challenges in the three

major battery components: anodes, electrolytes and cathodes. Mechanical and chemical degradation of electrodes associated with large volume changes during charging and discharging is a critical factor that limits their capacity and lifetime. However, the degradation mechanisms are not well-understood *quantitatively*, which is a critical obstacle in developing the next generation of LIBs. Optimal battery designs must balance requirements such as mechanical performance, minimizing electrochemical side reactions, controlling the formation of solid-electrolyte interface (SEI) layers and managing mass transport through the microstructure. The PIs, in collaboration with National Lab and industrial partners, are well positioned to address these issues. The proposed research is in full alignment with the State of Rhode Island's Science and Technology plan, which identifies energy and environment as one of the core-sectors on which the State's knowledge economy can be built.

Controlling mechanical and chemical degradation is the primary challenge in developing the next generation of higher energy density batteries. The development of failure resistant battery microstructures will require a fundamental understanding of the evolution of stress, deformation, damage, and electrochemistry in battery materials during cyclic charging and discharging. In addition, controlling the reactions at the electrode/electrolyte interface is critical for the formation of a stable SEI layer. We propose to tackle these issues using a combination of controlled experiments on model battery materials and practical composite electrodes, together with multi-scale computations. It should be noted that our main objective is not to develop new electrode materials; instead, it is to investigate the basic properties and phenomena that control the long term performance of the electrode materials, which can help battery developers in optimizing electrode microstructures and material formulations. Our effort is organized into two related thrusts, the objectives of which are: (i) Experiments and multi-scale modeling to understand deformation, mechanical behavior and evolution in practical battery microstructures during cyclic charging; (ii) Investigate the surface chemical reactions and the role of electrolyte additives on SEI formation and stability. Our investigations will be carried out on current electrode materials and materials that are considered to be promising for the next generation of high energy density LIBs, such as Si, Sn and Si-C for anodes, Li_2MnO_3 stabilized $LiMO_2$ composite cathodes.

The proposed research will lead to better understanding of mechanical and chemical degradation in LIB materials. The development of a fundamental understanding of the evolution of stress, deformation, damage, and electrochemistry in composite electrodes will assist in the development of failure resistant microstructures for lithium ion battery electrodes. Development of a structural and mechanistic understanding of interfacial surface films on electrode materials will allow systematic development of superior electrolyte formulations for the next generation electrode materials, which will help improve cycle life and calendar life of lithium ion batteries.

Center for Spintronics and Biodetection (CSB) - EPSCoR Implementation Award

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Students:	1 Postdoctoral Fellow(s), 9 Graduate(s), 3 Undergraduate(s)

Funding: $2,250,000 (Three years)

Traditional semiconductor electronics, which is based on the control of electron charges, cannot be further miniaturized beyond 2020 due to the limit of thermal management of charge dissipation. Using the spin of electrons, which can move information without moving charge and thus significantly reduce energy dissipation, is a potential candidate for electronic devices beyond 2020. Built upon the success of the Center for Spintronics and Biodetection (CSB), this renewal focuses on harnessing coherent spin states and their dynamics for high performance spintronic devices, as well as integration with novel, functionalized magnetic nanoparticles for the detection of biochemical molecules. CSB's research will provide fundamental insight into magneto-electronic phenomena with broad impact on diverse technologies including information storage, microwave communication and detection, and biomedical diagnostics. CSB's research activities are well aligned with the Materials Sciences and Engineering program under the Office of Basic Energy Science, and the State of Delaware's initiatives on developing scientific infrastructure (people and facilities) in the areas of biotechnology, environment, and nanoscience. CSB participants will include an interdisciplinary mix of post-docs, graduate and undergraduate students who will collaborate with scientists in academia, the Delaware Environment Institute, industry, and DOE National Laboratories and facilities, including using the Spallation Neutron Source (Oak Ridge National Laboratory) and National Synchrotron Light Source (Brookhaven National Laboratory), and the Center for Nanoscale Materials (Argonne National Laboratory) for fabricating and characterizing nanoscale magnetic heterostructures.

The project's objectives are:

1. Revealing fundamental physics of generation, manipulation, and detection of low dissipation spin current. These include the understanding of spin transport across interfaces, through materials, and the effects of spin-orbit coupling, exchange interaction, electron-electron interaction, and radio-frequency fields

2. Studying microwave and non-local spin torque induced spin dynamics in spintronic devices, and developing novel microwave devices such as microwave detectors.

3. Identifying and controlling fluctuations and noise in magnetic nanostructures to attain pico-Tesla magnetic field detectivity at low frequencies

4. Advancing magnetic nanotechnology for sensitive biodetection including synthesizing of stable monodisperse magnetic nanoparticles (NPs) with high moments for improved signal/noise ratio, and understanding of the interactions between functionalized NPs and the magnetic senor's surface and biological molecules

5. Education and mentoring of students and supporting State's science and technology developments

Nanoscale Materials and Architectures for Energy Conversion

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Students:	8 Graduate(s), 0 Undergraduate(s)
Funding:	$1,880,000 (Three years)

The Kentucky EPSCoR Program is an inter-university, multidisciplinary energy-related research cluster in nanomaterials for converting solar radiation and residual thermal energy to electrical energy and hydrogen. It creates a collaborative center of excellence based on research expertise in nanomaterials, architectures, and their synthesis. Fundamental processes of light absorption, charge separation/transport, and electron emission within nanostructured materials are examined to improve solar and thermal energy conversion processes.

The research strengthens and renews collaboration between the University of Louisville, University of Kentucky, and NREL and establishes collaboration with the DOE Solar Fuels hub. A new faculty member is hired (Dr. Jinjun Liu) for fundamental research studies using ultra-fast transient spectroscopy. The cluster enables mentoring of one junior faculty, one research scientist and eight graduate students. The program enhances the annual Kentucky renewable energy and energy efficiency workshop and makes a positive impact on several new energy research and development infrastructure initiatives.

Focus Areas:

1. Solar fuels: Photoelectrochemical water splitting and carbon dioxide reduction

   In the solar fuels theme, the outcomes include prediction of new semiconductor alloys based on dilute antimonides, a number of cost-effective strategies for nanowire arrays, and a strategy for obtaining ternary nitride alloys suitable for solar hydrogen. Specifically, in the renewal, we propose an aggressive strategy to synthesize ternary nitride alloys and new materials on nanowire array platforms on suitable substrates for studying their behavior for solar to fuels conversion.

2. Solar electricity: Dye-sensitized and organic hybrid solar cells

   In the solar electricity theme, the outcomes include new concepts and new understanding about charge separation and transport in nanostructured materials used in DSSCs and OPVs. In the renewal, using the developed conceptual understanding, new nanostructured materials assemblies will be studied for designing new assemblies for improving the efficiency of both DSSCs and OPVs.

3. Thermal energy conversion: Thermionic/thermoelectric tandem devices

   In the thermal energy conversion theme, a novel nanostructure architecture based on CCNT arrays is shown to be promising for field and TE processes. In addition, the synthesis of proposed materials, i.e., diamond nanocrystals at CCNT tips, was achieved. In the renewal, we propose to investigate the work function and TE process from n-type doped nanocrystals supported on suitable nanotip arrays beyond carbon. Most importantly, based on device level modeling, we propose several tandem device designs that combine both thermionic/thermoelectric and thermionic and light absorption to achieve efficiencies >30% for thermal energy conversion.

Thermochemical Conversion of Woody Biomass to Fuels and Chemicals - EPSCoR Implementation Award

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	Meulenberg, Robert, MAINE, UNIVERSITY OF
	Jensen, Bruce, MAINE, UNIVERSITY OF
	Austin, Rachael, BATES COLLEGE
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Students:	1 Postdoctoral Fellow(s), 5 Graduate(s), 7 Undergraduate(s)
Funding:	$1,860,000 (Three years)

Maine and its industries have identified more efficient utilization of biomass as a critical economic development issue. In Phase I, a research team was assembled, research equipment was implemented and expertise was demonstrated in pyrolysis, hydrodeoxygenation of pyrolysis oils, catalyst synthesis and characterization, and reaction engineering. Phase II will build upon this infrastructure to innovate reaction pathways and process engineering, and integrate new approaches for fuels and chemical production within pulp and paper and other industries within the state. This research cluster brings together chemists, engineers, physicists and students from the University of Maine, Bates College, Bowdoin College, and BioFine, LLC. The plan also builds upon collaborations with Oak Ridge National Laboratory and Brookhaven National Laboratory. The specific research projects within this proposal are of critical interest to the DOE - in particular the biomass program within EERE and the catalysis/chemical transformations program within BES.

Center for Integrated Computation and Analysis of Reconnection and Turbulence (CICART) - EPSCoR Implementation Award

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	Sullivan, Brian, NEW HAMPSHIRE, UNIVERSITY OF
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Students:	1 Postdoctoral Fellow(s), 4 Graduate(s), 0 Undergraduate(s)
Funding:	$2,250,000 (Three years)

CICART is a partnership between the University of New Hampshire (UNH) and Dartmouth College. CICART addresses two important science needs of the DOE: the basic understanding of magnetic reconnection and turbulence that strongly impacts the performance of fusion plasmas, and the development of new mathematical and computational tools that enable the modeling and control of these phenomena. The principal participants of CICART constitute an interdisciplinary group, drawn from the communities of applied mathematics, astrophysics, computational physics, fluid dynamics, and fusion physics. It is a main premise of CICART that fundamental aspects of magnetic reconnection and turbulence in fusion devices, smaller-scale laboratory experiments, and space and astrophysical plasmas can be viewed from a common perspective, and that progress in understanding in any of these interconnected fields is likely to lead to progress in others. The establishment of CICART has strongly impacted the education and research mission of a new Program in Integrated Applied Mathematics in the College of Engineering and Applied Sciences at UNH by enabling the recruitment of a tenure-track faculty member, supported equally by UNH and CICART, and the establishment of an IBM-UNH Computing Alliance. The proposed areas of research include the following topics: (A) Reconnection and secondary instabilities in large high-Lundquist-number plasmas, (B) Particle acceleration in the presence of multiple magnetic islands, (C) Gyrokinetic reconnection: comparison with fluid and particle-in-cell models, (D) Imbalanced turbulence, (E) Ion heating, and (F) Turbulence in laboratory (including fusion-relevant) experiments. These theoretical studies make active use of three high- performance computer simulation codes: (1) The Magnetic Reconnection Code, based on extended two-fluid (or Hall MHD) equations, in an Adaptive Mesh Refinement (AMR) framework, (2) the Particle Simulation Code, a fully electromagnetic 3D *P*article-*I*n-*C*ell (PIC) code that includes a collision operator, and (3) GS2, an Eulerian, electromagnetic, kinetic code that is widely used in the fusion program, and simulates the nonlinear gyrokinetic equations, together with a self-consistent set of Maxwell's equations.

Center for Interfacial Reaction Engineering - EPSCoR Implementation Award

Institution:	OKLAHOMA, UNIVERSITY OF
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	Gasem, Khaled A.M., OKLAHOMA STATE UNIVERSITY
	Wang, Sanwu, TULSA, UNIVERSITY OF
Students:	4 Postdoctoral Fellow(s), 7 Graduate(s), 3 Undergraduate(s)
Funding:	$2,901,363 (Three years)

Research at the Center for Interfacial Reaction Engineering will establish the scientific basis for a novel integrated catalytic technology, which can be used to efficiently refine complex fluids such as bio-oil and residual heavy oil fractions from petroleum cracking. Key elements of the new technology are multifunctional solid materials that serve as surfactants and as catalysts. These novel materials promote the formation of emulsions and thus separate mixtures into confined reaction environments. From their position at the liquid/liquid interface, these high surface area materials will simultaneously catalyze desired chemical reactions in both, organic and aqueous phases (see illustration below). After appropriate residence time, phase separation will occur automatically after removal of the surfactant-

catalyst. Inherent to this type of liquid phase processing will be moderate reaction temperatures and pressures, which will allow for energy-efficient operation.

Researchers at the Center for Interfacial Reaction Engineering will address all fundamental scientific aspects that are necessary to develop the materials and to engineer the processes. This research will deliver an entirely new class of materials and in-depth knowledge of the chemistry at the various interfaces between all classical states of matter. The characterization of the materials and the emulsions will require application of an array of techniques for bulk structural as well as surface and interface analysis. To monitor catalytic performance, advanced methods for vapor and liquid phase analysis will be used.

A potential outcome of the project is a technically viable solution for the processing of biomass and of heavy oils, which will alleviate the current pressing issues regarding energy and fuel supplies.

The multiple scientific tasks will require a multidisciplinary multi-institutional team, which will consist of experts in the fields of (i) surfactants, colloids and interfaces, (ii) thermodynamics of phase behavior, (iii) materials development, materials characterization and catalysis, (iv) spectroscopic investigation of interfaces, and (v) theoretical surface physics. The team is assembled to meet the theoretical and experimental challenges in investigating the phase chemistry and the catalytic chemistry at the macroscopic as well as the molecular level.

Development and Understanding of Multifunctional Nanostructured Magnetoelectric and Spintronic Materials - EPSCoR Implementation Award

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Students:	2 Postdoctoral Fellow(s), 8 Graduate(s), 2 Undergraduate(s)
Funding:	$2,430,000 (Three years)

Magnetoelectric (ME) multiferroics and spintronics combine standard microelectronics with spin-dependent effects that arise from interactions between electrons and magnetic field. The spin dependent phenomena become challenging at the nanoscale where new physical effects emerge affecting the spin injection, transport, and switching times. The goals of this project are CMOS device compatible Multifunctional Materials to meet the near future demand of miniaturization of Si based

technology and for the next generation technology beyond Si. Such a technology has been following Moore's law during last 4 decades (i.e. the number of transistors per integrated circuit (IC) doubles roughly every 24 months). For this advancement, however, the fundamental science and understanding is needed to develop high-k gate oxides (for 22 nm node technology and beyond), ME multiferroics, and dilute magnetic semiconductors (DMS). Such materials have the potential to form the basis of a new generation of energy efficient nanoscale electronic devices that are fast responding, have low power consumption and high integration density. In the present grant, the researchers are actively involved in the synthesis and characterization of various functional oxides and silicides to accomplish this goal.

Crystal Growth and Detector Development at Homestake for DUSEL Experiments- EPSCoR Implementation Award

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Students:	4 Postdoctoral Fellow(s), 14 Graduate(s), 8 Undergraduate(s)
Funding:	$2,974,378 (Three years)

The overall goal of the project is to perform material purification and crystal growth underground for Ultra-Low Background Experiments at the Sanford Underground Research Facility (SURF, previously called DUSEL) at Homestake, Lead, South Dakota. It was recommended by the National Research Council (NRC) that a ton-scale dark matter experiment and a ton-scale neutrinoless double beta decay experiment should be built to address critical questions about dark matter and neutrinos in this decade. Germanium crystals were used in the large scale dark matter and neutrinoless double beta decay experiments that recently reported a possible dark matter signature (CoGeNT) and the claimed discovery of neutrinoless double beta decay (Klapdor-Kleingrothaus), and as such represent a preferred material for use in future experiments. Thus, growth of high-purity germanium crystals is a key element in the success of these underground experiments. The growth of ultra-pure germanium crystals in an underground environment is a critical step in the underground experiments. However, much R&D needs to be done on the surface to grow detector-grade crystals. The objectives of this proposal, submitted on behalf of the CUBED collaboration including seven institutions in South Dakota in partnership with Los Alamos National Laboratory and Lawrence Berkeley National Laboratory, are: 1) to provide leadership so that the current South Dakota faculty who are interested in developing new detectors may fully participate in large-scale collaborations planned for SURF; 2) to implement R&D activities including

Monte Carlo simulation for material purification and crystal growth on the surface; 3) to construct an underground lab for materials purification and crystal growth; 4) to grow crystals to contribute to the ton scale dark matter and neutrinoless double-beta decay experiments; 5) to develop new detectors with the grown crystals; and 6) to train students, postdoctoral researchers, and technicians to be qualified workers in the state so that they can be active participants in the current (Majorana and LUX) and future ultra-low background experiments at SURF.

Neutron Scattering Research Network for EPSCoR States- EPSCoR Implementation Award

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	Sokolov, Alexi P., TENNESSEE, UNIVERSITY OF
Students:	4 Postdoctoral Fellow(s), 7 Graduate(s), 0 Undergraduate(s)
Funding:	$1,666,300 (Three years)

With the completion of the Spallation Neutron Source (SNS) and upgrading of the High-Flux Isotope Reactor (HFIR) at the Oak Ridge National Laboratory (ORNL) the state of Tennessee now leads the world in the capability to conduct neutron scattering research. This project aims at directing the great impact of these facilities to researchers in the EPSCoR states, Tennessee in particular, by creating a research collaboration network around these facilities. The plan consists of two parts: (1) Direct effort to increase the user base through the travel fellowship for graduate students and faculty from the EPSCoR states to use the neutron facilities at the ORNL, and through workshops and schools on the application of neutron scattering, and (2) Research collaborations among the core participants from UTK and other states making use of the neutron scattering facilities at ORNL.

The EPSCoR Travel Fellowship Program started in the Phase I of this grant has grown to support over 120 recipients per year including the workshop support, and is expected to grow further. This program is highly popular particularly among young researchers, and will continue to be the foundation of this project. We support several educational workshops, organize one by ourselves each year, and will continue to support several of such workshops. In addition we support the users through equipment for general users, and support of sabbatical leaves by researchers from other EPSCoR states.

The core research groups participating in this project include not only researchers from Tennessee but those from Kansas, South Carolina, Puerto Rico and Louisiana, making this project a national, rather than regional, enterprise. Collaborations that were seeded by this project have grown into two major projects, one in condensed matter physics and the other in soft matter sciences. Through this project we promote the use of neutron scattering, particularly in biological and life sciences and in energy sciences, and facilitate the DOE investment in this field to impact wide fields of science and engineering.

This project is administered through the Joint Institute for Neutron Sciences (JINS) of the University of Tennessee (UT). The new JINS building opened December, 2010, right next to the SNS, and houses much of the activities supported by this grant. JINS is jointly supported by both UT and ORNL, and participates in organizing workshops and schools to promote the use of neutron scattering.

Quantum Dot Sensitized Solar Cells Based on Ternary Metal Oxide Nanowires - EPSCoR Implementation Award

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	Pikal, Jon, WYOMING, UNIVERSITY OF
	Tang, Jinke, WYOMING, UNIVERSITY OF
Students:	4 Postdoctoral Fellow(s), 8 Graduate(s), 2 Undergraduate(s)
Funding:	$2,440,711 (Three years)

This joint effort on renewable energy research at the University of Wyoming addresses novel nanostructures, i.e., ternary metal oxide nanowires, for photovoltaic (PV) applications. Compared with simple binary materials, ternary metal oxides offer more freedom in the tuning of chemical and physical properties, which have the potential to optimize bandgap and energy level alignment in quantum dot (QD) sensitized solar cells. In addition, ternary oxides also exhibit better corrosion resistance than many binary materials. Therefore, combining ternary oxide nanowires with quantum dots will provide significant advantages for light absorption and carrier injection and transport in PV structures, and will create more stable devices with a longer lifetime.

The research objective of this proposal is to realize QD sensitized solar cells based on ternary metal oxide nanowires and study the physical and chemical mechanisms that govern device operations. We will especially investigate the synthesis of different ternary metal oxide nanowires, different QD assembly methods, and their influence on charge transport and solar cell performance . Our research plan consists of the following five sub-projects: (1) synthesis of ternary metal oxide nanowires, (2) synthesis of QDs and exploration of non-solution based QD deposition methods, (3) physical and electro-optical characterizations of fabricated solar devices, (4) device modeling and first-principle theoretical study of transport physics, and (5) investigation of long term stability issues of QD sensitized solar cells. This study will achieve a better understanding of carrier transport and recombination processes in ternary nanowire solar cells and have the potential to improve the performance of these nanomaterial-based PV devices.

This research effort will also initiate an important research direction in the jurisdiction. It will bring together researchers from different academic disciplines to work on one common scientific theme, and is a vital step toward the implementation and the eventual establishment of an outstanding, nationally competitive research program in energy-related nanomaterials in the state of Wyoming. Through this project we will also develop a fruitful collaboration between UW and DOE national labs such as NREL, which will benefit our long-term goal of establishing a sustainable research program in the renewable energy field.

Direct Utilization of Coal Syngas in High Temperature Fuel Cells - EPSCoR Implementation Award

Institution:	WEST VIRGINIA UNIVERSITY
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Principal Investigator:	Celik, Ismail, West Virginia University
Sr. Investigator(s):	Finlea, Harry, West Virginia University
	Kang, Bruce, West Virginia University
	Liu, Xingbo, West Virginia University
	Sabolsky, Edward, West Virginia University
	Song, Xueyan, West Virginia University
	Wu, Nick, West Virginia University
	Zondlo, John , West Virginia University
Students:	6 Postdoctoral Fellow(s), 11 Graduate(s), 0 Undergraduate(s)
Funding:	$1,950,000 (Three years)

In the phase I (about two years in duration) of the WV EPSCoR project we have established primary infrastructure that was necessary to conduct state-of-the-art fuel-cell research in terms of test benches, laboratories, computational capabilities, materials processing, and cell manufacturing capabilities. These capabilities have enabled us to carry out research leading to an understanding of the extent and nature of performance degradation caused by impurities/contaminants found in typical coal syngas. Laboratory experiments and theoretical calculations were carried out on SOFCs with H_2S, PH_3, HCl. More testing is currently underway. The results of our current work and data from the literature have shown that many trace species found in coal gas can cause severe performance degradation depending on their concentration, temperature, and cell materials and geometry, as well as cell operating conditions. In the second phase of this program we propose to continue the study along the same lines, but with more focus on mechanisms of degradation using more sophisticated in-situ as well as ex-situ measurement techniques. We will transfer this knowledge base into theoretical analyses and corresponding computational models to predict minimum tolerance levels of typical Ni-YSZ/YSZ/LSM cell for a range of contaminants. In addition, we will use these models to predict cell degradation under defined contaminant concentration with the objective of optimizing transport processes and materials used to prolong cell lifetime. Finally, we propose to extend this study to utilization of bio-gas in SOFCs to better position our research team for future competitive external funding.

Single-Molecule Spectroelectrochemistry of Interfacial Charge Transfer - EPSCoR State – National Laboratory Partnerships

Institution: ALABAMA, UNIVERSITY OF
Point of Contact: Pan, S., span1@bama.ua.edu
Principal Investigator: Pan, S.
Sr. Investigator(s): Hu, Dehong, PACIFIC NORTHWEST NATIONAL LABORATORY
Students: 1 Postdoctoral Fellow(s), 2 Graduate(s), 0 Undergraduate(s)
Funding: $542,115 (Three years)

The central goal of this project is to investigate the interfacial charge transfer dynamics of single fluorescent molecules (e.g., conjugate polymer and small organic dye molecules) at a semiconductor surface with ordered nanostructures using combined methods of electrochemistry and single molecule spectroscopy. Our study shows that the single molecule fluorescence blinking dynamics, their spatial distribution heterogeneities, and strong dependence on interfacial charge transfer to nanostructured TiO_2 electrodes. This study would potentially help understand the interfacial charge transfer dynamics in an organic photovoltaic (OPV) device, and ultimately empower us to confront challenges and problems prohibiting the development of efficient hybrid OPVs. Our accomplishments are shown as follows:

(1) Ordered TiO_2 nanostructures are designed and fabricated for studying interfacial charge transfer activities of single fluorescent polymer molecules (e.g., MEH-PPV, and P3HT) , and small molecules (BODiPY dyes). Single molecule spectroelectrochemistry has been used to provide valuable insights into the complex interactions among excited and charged species that exist in a hybrid OPV device environment.

(2) Heterogeneous photoinduced charge transfer activities of TiO_2 single crystal surface are investigated using combined methods of photoreduction for plasmonic antenna and surface-enhanced Raman spectroscopy. The Plasmon antennas of silver nanoparticles are used to help obtain Raman of dye molecules to reveal the interfacial charge transfer dynamics of the single crystal particles. Photoelectrochemical techniques and single molecule Raman are used to investigate how different surface doping methods would affect the spatial distribution of the plasmon antenna and single crystal facet dependences.

(3) A new method of probing redox reaction at single nanoparticle level has been invented using combined electrochemical and light scattering technique.

The ongoing project continues understanding interfacial charge transfer activities of single fluorescent polymer molecules in single TiO_2 nanotubes using fluorescence correlation spectroscopy and polarized fluorescence emission methods.

Progress towards "Picosecond x-ray diagnostics for third and fourth generation synchrotron sources" - EPSCoR State – National Laboratory Partnerships

Institution: DELAWARE, UNIVERSITY OF
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Sr. Investigator(s): Dufresne, Eric, ARGONNE NATIONAL LABORATORY
Students: 1 Postdoctoral Fellow(s), 2 Graduate(s), 0 Undergraduate(s)

Funding: $545,000 (Three years)

In this project, which begun during the last quarter of FY2011, the PI is forging a scientific partnership between the University of Delaware and the Advanced Photon Source (APS) at Argonne National Laboratory. The goal of this project is to develop a series of picosecond diagnostic tools for time-resolved x-ray studies. Three distinct time-resolved x-ray scattering experiments will be developed during the three year funding cycle of this grant: 1) X-ray switching through the generation of laser generated picosecond surface acoustic waves, 2) The construction of an x-ray pump-probe spectrometer for the study of x-ray induced structural dynamics, and 3) The study of x-ray induced structural dynamics through two-color x-ray pump-probe spectroscopy. These three projects, which currently support the work of two PhD graduate students, are in the early stages of design and construction.

The demonstration of an ultrafast x-ray switch through laser induced coherent surface acoustic waves will be the first experiment that will be performed with this partnership. This project aims to be able to slice the 100 picosecond x-ray pulse of the APS into picosecond bunches that are suitable for time-resolved studies. In the past year two scientific papers related to this grant have been published in peer reviewed scientific journals, and a third is currently being prepared for submission. In work published in J. Applied Physics (vol. **112**, pg. 013527 (2012)) we measured the optical phonon dynamics in a 20nm Bismuth thin film. This work represents the first step for producing an x-ray switch using the soft phonon mode in a Bismuth thin film. In work published in Applied Physics Letters (vol **100** pg 191903 (2012)), we measured the laser induced strain from a photo-excited metallic film on a crystalline substrate measured by time-resolved x-ray diffraction. This work, performed at the University of Delaware's picosecond x-ray facility, represents a significant step in the demonstration of the ultrafast x-ray switch. Further studies will be undertaken at Argonne. In particular, two general user proposals have been submitted to Argonne National Laboratory; one accepted at the Center for Nanoscale Materials (CNM) for fabrication, and a second to the APS for x-ray beamtime. If the user proposal to the APS is accepted, the first time-resolved x-ray experiments will commence during the winter of 2013 with an anticipated demonstration of the x-ray slicing by mid FY2013.

The other projects are currently in the design and construction stages at the University of Delaware. In particular, we are currently testing a laser-based x-ray source for producing picosecond x-rays at the APS, and have purchased a two-dimensional x- ray CCD detector. A general user proposal for these experiments will be submitted to the APS during the winter of 2013.

Fundamental fluid physics studies for energy efficiency and sustainability - EPSCoR State – National Laboratory Partnerships

Institution: IDAHO, UNIVERSITY OF
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McEligot, Donald M., IDAHO, UNIVERSITY OF
Tokuhiro, Akira T., IDAHO, UNIVERSITY OF
Xing, Tao, IDAHO, UNIVERSITY OF
Ferguson, James R., BOISE STATE UNIVERSITY
Stoots, Carl M., IDAHO NATIONAL LABORATORY

Students: 0 Postdoctoral Fellow(s), 5 Graduate, 0 Undergraduate

Funding: $584,961 (Three years)

The sustainability of a system is maximized when entropy generation is minimized; the issue of efficiency in practical systems must be thought of as how much entropy is generated. Consequently, the overall technical objective of this study is to address the scientific issue of obtaining basic understanding of local (pointwise) distributions of entropy generation rates S’” in characteristic wall shear flows, because fundamental understanding of entropy generation in such flows is a key to increasing energy efficiency and sustainability and, thereby, reducing fuel consumption, green-house gases and/or waste. For entropy generated by fluid friction, the rates are reasonably predictable for turbulent flows and pure laminar flows; the main difficulty now lies in prediction for flows undergoing so-called “bypass” transition from laminar to turbulent states (i.e., transition prematurely induced by strong freestream turbulence) in streamwise pressure gradients.

Prof. John Crepeau of the University of Idaho (UI) will serve as Project Director and coordinate the overall project. Dr. Carl M. Stoots, PI for the Idaho National Laboratory's (INL) unique Matched-Index-of-Refraction (MIR) flow system, will supervise its use by graduate students and recommend appropriate operating and measuring techniques for the necessary experiments. He and Profs. Ralph S. Budwig and Donald M. McEligot will conduct analyses of the experimental uncertainties of the proposed techniques. Existing MIR transition data will be employed to evaluate benefits and problems of these techniques for measuring S’” in bypass transition with pressure gradients and to quantify some necessary estimates. In conjunction with them, Prof. Budwig and students will develop new MIR experiments to measure S’” in the range of conditions needed and then the students will conduct the experiments at the INL. Profs. Akira Tokuhiro and Tao Xing (UI) and James R. Ferguson of Boise State (BSU) and students will provide computational fluid dynamic calculations to assist the experiment development and to be assessed with the consequent experimental data and Direct Numerical Simulation (DNS) results; their evaluation of transition models effective (and ineffective) in these cases will benefit the energy design community directly. As informal collaborators, Drs. L. Brandt and P. Schlatter at KTH Sweden and Dr. T. Zaki at Imperial College London and their students will provide results of DNS for bypass transition as guidance and to provide estimates of the magnitudes of terms not easily measurable. Dr. E. J. Walsh and students at the University of Oxford and the University of Limerick will extract values of S’” from DNS results and separate them into the contributions from the growing turbulent spots and surrounding unsteady laminar flow.

Development of this Idaho-based international team of experimental and computational fluid physicists will advance fundamental energy-oriented science and engineering research partnerships within the Idaho National Laboratory to the benefit of DOE programs in Nuclear Energy and Energy Efficiency. Some applications include nuclear and fossil power plants, turbine blade aerodynamics, heat exchangers, wind turbines, urban aerodynamics, fusion energy and underwater bodies. The coupled operation of this partnership will enhance the capabilities of the two Idaho academic institutions and INL to conduct internationally-competitive energy-related research. It will leverage ongoing efforts by young faculty at Oxford, Limerick, KTH, and Imperial College to expand the abilities and networks of the young faculty and students at the UI and BSU to enhance their recognition as contributing members of the international fluid physics community.

Exploiting the Use of Social Networking to Facilitate Collaboration in the Scientific Community - EPSCoR State – National Laboratory Partnerships

Institution: INFORMATION INTERNATIONAL ASSOCIATES, INC.,
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Sr. Investigator(s):
Bozdogan, Hamparsum, TENNESSEE, UNIVERSITY OF
Shankar, Mallikarjun, OAK RIDGE NATIONAL LABORATORY
Students: 1 Postdoctoral Fellow(s), 1 Graduate(s), 0 Undergraduate(s)
Funding: $554,769 (Three years)

Scientific collaboration has a number of characteristics that do not come into play in the social environment. For example, there are security and privacy issues around intellectual property. While social networking is totally freeform, scientific collaboration has more of a workflow nature. This research will examine these and additional differences that come into play in the scientific research area. The end objectives for the project are to determine how social networking concepts can be effectively applied to scientific collaboration and to identify or develop software applications to enable this capability.

Currently, scientific collaborations take on many forms, including face-to-face meetings, conference calls, teleconferences and ad hoc electronic or web based systems. With the rapid proliferation of social networking tools, there is currently an abundance of technologies that may lend themselves to a more robust, standardized method of facilitating scientific collaboration. In this project, we propose to identify and define the different types of scientific collaboration into broad classifications. We will then identify and define the requirements associated with each collaboration classification, and finally, we will define a general solution and show how it can be adapted to each classification.

IIa will use a straightforward research process to manage this project. The following steps will be used to develop the technical approach for researching the concept and to define a general solution for collaboration within the scientific community. Steps include collaboration classification analysis, technology survey, and identification of barriers to adoption of social media in the scientific community.

The research will also examine DOE's extensive Scientific and Technical Information holdings to identify collaboration patterns and explore the differences in collaboration based on technical research disciplines. This aspect of the research will be supported with advanced statistical analysis techniques and visualization methodology. The research will attempt to draw conclusions on how social media can improve collaboration in selected subject areas.

The long-term goal impact of the project is to help research scientists conduct collaboration and obtain answers immediately in real time rather than using conventional collaboration tools that take days or weeks to exchange ideas among researchers. The potential impact is the acceleration of the research process, making the results available to the scientific community sooner.

The proposed research will be performed by a team led by Information International Associates, Inc. (IIa) in Oak Ridge, TN with a team from the Department of Statistics, Operations and Management Science at the University of Tennessee at Knoxville. The Oak Ridge National Laboratory Computational Sciences and Engineering Division will be a non-funded collaborator on the research.

Materials Development for Boron Phosphide Based Neutron Detectors - EPSCoR State – National Laboratory Partnerships

Institution: KANSAS STATE UNIVERSITY
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Principal Investigator: Edgar, J.H.
Sr. Investigator(s): Payne, Stephen, LAWRENCE LIVERMORE NATIONAL LABORATORY
Students: 0 Postdoctoral Fellow(s), 2 Graduate(s), 0 Undergraduate(s)
Funding: $558,904 (Three years)

Boron phosphide (BP) behaves as a conventional semiconductor (its electrical properties can be controlled), thus it should be suitable for making electronic devices in a high structural quality and low residual impurity concentration form. Confirming this hypothesis will prove that BP is an excellent candidate for thermal neutron detectors. The thermal neutron capture cross-section of the boron-10 isotope is orders of magnitude larger than most elements; it is a highly effective at capturing neutrons. This neutron-capture reaction produces energetic lithium ions and alpha particles that generate charged particles (electrons and holes) in BP that can serve as the signal for the presence of neutrons. Unlike conventional semiconductors, both neutron capture and charge generation can occur in BP, so its detection efficiency can approach 100 %.

Epitaxial films of BP will be prepared by chemical vapor deposition on 4H-silicon carbide (0001) substrates, to facilitate control of its electrical properties. The high stability of SiC and its low lattice constant mismatch to BP will minimize the residual impurity concentrations in the films, produce high crystal quality films, and make high deposition rates (>10 microns/h) possible. This will enable the preparation of thick films with the best electrical properties possible, so all incident thermal neutrons can be captured. The deposition temperature, phosphorus and boron reactant ratio, and growth rates will be optimized to produce high rates and high quality electrical properties. Comparisons will be made with bulk BP crystals grown from solution, which have lower dislocation densities.

The electrical properties of BP will be controlled by intentional doping with impurities during deposition, specifically sulfur to modify the electron concentration in *n*-conductivity films. The doped films will be thoroughly characterized to establish the relationship between the dopant concentrations in the process gas and the solid as functions of process conditions (temperature, reactant ratio), and the dependence of the electrical properties (major charge carrier concentration and mobility) on the concentration and type of impurities present. Hall measurements will establish the dependence of the electron and hole mobilities on the impurity concentrations and specimen temperature.

Junction diodes will be fabricated and tested, to further explore the electrical properties of BP (charge carrier distribution and minority carrier lifetime) and the device performance (threshold voltage, reverse bias leakage current) in operation. This project will culminate in testing the detection efficiency under a thermal neutrons fluence, and evaluating any device degradation mechanisms.

Neutron detectors are widely employed by the DOE, in homeland security, particle physics, neutron diffraction, radiation monitoring, and astronomy. The ultimate devices enabled by this project will be more sensitive, have a higher energy resolution, better position and time resolution, be more robust, and lower cost than existing devices, and will substantially improve the DOE abilities to meet its programmatic needs.

Ab Initio Nuclear Structure and Reaction Calculations for Rare Isotopes - EPSCoR State – National Laboratory Partnerships

Institution: LOUISIANA STATE UNIVERSITY
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Principal Investigator: Draayer, J.P.
Sr. Investigator(s): Hayes, A.C., LOS ALAMOS NATIONAL LABORATORY
Students: 1 Postdoctoral Fellow(s), 2 Graduate(s), 0 Undergraduate(s)
Funding: $450,000 (Three years)

The purpose of this collaborative project is to advance basic nuclear physics research in partnership with Los Alamos National Lab staff, through the development of an innovative *ab initio* nuclear structure model with forefront predictive capabilities to address several fundamental questions, and specifically some issues of particular interest to the National Labs.

The project will advance an extensible microscopic framework for studying nuclear structure and reaction processes that capitalizes on advances being made in *ab initio* methods while exploiting symmetries – exact and partial, known to dominate the dynamics. As part of the project we have developed a symmetry-adapted and user-friendly, open-source shell-model code, and used the code to explore with externally provided realistic interactions derived from QCD considerations, the properties of nuclei far from stability. The code has been applied first for light systems so the currently available *ab initio* methods can be used to guide the development, but ultimately pushing towards heavier ones that will require symmetry guided winnowing decisions. The work will target strong as well as weak interaction processes as required, for example, in modeling astrophysical phenomena and probing fundamental symmetries in nature.

In this research, we will solve the quantum many-particle problem for nuclei, both on and off the line of nuclear stability, with unprecedented accuracy by designing and implementing a set of novel nuclear physics symmetry-based algorithms that address the limitation of current *ab initio* models, specifically, the explosive growth in computational resource demands with increasing size of the model space. This in turn will provide the nuclear physics community with the first accurate and microscopic treatment of strong and weak interaction cross sections.

Studies of interest will include rare neutron-rich isotopes to be accessed at the world-leading Facility for Rare Isotope Beams, proton-rich short-lived nuclei important for modeling X-ray bursts, as well as analysis of the noteworthy MiniBooNE neutrino oscillation experiment with a focus on neutrino-carbon scattering, but also with a view toward projected argon-based neutrino experiments. Furthermore, the collaboration will focus on several key problems related to energy and defense applications that are currently studied at the National Labs. The project is anticipated to provide first accurate cross sections that are crucial for the nuclear reactions of light isotopes taking place in the hot dense environment during the fusion burn to be achieved at the National Ignition Facility (NIF). An accurate description of such reactions will be vital for the success of the fusion ignition experiments, as the reactions can diagnose hydrodynamic instabilities at the interfaces of NIF capsules (that can significantly quench the fusion burn) as well as various dynamic aspects of the capsule implosion (that are key to successful inertial confinement fusion). Knowledge of the cross sections for similar exotic reactions in nuclear explosions would greatly enhance our weapons radiochemical analyses for stockpile stewardship. The proposed collaboration will involve training of graduate students and postdoctoral associates and will have far-reaching impacts on multiple disciplines including nuclear physics, astrophysics, electro-weak (neutrino) physics, and cosmology.

Searches for New Physics Phenomena in Hadronic Jet Production in the early ATLAS data - EPSCoR State – National Laboratory Partnerships

Institution: LOUISIANA TECH UNIVERSITY
Point of Contact: Wobisch, Markus, wobisch@latech.edu
Principal Investigator: Wobisch, Markus
Sr. Investigator(s): Begel, Michael, BROOKHAVEN NATIONAL LABORATORY

Students: 1 Postdoctoral Fellow(s), 1 Graduate(s), 0 Undergraduate(s)

Funding: $240,000 (Three years)

The Large Hadron Collider (LHC) at CERN in Geneva, Switzerland will explore the fundamental properties and interactions of matter in a yet unexplored energy regime. Of all processes with very large momentum transfers at a hadron collider, hadronic jet production is the process with the largest production rate. This feature makes jet production a unique process with unmatched sensitivity to test the Standard Model in previously unexplored regions of large energies. The proposed project plans to study the production rates and angular distributions of hadronic jets to search for New Physics phenomena beyond the Standard Model at the energy frontier using data taken with the ATLAS detector at the LHC at a center-of-mass energy of 8 TeV.

One fundamental ingredient for measurements of hadronic jets is a jet trigger with high efficiency and a sharp turn-on. A major part of the proposed project is therefore related to the ATLAS jet trigger. This work focusses on extending the functionality of the Level-2 jet trigger, to improve angular resolutions for jets and to increase the jet finding efficiency in multi-jet final states. The results will later be used to measure suited ratios of multi-jet cross sections which are sensitive to various classes of New Physics signatures while they have reduced sensitivity to correlated experimental and theoretical uncertainties. These measurements may result in discoveries which could be a revolution of our present picture of the physical world (such as the discovery of extra spatial dimensions). In the absence of such discoveries, the measurements will be able to rule out some New Physics models, or significantly restrict their parameter space.

The project will benefit from the Dr. Wobisch's expertise in measurements and phenomenological QCD analyses of jet data gained in the H1 experiment at the HERA collider and in the DØ experiment in Run II of the Fermilab Tevatron collider where Wobisch has produced outstanding results in the field of jet measurements and their interpretations in the context of QCD and New Physics models. Especially his experience gained for recent DØ multi-jet results will directly be applicable for the measurements proposed in this project.

The project will be performed in partnership with Dr. Michael Begel from Brookhaven National Laboratory (BNL). BNL is an active participant in the ATLAS Collaboration, the U.S. host laboratory for the experiment, and the site of the U.S. Tier 1 computing center for ATLAS which will store and process data from the experiment. BNL was also involved in the construction of the Liquid Argon Barrel Cryostat of the ATLAS detector. Dr. Begel is an expert on QCD physics in jet and photon production, and Dr. Begel and Wobisch have a long history of working together successfully on measurements and interpretations of jet data inside the DØ QCD working group and the DØ QCD editorial board. The combined expertise of Drs. Begel and Wobisch in conceptual, experimental, and theoretical aspects of jet physics will be a strong foundation for this project.

Making the Grid "Smart" through "Smart" Microgrids: Real-Time Power Management of Microgrids with Multiple Distributed Generation Sources Using Intelligent Control - EPSCoR State – National Laboratory Partnerships

Institution:	MONTANA STATE UNIVERSITY
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Principal Investigator:	Nehrir, M. Hashem
Sr. Investigator(s):	Marnay, Chris, LAWRENCE BERKELEY NATIONAL LABORATORY
	Hammerstrom, Donald, PACIFIC NORTHWEST NATIONAL LABORATORY
Students:	1 Postdoctoral Fellow(s) (10 months), 2 Graduate(s), 1 Undergraduate(s)
Funding:	$465,019 (Three years)

This Project is a collaborative research with two DOE National Laboratories, Lawrence Berkeley National Lab (LBNL) and Pacific Northwest National Lab (PNNL). The objective of the project is to investigate real-time power management strategies for microgrids using intelligent control. Microgrid is considered to be the cornerstone of the future "smart grid." It is defined as a collection of distributed generation (DG) sources, storage, and loads connected to a common bus, normally at the distribution- level. Microgrids can have a combination of conventional DG and alternative energy DG (AEDG) sources operating in grid-connected or stand-alone (islanded) mode to achieve the ultimate goal of maximum feasible energy sustainability, reliability, and efficiency while minimizing cost and undesired environmental impact (emissions).

Microgrid component sizing for specific applications will be conducted and the suitability of promising heuristic-based, biologically-inspired, multi-objective optimization techniques, such as particle swarm optimization (PSO) and genetic algorithms (GA), as well as multi-agent systems (MAS), for microgrid power management will be evaluated. An MAS-based energy management system will prioritize and control energy utilization among the various components connected to a microgrid to achieve optimum power delivery, taking into account technical factors, as well as issues such as environmental and economic, and historical data (e.g., renewable resource and load information). The project will also include balancing of generation and demand in islanded microgrids through demand response (load control) and islanding detection.

Nanoscale Studies of Pyroelectric and Thermoelectric Phenomena - EPSCoR State – National Laboratory Partnerships

Institution:	NEBRASKA, UNIVERSITY OF
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Principal Investigator:	Gruverman, Alexei
Sr. Investigator(s):	Ducharme, Stephen, NEBRASKA, UNIVERSITY OF
	Kalinin, Sergei V., OAK RIDGE NATIONAL LABORATORY
Students:	1 Postdoctoral Fellow(s), 3 Graduate(s), 0 Undergraduate(s)
Funding:	$600,000 (Three years)

The purpose of this project is to develop a versatile Thermo-modulation Electric-sensing Scanning Probe Microscope (ThE-SPM) system and apply it to dynamics studies and nanoscale mapping of pyroelectric, thermoelectric and photovoltaic properties of a variety of technological and biological materials. The

ThE-SPM system is an extension of conventional scanning probe microscopy (SPM), in which the temperature of a sample is modulated through the sharp SPM probe tip, and the resulting thermally generated currents recorded as the tip is scanned over the sample. The model samples that will be used for these studies include thin films of ferroelectric polymers polyvinylidene fluoride-trifluoroethylene (pVDF-TrFE) and ZnO-$BaTiO_3$ heterostructures.

The expected outcomes or the project include the following: demonstration of a new suite of functional nanoscale imaging and characterization methods to complement existing SPM capabilities; fundamental nanoscale studies of a number of thin films and nanostructures; nanoscale characterization and performance testing of pyroelectric and photovoltaic devices.

High Pressure X-Ray Absorption Studies on Correlated-Electron Systems - EPSCoR State – National Laboratory Partnerships

Institution:	NEVADA-LAS VEGAS, UNIVERSITY OF
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Principal Investigator:	Cornelius, Andrew L.
Sr. Investigator(s):	Booth, Corwin, LAWRENCE BERKELEY NATIONAL LABORATORY
Students:	1 Postdoctoral Fellow(s), 1 Graduate(s), 0 Undergraduate(s)
Funding:	$578,811 (Three years)

The project revolves around collaboration between the PI, Andrew Cornelius at University of Nevada, Las Vegas (UNLV) and National Laboratory Partner Corwin Booth at Lawrence Berkeley National Laboratory. This project intends to combine the collaborators of expertise to perform high-pressure x-ray absorption measurements. In addition, numerous other physical property measurements will be performed as required for a thorough understanding of the effect of pressure on correlated-electron systems.

Correlated-electron systems are so named because there are strong interactions between electrons unlike traditional metals such as copper that have weakly interacting “free electrons.” Studies on correlated-electron systems have wide ranging interest from defense related issues to future use in nanoscale devices. We strive to further the understanding of two important aspects of correlated-electron materials: energy and length scales. By using external pressure and low temperature to submit the systems to extreme conditions, we are allowed to drastically change the physical properties of the materials. Experimental results are a necessity for understanding these complicated materials and allow critical tests to theory.

This work will train scientists at the graduate student and postdoctoral level at UNLV and at national user facilities on measurements at extreme conditions. The study of strong electronic correlations in rare earth materials is of long standing DOE interest. A necessity for performing the wide set of proposed experiments requires the proposed collaboration along with others that are already in place. As there is a concern that there will be a shortage of quality candidates to man such laboratories in the future, it is a national necessity to train young scientists in these novel techniques. The research would continue our quest for a much needed thorough understanding of correlated-electron systems.

Manipulation of Phonons with Phononic Crystals - EPSCoR State – National Laboratory Partnerships

Institution:	New Mexico, University of
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Principal Investigator:	Leseman, Zayd
Sr. Investigator(s):	El-Kady, Ihab, SANDIA NATIONAL LABORATORIES
Students:	1 Postdoctoral Fellow(s), 2 Graduate(s), 1 Undergraduate(s)
Funding:	$585,252 (Three years)

The research objective of this proposal is to model, fabricate, and characterize Phononic Crystals (PnCs). This effort can be broken down by frequency regimes – THz PnCs and GHz and lower frequency PnCs. In order to capture the behavior of the THz PnCs continuum wave mechanics, a semi-classical formulation, and lattice dynamics theory will be utilized during the modeling stages. For fabrication of THz PnCs a novel nanofabrication technique for PnCs will be utilized - nanoFIBrication – that uses a focused ion beam (FIB) to make the inclusions in previously fabricated membranes. Characterization of these crystals will be carried out from cryogenic to elevated temperatures in an effort to determine changes in the thermal conductivities of the PnC versus that of the PnC's bulk matrix material. Tailoring the thermal conductivity of materials is a key step in creating high-zT materials. For the GHz and lower frequency PnCs, continuum wave mechanics only need to be utilized for modeling. Specifically, the Finite Element Method (FEM) and Finite-Difference Time Domain (FDTD) method will be used to model the PnCs. Fabrication of the PnCs in this frequency range will be accomplished using standard microfabrication techniques. Characterization of these PnCs will be accomplished by launching longitudinal waves in the PnC via piezoelectric crystals and subsequently transduced on the opposite side of the PnC. Using these techniques PnC based passive signal processing and logic circuits will be created lowering energy requirement for a variety of communications applications.

Interband Cascade Photovoltaic Cells - EPSCoR State – National Laboratory Partnerships

Institution:	OKLAHOMA, UNIVERSITY OF
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Principal Investigator:	Yang, Rui Q.
Sr. Investigator(s):	Santos, Michael B., OKLAHOMA, UNIVERSITY OF
	Johnson, Matthew B., OKLAHOMA, UNIVERSITY OF
	Klem, John F., SANDIA NATIONAL LABORATORIES
Students:	2 Postdoctoral Fellow(s), 3 Graduate(s), 1 Undergraduate(s)
Funding:	$600,000 (Three years)

In this project, we will perform basic and applied research to systematically investigate our newly proposed interband cascade (IC) photovoltaic (PV) cells. These cells follow from the great success of infrared IC lasers that pioneered the use of quantum-engineered IC structures. This quantum-engineered approach will enable PV cells to efficiently convert infrared radiation from the sun or other heat source, to electricity. Such cells will have important applications for more efficient use of solar energy, waste-heat recovery, and power beaming in combination with mid-infrared lasers. The objectives of our investigations are to: achieve extensive understanding of the fundamental aspects of the proposed PV structures, develop the necessary knowledge for making such IC PV cells, and demonstrate prototype working PV cells. This research will focus on IC PV structures and their segments

for utilizing the mid-infrared radiation (2-5 µm) emitted by heat sources (1,000-2,000 K) that are widely available from combustion systems. The success of this project will not only push PV technology to longer wavelengths, allowing for relatively low-temperature thermal sources, it will also generate new cutting-edge knowledge in the design and understanding of quantum-engineered semiconductor structures and devices.

Our investigations will relate to material quality, electrical and optical properties, and their interplay for the different regions of an IC PV structure. These fundamental aspects include: systematic knowledge about the carrier absorption and recombination processes over the mid-infrared spectral range; and how carrier transport is affected by tunneling and scattering mechanisms involving defects, phonons, and electron-electron interactions. The tasks involve: design, modeling and optimization of IC PV structures, molecular beam epitaxial growth of PV structures and relevant segments, material characterization, prototype device fabrication and testing. At the end of this program, we expect to demonstrate the concepts for IC PV devices with conversion efficiencies approaching 30% or higher.

Improving the Calendar Life and Safety of Lithium Ion Batteries: Development of Novel Electrolytes and Additives - EPSCoR State – National Laboratory Partnerships

Institution: RHODE ISLAND, UNIVERSITY OF
Point of Contact: Lucht, Brett L., blucht@chm.uri.edu
Principal Investigator: Lucht, Brett L.
Sr. Investigator(s): Abraham, Daniel P., ARGONNE NATIONAL LABORATORY

Students: 1 Postdoctoral Fellow(s), 2 Graduate(s), 0 Undergraduate(s)

Funding: $590,991(Three years)

High-power lithium-ion batteries for hybrid electric vehicle (HEV) applications are being studied as part of the U.S. Department of Energy's Applied Battery Research for Transportation (ABRT) program. Lithium-ion cells ranging in capacity from 1 mAh to 1 Ah, are being built and tested to determine suitable electrode-electrolyte combinations that will meet calendar life, safety, low-temperature performance, and cost goals of the ABRT program.

The ABRT program is currently focused on lithium-ion batteries for plug-in HEV (PHEV) systems. Topics of interest to the ABRT program include: (a) electrode materials that are new or modified versions of current chemistries, (b) novel electrolytes, or additives to current electrolytes, to enhance cell performance and life, (c) changes in cell testing conditions that include wider voltage windows and greater state-of-charge (SOC) swings, etc. The degradation mechanisms associated with various cell chemistries and testing conditions needs to be identified to determine suitable electrode-electrolyte combinations that will meet the target goals of PHEV batteries. The wider range of materials and testing conditions to be examined will be challenging because of the in-depth electrochemical and physicochemical diagnostic studies need to detail cell aging mechanisms. The knowledge gained from these studies will be valuable to the lithium-battery community, and especially to our colleagues in the battery industry.

Researchers at the University of Rhode Island, led by Prof. Brett Lucht, in collaboration with researchers at Argonne National Laboratory, led by Dr. Daniel Abraham, have been conducting analyses of the mechanism of electrolyte reactions with the surface of electrode materials for two years. This proposal is a significant expansion of this collaborative work. The proposed partnership will focus on the development of a mechanistic understanding of the electrochemical and thermal reactions of the

electrolyte with the surface of the electrodes (both anode and cathode) and the development of improved electrolyte formulations to increase the calendar life and safety of lithium ion batteries. Argonne National laboratory has significant experience with the development of novel battery materials, electrochemical analysis, and surface analysis. Researchers at the University of Rhode Island have a complementary experience base including synthesis of novel electrolytes and electrolyte additives, surface analysis and mechanistic organic and organometallic chemistry. This combination of experience is unique and will provide significant advances in the understanding of the basic materials chemistry of the electrolyte/electrode interphase. The reactions that generate and degrade the electrolyte/electrode interphase are one of the most critical aspects for calendar life performance of lithium ion batteries. Through this partnership, we will utilize our mechanistic insight of the limiting reactions of the current state-of-art (SOA) electrolyte to develop novel salts, solvents, and additives for the next generation electrolytes for lithium ion batteries. The development of the next generation of electrolytes for lithium ion batteries will provide a solution to the calendar life problems associated with current lithium ion battery technology and improve performance with the next generation of electrode materials.

Plasmon Mapping in Metallic Nanostructures and its Application to Single Molecule Surface Enhanced Raman Scattering: Imaging Electromagnetic Hot-Spots and Analyte Location - EPSCoR State – National Laboratory Partnerships

Institution:	TENNESSEE, UNIVERSITY OF
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Sr. Investigator(s):	Guiton, B., OAK RIDGE NATIONAL LABORATORY
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	Schatz, G., NORTHWESTERN UNIVERSITY
Students:	1 Postdoctoral Fellow(s), 2 Graduate(s), 0 Undergraduate(s)
Funding:	$450,000 (Three years)

We seek to characterize the electric field enhancements obtained when the localized surface plasmon resonance is excited in metallic nanostructures for use in single molecule surface enhanced Raman spectroscopy. These goals will be accomplished by combining optical spectroscopy measurements with electron energy loss spectroscopy, and single molecule imaging, in the aberration-corrected scanning transmission electron microscopes at Oak Ridge National Laboratory. This project has several high impact objectives: (1) Deeper understanding of the couplings that mediate the flow of energy between localized surface plasmons and surface bound molecules. This understanding will emerge from correlated optical microscopy, electron microscopy, and theoretical simulations of well defined nanostructures. (2) The first experimental mapping of the plasmonic “hot-spot” required for single molecule surface enhanced Raman scattering. Previous studies have inferred the existence of regions of high electric field enhancement but no direct experimental observation has been made. (3) The first experimental mapping of the location and position of the analyte molecule in the hot-spot. While it is assumed that the molecule must be located in the electromagnetic hot spot, the exact location and position of the molecule is unknown. We are particularly interested in plasmonic nanostructures important for single molecule surface enhanced Raman scattering because of their potential application to the study of heterogeneous catalysis and solar energy harvesting.

Study of Compatibility of Stainless Steel Weld Joints with Liquid Sodium- Potassium Coolants for Fission Surface Power Reactors for Lunar and Space Applications - EPSCoR State – National Laboratory Partnerships

Institution: TENNESSEE, UNIVERSITY OF
Point of Contact: Grossbeck, M. L., mgrossbe@utk.edu
Principal Investigator: Grossbeck, M. L.
Sr. Investigator(s): Qualls, A.L., OAK RIDGE NATIONAL LABORATORY

Students: 0 Postdoctoral Fellow(s), 1 Graduate(s), 0 Undergraduate(s)

Funding: $579,889 (Three years)

To make a manned mission to the surface of the moon or to Mars with any significant residence time, the power requirements will make a nuclear reactor the most feasible source of energy. To prepare for such a mission, NASA has teamed with the DOE to develop Fission Surface Power technology with the goal of developing viable options by 2013. The Fission Surface Power System (FSPS) recommended as the initial baseline design includes a liquid metal reactor and primary coolant system that transfers heat to two intermediate liquid metal heat transfer loops. Each intermediate loop transfers heat to two Stirling heat exchangers that each power two Stirling converters. Both the primary and the intermediate loops will use sodium-potassium (NaK) as the liquid metal coolant, and the primary loop will operate at temperatures exceeding 600°C. The alloy selected for the heat exchangers and piping is AISI Type 316L stainless steel.

The extensive experience with NaK in breeder reactor programs and with earlier space reactors for unmanned missions lends considerable confidence in using NaK as a coolant in contact with stainless steel alloys. However, the microstructure, chemical segregation, and stress state of a weld leads to the potential for corrosion and cracking. Such failures have been experienced in NaK systems that have operated for times less than the eight year goal for the FSPS. For this reason, it is necessary to evaluate candidate weld techniques and expose welds to high-temperature, flowing NaK in a closed, closely controlled system.

The goal of this project is to determine the optimum weld configuration for a NaK system that will withstand service for eight years under FSPS conditions. Since the most difficult weld to make and to evaluate is the tube to tube sheet weld in the intermediate heat exchangers, it will be the focus of this research. A loop of flowing NaK will be fabricated for exposure of candidate weld specimens at temperatures of 575 and 600°C, the expected temperatures within the intermediate heat exchangers. Since metal transfer from a high-temperature region to a cooler region is a predominant mode of corrosion in liquid metal systems, specimens will be placed at zones in the loop at the above temperatures to evaluate the effects of both alloy component leaching and metal deposition. Microstructural analysis and mechanical testing will be performed to evaluate weld performance.

The research will be coordinated with Oak Ridge National Laboratory (ORNL) where the weld samples will be prepared. In addition, ORNL will participate in the loop operation to assist in keeping the testing relevant to the project and to take advantage of the extensive experience in liquid metal research at ORNL.

Antibodies to Radionuclides: Engineering by Surface Display for Immunosensors- EPSCoR State – National Laboratory Partnerships

Institution: TULANE UNIVERSITY
Point of Contact: Blake, Diane A., blake@tulane.edu
Principal Investigator: Blake, Diane A.
Sr. Investigator(s): Bradbury, Andrew R.M., LOS ALAMOS NATIONAL LABORATORY
Students: 1 Postdoctoral Fellow(s), 1 Graduate(s), 0 Undergraduate(s)
Funding: $563,063 (Three years)

The techniques of antibody display, which permit molecular engineering of antibody structure and function, have the potential to revolutionize the way scientists generate binding proteins for specific applications. However, the skills required to efficiently use antibody display techniques have proven difficult to acquire without hands-on training and exchange of laboratory personnel. This research project, which has supported scientific exchange with the Bradbury Laboratory at Los Alamos National Laboratory, has brought important expertise in antibody display to the State of Louisiana while pursuing a project with direct relevance to the DOE's EM program.

Previous work in the Blake laboratory led to the development of monoclonal antibodies that bound tightly and specifically to chelated uranyl ions. These antibodies were subsequently formatted into sensors that provided accurate, near real-time data about the presence of U(VI) in groundwater samples. While these antibody-based sensors demonstrated their utility in the detection and quantitation of U(VI) in groundwater from a contaminated site, the protocol used in the field required precise pre-treatment of the environmental sample. During this EPSCoR project period, we have used antibody display techniques to re-engineer these anti-uranium antibodies to make our assay systems more convenient for field research activities. We will also use antibody display technology to generate new antibodies that recognize chelated plutonium.

The goals of this project are as follows:

1) To re-engineer existing monoclonal and recombinant antibodies to chelated uranium already available in the Blake laboratory so that the antibodies retain their binding to chelated uranium but decrease their binding to metal-free chelator;

2) To validate the re-engineered antibodies for near-real time analysis of uranium using the sensors and archived environmental samples already available in the Blake laboratory and to develop prototype lateral flow strips for metal ion analysis;

3) To utilize RNA from previous experiments and newly immunized animals to develop recombinant antibodies to chelated plutonium.

The antibodies to be developed and validated in this project will be of value to the DOE EM program in the development of new monitoring systems for the remediation of soil and groundwater. These novel reagents and sensors could also be used by on-site inspectors at suspected nuclear weapon production sites, or by homeland security to screen for the dispersal of uranium or plutonium in the aftermath of an event involving a suspected dirty bomb or other explosive device.

Importance and Relevance to DOE's Mission: The mission of DOE's EM program is the safe and successful clean-up of uranium mining sites, nuclear weapons production sites and weapons testing sites that are the legacy of 5 decades of Cold War. One of the priorities of this program is the remediation of

soil and groundwater; the anti-uranium antibodies to be re-engineered in this proposal have already been shown to assist in remediation efforts. The proposed studies will make these antibodies cheaper to produce (because the recombinant antibodies can be produced from bacterial cultures) and easier to use in the field (because the new antibodies will not be affected by the concentration of metal-free chelator in the final assays).The recombinant anti-plutonium antibodies to be developed herein could be transformative in monitoring efforts to remediate this radionuclide.

Two Photon Absorption Laser Induced Fluorescence for Neutral Hydrogen Profile Measurements - EPSCoR State – National Laboratory Partnerships

Institution: WEST VIRGINIA, UNIVERSITY
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Principal Investigator: Scime, Earl
Sr. Investigator(s): Hillis, Donald L., OAK RIDGE NATIONAL LABORATORY

0Students: 1 Postdoctoral Fellow(s), 1 Graduate(s), 0 Undergraduate(s)

Funding: $599,236 (Three years)

The magnitude and spatial dependence of neutral density in magnetic confinement fusion experiments is a key physical parameter, particularly in the plasma edge. Modeling codes require precise measurements of the neutral density to calculate charge-exchange power losses and drag forces on rotating plasmas. However, direct measurements of the neutral density are problematic. Tomographic imaging of hydrogenic plasmas in the H_α line (requiring extensive optical access) can provide a reconstructed source profile if the electron density and temperature profiles are well known. Neutral beam-based measurements can also provide some indication of the spatial distribution of neutrals in the plasma. In this work, we propose to construct a laser-based diagnostic capable of providing spatially resolved measurements of the neutral density in the edge of DIII-D plasmas. The diagnostic concept is based on two-photon absorption laser induced fluorescence (TALIF). By injecting two beams of 205 nm light (co or counter propagating), ground state hydrogen (or deuterium or tritium) can be excited from the n = 1 level to the n = 3 level at the location where the two beams intersect. Individually, the beams experience no absorption and therefore have no difficulty penetrating even dense plasmas. After excitation, a fraction of the hydrogen atoms decay from the n = 3 level to the n = 2 level and emit photons at 656 nm (the $H_\square$ line). Calculations based on the results of previous TALIF experiments in magnetic fusion devices indicate that a laser pulse energy of approximately 3 mJ delivered in 5 ns will provide sufficient signal-to-noise for detection of the fluorescence. In the last decade, TALIF measurements of hydrogen plasmas have become relatively common in the plasma processing industry. The rapid growth in TALIF measurements in processing plasmas is due to the availability of a new class of solid state pumped, tunable, frequency-doubled, high-power, low-maintenance lasers. The plasma physics group at West Virginia University (WVU) has a successful track record in the development of new laser induced fluorescence diagnostic systems for low temperature plasmas using tuanble lasers. In collaboration with the DIII-D engineering staff and experts in plasma edge diagnostics for DIII-D from Oak Ridge National Laboratory (ORNL), WVU researchers will design a TALIF system capable of providing spatially resolved measurements of neutral deuterium densities in the DIII-D edge. The laser systems will be specified, purchased, and assembled at WVU. Three different optical configurations of TALIF system will be tested on, DIII-D pedestal region relevant, hydrogen and deuterium discharges at WVU. At WVU an absolute calibration scheme based on TALIF on krypton gas will be designed and demonstrated. Detailed signal-to-noise calculations incorporating achieved TALIF laser parameters and modeling of actual DIII-D discharges will be prepared and used to design the optical and vacuum components

necessary to accomplish TALIF in the DIII-D edge region. The TALIF system will be moved to DIII-D for installation in collaboration with ORNL researchers.

Characterizing Synthetic and Natural Spider Silk Fibers Using X-ray and Neutron Diffraction - EPSCoR State – National Laboratory Partnerships	
Institution:	WYOMING, UNIVERSITY OF (with a subcontract to Utah State University)
Point of Contact:	Lewis, Randolph V., randy.lewis@usu.edu
Principal Investigator:	Lewis, Randolph V.
Sr. Investigator(s):	Benmore, Chris J., ARGONNE NATIONAL LABORATORY
	Yarger, Jeffrey L., ARIZONA STATE UNIVERSITY
Students:	0 Postdoctoral Fellow(s), 4 Graduate(s), 0 Undergraduate(s)
Funding:	$600,000 (Three years)

Spider silks have the potential to provide new bio-inspired materials for numerous applications in Bioenergetics and products ranging from protective clothing to artificial ligaments and tendons. A number of spider silk genes have been cloned and sequenced by the Lewis laboratory revealing the basis for understanding the key elements of spider silk proteins with respect to their materials performance. In particular, specific amino acid motifs have been identified which have been conserved for over 125 million years in all spiders that use their silk to physically trap prey. The key element in taking the next step toward generating bio-based materials from spider silks will be to move from the current descriptive data to predictive knowledge. No one has systematically varied the sequence motifs in the spider silk proteins and determined how this influences the mechanical properties of the resulting fibers. Also no one has systematically been able to study single spider silk fibers to determine key structural elements.

Current efforts are focused on mimicking spider silk through synthetic proteins. In developing synthetic silk fibers, we first need to understand the complete secondary and tertiary structure of natural silk so that we can compare synthetic constructs to the natural material. Being able to compare the structure on a single fiber level is critical to the future of molecular directed mimic development because we can vary mechanical properties by different spinning methods. Thus we need to be able to determine the correlations between structure and mechanical properties. In the past several years we have used recombinant DNA methods to generate synthetic spider silk proteins. We now have over 20 different proteins, which vary in the ratio of crystalline to amorphous regions as well as the protein sequences in both of those regions. Most of these have been spun into fibers and these fibers range in mechanical properties from those with elasticities and toughness values greater than dragline silk to those with values much less than the natural silks. The molecular basis for these differences cannot be determined using current methods. The new generation of synchrotron x-ray diffraction and neutron beamlines will allow, for the first time, determination of the molecular structure of silk fibers and synthetic mimics. We propose an exciting new collaborative research team working jointly between Argonne National Laboratory, Arizona State U. and the University of Wyoming to address the "characterization of synthetic and natural spider silk fibers using x-ray and neutron diffraction." Thus these new methodologies will provide understanding of current fibers and determine changes needed to produce fibers with specific properties.

The following specific aims are proposed:

• Synthesize spider silk fibers with molecular structures mimicking that of natural silks. Test the mechanical properties of these materials and compare them to natural silk fibers.

• Develop x-ray and neutron diffraction techniques to better determine the structure in amorphous and semi-crystalline biopolymers, such as spider silk fibers.

• Combine mechanical testing and structural x-ray and neutron diffraction data to develop a molecular understanding of the structure-function relationship in spider silk materials.

• Elucidate the role water plays in spider silk fiber formation and structure. Emphasis will be placed on combined neutron and NMR studies.

• Use solid-state Nuclear Magnetic Resonance (NMR) to characterize synthetic and natural spider silk materials that show potential as a biomimetic material or bio-inspired polymer architecture.

• Develop EPSCoR student and postdoctoral training and exposure to national laboratory facilities.

• Further develop scientific outreach and chemical education programs and research.

Accomplishment of these objectives are will provide new methodologies to determine protein fiber structures and correlate these structures with mechanical properties and provide broad training in molecular structure analysis to students.

EPSCoR Early Career Award – Miracles in Scattering Amplitudes: from QCD to Gravity

Institution:	BROWN UNIVERSITY
Point of Contact:	Volovich, Anastasia, anastasia_volovich@brown.edu
Principal Investigator:	Volovich, Anastasia
Sr. Investigator(s):	
Students:	1 Postdoctoral Fellow(s), 1 Graduate(s), 0 Undergraduate(s)
Funding:	$750,000 (Five years)

This research in the area of theoretical high energy physics is centered on the theory and phenomenology of scattering amplitudes in quantum field theories and gravity. Recently, remarkable advances have been made in this area, with broad spectrum of results ranging from new precision prediction of in QCD which will be very important for understanding LHC data to the miraculous structures in $N = 4$ Yang-Mills and $N = 8$ supergravity inspired by twistor space and on-shell methods. The improved ability to calculate scattering amplitudes directly challenges some of our basic premises in quantum gravity and moreover suggests that a new kind of unifying theory should exist. Moreover, our recent discovery of a very simple analytic formula of the first non-trivial multi-loop amplitude in Yang-Mills (which otherwise required a formidable calculation using traditional techniques) signals that a great vista of anticipated structure awaits exploration.

The goal of this research project is to deepen our understanding of gauge and gravity theories by exploring these hidden structures (ranging from integrability to twisters to the theory of motives), and using these rich structures as much as possible to aid practical calculations relevant to collider physics. These hidden structures not only help us calculate and make predictions for experimentally relevant processes but also lead to deeper understanding of fundamental properties of field and gravity theories.

Contributions may be expected in the fields of: QCD and Collider Physics; N=4 Yang-Mills and AdS/CFT; and Quantum Gravity.

EPSCoR Early Career Award – Growth and Properties of New Epitaxial Metal/Semiconductor Nanocomposites

Institution:	UNIVERSITY OF DELAWARE
Point of Contact:	Zide, Joshua, zide@udel.edu
Principal Investigator:	Zide, Joshua
Sr. Investigator(s):	
Students:	0 Postdoctoral Fellow(s), 2 Graduate(s), 0 Undergraduate(s)
Funding:	$750,000 (Five years)

This project aims to provide a new synthesis capability to the thin film electronic materials science community that allows for the incorporation of a variety of metal and semiconductor nanoparticles into a semiconductor matrix for use in thermoelectrics, optoelectronics, and other applications. The new method is a two-step process: First, a gas condensation process is used to make nanoparticles of desired material compositions with controlled morphology and size. Next, the nanoparticles are incorporated into a semiconductor matrix by a melt process called liquid phase epitaxy (LPE). This hybrid method offers more versatility in compositional variety and morphology than is currently accessible through the standard Molecular Beam Epitaxy (MBE) method and therefore provides a greater variety of materials for discovery.

EPSCoR Early Career Award – Electron Dynamics in Nanostructures in Strong Laser Fields

Institution:	KANSAS STATE UNIVERSITY
Point of Contact:	Kling, Matthias, kling@phys.ksu.edu
Principal Investigator:	Kling, Matthias
Sr. Investigator(s):	
Students:	0 Postdoctoral Fellow(s), 2 Graduate(s), 0 Undergraduate(s)
Funding:	$750,000 (Five years)

This project aims to investigate novel physical effects in nanomaterials in strong laser fields. The laser fields will be strong enough to pull out and accelerate electrons from the nanoparticles and to transiently modify the material's electronic properties. The project aims to advance the fundamental understanding of how the collective electron motion in strong laser fields is established, how its precise evolution depends on the driving light waveform, how the material properties are influenced by the strong field, and over which pathways and timescales the collective motion decays. The laser-driven collective electron dynamics can unfold on attosecond time scales (one attosecond is a billionth of a billionth of a second) and will be traced by employing attosecond nanoplasmonic streaking spectroscopy. The studies will focus on isolated dielectric, semiconductor and metal nanoparticles. The project can uncover new functionalities of nanomaterials and enable transformative photonic applications of nanostructured devices for the development of sustainable energy sources and ultrafast information and computation technology.

EPSCoR Early Career Award – Neutrino Oscillations in Supernovae

Institution: UNIVERSITY OF NEW MEXICO
Point of Contact: Duan, Huaiyu, duan@unm.edu
Principal Investigator: Duan, Huaiyu
Sr. Investigator(s):
Students: 1 Postdoctoral Fellow(s), 1 Graduate(s), 0 Undergraduate(s)
Funding: $750,000 (Five years)

At the end of the life of a massive star, its core collapses under its own gravity and the star explodes as a supernova. Supernovae are crucial to the chemical evolution of the universe. They disseminate heavy elements into the Interstellar Medium inside which new generations of stars are born. Although supernovae have been observed in the last several decades, only recently, with the advances of computing technologies and the development of multi-dimensional supernova simulations, is the explosion mechanism of a supernova finally (close to being) understood. However, the recent development of neutrino mixing adds a new twist to this puzzle. Neutrinos interact very weakly with ordinary matter but carry away 99% of the total energy of a supernova. The electron-flavor neutrinos and antineutrinos play pivotal roles in supernova physics. It has been established by experiments that neutrinos and antineutrinos of the electron flavor can transform or oscillate into neutrinos of other flavors and vice versa. In this project, we will take inputs from supernova simulations, perform large-scale numerical simulations of neutrino oscillations in supernovae, and investigate the potential impacts of neutrino oscillations on supernova physics. By studying neutrino oscillations in supernovae, we will complete an important piece of the supernova puzzle and help answer some fundamental questions such as ones about the origin of the elements.

EPSCoR Early Career Award – Modeling of Photoexcited Process at Interfaces of Functionalized Quantum Dots

Institution: NORTH DAKOTA STATE UNIVERSITY
Point of Contact: Kilina, Svetlana; svetlana.kilina@ndsu.edu
Principal Investigator: Volovich, Anastasia
Sr. Investigator(s):
Students: 1 Postdoctoral Fellow(s), 1 Graduate(s), 1 Undergraduate(s)
Funding: $750,000 (Five years)

The main obstacle impeding the path towards development of efficient quantum-dot (QD) based materials for solar energy conversion and lighting applications is a limited understanding of fundamental process that occur at the surfaces and interfaces of these nanomaterials subsequent to photoexcitation. The objective of this project is to fill the gap in the present understanding of the role of quantum-dot surfaces in light-driven physicochemical processes by establishing state-of-the-art computational methods capable of describing photoexcitation in the nanosized systems and their interfaces at the atomistic level. Such methods will allow for a systematic theoretical analysis on the effects of a soft layer of organic ligands and/or a shell of a different semiconductor covering the QD surface on the morphology, electronic structure, optical response, charge/energy transfer, and excitation dissipation in quantum dots. This will also provide insight into the extent to which we can control radiative and

nonradiative process and electronic transport in these systems by chemical modification of the QD surfaces. The acquired theoretical knowledge will allow for a better explanation and interpretation of experimental data and will facilitate rational design of new nanostructures with desired optical, transport, and light harvesting properties that are fundamental to a myriad of clean energy technologies.

EPSCoR Early Career Award – Enhancing Metabolic Flux to Photosynthetic Biofuels

Institution: VANDERBILT UNIVERSITY
Point of Contact: Young, Jamey, j.d.young@vanderbilt.edu
Principal Investigator: Young, Jamey
Sr. Investigator(s):

Students: 0 Postdoctoral Fellow(s), 1 Graduate(s), 0 Undergraduate(s)

Funding: $750,000 (Five years)

Developing liquid transportation fuels that are both renewable and compatible with existing fuel infrastructure is a major research challenge of the next decade. Corn ethanol provides nearly all of the renewable fuel currently used in the U.S. However, attention is shifting to "advanced" biofuels that more closely resemble gasoline. Several recent studies have demonstrated the feasibility of producing advanced biofuels in engineered strains of photosynthetic cyanobacteria. These organisms could be used to produce liquid fuels directly from sunlight and CO_2 on land unsuitable for agriculture, thereby minimizing energy-intensive harvesting, transporting, and degrading of plant-derived feedstocks. However, cyanobacterial fuel productivity is currently too low for industrial feasibility. Therefore, this project will test new metabolic engineering approaches for maximizing carbon flux from CO_2 to biofuels in cyanobacterial hosts. Tools will be developed for analyzing carbon flux and engineering the metabolic pathways that result in biofuel production. This will be further optimized by reprogramming the "biological clock" that controls daily metabolic rhythms that may affect those metabolic pathways. This work will have an important positive impact on the development of bioprocesses that rely upon photosynthetic microorganisms. In addition, it will provide fundamental insights into the role of biological clock genes in regulating photosynthesis and carbon fixation in engineered cyanobacteria. This research will directly contribute to DOE's mission by advancing toward production of renewable fuels that do not compete with agriculture.