Light-Stimulated Epitaxy of Novel Semiconductor Alloys and Heterostructures

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The realization of new semiconductor alloys and heterostructures is critical to materials research efforts, but kinetic limitations often impede the low temperature growth of such systems. Innovative approaches designed to tailor specific growth processes are needed to overcome these longstanding challenges. The principle objective of this research is to use light as an additional free parameter to control adatom dynamics. Specific goals of the project are to 1) expand our basic understanding of how photons affect semiconductor growth by molecular beam epitaxy, 2) selectively stimulate and manipulate surface processes that lead to atomistic growth control, and 3) systematically advance the boundaries of semiconductor synthesis and investigation. By establishing pathways that surmount current material synthesis constraints, this work will impact the development of advanced approaches to access new growth regimes, facilitate the exploration of novel materials systems and drive breakthroughs in photovoltaics and solid-state lighting technologies.

This research was selected for funding by the Office of Basic Energy Sciences.

Molecular and Structural Probes of Defect States in Quantum Dot Photovoltaics

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The objective of this research on quantum confined nanocrystals is to develop a fundamental understanding of the chemical properties of ligand-nanocrystal interfaces that will enable the control of defect-driven charge recombination in these systems. With this control, quantum confined nanocrystals may represent a cost effective means of absorbing light over the full solar spectrum for the production of electricity and fuels from sunlight. New spectroscopic techniques will be developed in this project that allow a direct correlation of molecular structural information about the ligand-nanocrystal interactions with the corresponding density and energetic distribution of surface defects and the influence that these defects have on charge transport and recombination. The insight that is gained will provide a molecular basis for the rational development of novel pathways for the of use quantum dots in systems for solar energy transduction.

This research was selected for funding by the Office of Basic Energy Sciences.

Exploring Efficient Data Movement Strategies for Exascale Systems with Deep Memory Hierarchies

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This project will enable scientific applications to prepare for exascale architectures without significantly increasing the programming complexity, while achieving at the same time the highest performance possible within tight power budgets. Dramatic changes in memory architecture will lead to multi-level memory hierarchies and possibly heterogeneous main memory. This project involves the development of programming constructs that enable applications to use deep memory hierarchies that are heterogeneous both in technology and architecture.

This research was selected for funding by the Office of Advanced Scientific Computing Research.

Mapping Interactions in Hybrid Systems with Active Scanning Probes

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The goal of this research is to investigate nanoscale interactions in hybrid systems by harnessing the precision and flexibility of scanning probe microscopy. Projected applications in areas such as energy conversion, opto-electronics, and spintronics will involve hybrid nanosystems composed of two or more materials or nanostructures that interact electrically, optically, or magnetically. Progress in understanding these interactions has been held back by the difficulty of accurately and efficiently positioning the system components with nanometer precision. To overcome this challenge, this work will employ cantilevers with integrated active magnetic and optical components. These active probes will be controllably scanned in proximity to metal or semiconductor nanoscale structures, essentially creating a highly tunable and versatile hybrid system. This technique will allow detailed studies of interactions between optical resonators and plasmonic or spintronic nanostructures or between dynamic ferromagnetic elements and quantum-confined electron spins. The planned research offers a significant increase of flexibility and efficiency for investigating hybrid systems over traditional nanoassembly, accelerating progress towards future technology.

This research was selected for funding by the Office of Basic Energy Sciences.

Catalyst Design for Small Molecule Activation of Energy Consequence

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This project targets the conversion of ubiquitous small molecules (e.g. NO, CO, H_2O) into viable precursors to synthetic fuels. Current state of the art catalyst design has not directly targeted transition metal complexes capable of mediating the multi-electron redox processes necessary to reduce the overpotential (energy loss) required to achieve efficient activation of small molecule substrates. In this vein, a new strategy has been developed for the assembly of polynuclear architectures, allowing for the construction of tunable polymetallic centers that assemble easily within a pre-organized template (conferring stability, selectivity and tunability) that can effect multi-electron redox processes for reactions. Catalyst development has commenced with the following target design elements: (1) catalysts feature multiple transition metal ions in the same reaction space to greatly expand accessible molecular redox capabilities; (2) catalysts are assembled in a polynucleating ligand framework that permits control over the cluster morphology as well as the local steric and electronic environment of the transition metal ions within the cluster. The high tunability of the catalyst composition (metal content) and geometric flexibility has permitted a rigorous assessment of electronic-structure-to-function relationship to be developed, further guiding synthetic efforts to realize more potent catalysts. The numerous permutations possible showcase the high degree of generality to this approach with many synthetic handles to tune redox and reaction chemistry. Trinuclear complexes have been synthesized featuring homo- and hetero-trinuclear cores featuring a variety of first row transition metal ions (Mn→Ni). The trinuclear units themselves can be assembled into larger molecular frameworks, giving rise to new materials with redox-programmable dimensionality and expanded redox flexibility. The molecular polynuclear platforms have been shown to successfully mediate multi-electron redox processes in a cooperative fashion without requiring strong chemical reductants or oxidants. The reactive molecular complexes are being used to activate and break down the robust bonds within typical waste stream small molecules (e.g., greenhouse gases) and convert them into value-added commodity chemicals. Ultimately, the catalysts developed by this approach will be required to convert energy acquired via renewable resources into synthetic fuels as an energy storage mechanism.

This research was selected for funding by the Office of Basic Energy Sciences.

One-Pot Catalytic Conversion of Biomass and Alkanes: Kinetically Coupling Deoxygenation and Dehydrogenation Pathways

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Biomass and natural gas will progressively replace petroleum and coal as feedstocks for energy carriers in the future. As precursors to liquid fuels, natural gas and biomass lie at opposite ends of the chemical spectrum. Natural gas is inert and its chemical conversion involves the removal of hydrogen while biomass contains oxygen that must also be removed. The long-term prospect of this research is the realization of a one-step catalytic conversion for both biomass and natural gas to hydrocarbon fuels by kinetically coupling biomass deoxygenation and alkane-dehydrogenation pathways. In essence, alkanes may serve as a hydrogen carrier for biomass deoxygenation while biomass-derived oxygenates may serve as the oxygen carrier for removing hydrogen from alkanes. Over zeolites, hydrogen removal steps limit alkane conversion. That is advantageous to the proposed cooperative reactions because the hydrogen-desorption bottleneck and resulting high concentration of hydrogen on catalytic surfaces will enable the deoxygenation of biomass-derived compounds. The fundamental research will entail the study of kinetics, mechanisms, and catalytic site architecture and electronic requirements for bifunctional catalysts constructed with transition metal carbides and zeolites. These catalysts are hypothesized to concurrently accomplish C-H bond activation, deoxygenation, and carbon chain growth chemistries. Chemical and structural characterization of the catalyst will be combined with transient and steady state kinetic measurements and isotopic tracer methods to probe the identity, reversibility, and kinetic relevance of elementary steps involved in concurrently processing methane and carbohydrate molecules that mimic biomass-derived fragments. This research effort will lead to fundamental advancement in the science of catalysis and the practical use of simple hydrogen-rich alkanes in biomass deoxygenation reactions.

This research was selected for funding by the Office of Basic Energy Sciences.

Detection and Attribution of Regional Climate Change with a Focus on the Precursors of Droughts

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The goal of this project is to improve understanding of the nature and causes of past changes in droughts to identify potential onset of future drought. The problem of identifying a component forced by climate change is typically addressed using established statistical detection and attribution (D&A) techniques. These techniques identify the characteristic "fingerprints" associated with climate change and connect them to likely causes in the system. However, these techniques have seen little application in drought research because of the noisy nature of the observations in this field. This project, instead of solely focusing on changes in drought characteristics, will investigate the naturally driven and externally forced components of known large-scale drought precursors such as specific ocean temperature patterns or poleward shifts in atmospheric circulation. The research will include an analysis of drought behavior in various climate model simulations and observations; a D&A-derived technique to investigate the temporal changes in major oceanic precursors; an uncertainty quantification analysis based on the 1998-2003 drought; and a rigorous D&A analysis of drought-promoting changes in atmospheric circulation patterns. This research will improve the understanding of drought mechanisms, establish new avenues in regional D&A research, and examine the sensitivity of the results to specific sources of uncertainties in the climate models, in measurements, in the climate drivers, and in the D&A methods. Ultimately, this work will provide scientific underpinning to inform decisions on how society might adapt to droughts in a changing climate.

This research was selected for funding by the Office of Biological and Environmental Research.

Spin Wave Interactions in Metallic Ferromagnets

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Dynamic excitations in ferromagnetic materials known as spin waves play a key role in a range of intriguing phenomena. The goal of this project is to investigate two main directions related to spin dynamics in metallic ferromagnets, namely the interactions between spin polarized currents and propagating spin waves and the interplay between spin waves and lattice vibrations (phonons) in thermally driven spin effects. Brillouin light scattering, a technique that is sensitive to both spin wave excitations and phonons, will be used to explore the fundamental nature of these effects.

This research was selected for funding by the Office of Basic Energy Sciences.

Searching for Dark Matter Axions with New High-Frequency Tunable Microwave Cavities

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The axion is a hypothetical particle that solves the strong-CP problem in nuclear physics and may be the dark matter of the universe. The Axion Dark Matter eXperiment (ADMX) and its sister experiment ADMX-High Frequency (ADMX-HF) are designed to detect axions by using large microwave cavities immersed in a strong magnetic field to resonantly convert the axion's rest mass into detectable photons. The current microwave cavity structures used, based on copper plated cylinders, limit the search to axions with masses corresponding to photons below 2 GHz. This research effort will investigate the use of new high-frequency tunable microwave cavities based on multi-post geometries and new thin film superconducting walls to boost the accessible volume and resonant factor of cavities above 2 GHz. Using these new cavity structures in ADMX and ADMX-HF will allow for axion dark matter searches in the previously inaccessible mass range of 2-10 GHz, greatly increasing the possibility of discovery.

This research was selected for funding by the Office of High Energy Physics.

Tracking for the New Muon g-2 Experiment

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There is a discrepancy between the measured and expected values of an intrinsic property of the muon, its magnetic dipole moment. The discrepancy could be one of the first indications of new physics beyond the current standard model. A new experiment will be conducted at Fermilab to test this discrepancy. The Fermilab experiment will measure the anomalous magnetic dipole moment of the muon, referred to mathematically as g-2, to a precision of 140 parts per billion. The goal of this project is to design and construct new tracking detectors for the Fermilab experiment to measure the trajectories of the decay products of the muon. The tracking detectors will help constrain systematic uncertainties in the measurement of g-2 and help rule out the possibility that the discrepancy is due to a problem with the measurement. This project will define the requirements of the tracking detectors, build prototype detectors to demonstrate the requirements are achievable, construct the final system in collaboration with several US and international institutions, and finally, analyze the first data from the new detectors. The tracking detectors will also expand the scope of the muon g-2 experiment by allowing a search for new intrinsic properties of the muon such as an electric dipole moment.

This research was selected for funding by the Office of High Energy Physics.

Multiphasic Soft Colloids: From Fundamentals to Application of Energy Sustainability

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The goal of this research project is to develop a fundamental understanding of the structure, dynamics and interaction of multiphasic soft colloidal systems for the design of novel materials with desirable properties. Multiphasic soft colloids represent a new class of macromolecules with two or more different functional groups at the periphery. Their structural heterogeneity establishes interactions that are directional in nature, which when extended to larger length scales offer great potential for novel emergent properties. Exploitation of these colloids as a platform for the development of new functional materials for energy applications requires quantitative understanding of the relationship between the chemical structure, interaction and spatial arrangement of these systems in their collective functional state. The planned research will use a synergistic approach, integrating material design and synthesis at the Center for Nanoscale Materials Science, advanced neutron scattering tools at the Spallation Neutron Source, and multi-scale simulations using the computational resources at the National Center for Computational Science at Oak Ridge National Laboratory. The knowledge gained from this program will provide the scientific foundation required for the development of exquisitely designed, multi-functional soft colloidal materials with properties and functions that address DOE's mission to develop advanced energy technologies including fuel cells, membranes for gas and liquid separation, organic light emitting diodes and photovoltaics and supercapacitors. Theory and computational algorithms developed for the interpretation of scattering data for this project will greatly benefit the larger soft condensed matter science community.

This research was selected for funding by the Office of Basic Energy Sciences.

Data Exploration at the Exascale

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This project explores important challenges related to preserving the ability of scientists to conduct exploratory analysis of data resulting from scientific simulations at the exascale. Because of severe constraints on the amount of data that can be saved from exascale supercomputers, it will be necessary to perform most of the data analysis during the run of a simulation and to sharply reduce the volume of the data that are stored, perhaps reducing the integrity of the data that are available for exploratory analysis after the simulation ends. Empirical methods will be used to characterize various approaches to data reduction in terms of data integrity, providing guidelines for scientists. This project will also research ways to visually represent loss of data integrity and resulting uncertainty.

This research was selected for funding by the Office of Advanced Scientific Computing Research.

In-situ Monitoring of Dynamic Phenomena During Solidification

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This project focuses on the ability to visualize experimentally and model theoretically the melting and solidification processes of metal alloy materials, even while at elevated temperatures. This project will use novel tools and unique probes, such as synchrotron x-ray and proton radiography and tomography, at National Laboratory Facilities that have not yet been used in the United States for this purpose. Modeling these processes will enable the prediction of the microscopic structure of metal alloys, even under harsh environments, and will allow for new understanding of a range of energy materials, such as wind turbine blades and lithium rechargeable batteries.

This research was selected for funding by the Office of Basic Energy Sciences.

Development and Characterization of Improved Disruption and Runaway Electron Mitigation Systems

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The goal of this research is to develop techniques to mitigate disruptions in large magnetic fusion devices. In these devices, called tokamaks, a portion of the containing magnetic field is generated by an electrical current flowing in a high temperature plasma (ionized gas). A disruption is a rapid loss of this current that produces a significant heat load to the walls of the plasma chamber. Disruptions are a major challenge for large tokamaks such as the international ITER device under construction because they can affect availability and performance. The focus of this effort is to maximize the efficiency of the proposed disruption mitigation schemes. It will test fusion-power-plant relevant designs and technologies that could be applied on ITER. Two of the more promising techniques for disruption mitigation are gas injection and shattered pellet injection. Both methods inject large numbers of particles to benignly dissipate the plasma energy. Shattered pellet injection is a new technique involving the injection of a large frozen hydrogen or neon pellet that is shattered by impacting a hard surface inside the tokamak. The solid fragments are expected to penetrate deeper into the plasma than gas, improving the material assimilation and removing the energy faster. These techniques will be studied on the DIII-D National Fusion Facility at General Atomics in San Diego. The solid/gas mix during the injection may be improved by modifying the shattering method and thus improving the efficiency of this technique. A new diagnostic system to characterize the efficiency of the assimilation of the injected particles will also be designed and tested. Finally, additional tunable injection systems will be installed to study simultaneous particle injection at different locations since the injection may have to be done through multiple systems on ITER to spread out the energy distribution.

This research was selected for funding by the Office of Fusion Energy Sciences.

Computational Fluid Dynamics Facility to Support Targets for the 12 GeV Program at Jefferson Laboratory

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This project will establish a computational fluid dynamics (CFD) research program at the Thomas Jefferson National Accelerator Facility (TJNAF) to investigate and standardize the performance of liquid hydrogen targets for nuclear physics experiments. Liquid hydrogen has long been a standard target material for fixed-target nuclear physics experiments at accelerator facilities worldwide. In the near future, experiments using very high intensity electron beams will require the removal of beam-deposited heating of up to an order of magnitude beyond that which has been achieved with previous targets. Through CFD simulations, it should be possible to reduce target boiling effects by more than an order of magnitude, which will be crucial for the reduction of systematic errors in planned high beam intensity experiments. In this CFD research program, a range of experimental target designs will be simulated and optimized, including the 5000 W target envisioned for the possible ultra-high precision MOLLER (Measurement Of a Lepton-Lepton Electroweak Reaction) experiment at TJNAF, which proposes a precision study of high-intensity polarized electron-electron scattering. This CFD research program will also analyze safety issues and will develop standard procedures for operating liquid hydrogen targets in the safest manner feasible.

This research was selected for funding by the Office of Nuclear Physics.

Precision Measurements with Low Energy Neutrons

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The purpose of this project is to measure fundamental properties of low-energy neutrons. We will contribute to three experiments that will be performed at the Oak Ridge National Laboratory Spallation Neutron Source, NPDGamma, Nab, and nEDM (neutron Electric Dipole Moment). The NPDGamma experiment will characterize the role of the weak force in interactions between neutrons and protons. The Nab experiment will measure correlations in the decay products of the neutron. In the third experiment, namely nEDM, the electric dipole moment of neutron, which is indicative of the separation of positive and negative charge of the neutron, will be sought. This is predicted in the Standard Model to be extremely small. If observed at the limit of sensitivity of the nEDM experiment, it would be a clear signature of physics beyond the Standard Model and might explain the deficiency of antimatter in the observable universe. All three experiments require precise magnetic fields to manipulate the spin of neutrons and helium-3 nuclei. We have developed a technique for calculating the optimal windings for such coils based on their geometry and magnetic field requirements. We will construct these coils as three-dimensional printed circuits. We will use a robotic arm to cut the exact traces of each circuit according to our calculations.

This research was selected for funding by the Office of Nuclear Physics.

Stochastic Simulation of Complex Fluid Flows

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Computational fluctuating hydrodynamics is a relatively new and actively growing area of computational fluid dynamics. Its growth is stimulated by advances in micro- and nano-manufacturing technologies and the development of novel materials such as nanofluids. Thermal fluctuations affect fluid flows at small scales and need to be included in state-of-the-art algorithms for fluid dynamics in a way that is consistent with statistical mechanics. This project explores new fields where there are few, if any, computational tools available for scientific studies in this area.

This research was selected for funding by the Office of Advanced Scientific Computing Research.

Vibrational Spectroscopy of Transient Combustion Intermediates Trapped in Helium Nanodroplets

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The objective of this research is to isolate and stabilize transient intermediates and products of prototype combustion reactions. This will be accomplished by Helium nanodroplet isolation (HENDI) spectroscopy, a novel technique where liquid helium nanodroplets freeze out high energy metastable configurations of a reacting system, permitting infrared spectroscopic characterizations of products and intermediates that result from hydrocarbon radical reactions with molecular oxygen and other small molecules relevant to combustion environments. The majority of these transient species have never been directly observed in traditional spectroscopy experiments. HENDI spectroscopy will be used to carry out the first direct observation of the elusive hydroperoxyalkyl radical (QOOH) and its oxygen adducts (O_2QOOH), important in the low temperature hydrocarbon oxidation chemistry associated with homogeneous charge compression ignition (HCCI) engines. HENDI will also be used to probe the outcome of the self reactions of resonantly stabilized free radicals, which are important in the earliest stages of soot formation. Thus, these studies may lead to an improved understanding of the detailed mechanisms of hydrocarbon combustion resulting in more accurate predictive combustion models. Furthermore, mid-infrared spectral signatures of important combustion intermediates will be obtained to develop laser diagnostic tools for modern chemical kinetics studies.

This research was selected for funding by the Office of Basic Energy Sciences.

Rational Design and Nanoscale Integration of Multi-Heterostructures as Highly Efficient Photocatalysts

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The combination of dissimilar materials with nanometer-scale dimensions can enable exciting opportunities to precisely control their electronic and optical properties and to create a new generation of integrated material systems with functional properties not possible in individual components. This project will design and synthesize complex nanostructures of dissimilar materials that integrate a nanoscale photovoltaic device with two distinct redox nanocatalysts. The interaction of light with these nanostructures creates electron-hole pairs that are quickly separated and transported to the integrated nanocatalysts to enable thermodynamically unfavorable redox reactions. Systematic studies will be carried out to develop general strategies for the synthesis of such complex nanostructures and to investigate their fundamental electronic, optical, and photocatalytic properties. The rational design of nanoscale architectures and seamless integration of multiple functional components in a single nanostructure can enable efficient optical absorption, charge generation, separation, transportation and utilization for productive redox chemistry. It therefore has the potential to enable a new generation of highly effective photocatalysts for efficient harvest and conversion of solar energy into chemical fuel.

This research was selected for funding by the Office of Basic Energy Sciences.

Neutrino Oscillations in Supernovae

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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.

This research was selected for funding by the Office of Nuclear Physics and the DOE Experimental Program to Stimulate Competitive Research.

Repurposing the Saccharomyces Cerevisiae Peroxisome for Compartmentalizing Multi-Enzyme Pathways

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To replace fossil fuels and other chemicals with biofuels and biomaterials from renewable sources, microbes can be engineered to alter their metabolism to maximize production of the desired chemicals. To do this, biosynthetic pathways from other species are added to a host organism, often resulting in the accumulation of new chemical compounds that are detrimental to the engineered microbe. Thus, a major challenge in microbial engineering is to enable high-yielding biofuel production without affecting the microorganism's health. One solution to this problem is to spatially separate engineered metabolic pathways from the rest of the metabolic machinery within the microbial cell. In fact, many organisms already use subcellular compartments, called organelles, to isolate cellular functions by encapsulating components within impermeable membranes. The goal of this research is to repurpose one of these organelles, specifically the peroxisome, for use in engineered yeasts. The peroxisome is unique in that it is not necessary for healthy cellular growth in most environmental conditions. Therefore, this organelle can serve as a minimal compartment where unnecessary components are replaced by desired ones. This research will determine how the peroxisome can be specialized for encapsulating synthetic metabolic processes that can facilitate the production of biofuels to address DOE's mission, moving forward to the development of renewable energy sources.

This research was selected for funding by the Office of Biological and Environmental Research.

Containment Domains: Programming and Execution Model Support for Resiliency

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Extreme-scale computing hardware cannot be effectively harnessed for scientific discovery unless severe reliability obstacles are overcome. The combination in future fabrication technology of a growing number of components and the decreasing inherent reliability of components will result in error and fault rates orders of magnitude higher than those in petascale systems today. This project will use *containment domains* for enabling scalable resiliency with low performance and power overheads. Containment domains are resiliency-specific programming constructs for combining high-level information and structure from the application with runtime information and services in the execution model.

This research was selected for funding by the Office of Advanced Scientific Computing Research.

Particle Physics at the Cosmic, Intensity, and Energy Frontiers

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Major efforts at the Intensity, Cosmic, and Energy frontiers of particle physics are rapidly furthering our understanding of the fundamental constituents of Nature and their interactions. The overall objectives of this research project are (1) to interpret and develop the theoretical implications of the data collected at these frontiers and (2) to provide the theoretical motivation, basis, and ideas for new experiments and for new analyses of experimental data. Within the Intensity Frontier, an experimental search for a new force mediated by a GeV-scale gauge boson will be carried out with the A' Experiment (APEX) and the Heavy Photon Search (HPS), both at Jefferson Laboratory. Within the Cosmic Frontier, contributions are planned to the search for dark matter particles with the Fermi Gamma-ray Space Telescope and other instruments. A detailed exploration will also be performed of new direct detection strategies for dark matter particles with sub-GeV masses to facilitate the development of new experiments. In addition, the theoretical implications of existing and future dark-matter-related anomalies will be examined. Within the Energy Frontier, the implications of the data from the Large Hadron Collider will be investigated. Novel search strategies will be developed to aid the search for new phenomena not described by the Standard Model of particle physics. By combining insights from all three particle physics frontiers, this research aims to increase our understanding of fundamental particle physics.

This research was selected for funding by the Office of High Energy Physics.

Bond Formation and Catalysis by Base-metal Unsaturated Isocyanides

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The goal of this project is to use the inexpensive, middle 3d-transition metals, manganese and cobalt, as high-efficiency reagents and catalysts for chemical-bond formation. A specific aim of this research is the development and mechanistic elucidation of manganese-based electrocatalysts for carbon dioxide (CO_2) reduction and fixation. Efficient activation and recycling of atmospheric CO_2 remains a significant contemporary challenge as global demand for carbon-based fuel sources continues to increase. Experiments and studies of this project focus specifically on the development and mechanistic elucidation of a new, manganese-based system for electrochemical reduction of CO_2 to water and carbon monoxide (CO). The new manganese catalysts proposed here feature *m*-terphenyl isocyanides as supporting groups. These isocyanides and their transition metal complexes represent a new class of molecular species that are inspired from classic, binary transition-metal carbonyls, which are by themselves catalysts for important chemical transformations. The *m*-terphenyl isocyanide complexes studied in this project offer a robust, but highly modular, platform for electrocatalyst development and optimization. Such ligand-directed control is lacking in metal carbonyl systems. In addition, the protective and tunable nature of *m*-terphenyl isocyanides allows for detailed assessment of the elementary steps operative in CO_2 reduction processes. The second aim of this research concerns the elucidation of new bond formation processes using cobalt isocyanide-containing molecules. The chemical properties of recently discovered and unique cobalt *m*-terphenyl isocyanide complexes will be especially applied to CO_2 remediation.

This research was selected for funding by the Office of Basic Energy Sciences.

Providing the Roadmap for New Element Discoveries and New Chemistries of the Heaviest Elements

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Transactinides are the heaviest elements at the bottom of the periodic table, and each must be produced artificially using nuclear fusion reactions between a projectile and target. In the 2000s, the most important projectile for forming heavy elements has been ^{48}Ca because of its large excess of neutrons. All possible elements that can be formed with ^{48}Ca projectiles have already been discovered, and it is not clear which other projectile could be used to discover the next new element. This project will systematically study the interactions of a variety of projectiles, most importantly ^{50}Ti and ^{54}Cr, in nuclear reactions with much higher production rates than those used for transactinides. This will help determine the most important influences on production rate with the goal of aiding in the discovery of the next new element. Additionally, this project will work to develop new extraction chromatography systems and implement new automated equipment to investigate the physical chemistry of the heaviest elements. These efforts will help guide heavy element research in the coming decade as scientists attempt to expand the limits of the periodic table.

This research was selected for funding by the Office of Nuclear Physics.

Ultrafast X-ray Studies of Intramolecular and Interfacial Charge Migration

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Chemically engineered devices play an increasingly important role in the development of sustainable energy production and storage solutions. Molecular assemblies can harvest sunlight and use the absorbed energy to produce electricity or to catalyze chemical reactions. This project addresses the need for an atomic-level understanding of light-induced charge generation and migration in molecular networks, in polymer blends, and at organic-inorganic interfaces. Understanding these processes is a prerequisite to exploit the potential of molecular-electronics-based energy solutions. Experimental techniques using intense, ultrashort x-ray pulses will monitor the light-induced creation and transport of charges in complex molecular systems in real time and from the perspective of specific atomic sites. The objective is to provide a predictive understanding of the most fundamental working principles and bottlenecks of molecular electronic function.

This research was selected for funding by the Office of Basic Energy Sciences.

Modulating Thermal Transport Phenomena in Nanostructures via Elastic Strain at Extreme Limits of Strength

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Nanoscale materials fabricated with nearly pristine crystal structure are often endowed with ultra-strength behavior, where material failure occurs at a significant fraction of its ideal limit. The thermal conductivity exhibited by such materials is also uniquely affected by the high surface-to-volume ratio at the nanoscale. The juxtaposition of the vastly increased dynamic range of elastic strain available in ultra-strength nanomaterials and altered thermal transport shows promise for tunable thermal properties. This project aims to exploit these properties of high-strength nanostructures to elucidate the coupling between large mechanical strains and thermal conductivity (both electron and phonon) leading to better understanding and control of the thermal performance in these materials. Unique fabrication methods to produce nanosized, quasi-defect-free single crystals and modern nanomechanical testing will be used to identify the size-dependent dynamic range of elastic strain and understand deformation mechanisms near the ideal limit. Identifying and quantifying thermal transport phenomena as a function of mechanical strain in these nanostructures will open the door to using elastic strain engineering in high-strength nanomaterials to tune thermal transport. The results of these investigations will be used to improve the performance, efficiency, and versatility of advanced thermal management and energy conversion devices with tunable response.

This research was selected for funding by the Office of Basic Energy Sciences.

Holography, Gravity and Condensed Matter

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Holographic duality is a set of a sophisticated theoretical ideas and tools that has been developed over the last decade as part of string theory. The goal of this project is to harness the insights afforded by holographic duality to shed light on challenging theoretical problems in the physics of exotic materials by dually reformulating the problems in terms of the seemingly unrelated dynamics of gravitating spacetimes. At the same time, this project will investigate novel phenomena in fundamental gravitational physics inspired by a condensed matter perspective. Experiments over the past three decades have uncovered families of materials deviating from the textbook behavior of metals. It has proved difficult to understand these materials with conventional theoretical techniques because the electrons in the metals are all strongly quantum entangled with one another. Holographic duality is able to reformulate the dynamics of certain such strongly correlated phases of matter as the gravitational ripples of a black hole event horizon. This project will use and develop further holographic techniques to obtain controlled theoretical descriptions of so-called quantum critical metals and of phases of matter exhibiting `fractionalized excitations,' wherein the electron appears to break up into multiple pieces. Novel experimental probes will be proposed. By combining the physical intuition of traditionally distinct arenas of physics, spacetime physics and condensed matter, this project has the potential to uncover new approaches to critical problems in both fields that have remained stubbornly present for many years.

This research was selected for funding by the Office of High Energy Physics.

Model-Data Fusion Approaches for Retrospective and Predictive Assessment of the Pan-Arctic Scale Permafrost Carbon Feedback to Global Climate

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Land areas spanning the northern high latitudes currently store enormous quantities of carbon as frozen organic matter in the region's soils and peatlands. The long-term fate of this carbon will be determined by changing temperatures already observed in these environments. These same environments are projected to warm faster than most other places on Earth over the next century. Rising temperatures will result in more and faster thawing of frozen organic matter. Once thawed, this carbon-rich material is subject to degradation by microbial organisms and/or transport through runoff to aquatic systems. Coupled with these anticipated changes is the role of disturbance from fire, invasive species, and the changing land surface resulting from soil thaw. The combination of global change and disturbance will alter historic patterns of carbon cycling with potentially large additions of greenhouse gasses to the atmosphere, thereby further increasing temperatures. The current scientific understanding of these processes in northern environments is quite limited and the existing knowledge is not consolidated in any one place or system. Data and information exist in different forms and in different places, ranging from satellite-based measurements to individual cores of soils taken for various research purposes. This project intends to survey, integrate, model and evaluate existing information on key processes that control the transfer of carbon from frozen organic material to atmospheric greenhouse gasses (mostly carbon dioxide and methane). The increased understanding that is expected from this project will help to design and implement future state-of-the-art scientific activities by providing priorities to different research areas and also will inform future decisions regarding energy and natural resources of the Arctic.

This research was selected for funding by the Office of Biological and Environmental Research.

Utilization of Protein Film Electrochemistry to Characterize the Mechanisms Imparting Aerotolerance and Bidirectionality in Soluble, Multimeric [NiFe]-Hydrogenases

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The overall goal of this research is to better understand how structural features control functional aspects of an important class of enzymes called soluble [NiFe]-hydrogenases. These enzymes mediate a reversible two-electron reduction of protons to form hydrogen gas. Studies of these enzymes may lead to improvements in bio-hydrogen production/utilization. Additionally, they serve as models for more complex multielectron redox enzymes such as those involved in nitrogen and carbon dioxide reduction. Two properties of [NiFe]-hydrogenases relevant to energy applications will be investigated: (1) What structural features influence the catalytic bias of the enzyme? and (2) What structural features determine the susceptibility of these enzymes to inactivation by molecular oxygen? [NiFe]-hydrogenases with a broad range of activities will be isolated from biologically diverse sources and characterized using a technique called protein film electrochemistry. Structural variants of these enzymes with precisely targeted changes will also be generated, characterized and compared with the results for the wild type enzymes to address the two questions above. The comprehensive understanding of the structural features controlling catalytic properties that result from this research can guide the development of improved redox enzymes and/or other novel bio-inspired catalysts.

This research was selected for funding by the Office of Basic Energy Sciences.

Graphene Membranes with Tunable Nanometer-Scale Pores

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Graphene, a one-atom thick membrane of hexagonally bonded carbon atoms, is one of the strongest materials known and is impervious to the diffusion of even helium gas. The potential for creation of tunable nanometer-scale pores in graphene, combined with its other properties, make it a promising material for improving selectivity, permeability, and energy efficiency in a diverse range of membrane separation and sensing applications. The objectives of this work are to (1) systematically study the effect of ion irradiation, nitrogen doping, and chemical oxidation to create tunable, nanometer-scale pores in single and multilayer graphene membranes and (2) elucidate the transport characteristics of the resulting membranes. High-resolution imaging will be used to study the pore structures, and transport measurements will be performed on large-area membranes as well as on single pores. The study will result in fundamental understanding of the relationship between fabrication methods, pore structures, and transport properties of graphene membranes, which may lead to significant advances in a wide range of separations applications.

This research was selected for funding by the Office of Basic Energy Sciences.

Modeling Astrophysical Explosions and the Nucleosynthesis of the Heavy Elements

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The heavier elements in the Universe were created and dispersed in the supernova explosion of stars, within which are realized extreme conditions for nuclear and neutrino processes. Astrophysical experiments provide a rich and constraining data set, but our theoretical understanding of supernovae and heavy element production remains incomplete. The goals of this project are to advance numerical simulations of astrophysical explosions and use them to connect the nuclear theory of supernovae to current and future experimental programs. The focus is on applying high performance computing to model the transport of radiation (both neutrino and electromagnetic) in core collapse supernovae and the outflows from neutron star mergers. General aims of this work include (1) further defining the explosive astrophysical environments that govern the nucleosynthesis of heavy and rare isotopes; (2) providing the means to test supernova explosion/nucleosynthesis calculations against the spectroscopic data from optical and x-ray telescopes; (3) preparing the way for more realistic treatments of neutrino interactions, with the ultimate goal of making supernovae a testing ground for probing fundamental neutrino physics; and (4) advancing the applicability of large scale computing to solve problems in nuclear physics, through the development of parallel algorithms of the type incorporated in our simulation codes.

This research was selected for funding by the Office of Nuclear Physics.

Large-Scale Modeling of Intense Short-Pulse Laser Interaction for HEDLP

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The objective of this research is to develop an integrated description of Petawatt-class laser-matter interactions that covers plasma physics from near-vacuum up to 1000x solid density, resolving time scales from sub-femto- to nanoseconds, i.e., from below the laser period to the hydrodynamic response time of heated targets. Studying nonlinear many-body physics in the laboratory at the relativistic limit - driven by intense, short laser pulses - is a grand challenge. It relates High Energy Density Laboratory Physics (HEDLP) to fundamental astrophysical problems like gamma-ray bursts and the origin of cosmic rays, and it has applications ranging from fusion energy to controlled amplification of desirable radiation or particle beams. Computer modeling is an essential part of the design and interpretation of HEDLP experiments. The key difficulty arises from the many physical scales involved. These are set by microscopic physics in solid-density plasma on the one hand, e.g., filamentation of the laser beam in blow-off plasma, and the macroscopic interaction volumes and times on the other. Currently, there is no self-consistent computer model available, and physics understanding of kinetic transport is incomplete. The proposed research will close this gap with a theoretical approach to understanding the fundamental kinetic physics of laser interaction and electron transport near critical density, integrating all essential physics that affect the outcome of a short-pulse laser-matter interaction experiment. This approach goes beyond the current paradigm of combining hydrodynamic models with separate laser absorption physics and electron-transport models. It will also be synergistic with several ongoing efforts on high-energy-density physics, e.g., fast-ignition of inertial confinement fusion targets.

This research was selected for funding by the Office of Fusion Energy Sciences.

Modeling of Photoexcited Process at Interfaces of Functionalized Quantum Dots

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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.

This research was selected for funding by the Office of Basic Energy Sciences and the DOE Experimental Program to Stimulate Competitive Research.

Electron Dynamics in Nanostructures in Strong Laser Fields

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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.

This research was selected for funding by the Office of Basic Energy Sciences and the DOE Experimental Program to Stimulate Competitive Research.

Probing High Temperature Superconductors with Magnetometry in Ultrahigh Magnetic Fields

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The objective of this research is to investigate the high-field magnetic properties of high temperature superconductors, materials that conduct electricity without loss. A technique known as high-resolution torque magnetometry will be developed to directly measure the magnetization of high temperature superconductors. This technique will be implemented using the 100 Tesla pulsed magnetic field facility that is part of the National High Magnetic Field Laboratory at Los Alamos National Laboratory. This research will address unanswered questions about the interplay between magnetism and superconductivity, determine the electronic structure of high temperature superconductors, and shed light on the mechanism of high temperature superconductivity and on potential applications of these materials in areas such as energy generation and power transmission.

This research was selected for funding by the Office of Basic Energy Sciences.

Optimal Cosmological Measurements with Weak Gravitational Lensing

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Weak gravitational lensing is the most direct way to observe distributions of dark matter in the universe. Weak gravitational lensing can also be used to study dark energy, which causes accelerated expansion of the universe and a slowing of the growth of large-scale structures (such as galaxy clusters) containing dark matter. Several large astronomical imaging surveys have been planned to measure weak gravitational lensing more precisely than ever before, eventually culminating in the Large Synoptic Survey Telescope (LSST). These imaging surveys gain in power when combined with spectroscopic surveys like the ongoing Baryon Oscillation Spectroscopic Survey (BOSS). The purpose of this project is to carry out measurements of weak gravitational lensing and then combine these results with other cosmological observations to identify optimal ways of constraining cosmological parameters and the nature of dark energy. The results will ensure that next-generation dark energy experiments realize their full potential.

This research was selected for funding by the Office of High Energy Physics.

Computational Modeling and Design of Radiation-Tolerant Materials for Fusion

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In nuclear fusion environments, materials are subjected to extreme conditions of radiation, temperature and mechanical load. Over time, this results in performance degradation to extents that may render these materials unsuitable for the purpose for which they were originally designed. The objectives of this research are to use theory, modeling and simulation to predict materials performance over the expected lifetime of fusion devices. This will result in an economical yet scientifically based way to test different design alternatives, suggest component improvements, and provide fusion plant design optimization. This research will advance the current state of the art in computational modeling one step further toward a `materials-by-design' strategy for energy applications.

This research was selected for funding by the Office of Fusion Energy Sciences.

Metabolism and Evolution of a Biofuel-Producing Microbial Coculture

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Some microbes can convert renewable resources such as carbohydrates and sunlight into biofuels. Therefore, they offer an urgently needed alternative to non-renewable fuels. Most research efforts in this area have focused on genetically engineering individual microbial species to improve biofuel production. However, a lesson can be taken from nature, where multiple microbial species help each other to thrive on food sources such as plant residues that the individual species can not use on their own. Furthermore, mixtures of specialized microbes can sometimes outperform a single engineered strain for producing chemicals of value to society. This research will make use of a mixture of two microbial species (a coculture) that work together using sugar and energy from sunlight to produce more hydrogen gas biofuel than either microbe could by itself. A major challenge in using cocultures is ensuring that the different species maintain a long-term cooperative relationship. This research will stabilize such cooperation by forcing each microbe to provide a nutrient that the other requires to survive. This approach enables experiments that will decipher how the metabolisms of the two species interact and thereby how they can be optimized for biofuel production. Studying the evolution of the microbes in the coculture will also lead to the discovery of traits that enhance biofuel production. This information will ultimately lead to the design and engineering of tailor-made microbial mixtures for the economical production of hydrogen gas and other biofuels from renewable resources.

This research was selected for funding by the Office of Biological and Environmental Research.

A Ruler To Measure The Universe: Probing Dark Energy with Baryon Acoustic Oscillations

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Understanding the acceleration of the expansion of the Universe and the nature of the "dark energy" responsible is one of the principal challenges in cosmology today. This research aims to constrain the properties of this dark energy with large astronomical surveys, using sound waves frozen in the early Universe (baryon acoustic oscillations or BAO) as a ruler to measure the expansion of the Universe. This work organized along two themes. The first is an analysis of currently ongoing surveys like the Baryon Oscillation Spectroscopic Survey (BOSS) to obtain precision measurements of the acceleration of the Universe. BOSS will survey 1.5 million galaxies by 2014 and will produce the definitive low redshift BAO measurement, improving on current constraints by factors of two and more. The second theme of this work is to develop techniques to enable the next generation of these surveys to achieve their full potential in terms of precision measurements.

This research was selected for funding by the Office of High Energy Physics.

Nuclear Physics on the Road to FRIB: Enhancing Direct-Reaction Measurements Through High-Resolution Coincidence Experiments

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"What is the origin of the elements in the cosmos? What are the nuclear reactions that drive stars and stellar explosions?" - These are among the priority questions highlighted by the Nuclear Science Advisory Committee. A powerful tool in addressing such questions is to study nuclear reactions using beams of exotic, short-lived nuclei to understand how nuclear properties evolve with proton- and neutron-number and to help determine the role exotic nuclei play in generating energy and synthesizing elements in exploding stars. The focus of this research is to significantly enhance the sensitivity of direct-reaction experiments on exotic nuclei by simultaneously measuring the gamma rays and charged particles that are emitted during the reaction process. Specifically, these measurements will be performed by coupling the resolving power of Gammasphere and ORRUBA (Oak Ridge Rutgers University Barrel Array), two of the highest efficiency and resolution arrays for detecting, respectively, gamma rays and charged particles from nuclear reactions. This powerful system will use beams of rare nuclei produced at the ATLAS (Argonne Tandem Linac Accelerator System) facility (Argonne National Laboratory) to significantly increase the experimental sensitivity required to study these exotic reaction processes. The resulting sensitivity gain will improve the extrapolation of nuclear structure models to even more exotic nuclei and enhance the reliability of calculations that simulate creation of heavy elements in supernovae. The experience gained through these studies will become a stepping-stone to the next-generation of experiments that could be performed at a future Facility for Rare Isotope Beams (FRIB).

This research was selected for funding by the Office of Nuclear Physics.

Spontaneous Generation of Rotation in Tokamak Plasmas

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The tokamak is one of the most promising fusion energy concepts. Tokamaks have demonstrated excellent performance in a variety of regimes, and the values of several figures of merit (the stored energy and the time that the injected energy remains within the machine) improve considerably in the presence of plasma rotation. The plasma can rotate freely because the tokamak has axial symmetry, i.e., it is doughnut shaped. In most experimental tokamaks, rotation is generated externally by injecting neutral particles at high speed that collide with the plasma. This injection mechanism is inefficient in the large tokamaks that are needed for energy production, making the spontaneous rotation observed in the absence of external momentum injection an attractive alternative. This spontaneous rotation may seem counter-intuitive because tokamaks are symmetric and do not have an obvious preferred direction. The problem is subtle and requires understanding of the delicate symmetries in an axisymmetric plasma. The objectives of this project are to develop the theoretical and numerical tools to study and predict spontaneous rotation in tokamaks and, using these tools, to design new configurations that exploit spontaneous rotation to improve performance. The theoretical results obtained during the research will be checked against experimental observations systematically to validate these completely new modeling tools. With the new insights gained, a tokamak that will rotate to high speed in the absence of external momentum sources will be designed. No previous tokamak has been built to optimize rotation in the absence of external injection, and this new design criterion may open new avenues to better performance.

This research was selected for funding by the Office of Fusion Energy Sciences.

Improved Sensitivity and Utility of Metaproteomics Analyses

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Microbial communities are found in virtually any environment. Understanding the relationship between microbes and their environment is key to the Department of Energy's goal of manipulating microorganisms for biofuel production. Microorganisms use proteins as a means to interact with their natural environments and digest their food to grow and survive. Therefore, analyzing proteins from microbial communities facilitates understanding the relationship between microbes and their environment. Mass spectrometry is a powerful technique to identify proteins in complex biological samples such as the microbes that constitute an environmental community. The objective of this project is to develop novel computational methods to dramatically improve the ability to detect and identify new proteins in these complex samples. Current protein identification methods require the use of protein databases to infer the function of the proteins present in the sample under study. The methods that will be developed in this project take advantage of the similarity among proteins that perform comparable functions in different organisms, circumventing the need for protein databases. These studies will focus on the cow rumen environment, where the microbial community degrades a variety of renewable resources such as plant residue. A final goal of the project is to improve the ability to identify the species of origin for newly discovered proteins within the cow rumen bacterial community. In a natural environment with thousands of different organisms present, this complex process is crucial for understanding the specialized roles that individual microbes play within the community and how they convert plant material into biofuels.

This research was selected for funding by the Office of Biological and Environmental Research.

Systems Approach to Engineering Cyanobacteria for Biofuel Production

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Most of the energy consumed in the U.S. is derived from non-renewable fuels (petroleum and natural gas), with a significant fraction of this energy being used for transportation. To reduce the amount of oil used to satisfy transportation energy needs in the U.S. and to alleviate our dependence on foreign sources of oil, renewable sources of transportation fuels are needed. Cyanobacteria offer a promising route for directly converting solar energy and carbon dioxide into biofuels. Certain cyanobacterial strains can be engineered to produce butanol, a biofuel that is compatible with the existing infrastructure for fuel transportation and use. The objectives of this research are to integrate computational modeling and experimental approaches to guide the engineering of cyanobacteria with improved butanol production. New computational approaches will be developed to facilitate the design of experiments, predict their outcomes, and evaluate the results. In this way, this project will identify genetic engineering strategies for improving butanol production in cyanobacteria. Experiments will subsequently be performed to construct and evaluate new engineered cyanobacterial strains. The developed approaches will be systematically applied to identify engineering strategies for improving production of a variety of biofuels in five other microorganisms, supporting the U.S. Department of Energy's mission for developing renewable ways of producing advanced biofuels.

This research was selected for funding by the Office of Biological and Environmental Research.

Early Time Dynamics in Heavy-Ion Collisions

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Currently, there is no dynamic model to describe the evolution of a "Quark-Gluon Plasma," the system created just after the collision of two heavy ions during experiments at the Relativistic Heavy-Ion Collider (RHIC) and the Large Hadron Collider (LHC). After the collision, the plasma initially is far from equilibrium. It consists of many particles that interact strongly and therefore cannot be simulated with any known existing technique. However, for reasons not fully understood, the plasma eventually comes into equilibrium, at which point it can be described using hydrodynamics. The aim of this project is to model the initial, pre-equilibrium stage following a collision of heavy nuclei together with its coming into equilibrium. To achieve this, a recent development from string theory known as gauge/gravity duality is employed to model the two approaching nuclei as two approaching gravitational shock waves in a space-time that has a negative cosmological constant (known as Anti-de-Sitter). To study the equilibration of the plasma, it will be simulated by solving Einstein's equations for this problem in general relativity numerically. Once the numerical results are available, it will be possible to extract important information such as when the plasma can be described by hydrodynamics and what its local pressure and fluid velocities are. This information will help to eliminate many unknowns in current hydrodynamic models of experimental data from the RHIC and the LHC, thus opening the door to extract precision information about material properties (such as the viscosity) of the underlying fundamental theory of strong interactions, Quantum Chromodynamics.

This research was selected for funding by the Office of Nuclear Physics.

Combining Scanning Probe Microscopy and Synchrotron Radiation for Nanoscale Imaging with Chemical, Electronic and Magnetic Contrast

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The objective of this research is to develop a novel, high-resolution microscopy technique for imaging of nanoscale materials with chemical, electronic, and magnetic contrast. It will combine the sub-nanometer spatial resolution of scanning probe microscopy with the chemical, electronic, and magnetic sensitivity of synchrotron radiation. The proposed development will drastically increase the spatial resolution of current state-of-the-art x-ray microscopy from only tens of nanometers down to atomic resolution. The technique will enable fundamentally new methods of characterization, which will be applied to the study of energy materials, nanoscale magnetic systems, and site-specific heterogeneous catalysis. A better understanding of these phenomena at the nanoscale has great potential to improve the conversion efficiency of quantum energy devices, lead to advances in future data storage applications, and yield more efficient catalytic reactions.

This research was selected for funding by the Office of Basic Energy Sciences.

Assembling Microorganisms into Energy Converting Materials

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This project will integrate microorganisms capable of reversible energy transduction in response to changing relative humidity with non-biological materials to create hybrid energy conversion systems. While plants and many other biological organisms have developed structures that are extraordinarily effective in converting changes in relative humidity into mechanical energy, engineered energy transduction systems rarely take advantage of this powerful phenomenon. Owing to their micrometer-scale dimensions, bacterial spores are amenable to integration into macroscopic structures with desired micro-architectures through directed- or self-assembly. Thus, the objective is to create robust and scalable energy conversion materials using bacterial spores as the key biomolecular material responsible for energy conversion. A suite of experimental platforms including atomic force microscopy and micro-electromechanical systems will be used to investigate (1) how to assemble hybrid spore-rubber latex structures that efficiently generate electricity by converting energy from evaporation of water and (2) how the interaction between water and spore nanostructure imposes limits on energy conversion. Progress can provide opportunities to tap into new forms of renewable energy and environmentally friendly energy storage.

This research was selected for funding by the Office of Basic Energy Sciences.

Dielectric Ceramics in Nanosheet Form

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Dielectric ceramic materials have properties that make them important components in a wide range of technologies, including capacitors, microwave communication systems, power conditioning, and thermoelectrics. The aim of this project is to create and study these ceramics as freestanding nanosheets, a non-natural form of these materials. Nanosheets are characterized as being fewer than ten nanometers in thickness and up to tens of micrometers in lateral dimensions. This "two-dimensional" morphology provides a unique opportunity to better understand the properties of dielectric ceramics down to monolayer thickness and to examine the roles of surface functionalization and interface interactions in these systems. This project includes the preparation of $MTiO_3$ and $MRuO_3$ nanosheets (M = metal) using innovative synthetic strategies, characterization of their dielectric and ferroelectric properties, and the development of solution-based processing methods that can lead to hybrid materials containing nanosheet components.

This research was selected for funding by the Office of Basic Energy Sciences.

From Cosmological Observations to Fundamental Interactions

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This research spans a wide range of topics within cosmology and has the purpose of enabling us to learn about very fundamental physics from astronomical observations. In the first part, techniques known as 'effective field theory' will be used to study the effects of processes that took place in the very early phase of the history of our Universe when it expanded rapidly and enormously, the very beginning of the Big Bang. These effects propagate during the development of the Universe over time and result in properties that can be observed today through various astronomical measurements. The improved precision of these measurements renders inadequate the previous analysis techniques. This calls for a new tool, 'effective field theory,' which has a proven track record in the particle physics context but has not yet been fully applied to cosmological physics. This tool allows the study of all possible interactions relevant during early inflation towards the determination of their resulting imprint on the current Universe. Additionally, it allows a study of the effect of compact dense concentrations of matter on the development of structures in the Universe such as galaxies. The second part of the program will apply directly to the astronomical data the theoretical understanding realized via the first part. This entails a development and application to data of new analysis techniques aimed at the search for new signatures of early inflation. One such technique is the analysis of the statistics of the so-called 'primordial perturbations.' By using these sophisticated techniques to quantify the effects of inflation on what we may see today, this research program will allow scientists to use current and future astronomical data to explore the remarkable window onto what happened in the mysterious and enigmatic birth of our Universe.

This research was selected for funding by the Office of High Energy Physics.

Engineering High Field Superconducting Materials for Frontier Accelerator Technology

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The objective of this project is to transform high-field superconductors, particularly $Bi_2Sr_2CaCu_2O_x$, a high-temperature superconducting material that has magnetic field upper limits surpassing 100 Tesla at 4.2 K and can be fabricated into a multifilamentary round wire, to practical magnet conductors that can be used to generate fields above 20 Tesla for the next generation of accelerators. Studies will focus on (1) understanding the micro- and nano-structures that produce high critical current density J_c in long-length conductors through extensive electromagnetic measurements and innovative micro-structural characterizations; (2) advancing high-temperature superconducting magnet engineering through designing, fabricating, and testing $Bi_2Sr_2CaCu_2O_x$ insert coils that reach 30 Tesla in a useful aperture of >30 mm. This research will result in a high-performance, 20-50 Tesla class conductor for the next generation of accelerators and spectrometers for medical imaging and advanced materials research. The fundamental understanding gained of superconductor synthesis and how nanostructure underpins the superconducting property will provide insights for the development of a large class of superconducting materials for magnet and energy applications.

This research was selected for funding by the Office of High Energy Physics.

Advanced Simulation Tools for Muon-Based Accelerators

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The objective of this project is to develop new modeling tools based on modern software frameworks, G4beamline and COSY Infinity, and to incorporate the most accurate theoretical calculations and experimental data available for crucial and not-yet-considered physics processes specific to muon accelerators. This study will substantially enhance the confidence that the tools used in assessing the feasibility of a muon collider or a neutrino factory will accurately represent the performance of a real machine. This work is critical to the support of long-range exploratory physics work aimed at developing new concepts. To pursue the computationally intensive analysis techniques required by this research, high-performance computing and general-purpose computation on graphics processing units will be employed. Tools developed during the project will be used on a daily basis to perform simulations that explore, evaluate, and validate the design of a muon collider that is the centerpiece of the national Muon Accelerator Program. Computer codes will be made accessible to the scientific community and will also be applicable to other existing and future muon facilities.

This research was selected for funding by the Office of High Energy Physics.

Trimodal Tapping Mode Atomic Force Microscopy: Simultaneous 4D Mapping of Conservative and Dissipative Probe-Sample Interactions of Energy-Relevant Materials

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This project aims to develop a multifrequency atomic force microscopy method with which it will be possible to perform rapid measurements of the conservative and dissipative forces between a sharp probe and a sample surface simultaneously as the sample topography is recorded. The new technique will have four-dimensional capabilities, allowing force measurement as a function of the three spatial coordinates and vertical velocity of the probe. The method will be applied to characterize the deformation-dependent electromechanical response of fuel-cell alkaline anion exchange membranes under accelerated degradation conditions as a function of temperature, relative humidity, and mechanical strain. The project will include both experimental and computational activities and will enable the use of a unique scanning probe technology to study the mechanisms through which fuel cell and battery materials degrade and to quantify their loss in performance along the way. Such understanding will be useful in the development of new, better performing materials or in providing guidance in extending the useful life of existing materials.

This research was selected for funding by the Office of Basic Energy Sciences.

Deciphering the Genetic and Molecular Underpinnings of Carbohydrate-Degrading Systems in Ruminal Bacteria

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Biofuels like ethanol can be obtained from cellulose present in plant cell walls. A challenge in the production of biofuels is the efficient breakdown of cellulose into simple sugars. Current industrial approaches rely on cocktails of cellulose-degrading enzymes. These strategies can be improved by identifying and characterizing more active enzymes. Arguably the most optimized natural cellulose degrading system is found in the rumen of domesticated cows. The rumen contains a diverse group of bacteria with highly active enzymes that digest cellulose in feed and convert this energy source into nutrients usable by the cow. This research will characterize the mechanism through which three bacteria from the rumen degrade cellulose. Each of these bacteria employs different strategies for cellulose degradation and will provide contrasting models that can increase our understanding of this fundamental process. This work will leverage existing genomic sequences for these bacteria to identify the genes and enzymes relevant for cellulose degradation. Importantly, these enzymes will be purified and biochemically tested for their capacity to degrade cellulose. Novel enzymes characterized in this way will not only expand our current set of cellulose-degrading enzymes but will also provide insights into how these specialized microbes accomplish cellulose degradation in natural systems. The results of this research will advance the DOE mission for the production of advanced biofuels.

This research was selected for funding by the Office of Biological and Environmental Research.

Linking the Codependence of Grain Boundary Structure and Density to Defect Evolution Mechanisms During Radiation Damage

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Development of materials that can withstand high doses of radiation is a key goal for the future of nuclear reactor operation. There has been an increased interest in nanocrystalline materials as candidates for nuclear reactor components because of their increased strength and theoretical resistance to radiation damage, but there is still not agreement about how grain boundary structure and proximity influence the development of damage. The objective of this work is to develop an understanding of the mutual dependence of damage accumulation on atomic scale grain boundary structure and density during irradiation. An in-situ transmission electron microscopy (TEM) approach will be taken to measure damage evolution kinetics during irradiation of model nanocrystalline materials. This technique will be used in conjunction with high-resolution analytical tools to elucidate structure and composition of these selected materials following irradiation. The information gained from these in-situ and ex-situ studies will yield mechanistic understanding of defect incubation and clustering that occurs during irradiation. These experiments will be enhanced by simulations for a more complete understanding of fundamental mechanisms at time and length scales that would otherwise be inaccessible with experimental techniques. The results obtained from this research will give rise to a predictive understanding of microstructural features in candidate materials for future advanced nuclear energy applications.

This research was selected for funding by the Office of Basic Energy Sciences.

Jet Probes of a New State of Matter

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The past decade has seen remarkable success in nuclear science at the high-energy frontier. Breakthroughs in the identification and initial characterization of a new state of matter, the quark-gluon plasma (QGP) produced at the Relativistic Heavy Ion Collider (RHIC), have been a highlight of this program. Today, there is a need for theoretical research that can elevate the investigation of nuclear matter under extreme conditions to a new level of precision and fully use the RHIC and the Large Hadron Collider (LHC) experimental heavy ion capabilities. This project will advance the theory of jets in nuclear collisions and employ these jets as powerful probes of the strongly interacting plasma. Our goal is to develop new tools for precision in-medium jet studies based on next-to-leading order perturbative Quantum Chromodynamics (QCD) and Soft Collinear Effective Theory (SCET). We will identify experimental observables that can differentiate between competing paradigms of particle production and interaction in the QGP. The expected outcome of this project will be a significant reduction of the current large uncertainty in the determination of plasma properties such as density, opacity, and transport coefficients.

This research was selected for funding by the Office of Nuclear Physics.

Regularized Finite Element Formulations for Shear Band Instabilities in Metals

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This project aims for an improved understanding of material instabilities in the development of advanced materials. A striking manifestation of instability in solids is the existence of shear bands, the localization of shear strain into narrow bands during high-speed deformation of metals such as those that occur in impact or blasts. Shear bands are indicators of irreversible damage that eventually cause fracture. New multiscale algorithms will be developed for enabling realistic, physics-based predictive models of materials fracture using high-performance computers. By understanding the true mechanisms that drive materials fracture, this research could aid in tackling important issues such as creation of more durable “green" materials; geologic sequestration of contaminants such as carbon dioxide in the fractured seabed; fracture of ice sheets in polar regions and their effect on global climate change; and the design of infrastructure that is resilient to natural disasters and man-made hazards.

This research was selected for funding by the Office of Advanced Scientific Computing Research.

Precision Measurement of Electron Antineutrino Disappearance in the Daya Bay Experiment

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Experimental observations have established that neutrinos undergo transitions from one type to another as they travel. The Daya Bay reactor neutrino experiment has recently observed the disappearance of electron-type antineutrinos from reactor cores at the Daya Bay Power Plant located in China. This observation allowed Daya Bay to make a measurement of the neutrino mixing parameter ϑ_{13}, which was previously only known to be small in comparison to the other neutrino mixing parameters. Daya Bay continues to take data and will improve upon this measurement in the near future. The Daya Bay antineutrino detectors are located underground to shield them against cosmic ray muons, and a veto system is used to detect cosmic muons that could produce background events. This program will focus on the study of cosmic muon-induced backgrounds at Daya Bay with a goal of achieving the lowest possible level of background-related systematic uncertainty on the disappearance measurement. Additionally, data from the veto system will be used to make measurements of the muon flux and the production of neutrons and radioactive nuclei by cosmic muons. These measurements will be of general interest to other experiments that are sensitive to cosmic muon-induced backgrounds such as neutrinoless double β decay and dark matter searches.

This research was selected for funding by the Office of High Energy Physics.

Periodicity and the Role of the 5f-Electrons at Protactinium

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The assessment and development of viable alternative nuclear fuel cycles for nuclear energy systems relies on our ability to rationally and deliberately control the molecular level chemical behavior of these systems. The actinides (thorium, protactinium, uranium, plutonium) are major chemical components of these complex systems. Controlling and predicting their chemistry can be accomplished through a fundamental understanding of how these elements form molecular complexes or chemical bonds. The difficulty in describing the chemistry of actinide bonding arises from our lack of knowledge regarding the particular contributions to bond formation each of the actinide electronic orbitals makes to the molecular bond. Differing contributions to molecular bonding from different electronic orbitals vastly changes the structure, geometry, reactivity and stability of molecular complexes. In the actinide elements the electronic orbitals of interest in bond formation are the f-orbitals, the orbitals that define them as actinides, and the d-orbitals that drive the chemistry of the transition metals. The aim of this research program is to investigate the contributions of the f and d orbitals to actinide bonding by focusing on the second actinide element, protactinium. Protactinium is uniquely situated at the electronic intersection of actinide-f and transition metal-d chemistries, its 5f and 6d orbitals are nearly identical in energy. The small differences in the orbital energies at protactinium, in contrast to later actinides such as plutonium, make it the ideal candidate to study and quantify how the differing orbital interactions and contributions manifest themselves in the geometry, structure and reactivity of actinide complexes. Invaluable insight for rational manipulation, modeling, and controlling the chemistry and bonding across the entire actinide series will be obtained by coupling the results of this study of protactinium's coordination chemistry, structural, and spectroscopic properties with the established periodic trends in electronic structure and bonding in the early actinides and transition metals. The knowledge and understanding derived from this study of the chemistry of protactinium bonding will provide the basis upon which to unify our understanding of electronic and bonding interactions across the entire periodic table.

This research was selected for funding by the Office of Basic Energy Sciences.

Free Radical Reactions of Hydrocarbons at Aqueous Interfaces

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Chemical reactions that occur at hydrocarbon/water and electrolyte interfaces govern a wide array of environmentally and technologically important processes, including electrochemistry, aerosol photo-oxidation, cloud chemistry, corrosion, and heterogeneous catalysis. Hydrocarbon free radicals, formed at these interfaces, play important roles in the chemistry as initiators or propagators of surface reactions or as reactive intermediates. Two experimental techniques will be used in new ways to examine the surface chemistry of hydrocarbon free radicals at gas/liquid interfaces. The atomic and molecular changes at the surface of micron-sized droplets will be measured by ambient pressure X-ray photoelectron spectroscopy. A surface sensitive mass spectrometer will be used to make kinetic measurements of reaction rates and product distributions. The objective of this research is provide a molecular description of the reaction pathways that lead to either bulk solvation of an organic molecule or its removal from the interface through decomposition into gas phase products. These interfacial processes are important for understanding and eventually predicting the environmental fate of hydrocarbon byproducts of energy use and consumption.

This research was selected for funding by the Office of Basic Energy Sciences.

In Situ Scanning Force Microscopy Studies of Cross-coupled Domains and Domain Walls

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The objective of this project is to explore the nanoscale emergent phenomena and to understand the unconventional properties of cross-coupled domains and domain walls in multiferroics, where both ferroelectricity and magnetism coexist. The giant magnetoelectric effect due to coupled ferroic orders in multiferroics is of both fundamental and technological interest and is promising for energy-efficient multifunctional applications. The presence of domains and domain walls is a distinguishing feature of any ferroic order; their responses to external stimuli determine the macroscopic properties and the functionalities of ferroic materials. To address the challenges and to directly visualize the cross-coupled domains and domain walls and their responses to the applied electric and magnetic fields, this project will develop a unique, high-resolution and high-sensitivity in situ scanning force microscopy (SFM). The real space imaging of domains and domain walls by SFM aims to fundamentally understand the nature of magnetoelectric cross-coupling in representative multiferroic and magnetoelectric materials.

This research was selected for funding by the Office of Basic Energy Sciences.

Advanced Seeding, Beam Manipulation and Beam Diagnostic Techniques for Next Generation X-ray Free Electron Lasers

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X-ray free electron lasers can provide tunable high-power coherent radiation that enables forefront sciences in various areas. This project aims to develop critical techniques that will greatly enhance the capability of next-generation X-ray free electron lasers in delivering X-ray pulses with narrower bandwidth (close to Fourier transform limit) and shorter pulse width (less than 1 femtosecond, or 10^{-15} seconds). These ultra-short, ultra-narrowband X-rays will allow four-dimensional visualization of molecular and atomic dynamics, offering new possibilities of studying ultra-fast processes at the atomic and molecular level. The research will focus on (1) studying advanced seeding and beam manipulation techniques that promise generation of fully coherent X-ray pulses at a wavelength of about 1 nm, (2) pursuing advanced techniques to mitigate coherent synchrotron radiation and other collective effects for generation of ultra-short electron bunches, and (3) developing novel methods to measure ultra-short electron bunches. The outcome of this research should enhance the core capabilities of accelerator-based X-ray light sources and potentially open up many new opportunities for X-ray sciences.

This research was selected for funding by the Office of Basic Energy Sciences.

Photon-Electron Interactions in Dirac Quantum Materials

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The objective of this research is to understand and control electron, photon, and phonon interactions in new classes of Dirac quantum materials such as graphene and topological insulators. These materials have unusual physical properties that hold promise for novel energy harvesting technologies. The proposed work will investigate the fundamental and technical aspects of these materials using the combination of ultrafast optical spectroscopy and electrical transport measurements. Spatially and temporally resolved photocurrent measurements will allow exploration of the novel electronic response of these materials to optical excitation. This includes energy transport by non-equilibrium Dirac quasiparticles, carrier distribution and dynamics of topologically protected spins, and spin and valley Hall effects. The resulting fundamental understanding may lead to new energy-efficient applications in high-speed electronics, dissipation-free spintronics, and photovoltaics.

This research was selected for funding by the Office of Basic Energy Sciences.

Computational Bayesian Framework for Quantification and Reduction of Predictive Uncertainty in Groundwater Reactive Transport Modeling

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Subsurface environmental systems, in which intricate biogeochemical processes interact across multiple spatial and temporal scales, are open and complex. Understanding and predicting system responses to natural forces and human activities is indispensable for environmental management and protection. However, predictions of the subsurface system are inherently uncertain, and uncertainty is one of the greatest obstacles in groundwater reactive transport modeling. The goals of this project are to (1) develop new computational and mathematical methods for quantification of predictive uncertainty and (2) use the developed methods as the basis to develop new methods of experimental design and data collection for reduction of predictive uncertainty. The proposed computational Bayesian framework is general and compatible with other widely used reactive transport models and numerical codes, so the advances can be easily applied to gain insights into subsurface biogeochemical processes that occur across a wide range of field sites and environmental conditions.

This research was selected for funding by the Office of Biological and Environmental Research.

Enhancing Metabolic Flux to Photosynthetic Biofuels

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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.

This research was selected for funding by the Office of Biological and Environmental Research and the DOE Experimental Program to Stimulate Competitive Research.

Next-Generation Optimization under Uncertainty: Structure-Oriented Algorithms

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With the advent of the smart grid, renewable technologies, and carbon emission programs, a key concern is the coordination of national infrastructures such as the electricity, natural gas, and water supply network systems. Anticipating and mitigating uncertainty of weather, demands, and contingencies in a more integrated environment are necessary to maximize resource efficiency and prevent cascading failures that can ultimately lead to catastrophic shortages of supplies. This project will develop scalable high-performance computing algorithms that will aid the design and real-time dispatch operations of national energy infrastructure systems.

This research was selected for funding by the Office of Advanced Scientific Computing Research.

Understanding Liquid Argon Neutrino Detectors: Moving from Art to Science

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One of the most surprising and important developments in particle physics in the last decade has been the discovery that neutrinos can change from one type to another and hence must have mass. A new generation of experiments are needed to investigate this phenomenon of neutrino oscillation and its implications. To pursue this physics, large liquid argon (LAr) time projection chambers (TPCs) are particularly intriguing detector options because they can image particle trajectories with stunning detail and precision. One challenge posed by LAr TPCs is that few neutrino events have ever been fully reconstructed in such devices, which makes it difficult to estimate their performance on complex neutrino interactions. To quantify the capabilities of such detectors for neutrino physics, this research will focus on the analysis of data collected in the exposure of modestly-sized LAr TPCs to intense particle beams at Fermilab. The goals are to build expertise with this very promising technology, to inform the design of potential future long-baseline neutrino detectors, and to provide an improved understanding of nuclear effects that complicate low energy neutrino interactions.

This research was selected for funding by the Office of High Energy Physics.

Search for New Physics and Upgrade of the Muon Spectrometer at ATLAS

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The very successful operation of the Large Hadron Collider (LHC) in the first two years has enabled physicists to venture far into unexplored territories of the Tera-electron-volts energy scale and has provided unique opportunities to make fundamental discoveries in particle physics. This research will focus on searching for new physics with vector gauge boson pairs or lepton pairs with the ATLAS (A Toroidal LHC ApparatuS) experiment. These studies could provide insights to the source of electroweak symmetry breaking or the existence of new dynamics and new force carriers. In order to maximize the discovery potential at the energy frontier, this project also aims to improve the performance of the ATLAS muon spectrometer by developing an upgrade strategy for the forward muon trigger system for future high energy and high luminosity physics programs at the LHC.

This research was selected for funding by the Office of High Energy Physics.

Growth and Properties of New Epitaxial Metal/Semiconductor Nanocomposites

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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.

This research was selected for funding by the Office of Basic Energy Sciences and the DOE Experimental Program to Stimulate Competitive Research.