Biomimetic Templated Self-Assembly of Light Harvesting Nanostructures

Dr. Alfredo Alexander-Katz, Assistant Professor
Department of Materials Science and Engineering
Massachusetts Institute of Technology
Cambridge, MA 02139

Inspired by the most efficient light-harvesting antenna found in nature called the chlorosome, this project will explore and understand from a theoretical perspective templated supramolecular self-assembly of natural and synthetic organic chromophores. Of particular interest is the self-organization of such organic dyes in block copolymer matrices. This system is meant to mimic elements present in naturally occurring light-harvesting nanostructures and transfer them to synthetic systems to identify under what conditions it is possible to self-assemble (or even perfect) such remarkable nanostructures. Through development of theoretical models and by performing simulations over a wide range of copolymer parameters and dye chemistries, a fundamental understanding of this system will be achieved. Since block copolymers offer the opportunity to control supramolecular assembly morphology and spatial localization, this knowledge could lead to new mesoscale materials that have enhanced transport properties and potentially could direct the flow of energy. This has many potentially transformative applications in which photon harvesting and energy conversion are key elements, such as solar cells and thermoelectric materials.

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

Adsorbate Interactions in Catalytic Trend Studies

Dr. Thomas Bligaard, Senior Staff Scientist
SUNCAT Center for Interface Science and Catalysis
Chemical Sciences Division
Photon Science Directorate
SLAC National Accelerator Laboratory
Menlo Park, CA 94025

There is a constant drive toward more energy- and resource-efficient technologies, for example related to the use of natural gas or biomass, and new sustainable energy processes. A key element in most novel energy technologies is the need for new, efficient catalysts made from Earth-abundant materials. The atomic-scale design of catalytic materials with tailored properties represents a scientific grand challenge. Computational catalyst search approaches leveraging electronic structure theory based atomic-scale simulations coupled with kinetic models constitute a promising avenue for future catalyst discovery efforts. To reliably address detailed catalytic properties, such as product selectivity, the simulation accuracy needs to be improved significantly. The absence of suitable models for reliably including interactions between adsorbates presents a leading contribution to the inaccuracy in computational catalysis trend studies. This project aims to improve the fundamental understanding of the interactions between adsorbed atoms and molecular fragments on transition metal surfaces and devise models to include these interactions in catalytic trend studies. The scientific insights and the set of tools established in this project aim to create a break-through in obtaining quantitative agreement between theoretical catalysis studies and experimental measurements and could potentially become a cornerstone in establishing an accurate and reliable “Catalyst Genome”.

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

Integrating Advanced Software and Statistical Methods for Spectroscopic Dark-Energy Surveys

Dr. Adam S. Bolton, Assistant Professor
Department of Physics and Astronomy
University of Utah
Salt Lake City, UT 84112

The physical nature of the dark energy (DE) that drives the present-day accelerated expansion of the universe is one of the most fundamental mysteries in science. All current experimental prospects for understanding DE are found in observational cosmology, and rely on the measurement of cosmological Doppler shifts ("redshifts") with telescopes and spectrographs. This research will develop and implement next-generation software algorithms and statistical methods for the optimal analysis of data from spectroscopic DE experiments, integrating all levels from raw detector pixels to high-level DE science with: (1) calibration methods for determining and representing the relationship between electromagnetic stimulus and detector response; (2) extraction methods for the lossless compression of raw detector data into one-dimensional spectra of galaxies and quasars; (3) classification and redshift-measurement methods based on hierarchical Bayesian statistics; and (4) DE parameter-measurement methods incorporating the full information content of the experimental data. This work will enable spectroscopic DE surveys to maximize their efficiency and realize their full power in illuminating the dark sector of the universe.

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

Energy-Efficient Parallel Graph and Data Mining Algorithms

Dr. Aydın Buluç, Computational Research Scientist
Complex Systems Group
Computational Research Division
Computing Sciences Directorate
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

Data are fundamental sources of insight for experimental and computational sciences. The Department of Energy (DOE) acknowledges the challenges posed by fast-growing scientific data sets and more complex data. The graph abstraction provides a natural way to represent relationships among complex fast-growing scientific data sets. On future exascale systems, power consumption is of primary concern yet existing graph algorithms consume too much energy per useful operation due to their high communication costs, lack of locality, and inability to exploit hierarchy. This project explores methods to increase the energy efficiency of parallel graph algorithms and data mining tasks. A new family of algorithms will be developed to drastically reduce the energy footprint and running time of the graph and sparse matrix computations that form the basis of various data mining techniques. This project will also exploit the well-known duality between graph and sparse matrices to develop communication-avoiding graph algorithms that consume significantly less power. This project is relevant to DOE mission-critical science including bioinformatics and genomics with particular emphasis on plant genomics that can result in better biofuels through efficient genetic mapping, climate science where recent graph-based methods show increased accuracy in hurricane predictions, and combustion science where graph search techniques are used to analyze extreme-scale simulation data.

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

Develop On-Demand Nanoplasmonic Device Concepts in a Semiconductor Compatible Hybrid System

Dr. Cheng Cen, Assistant Professor
Department of Physics
West Virginia University
Morgantown, WV 26506

The objective for this project is to develop an on-demand nanoplasmonic platform that combines emerging oxide nanoelectronics with a low-loss semiconductor-friendly plasmonic material – graphene. In the heterostructures of graphene/$LaAlO_3$/$SrTiO_3$, the nanoscale conducting structures at $LaAlO_3$/$SrTiO_3$ interfaces reversibly patterned by conducting atomic force microscope (c-AFM) will be used to spatially modulate the chemical potential in the top graphene layer and provide dynamic confinement and manipulations of plasmon modes in graphene. Various rewritable nanoplasmonic devices, including waveguides, active modulators, on chip light source and sensors, will be explored by c-AFM lithography and in-situ near field scanning optical microscopy. The successful development of such hybrid plasmonic platform will enable creation of on demand nanoplasmonic devices in one single step and can potentially lead to tantalizing applications in single molecule spectroscopy, scalable solid state quantum information processing and novel plasmon probes for various interesting material quanta in condensed matter physics.

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

Exploring Fundamental Physics through New Measurements of the Cosmic Microwave Background Polarization

Dr. Clarence L. Chang, Assistant Scientist
Astrophysics and Cosmology Group
High Energy Physics Division
Physical Sciences and Engineering Directorate
Argonne National Laboratory
Lemont, IL 60439

The Cosmic Microwave Background (CMB) is the relic radiation from 400,000 years after the Big Bang. The CMB is an image of the early universe and a unique window into fundamental physics. The goal of this research program is to measure a faint signal embedded in the polarization pattern of the CMB. This signal, called "B-modes," has never been seen and will explore two scientific topics. The first topic is the nature of inflation, the theorized rapid exponential expansion of the early universe, taking place between 10^{-36} and 10^{-32} seconds after the Big Bang. CMB "B-modes" are the unique probe of this physics. Interestingly, the physics of inflation connects directly to our understanding of physics at high energies. Inflation is expected to take place at energies of about 10^{16} GeV, the same energy scale favored by Grand Unified Theories of Particle Physics. The second scientific goal of this program is to use CMB "B-modes" to measure the mass of the neutrinos. It is well understood that neutrinos are massive, however, the value of the neutrino mass is currently unknown. This award will support a program pursuing these science objectives through two research activities. The first activity is analyzing data from the South Pole Telescope polarization (SPT-Pol) experiment, a recently deployed CMB polarimeter on the South Pole Telescope. SPT-Pol uses a focal plane comprised of custom designed and fabricated detectors using superconducting technology. With this focal plane, SPT-Pol will be able to make the first observations of CMB "B-modes." The second activity is the development of new superconducting detector technology for next generation CMB experiments. This technology would enable the construction of future CMB instruments that will be 10-100 times more powerful than the current state-of-the-art South Pole Telescope-Polarization (SPT-Pol)

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

The Higgs Frontier

Dr. Clifford W. Cheung, Assistant Professor of Theoretical Physics
Department of Physics
California Institute of Technology
Pasadena, CA 91125

The recent discovery of a new particle consistent with the Higgs boson completes the table of the fundamental particles predicted in the Standard Model (SM) of particle physics. The aim of this research is to determine the implications of present and future Higgs measurements for fundamental physics at the energy, intensity, and cosmic frontiers. At the Energy Frontier, modified Higgs properties are a smoking gun for new weak scale particles. The proposed work will establish a systematic mapping between observed Higgs properties and simplified models of new physics. In turn, these effective theories will be used to hone targeted searches for new weak scale particles, and address fundamental questions about vacuum stability and grand unification. At the Intensity Frontier, numerous hidden sector models couple to the SM through the Higgs boson or closely related particles. The proposed work will explore the ramifications of Higgs properties for hidden sectors and their phenomenology at high intensity probes like B-factories, fixed target experiments, and neutrino observatories. At the Cosmic Frontier, the Higgs boson critically affects direct detection constraints for many models of weakly interacting massive particle (WIMP) dark matter (DM). Intriguingly, these theories presently lie at the experimental tipping point between observation and exclusion. The proposed work will utilize simplified models of DM to help exclude the majority of thermal relic WIMP DM theories within the next generation of direct detection experiments. This work will also study the cross-correlations between DM direct detection and Large Hadron Collider (LHC) limits, and the implications of Higgs measurements for early universe cosmology. Key elements of this research proposal employ a simplified model framework, defined here to be the SM augmented by the handful of new particles relevant to a given observation. From a purely theoretical perspective, simplified models are advantageous because they eliminate extraneous states and parameters which typically accompany ultraviolet completions; experimentally, they are observationally inclusive, and have been actively adopted by experimentalists at the LHC in a variety of direct searches for new physics.

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

Experiments and Simulations of Hypervelocity Impact Plasmas

Dr. Sigrid Close, Assistant Professor
Department of Aeronautics and Astronautics
Stanford University
Palo Alto, CA 94305

Hypervelocity particles, including meteoroids and space debris with masses smaller than 1 microgram, routinely impact spacecraft. Upon impact, a particle vaporizes and ionizes itself and part of the spacecraft surface, producing a dense plasma that expands and radiates electromagnetic energy. However, the behavior of the resulting plasma and its potential to produce a spacecraft anomaly remains unknown. This research effort will investigate plasmas generated by hypervelocity impacts in order to characterize the behavior of the expanding plasma and its interactions with the ambient environment. The project will include experimental campaigns to be conducted at a dust accelerator facility that can accelerate particles up to 60 km/s, which is representative of meteoroid speeds, and at a light gas gun facility that can accelerate larger projectiles up to 7 km/s, which is representative of orbital debris. The experiments will use plasma, optical and radio frequency sensors to characterize the dynamics and associated emission resulting from hypervelocity impact plasmas. This project will also combine the collected data with results from numerical simulations using particle-in-cell (PIC) and smoothed particle hydrodynamics (SPH) techniques. The results from both experimental measurements and simulations will provide a new understanding of the mechanism for the onset of instabilities and turbulence that can lead to radio frequency emission by these plasmas.

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

Extreme Expression of Cellulases in Poplar

Dr. Heather D. Coleman, Assistant Professor
Department of Biology
Syracuse University
Syracuse, NY 13244

Cellulose, the major component of plant cell walls, is composed of long chains of sugars linked together. Plant cellulosic biomass (stalks, trunks, stems, and leaves) provide a vast, untapped source of sugars that can be fermented to produce biofuels. Sugars are extracted from biomass using enzymes (cellulases) that break down cellulose. However, a major roadblock to developing an economically viable cellulosic biofuel production process is the cost of those enzymes, typically produced and purified using bacteria or fungi. An alternative and potentially more economic approach is to produce the enzymes within the plant itself. The goal of this research is to implement a new genetic engineering technology to produce large amounts of exogenous cellulases into poplar cells. This technology allows the researcher to control the production of the enzymes within the plant using an inducer substance that triggers the rapid accumulation of the cellulases. The transformation of poplar trees using this approach will increase the efficiency of converting cellulose to fermentable sugars and will increase our understanding of plant cell walls. Furthermore, the cellulases produced by these transformed trees could be purified in a cost-effective way, paving the way for developing a sustainable alternative for the production of biofuels from woody feedstocks.

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

First Principles Predictions of Phase Stability in Complex Oxides

Dr. Valentino R. Cooper, Research and Development Staff Member
Advanced Materials Group
Materials Sciences and Technology Division
Physical Sciences Directorate
Oak Ridge National Laboratory
Oak Ridge, TN 37831

The goal of this project is to use first principles methods to predict materials with enhanced properties that *can be synthesized* and remain *active under device relevant conditions*. Theory and computation have become an integral part of the materials discovery process. Theory and computation have become an integral part of the materials discovery process. Electronic structure methods, for example, excel at the prediction of macroscopic properties in materials that have yet to be grown. Unfortunately, predictions of synthesizability and operability are less straightforward. Temperature, pressure and the stability of competing phases are amongst the litany of factors that determine whether a material can be made or will exhibit favorable properties under the required operating conditions. This project aims to develop and implement robust, high-throughput computational approaches for exploring phase stability to facilitate the prediction-to-synthesis process. Addressing this challenge will require strong synergy between (i) electronic structure calculations for properties predictions, (ii) phenomenological/empirical models for examining phase stability as related to competing secondary structures and temperature- and pressure-dependent transitions and (iii) experimental validation. The abundance of possible cation chemical identities and arrangements makes complex perovskite oxides an ideal playground for these studies, especially since this variability gives rise to both a wide array of physical, chemical, electrical and magnetic properties as well as to possible competing structures. In this vein, this project is focused on the identification of solid solutions of complex oxides with enhanced piezoelectric properties. These materials are fundamentally important in many modern technologies such as high-resolution ultrasound machines and fuel injectors in clean burning and efficient diesel engines. It is anticipated that more responsive, lead-free materials may enable new and exciting technologies. Equally important is the fact that the framework implemented in this project will be applicable to a wide range of materials; thus having a broader impact for accelerating the design and experimental realization of novel materials.

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

Fast, Dynamic, and Scalable Algorithms for Large-Scale Constrained Optimization

Dr. Frank E. Curtis, Assistant Professor
Department of Industrial and Systems Engineering
Lehigh University
Bethlehem, PA 18015

Scientists and engineers are constantly faced with the task to optimize an objective subject to physical, environmental, or resource constraints. The technique of using mathematical models to formulate and find real solutions of such problems is known as mathematical optimization, a process that has become invaluable for design and discovery in numerous scientific fields. This project will involve the development and implementation of high-performance computing algorithms for solving cutting-edge optimization problems. These include problems that involve (1) data uncertainties, such as those in the future supply, demand, and capacity of a given power system, (2) extreme numbers of alternatives, such as in the design of electrical power grids to avoid network vulnerabilities, and (3) real-time decisions, such as in the control of chemical reactors. The key features of these new algorithms are that they will be fast, dynamic, and scalable to meet the computational requirements of scientists and researchers working to optimize large-scale, complex systems.

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

Multiple Coupled Potential Energy Surfaces with Application to Combustion

Dr. Richard Dawes, Assistant Professor
Department of Chemistry
Missouri University of Science and Technology
Rolla, MO 65409

Hydrocarbon combustion involves the dynamics of numerous small radicals such as HO_2, HCO, and HOCO. Dynamical calculations for these relatively simple systems are very sensitive to the detailed topography of their global potential energy surfaces (PESs). The objective of this research is to develop general strategies for robustly convergent electronic structure theory for global multichannel reactive surfaces, particularly for molecular systems important to combustion. Combining advances in ab initio methods with automated interpolative PES fitting allows the construction of high-quality PESs incorporating thousands of high level data to be done rapidly through parallel processing on high-performance computing (HPC) clusters. This project will benefit the combustion community by facilitating rapid and routine development of global PESs and subsequent dynamics studies.

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

From Quarks to the Cosmos: Ab Initio Studies in Nuclear Physics

Dr. William Detmold, Assistant Professor
Department of Physics
Massachusetts Institute of Technology
Cambridge, MA 02139

The Standard Model provides the basis for our understanding of the world at the smallest scales. A central part of the Standard Model is Quantum Chromodynamics (QCD), which describes the strong interactions between quarks and gluons, interactions that bind them together into protons and neutrons and, ultimately, into nuclei. A central goal of nuclear physics is to understand the mechanisms and consequences of these interactions. Because of their complexity, the equations describing QCD can so far only be solved numerically using supercomputers. This research will expand the regimes in which these numerical methods can be applied, enabling Standard Model investigations of central questions in nuclear physics. In particular, the spectrum, structure and decays of light nuclei and hyper-nuclei (exotic cousins of nuclei that contain so-called strange quarks) will be computed, providing important comparisons for contemporary experiments at Thomas Jefferson National Accelerator Facility and other laboratories around the world. In addition, the research will investigate the two-body and three-body interactions between protons, neutrons and hyperons (particles similar to the proton but containing strange quarks) that play crucial roles in the dense interiors of supernovae and neutron stars.

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

Neutrinoless Double-Beta Decay Searches and Other Fundamental Physics Measurements with Ultra-Low Background Enriched-Germanium Detectors

Dr. Jason A. Detwiler, Assistant Professor
Department of Physics
University of Washington
Seattle, WA 98195

The goal of this research is to search for neutrinoless double-beta decay, weakly-interacting massive particle dark matter, solar axions, and other rare processes using germanium detectors. Detection of any of these physics particles and processes would have vast implications for our understanding of nature; from our description of the fundamental particles and their interactions, to hints toward grand unification of the forces of nature, to the potential resolution of the unexplained excess of matter over antimatter in the observable universe. Central to this effort will be research on the Majorana Demonstrator project, which is under construction at the Sanford Underground Research Facility in Lead, South Dakota. This project will support participation in the construction and commissioning of the enriched germanium detector modules, in detector operations and data taking, and coordination of the data analysis effort. A detector research and development laboratory will also be set up at the University of Washington to make auxiliary measurements to further constrain potential backgrounds in the Majorana Demonstrator experiment, and to prototype and evaluate detector upgrades that will enable future, more sensitive experiments.

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

Edge Pedestal Structure Control for Maximum Core Fusion Performance

Dr. Ahmed Diallo, Staff Research Physicist
National Spherical Torus Experiment Upgrade
Plasma Science and Technology Department
Princeton Plasma Physics Laboratory
Princeton, NJ 08543

The anticipated performance of future fusion reactors such as ITER and a Fusion Nuclear Science Facility (FNSF) will rely on controlling the edge of the plasma. The edge plasma region is especially important since the plasma temperature rises very rapidly over a short distance in this region, and high plasma temperature is essential to maximizing fusion power. If the edge is not controlled properly, edge-localized instabilities can rapidly transport heat from the core and deposit large bursts of energy onto plasma-facing components. These energy bursts can damage the components, and the component materials can pollute the plasma and reduce the fusion power. The edge region of the plasma where the temperature changes most rapidly is typically a few centimeters wide and is referred to as the pedestal. This research project is aimed at understanding the physical mechanisms governing the pedestal during its formation, and subsequently, at demonstrating how to control the pedestal on National Spherical Torus Experiment-Upgrade (NSTX-U) at the Princeton Plasma Physics Laboratory. To achieve this goal, the project is divided into two major phases. First, this research will establish how the edge is formed and evolves before destabilizing the plasma by analyzing the evolution of pedestal density and temperature profiles. Once the evolution of the pedestal is understood, the second phase will consist of controlling it through the use of a combination of stimulated particle expulsion and external fueling actuators (e.g., granule injectors or radio frequency waves) to increase or reduce the density of the pedestal. When the appropriate level of expulsion and/or fueling is determined, it will be integrated onto NSTX-U for optimum plasma operation as part of the final phase. The successful demonstration of this edge control is paramount to achieve maximum fusion power and efficiency and will provide the knowledge base for extending advanced edge control techniques to next-step fusion devices.

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

The Nature of the Spin Dependent Surface Chemical Bond: Spin-Polarized STM Studies of Metal-Organic Interfaces

Dr. Daniel B. Dougherty, Assistant Professor
Department of Physics
North Carolina State University
Raleigh, NC 27695

This project applies spin polarized scanning tunneling microscopy and spectroscopy to characterize interactions between organic molecular materials and magnetic surfaces. Using this novel and spin-resolved technique allows single molecule imaging resolution to be combined with magnetic sensitivity. By simultaneously mapping the spin-polarized density of electronic states and adsorption geometry of organic molecules on magnetic surfaces, the project aims to observe the magnetic impacts of metal-organic interfacial interactions. These interactions can imprint magnetic properties on otherwise non-magnetic molecules or can be used to modify intrinsic molecular magnetism. Goals of the project include understanding how magnetic interactions at metal-molecule interfaces are determined by molecular geometry, binding location on the surface, and molecular magnetism. This information could help the optimization of interfaces in organic spintronic devices that may be used for information storage and computing applications.

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

Solution-Based Adaptivity as a Paradigm for Computational Fluid Dynamics

Dr. Krzysztof J. Fidkowski, Assistant Professor
Department of Aerospace Engineering
University of Michigan
Ann Arbor, MI 48109

Computational simulations of physical phenomena inherently introduce numerical errors due to space and time discretization. Successful predictive science and engineering requires both robust control of this numerical error and an adaptive method that ensures the appropriate amount of resolution for efficient calculations. This project addresses both of these aspects through innovations in error estimation and discretization adaptation. New techniques will be developed to efficiently estimate error and to ensure resolution of important areas of a computational domain, without wasting resources on features that do not affect accuracy. These methods will bring together recent advances in numerous computational areas, including high-order accurate finite elements, a-posteriori error estimation, model reduction, and approximation space optimization. While adaptive methods apply to many different computational simulations, the project will stay grounded with a practical Department of Energy application, thermal hydraulics. In this application, access to inexpensive high-fidelity adaptive computations will yield more reliable analysis, improved designs, and accurate uncertainty propagation.

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

Atomically Defined Edge-Doping of Graphene Nanoribbons for Mesoscale Electronics

Dr. Felix R. Fischer, Assistant Professor
Department of Chemistry
University of California, Berkeley
Berkeley, CA 94704

The outstanding transformative potential of graphene, an infinite two-dimensional sheet of carbon atoms tightly packed into a honeycomb lattice, has been recognized mostly due to its exceptionally high electric conductivity, thermal conductivity, and tensile strength. These undeniably very desirable properties, however, represent only a very small facet of the true potential of all-carbon based materials and its promise to revolutionize the field of molecular electronics. Graphene's most unusual characteristics emerge when the infinite macroscopic sheet is scaled down to nanometer dimensions. The exploration, realization, and implementation of its truly exotic electronic and magnetic properties rely on the development of innovative synthetic strategies that provide atomically precise control over the self-assembly of mesoscale objects. The central objective of this research is to develop the crucial chemical tools required to synthesize and to fine-tune the physical properties of graphene nanoribbons (GNRs) with atomic precision. The innovative techniques and the expanded knowledge will be used to rationally tailor desired physical properties and function into nanometer-scale molecular electronic devices; e.g. transistors as logic gates in computing, data storage media based on electrically gated spin valves, or molecular amplifiers, all fabricated from readily available molecular building blocks into atomically defined GNRs.

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

The Origin of Heavy Elements: Connecting Laboratory Nuclear Astrophysics with Astronomical Observations through Nucleosynthesis Modeling

Dr. Carla Fröhlich, Assistant Professor
Department of Physics
North Carolina State University
Raleigh, NC 27695

One of the fundamental questions about our origin and the origin of the cosmos around us is where and how the chemical elements are made. Supernovae, the violent deaths of stars, play an important role in this: Almost all of the elements are created in stars and dispersed in supernova explosions. Our theoretical understanding of supernova explosions and of the creation of heavy elements is still incomplete. However, nuclear experiments and astronomical observations provide a multifaceted set of constraints. The goals of this project are to advance the simulations of nucleosynthesis in astrophysical explosions and to use them to connect current and future experimental efforts in nuclear physics with astronomical observations. The focus of this project is on modeling nucleosynthesis in core-collapse supernovae and similar astrophysical environments. General aims of this project include refining the conditions in supernovae and the associated nucleosynthesis of heavy and rare isotopes, providing the means to test theoretical predictions and experimental results in nuclear physics against data from optical and X-ray telescopes, and preparing for future experimental efforts in nuclear physics.

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

Predictive Theory of Topological States of Matter

Dr. Liang Fu, Assistant Professor
Department of Physics
Massachusetts Institute of Technology
Cambridge, MA 02139

Topological states of matter are novel quantum phases that exhibit universal and quantized properties arising from topological properties of many-body quantum wavefunctions. In recent years, predictive theory has played a leading role in the discovery of topological states in a variety of quantum materials. The goal of this research is to develop the theory for new topological states of matter in crystalline solids and predict/propose their material realizations. This research will determine novel quantum properties of topological materials, shed new light on the competition between electron localization and itinerancy in solids, and enable potential applications in tunable quantum electronics.

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

Probing Chromophore Energetics and Couplings for Singlet Fission in Solar Cell Applications

Dr. Etienne Garand, Assistant Professor
Department of Chemistry
University of Wisconsin-Madision
Madison, WI 53715

The goal of this project is to provide a molecular-level understanding of paths for improving alternative sources of energy, including an improved efficiency of dye-sensitized solar cells. Here, the mechanisms and molecular requirements for efficient exciton multiplication through singlet fission are explored using high-resolution anion photoelectron spectroscopy to probe clusters and covalently-bonded dimers of organic chromophores. The experiments are capable of observing directly the singlet, triplet, and charge transfer states involved in singlet fission and determining precisely their energetics, vibrational structures and couplings. More specific aims are (1) to probe the evolution of the electronic structure as a function of cluster size in order to understand singlet fission in crystals, (2) to explore the relationship between the nature of linkers and the electronic structure in covalently-bonded chromophore dimers, and (3) to highlight the differences, including exciton delocalization and the effects of solvent interactions, between the crystalline species and the isolated covalently-bonded dimers.

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

Simulation of Correlated Lattice and Impurity Systems Out of Equilibrium

Dr. Emanuel Gull, Assistant Professor
Physics Department
University of Michigan
Ann Arbor, MI 48109

Correlated quantum systems out of equilibrium exhibit a wealth of intriguing and unexpected quantum phenomena. Theoretical understanding of these phenomena lags far behind current experimental capabilities, as standard analytic approaches routinely fail and a solution of the quantum mechanical equations of motion precise enough to describe correlation physics is not available. In this project, unbiased and numerically exact methods for numerically simulating correlated quantum impurity and lattice models out of equilibrium will be developed based on continuous-time quantum Monte Carlo algorithms. These methods will be used to systematically study the physics of correlated quantum systems in non-equilibrium situations.

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

Design Synthesis and Characterization of Triptycene-Containing Macromolecules with Hierarchically Controlled Architectures as Functional Membrane Materials for Energy Applications

Dr. Ruilan Guo, Assistant Professor
Department of Chemical and Biomolecular Engineering
University of Notre Dame
Notre Dame, IN 46556

Rising energy demands, limited supplies and an increasing awareness of environmental factors make innovative energy technologies that explore renewable, clean energy resources or enable environmentally sustainable and efficient ways to use fossil fuels highly desirable. In many cases, the critical component has been efficient chemical separation, such as gas separations in carbon capture and selective ion transport in fuel cells and osmotic power applications. Membrane technology, which takes advantage of materials selectivity rather than energy to perform separations, is a promising approach because of its low energy consumption, environmental friendliness, modularity, and reliability. This project addresses the growing need for revolutionary macromolecular membrane materials applicable for a broad range of critical membrane mediated technologies. The objective of this research is to design and develop a new platform of high performance functional polymeric membranes with hierarchically controlled architectures derived from three-dimensional, shape persistent triptycene molecular units. These polymers possess rich structural hierarchy and versatile chemistry that enables the polymers to organize into unique spatial arrangements using novel chain threading and interlocking self-assembly concepts. Accomplishment of the planned research would enable the identification of the critical structural and topological variables over multiple length scales needed for fast and selective molecular separation and transport. The separations to be addressed have the potential to be of enormous significance in the U.S. quest to more efficiently exploit fossil fuel resources and to address the grand challenges in carbon capture.

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

State-of-the-Art Microscopic Computations of Weak Processes in Nuclei

Dr. Gaute Hagen, Research and Development Staff Member
Nuclear Physics Theory Group
Physics Division
Physical Sciences Directorate
Oak Ridge National Laboratory
Oak Ridge, TN 37831

Electroweak processes such as beta decay in atomic nuclei address fundamental questions such as: "*What are the mechanisms for the production of elements heavier than iron? What is the nature of the neutrino? What is the electroweak charge distribution in nuclei*?" Beta decay rates are crucial input for nucleosynthesis simulations that aim at determining the origin of elements, and also for understanding the nature of the neutrino ("Is the neutrino its own anti-particle?"). The aim of the planned research is to address these questions by state-of-the-art microscopic computations of weak nuclear decays with quantified uncertainties. By developing novel extensions of the coupled-cluster method, this research will make predictions of properties of medium-mass, neutron-rich nuclei at a microscopic level. The planned research will be relevant for the future experiments aimed at measuring the weak charge distribution in Calcium-48 at Jefferson Lab, neutrinoless double-beta decay experiments with the Majorana Demonstrator, and beta decay lifetimes for astrophysically relevant exotic nuclei such as Nickel-78 and Tin-132 studied at the Facility for Rare Isotope Beams (FRIB). These advanced calculations, based on two- and three-nucleon interactions, will shed new light on the microscopic mechanisms behind weak decays such as neutrinoless double-beta decay, and will help constrain nuclear forces.

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

The Multiconfiguration Time-dependent Hartree Fock (MCTDHF) Method for Interactions of Molecules with Strong Ultrafast High-Energy Laser Pulses

Dr. Daniel J. Haxton, Staff Scientist
Atomic, Molecular, and Optical Theory Group
Chemical Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

Recent advances in laser technology have enabled an entirely new class of experiments involving ultrafast laser pulses. These pulses can be used to excite, probe, and ultimately control atoms and molecules on the time scale of electronic motion. Theoretical modeling is crucial for designing such experiments and explaining the results. However, it is difficult to calculate what happens to a molecule exposed to intense, short laser pulses and there are no established methods to do so, even with a supercomputer. Recently the Multiconfiguration Time-Dependent Hartree-Fock (MCTDHF) method has been shown to be viable for this purpose. The goals of this research problem are to further develop and apply the MCTDHF method to small systems (atoms and diatomic molecules) that are under investigation in current experiments. Additional capabilities will be implemented to apply the method to studies of the light-induced dynamics of larger, polyatomic molecules.

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

Neutron Scattering Instrumentation Research and Development for High Spatial and Temporal Resolution Imaging at Oak Ridge National Laboratory

Dr. Jason P. Hayward, Assistant Professor
Department of Nuclear Engineering
The University of Tennessee
Knoxville, TN 37996

This project will exploit recent advances in optoelectronics to develop new concepts for position sensitive area detectors with orders of magnitude higher spatial and temporal resolution and to apply this new capability to map Li distribution in an operating Li-air cell. Success in this research will be transformational to neutron imaging, a powerful tool to investigate materials for such applications as fuel cells, energy storage, hydrogen storage and nuclear technology. The higher time resolution of the detectors will make it possible to efficiently carry out Bragg edge (or energy selective) imaging at high intensity pulsed sources like the Spallation Neutron Source. The processes, knowledge and algorithms developed will allow for spatially (1 micron) and time resolved (100 ns) high throughput neutron transmission imaging in large areas at reasonable costs in the near term. In addition to neutron imaging these detectors will greatly benefit single crystal Laue diffraction for macromolecular research.

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

High Performance Toolkit for Photon Science

Dr. Alexander Hexemer, Staff Scientist
Experimental Systems Group
Advanced Light Source
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

Light sources are Basic Energy Science facilities that serve thousands of researchers per year. These facilities are currently generating scientific data faster than can be analyzed using the computational methods of the past, so that scientific discovery is limited by the inability to rapidly analyze large data sets. The high performance toolkit will accelerate the rate of scientific discovery by enhancing the rate at which data can be analyzed. The main focus will be to develop and expand tools for analyzing large volumes of light source data. All tools in the toolkit will be optimized for parallelization on multiple central processing units (CPU), graphical processor units (GPU), and hybrid CPU/GPU multicore architectures. This will decrease analysis times by several orders of magnitude while simultaneously permitting larger data sets to be processed. An easy-to-use graphical user interface will be developed for the toolkit that can be easily accessed by a broad scientific audience.

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

High Precision Event Simulation for the LHC

Dr. Stefan Hoeche, Associate Staff Scientist
Theoretical Physics Department
Elementary Particle Physics Division
Particle Physics and Astrophysics Directorate
SLAC National Accelerator Laboratory
Menlo Park, CA 94205

Particle physics has entered a new era with the discovery of an elementary boson at the European Center for Nuclear Research (CERN) Large Hadron Collider (LHC). To determine the properties of the new particle and to search for signatures of physics beyond the Standard Model (SM) it is crucial to obtain reliable predictions for both signal and background reactions. Monte-Carlo event generators produce such predictions fully differentially at the level of observed particles. They rely on various models to cope with the many-body dynamics of the problem and with the non-abelian, nonlinear nature of Quantum Chromodynamics (QCD), the quantum-field theoretical model of the strong nuclear force. Dependence on the model parameters is one of the main uncertainties affecting measurements and searches at the LHC. Whenever possible such dependence must be reduced or eliminated. Strong interactions are omnipresent at the LHC, leading to the production of collimated sprays of hadrons, called jets, which enter the particle detectors. The simulation of jet dynamics in general purpose event generators is based on perturbation theory, with calculations carried out as an expansion in the strong coupling constant, α_s. In order to produce hadron level events suitable for passing through a detector simulation, certain terms in the expansion must be summed to all orders, which is achieved using parton shower algorithms. Parton showers are universal, but only approximate the exact higher-order perturbative QCD result for any given reaction, thus giving rise to large uncertainties. A major step forward in reducing these uncertainties will be achieved in this project by combining parton showers with exact next-to-next-to-leading order perturbative QCD calculations. Furthermore, the precision of the parton shower itself will be increased by including the full color dependence of splitting operators in the soft gluon limit. These developments will greatly enhance the discovery potential of the LHC.

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

Quest for a Top Quark Partner and Upgrade of the Pixel Detector Readout Chain at the CMS

Dr. Andrew G. Ivanov, Assistant Professor
Physics Department
Kansas State University
Manhattan, KS 66506

With the recent discovery of a new particle consistent with the Higgs boson, high energy physics has reached an important milestone. The Higgs boson completes the table of the fundamental particles predicted in the Standard Model (SM) of particle physics. Nonetheless, the partner of the top quark is the most anticipated candidate to be discovered next, where its existence is required in any "natural" extension of the model. The research focuses on expanding the current studies at the Compact Muon Solenoid (CMS) Experiment at the Large Hadron Collider (LHC) at the European Center for Nuclear Research (CERN) in Geneva, Switzerland on searches for top partners that have not yet been fully explored at CMS. In order to maintain a large potential for new physics discovery, the project also aims to improve the performance of the CMS Pixel Detector system by upgrading the data acquisition readout chain needed for future high energy and high luminosity physics runs at the LHC.

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

New Data on Neutron Reactions Relevant to Basic and Applied Science

Dr. Marian Jandel, Staff Scientist
Nuclear and Radiochemistry Group
Chemistry Division
Chemistry, Life, and Earth Sciences Directorate
Los Alamos National Laboratory
Los Alamos, NM 87545

Precise experimental data on nuclear reactions are essential for an improved understanding of a wide range of basic and applied problems in nuclear physics, including nucleosynthesis, weak interaction physics, dark matter detection, nuclear reactor operation, nuclear forensics, nuclear nonproliferation, and stockpile stewardship. In this project, new experimental methods and data analysis techniques will be developed to enable the determination of high-precision capture and neutron-induced fission cross sections, through detailed measurements of capture gamma rays and prompt fission gamma rays. These experiments will be performed at the Detector for Advanced Neutron Capture Experiments (DANCE) facility at the Los Alamos Neutron Science Center (LANSCE), which can measure these cross sections over almost seven orders of magnitude of incident neutron energy. New correlated data from these measurements will provide insights into the physics of the electromagnetic decays of nuclei, nuclear fission, and properties of excited nuclei. In addition, challenging measurements of neutron-induced reactions on short-lived nuclei will be carried out at DANCE and at the Lead Slowing-Down Spectrometer (LSDS), once suitable radioactive targets become available.

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

Mechanical Performance of HTS Superconductors for HEP Applications

Dr. Matthew C. Jewell, Assistant Professor
Materials Science Center
University of Wisconsin-Eau Claire
Eau Claire, WI 54702

Recent advances in the current-carrying capacity of high temperature superconductors (HTS) have focused the superconducting community on two primary materials of choice, $Bi_2Sr_2CaCu_2O_{8+x}$ (known as Bi-2212 or a type of bismuth strontium calcium copper oxide) and rare earth (Re) based coated conductors, $ReBa_2Cu_3O_{7-x}$ (known as ReBCO or rare-earth barium copper oxide). HTS development projects funded by the Department of Energy in recent years have not only led to significant improvements in the critical current density (Jc) of these conductors, but, particularly in the case of Bi-2212, have elucidated several key mechanisms blocking the current flow and provided optimism that further Jc improvements are achievable. However, the mechanical parameter space in which each conductor can operate has received significantly less attention. The objective of this work is to define the mechanical operating envelope of current Bi-2212 and ReBCO conductor designs, specify the microstructural origins of degradation in each conductor type, and provide feedback to the ongoing critical current enhancement efforts underway for each conductor type to ensure that the conductors developed are mechanically robust in addition to having high critical current performance. These efforts will also provide magnet builders with maximum flexibility in selecting a coil-winding route without being limited by present technical challenges such as delamination of the ReBCO conductor during thermal cool-down.

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

Emergence of High Tc Superconductivity Out of Charge and Spin Ordered Phases

Dr. Eun-Ah Kim, Assistant Professor
Department of Physics
Cornell University
Ithaca, NY 14853

How to understand and control high Tc superconductivity (HTSC) is among the most fundamental and pressing challenges in modern condensed matter physics. Recent experiments have revealed striking universality among copper-based and iron-based HTSC: the superconductivity emerges out of phases in which electron's charge and spin are spontaneously organized in orderly patterns bearing lower symmetry than the symmetry of the host lattice. However, little is known about how these orderly patterns form and what role they play in HTSC. The mechanism and the role of the observed charge and spin patterns in HTSC is the key objective of this research. In this project a "middle-up/down approach" is taken, applying theoretical perspectives directly to the analysis of experimental data and using the results as input to microscopic models to be studied using various analytical and computational methods. This approach enables theoretical guidance and supports cutting edge experimental efforts. The outcome, elucidating how HTSC emerges from charge/spin ordered phases, will provide insight into the mechanism of HTSC. More broadly, it will offer insights into how endless possibilities emerge in correlated systems and how we could control them.

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

Concrete Ingredients for Flexible Programming Abstractions on Exascale Systems

Dr. Sriram Krishnamoorthy, Staff Scientist
High Performance Computing Group
Computational Sciences and Mathematics Division
Fundamental and Computational Sciences Directorate
Pacific Northwest National Laboratory
Richland, WA 99352

Exascale systems are expected to have a very dynamic execution environment due to architectural heterogeneity, variable data access latencies, system noise, and fault management. Difficulties in programming such systems have led to a renewed interest in abstractions for finer-grained concurrency. This project will develop algorithms that target finer-grained concurrency, irregular data structures, and flexible data movement and synchronization semantics. The effectiveness of the algorithms designed will depend on the specific system architecture and status of the execution environment at a particular point in time. To this end, the project will identify and characterize the key performance characteristics of the algorithms developed.

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

Compiler and Run-Time Approaches to Enable Large Scale Irregular Programs

Dr. Milind Kulkarni, Assistant Professor
School of Electrical and Computer Engineering
Purdue University
West Lafayette, IN 47906

Irregular algorithms, which feature unpredictable accesses to data structures, are becoming increasingly common in high performance computing. The defining characteristics of irregular applications, their dynamic, unpredictable, data-dependent access patterns and data layouts, make achieving high performance on large scale systems difficult. This project will develop techniques that can address the communication, locality and scalability challenges that emerge as irregular applications are deployed on exascale systems. The research work will deliver a system that can (a) transform irregular applications to improve their locality and computational intensity, while reducing communication needs; and (b) perform run-time scheduling and tuning to optimize the application for a specific system. This system will allow programmers to easily deploy irregular applications that scale to exascale platforms without the need of hand-optimizing and hand-tuning their codes.

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

Microscopy of Electrostatic Field Effect in Novel Quantum Materials

Dr. Keji Lai, Assistant Professor
Physics Department
University of Texas at Austin
Austin, TX 78712

The objective of this research is to explore the nanoscale electronic properties when charge carriers are electrostatically modulated in advanced quantum materials, such as complex oxides, layered chalcogenides, and organic semiconductors. By combining electrolytic gating, a method that produces an unprecedented electric field effect, with scanning microwave impedance microscopy that probes sub-surface phenomena, this project aims to establish a new kind of useful imaging methodology as well as to answer many pressing questions in technologically important materials. Specifically, the research will (1) spatially resolve electronic phase transitions induced by density modulation; (2) compare the underlying physics between bulk chemical doping and surface electrostatic doping; and (3) investigate the microscopic origin of sub-threshold behaviors in novel field-effect transistors.

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

Developing Synthetic Biology Tools to Engineer Plant Root System and Improve Biomass Yield and Carbon Sequestration

Dr. Dominique Loque, Biological Engineer, Staff Scientist,
and Director of the Cell Wall Engineering Group
Joint BioEnergy Institute
Physical Biosciences Division
Biosciences Directorate
Lawrence Berkeley National Laboratory
Berkeley, CA

Dedicated crops for bioenergy production must be grown in marginal environments to avoid competition with food crops that are cultivated in high-quality arable land. However, nutrient and water availability is very low in these marginal environments. Therefore, energy crops must be engineered to improve their ability to extract those vital elements from poor soils so they can reach their full yield potential without the cost and environmental impact of chemical fertilization. The root system not only anchors a plant to the ground but is responsible for acquiring essential mineral nutrients and water and for maintaining interactions with the soil environment, all critical for plant growth. In spite of their importance for biomass accumulation, plant roots are relatively understudied and few engineering tools area available to better understand and improve root function. This project will address this need by developing “universal” root expression tools that are functional across a broad range of plant species. These tools will be used to engineer metabolic pathways that will be designed to optimize nutrient acquisition by energy crops such as switchgrass and Camelina. This research will deliver a diversity of building blocks for plant root engineering that will be instrumental in advancing DOE goals for sustainable production of bioenergy.

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

Resolving Reactor Antineutrino Anomaly with Strong Antineutrino Source

Dr. Jelena Maricic, Assistant Professor
Department of Physics and Astronomy
University of Hawaii
Honolulu, HI 96822

An intriguing, nearly three-sigma indication of the electron antineutrino disappearance at less than 100 m distance from the nuclear reactor core has recently been revealed. The effect was named a reactor antineutrino anomaly (RAA). The disappearance may be due to reactor neutrinos oscillating into another neutrino type. However, oscillation into either muon or tau neutrinos cannot happen at any detectable level in less than 100 m. Therefore, electron antineutrinos may be oscillating into a new, yet undiscovered, fourth neutrino type that is 'sterile', does not interact with ordinary matter, thus cannot be observed directly. All analyzed data combined, point to the oscillation length of less than 10 m between electron antineutrinos and sterile neutrinos. The objective of this research is to test the sterile neutrino oscillation hypothesis in a complimentary way: deploy a massive 76000 curie electron antineutrino source (cerium-144 and praseodymium-144) in the veto region of a giant, 1 kiloton antineutrino detector called Kamioka Liquid Scintillator Antineutrino Detector (KamLAND). The project is called CeLAND. It will search for the sterile neutrino oscillation in 3-16 m range and probe the majority of the oscillation phase space suggested by the RAA with 95% confidence level. Demonstrating the existence of fourth particle generation, sterile neutrinos would be one of the most dramatic discoveries of physics beyond the Standard Model. The resolution of RAA will in any case provide a valuable cross-check of the validity of the reactor antineutrino flux calculations.

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

Electron Microscopy with Vortex Beams Carrying Orbital Angular Momentum

Dr. Benjamin J. McMorran, Assistant Professor
Department of Physics and Materials Science Institute
University of Oregon
Eugene, OR 97403

The goal of this project is to develop new electron microscopy capabilities using electron vortex beams. Electron microscopy is one of the most widely used tools for studying energy-related materials at atomic length scales, yet the information that it can typically provide is limited by the types of physical interactions occurring between the electron beam and the sample. Electron vortex beams can interact with matter in new ways compared to conventional electron beams because they possess unique orbital, magnetic, and wave properties. This project investigates methods for using the electron vortex beam to directly probe magnetization and electronic orbital structure within materials. Methods will also be explored for using these beams to enhance image contrast of carbon-based materials at the nanoscale. To accomplish these goals, the project will advance a new technique of using nanofabricated electron optical structures to produce electron vortex beams inside existing microscopes.

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

Room Temperature Electrochemical Upgrading of Methane to Oxygenate Fuels

Dr. William E. Mustain, Assistant Professor
Department of Chemical, Materials and Biomolecular Engineering
University of Connecticut
Storrs, CT 06269

With recent discoveries of vast amounts of shale methane deposits in Pennsylvania and the Dakotas, and the introduction of renewable biogas to the market, the availability of methane in the United States is at an all-time high. High petroleum prices and an increased emphasis on domestic energy security will make methane-to-fuels (MTF) processes even more important in the near-future than they are today. Current MTF processes are initiated through the steam reforming of methane to syngas ($CO + H_2$), followed by catalytic re-reduction of CO by H_2 to hydrocarbon and oxygenate fuels. Unfortunately, the large heat requirements and high temperatures (900-1100^oC) of steam reforming makes the process expensive, the reaction selectivity poor, and the implementation complicated with complex heat integration schemes, costly gas separations, and limited available materials that can withstand severe stress. In addition, the steam reforming process produces a significant amount of CO_2. The objectives of this research are to understand the underlying mechanisms for the direct electrochemical conversion of methane to syngas at room temperature, and develop new electrocatalysts that convert methane to methanol at room temperature ($T < 40^oC$) with high selectivity (> 90%) to overcome the limitations of existing MTF processes. Methanol was selected as the target molecule because it can be used directly as an energy source and it is the primary precursor for the manufacture of many commodity chemicals, making it one of the most produced and important industrial chemicals in the world. This project will have far reaching applications by providing a new pathway for the electrochemical synthesis of complex oxygenates and long-chain hydrocarbons through the formation of new C-O and C-C bonds.

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

Methane Oxidation in the Rhizosphere of Wetland Plants

Dr. Rebecca B. Neumann, Assistant Professor
Department of Civil and Environmental Engineering
University of Washington
Seattle, WA 98195

Methane is a potent greenhouse gas, with a global warming potential 20-times larger than that of carbon dioxide. The objective of this project is to improve predictions of future methane emissions. The project will examine the conversion of methane to carbon dioxide, i.e., methane oxidation, within the soil zone surrounding roots (the rhizosphere) of wetland plants. Wetlands are the largest natural source of methane to the atmosphere, and a majority of methane emitted by wetlands travels from soil through plants to the atmosphere. Plants also support the movement of atmospheric oxygen into the soil where it can oxidize methane; up to 90% of the methane produced in wetlands can be converted to carbon dioxide in this way. However, the process is not well captured by most computer models where oxidation of methane is simply set to a constant percentage. In reality, the percentage of methane oxidized in the rhizosphere is dynamic, responding to soil and water chemistry and to plant traits and behavior. As the climate changes, plant species composition, plant behavior, and subsurface chemistry will change, altering the fraction of methane oxidized within wetlands. Thus, understanding the dynamic response of methane oxidation to these expected climate-induced changes is key to accurately predicting future methane emissions. This project will study the potential for future changes in methane oxidation using a combination of field measurements, laboratory experiments and modeling investigations informed by field and laboratory results. Outcomes include a quantitative and predictive understanding of the interaction between plant behavior and methane oxidation in wetlands, an improved representation of methane oxidation in computer models, and an enhanced appreciation of how changes to the climate system will impact methane emissions from wetlands. These outcomes address one of the scientific drivers for the Biological and Environmental Research program at DOE: "discovering the physical, chemical, and biological drivers and environmental impacts of climate change."

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

Engineering Anaerobic Gut Fungi for Lignocellulose Breakdown

Dr. Michelle A. O'Malley, Assistant Professor
Chemical Engineering Department
University of California, Santa Barbara
Santa Barbara, CA 93106

Renewable biofuels derived from plant biomass (stems, stocks, and leaves, mainly composed of cellulose and lignin) are attractive alternatives to petroleum-based fuels. To produce biofuels, enzymes are used to break down cellulose into simple sugars, which are then fermented into fuels such as ethanol and butanol. However, because the structure of cellulose is a tightly bound network of crystalline cellulosic fibers and lignin, existing biomass degrading enzymes are not very efficient. New technologies to break down plant material into sugar can be developed by studying how microbes digest lignocellulose in biomass-rich environments, such as the digestive tract of large herbivores. Anaerobic fungi that live in the absence of oxygen and are native to the gut and rumen of these animals, have evolved powerful enzymes to degrade plant biomass. This project will develop new experimental tools to engineer anaerobic fungi for lignocellulose breakdown and biofuel production. To accomplish this goal, a panel of anaerobic fungi will be isolated from different herbivores and screened for their ability to degrade several types of lignin-rich grasses and agricultural waste. Focusing on a model anaerobic fungus, the basic metabolic processes that control enzyme production will be determined. This information will be used to develop new genetic engineering strategies to manipulate gut fungi at the molecular level. Understanding the biology of these anaerobic organisms will result in the development novel platforms for biofuel production.

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

Neutrino Physics with SNO+

Dr. Gabriel D. Orebi Gann, Assistant Professor
Department of Physics
University of California, Berkeley
Berkeley, CA 94704

Neutrinos are unique in the Standard Model of particle physics, with masses many orders of magnitude below any other known fundamental particle. The reason for this is not yet understood, but could shed light on critical questions such as the absence of antimatter in our matter-dominated Universe. Perhaps the most fundamental question in neutrino physics lies in the very nature of the neutrino: the neutrino is the only known fermion with the potential to be its own antiparticle. Sudbury Neutrino Observatory or SNO+ is a neutrino experiment with a broad physics program, the primary goal being a search for the phenomenon of neutrinoless double beta decay, a process possible only if the neutrino is indeed its own antiparticle. Such a discovery would re-write our understanding of particle physics, including introducing the need for a new mechanism for generating particle mass, and also place limits on the as-yet-unknown neutrino mass. SNO+ will also detect neutrinos from diverse sources such as the Sun, nearby supernovae, and from within the Earth itself. This proposal requests support for a targeted plan of optical calibrations of the SNO+ detector. A well-understood, stable source of light will be developed using the "Cherenkov effect", with the goal of measuring and monitoring the efficiency of SNO+ light sensors independently of the other optical properties of the detector. The work to be done under this award will provide SNO+ with a precise model for the detector response, allowing an enhancement in the accuracy of predictions for real data, thus improving the sensitivity of the experiment. Also supported is the implementation of these calibrations in physics analyses, involvement in all levels of analysis activities, and leadership in SNO+ science.

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

Search for the Higgs and Physics Beyond the Standard Model with the CMS Electromagnetic Calorimeter

Dr. Toyoko Jennifer Orimoto, Assistant Professor
Department of Physics
Northeastern University
Boston, MA 02115

Understanding the origins of electroweak symmetry breaking and probing the possibilities of new physics at the Energy Frontier is one of the primary goals of high energy physics. The recent Higgs boson discovery by the Large Hadron Collider (LHC) experiments at the European Center for Nuclear Research (CERN) in Geneva, Switzerland signal a new era in particle physics and brings us closer to achieving these goals. The most critical next steps in the Compact Muon Solenoid (CMS) Experiment's physics program include the characterization of this new particle by studying whether it exhibits the expected properties of a Standard Model (SM) Higgs boson, whether additional Higgs particles exist, or if any deviations from the model indicate the presence of new physics. The project further aims to maximize these studies by improving the data acquisition and performance of the CMS Electromagnetic Calorimeter system to enhance the high energy resolution needed for observing the Higgs boson.

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

Non-Centrosymmetric Topological Superconductivity

Dr. Johnpierre Paglione, Assistant Professor
Department of Physics
University of Maryland
College Park, MD 20742

Topological insulators are a newly discovered class of materials with strong potential for impact in both fundamental science and future technologies. Differing from conventional insulators by the presence of a robust metallic surface state, these materials offer possible new avenues for technologies such as spintronics and quantum computation. Coupling these states with the perfect conductivity found in a superconductor has the potential to not only help elucidate new physics, but also to establish the groundwork for new technologies that combine the unique features of each state of matter. This program is focused on the synthesis, characterization, and optimization of a new family of materials with promise of being both topological insulators and superconductors simultaneously, allowing for investigations of the interplay between these two states of matter in the same material system.

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

A Multiscale Reduced-Order Method for Integrated Earth System Modeling

Dr. George Shu Heng Pau, Research Scientist
Hydrogeology Department
Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

Earth system models are increasingly used as predictive tools for decision support and policy making to mitigate the effects of climate change. Considerable effort has been invested to improve the accuracy of these models by incorporating physical processes with vastly different spatial and temporal scales, leading to multiscale earth system models. For example, small-scale cloud-resolving models are embedded in coarse-scale climate atmospheric models to improve the modeling of precipitation. However, these embedded multiscale models are typically very slow to calculate and evaluate, even with the use of supercomputers. This project will build a new kind of climate model, a so-called "reduced-order" model, made up of statistical approximations or "surrogates" for multi-scale processes that can be solved much more quickly than a full climate model. The reduced-order model will be constructed numerically using a combination of techniques from applied mathematics and computer science. New linking or "coupling" approaches that exploit the computational efficiency of reduced-order models will be developed to bridge component and sub-component models of different scales. This project will also efficiently estimate the uncertainties and errors of the reduced-order model, enabling objective quantification and adaptive improvement of the model fidelity. The efficiency gains from using a reduced-order model will enable rigorous characterization of uncertainties in the predicted outcomes and improve confidence in the predictive capabilities of Earth system models. The example or test case chosen for this project is a "surrogate" Arctic permafrost model that will approximate the full-blown land model under development for the DoE sponsored Next Generation Ecosystem Experiment (NGEE).

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

Application of Next-Generation Sequencing to Engineering mRNA Turnover in Cyanobacteria

Dr. Brian F. Pfleger, Assistant Professor
Chemical and Biological Engineering Department
University of Wisconsin-Madision
Madison, WI 53715

The ability to control gene expression in microorganisms is essential for biotechnology applications such as renewable fuel production and carbon dioxide fixation. To carry out their function, genes coded in the DNA must be transcribed into a messenger RNA (mRNA), which is translated into a protein with biological activity. While the processes of transcription and translation are well understood in many organisms, much less is known about the stability of the mRNA and how its life span affects gene expression. Thus, genetic engineering tools used to express foreign genes in microbes rarely consider key factors that influence mRNA stability. The goal of this project is to fill this gap in knowledge for a model photosynthetic bacterium, a cyanobacterium. Using the latest DNA sequencing technologies, this research will identify mRNA sequence features that affect the rate of mRNA turnover. Those features will be used to design strategies for altering mRNA stability and to improve oil production in cyanobacteria. The planned experiments will leverage the DOE Joint Genome Institute DNA and RNA sequencing capabilities and will contribute data for the computational infrastructure provided by the DOE Knowledgebase. The knowledge gained from this project will help the development of more accurate gene expression models and will facilitate metabolic engineering projects needed to advance toward the sustainable production of biofuels.

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

Energy Transport in High-Energy-Density Matter

Dr. Yuan Ping, Staff Scientist
High Energy Density (HED) Section
Physics Division
Physical and Life Sciences Directorate
Lawrence Livermore National Laboratory
Livermore, CA 94550

This project aims to provide high-quality data on critical energy transport properties of high-energy-density (HED) matter. Transport processes, such as thermal and electrical conduction, radiation, viscosity, electron-ion equilibration and particle stopping, determine the mechanisms and rates of energy transfer and redistribution within HED matter. These energy partition pathways must be properly diagnosed and understood in order to develop and benchmark next-generation advanced models for extreme HED conditions such as those found in Inertial Confinement Fusion (ICF). Energy transport not only affects capsule performance in ICF central hot-spot ignition, but also is important in advanced ICF schemes including fast ignition and shock ignition. At present, very little data exist in the relevant regimes because these extreme conditions are difficult to create and to measure. A suite of recently developed novel x-ray and optical techniques can now enable the challenging measurements, in particular, on thermal conductivity, electrical conductivity and viscosity. The data will also impact many other fields where HED science plays a crucial role, such as studies of geophysical phenomena, planetary formation, and astrophysical objects.

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

Examination of Actinide Chemistry at Solid-Water Interfaces to Support Advanced Actinide Separations

Dr. Brian A. Powell, Assistant Professor
Department of Environmental Engineering and Earth Sciences
Clemson University
Clemson, SC 29634

The study of the chemical and physical properties of actinide bonding and reactivity is essential for the development of an improved nuclear fuel cycle and to understand how the actinides move through the environment. This work will examine the fundamental chemical properties of actinide elements in aqueous solutions and at solid-water interfaces. Sorption of actinides to solid surfaces such as minerals and soils can limit the movement of actinides in the environment and sorption to engineered solids can facilitate separation of actinides from other waste materials within the nuclear fuel cycle. Understanding and quantifying actinide bonding and reactivity at solid-water interfaces is needed for a wide range of applications such as advanced actinide separation schemes, waste treatment and disposal, understanding actinide behavior under geologic repository conditions, and determining the performance of actinide bearing wastes and waste facilities. A novel aspect of this work will be to examine sorption processes on a mechanistic basis and quantify the data using a standard thermochemical construct as opposed to the empirical methods commonly employed. The overarching objectives of this work are to provide a mechanistic conceptual model and a quantitative sorption model describing actinide behavior at solid-water interfaces based on a molecular level understanding of the chemical processes involved. Particular attention will be focused on understanding underlying mechanisms of actinide sorption to differing solid phases, understanding underlying mechanisms behind frequent observations of hysteretic sorption and understanding the potential formation of ternary actinide-ligand-surface complexes. The ability to predict distribution of the actinides between aqueous and solid phases in the presence of various organic ligands represents a step towards the development of unique, organic solvent free separation systems based on solid-liquid partitioning and will also improve models of actinide behavior in natural systems containing naturally occurring organic ligands.

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

Neutron Scattering Investigation of the Relationship between Molecular Structure, Morphology and Dynamics in Conjugated Polymers

Dr. Danilo C. Pozzo, Assistant Professor
Department of Chemical Engineering
University of Washington
Seattle, WA 98195

The overarching goal of this project is to develop structure-property relationships for conjugated polymers, an important new class of materials used in applications such as organic solar cells, thermoelectric energy conversion, flexible displays incorporating organic light emitting diodes, conductive and electrochromic coatings, supercapacitors and chemical sensors. These polymers offer several advantages including simplified processing from solution, the use of abundant raw materials, flexible form-factors and a capacity to fine-tune semiconductor energy levels. Unfortunately, unmodified conjugated polymers are generally insoluble and hence difficult to process. To overcome this problem, the polymers are chemically modified by attaching chemical side-groups to their backbones to boost solubility in processing solvents without significantly affecting their properties. However, these steps can impact the ultimate performance of the polymers. Currently, predictive knowledge is lacking on how the specific molecular structure of the side-groups affects polymer self-assembly and charge propagation in nanostructured phases or in the solid-state. To address this gap, neutron scattering experiments (elastic and quasi-elastic) will be employed to probe the nanostructure and the system dynamics along with simultaneous (in-situ) dielectric spectroscopy and rheology to understand and develop structure-property relationships. Experiments will be complemented by molecular simulations to gain predictive knowledge on the relationship of chain structure, microstructure, and time-dependent relaxation processes with the macroscopic properties of the materials.

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

Computational Design of Graphene-Supported Nanocatalysts

Dr. Ashwin Ramasubramaniam, Assistant Professor
Department of Mechanical and Industrial Engineering
University of Massachusetts, Amherst
Amherst, MA 01003

The goal of this project is to develop a systematic computational approach for the rational design and evaluation of nanoscale transition-metal catalysts supported on graphene, a two-dimensional sheet of carbon atoms arranged in a honeycomb lattice. The use of graphene supports, as compared to carbon nanotubes or carbon black, has been experimentally shown to enhance significantly the catalytic activity of metal nanoclusters in fuel cell electrodes. However, there is not yet a clear mechanistic understanding of the role played by graphene supports in improving catalyst performance. This project will develop and implement computational models to understand and predict electronic interactions between transition-metal nanoclusters and graphene supports, taking into account complexities that arise in practice from statistical variations in cluster size and morphology, quantum size effects at the nanoscale, and the presence of physical and chemical defects in graphene. Model transition metal and graphene catalyst systems will be employed for statistical sampling of selected reactions pathways to probe the influence of substrate–cluster interactions on reaction thermodynamics and kinetics. The fundamental understanding gained from these studies could guide the rational design of superior, graphene-supported, transition-metal nanocatalysts with potential applications in energy conversion pathways for alternative fuels.

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

Mid-rapidity Di-lepton Measurements at RHIC with the Muon Telescope Detector at STAR

Dr. Lijuan Ruan, Physicist
STAR Group
Physics Department
Nuclear and Particle Physics Directorate
Brookhaven National Laboratory
Upton, NY 11973

An important task in today's relativistic heavy ion physics is to study the fundamental properties of the Quark Gluon Plasma (QGP), including the temperature, density profile, and color screening. Data taken over the last decade have demonstrated that the Relativistic Heavy Ion Collider (RHIC) has created the QGP, a hot, dense medium with partonic degrees of freedom. However, the initial temperature of the QGP is not well constrained by previous experimental results and estimates dependent on models have large uncertainties. The planned study will measure the decay of different quarkonium states into two muons. These bound states of two heavy quarks are predicted to melt before decaying at very different temperatures in the QGP. The dissociation of the states depends on the color screening length of the QGP and quarkonium binding energies, that is, how strongly the different colored quarks are screened from each other in the QGP. In addition, measurements of muon-electron correlations from heavy flavor decay will help remove the dominant background for an alternative method of determining the QGP temperature based on the measurement of thermal radiation. With these new techniques, the planned measurements will provide direct information on the temperature and the characteristics of the color screening in the QGP created at RHIC.

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

Hadronic Parity Violation in Few-Nucleon Systems

Dr. Matthias R. Schindler, Assistant Professor
Department of Physics and Astronomy
University of South Carolina
Columbia, SC 29208

The objective of this research is the detailed and model-independent analysis and interpretation of the parity-violating component of the interactions between nucleons. Resulting from the interplay of weak and strong interactions between quarks, the constituents of the nucleons, parity violation in nucleon interactions offers a unique probe of the forces and mechanisms that bind the quarks into nucleons. Despite several decades of experimental and theoretical efforts, hadronic parity violation is still poorly understood. Recent progress on high-intensity neutron sources, for example at the Spallation Neutron Source at Oak Ridge National Laboratory, makes it possible to study parity violation in few-nucleon systems. This project will apply modern theoretical techniques to find a consistent description of parity-violating interactions in a collection of different experiments, and will also establish connections to lattice gauge theory and parity violation in more complex systems.

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

Dynamics of Emergent Crystallinity in Photonic Quantum Materials

Dr. Jonathan Simon, Assistant Professor
Department of Physics
University of Chicago
Chicago, IL 60637

Photons make fantastic information carriers because they pass through one another nearly unimpeded. For this same reason, a material composed solely of photons is virtually unheard of: unlike atoms, photons simply do not collide enough to order spontaneously. This work aims to synthesize and study the very first “optical material” by indirectly engineering collisions between photons through the real scattering of photons off of highly excited atoms. The fabric of these exotic materials is predicted to froth with quantum foam churned up by a many-body Heisenberg uncertainty principle. Stirring this foam and watching it swirl and settle will provide insight into the properties of a forthcoming generation of engineered materials whose bizarre properties arise due to quantum mechanics. In particular, the work will have immediate implications for quantum computing and quantum communication, as well as the structure, heat capacity, and conductivity of low dimensional electronic systems.

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

Decoupling the Electronic and Geometric Parameters of Metal Nanocatalysts

Dr. Sara E. Skrabalak, Assistant Professor
Department of Chemistry
Indiana University
Bloomington, IN 47405

Central to many industrial processes (e.g., petroleum refining) and the realization of new energy platforms (e.g., fuel cells and biomass conversion) is heterogeneous catalysis. The performance of a catalyst is governed by interplay between electronic and geometric factors, but controlling these parameters to achieve efficient catalysis remains a grand challenge. The central objective of this research is to decouple the electronic and geometric parameters of nanoscale metal catalysts for independent manipulation through the design and use of new architecturally-controlled bimetallic nanocrystals. The binary composition of the structures will provide a means of electronic control while the shape of the nanocrystals will provide geometric control. Independent selection of these features in new architecturally-controlled nanostructures will allow the electronic and geometric parameters of metal nanocatalysts to be effectively decoupled for independent manipulation. Initial experiments are directed toward new nanocatalysts for formic acid electroxidation, but it is anticipated that novel architecturally-controlled bimetallic nanocrystals will be designed, synthesized, and applied to other chemical transformations requiring advances in catalysis. Validation of new catalysts designs can bring unprecedented efficiency to many chemical processes and conserve both natural resources and economic capital which are requisite for a sustainable future.

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

Nanostructured Colloidal Self-Assembly and Controlled Alignment of Anisotropic Nanoparticles

Dr. Ivan I. Smalyukh, Assistant Professor
Department of Physics
University of Colorado
Boulder, CO 80309

Harvesting, storage, and conversion of energy among its different forms strongly depend on available materials and their properties. Self-assembly of nano-sized functional units is an exceptionally promising way of designing inexpensive artificial composite materials with new macroscopic physical behavior and properties. The main objective of this project is to explore self-organization of anisotropic nanoparticles into colloidal composites with tunable ordered structures. The research will focus on understanding and control of self-assembly of metal and semiconductor nanoparticles, as well as on material behavior arising from their ordered self-organization and alignment. Fundamental studies of shape-dependent colloidal interactions and ordering of quantum dots and plasmonic metal nanoparticles will reveal underpinning physical mechanisms that guide mesoscale morphology and ultimately determine material properties of the self-assembled composites. These properties will be characterized and correlated with hierarchical structures and composition. Analytical and numerical modeling of colloidal interactions and material properties will provide important insights at different stages of this project. This research may enable new, cheaper, and more efficient renewable energy technologies, a new breed of energy-efficient information displays and consumer devices, as well as a fertile ground for new basic science.

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

Transition Metal Oxides Spinel Nanomaterials for Supercapacitor Reactions

Dr. Xiaowei Teng, Assistant Professor
Chemical Engineering Department
University of New Hampshire
Durham, NH 03824

The principal means for storing energy generated off-peak for later on-peak usage currently leave a void between overall storage capability and power delivery. Supercapacitors as a class of energy storage devices are able to fill the energy and power gap between batteries and electrostatic capacitors. The proposed work is to investigate the charge-storage mechanisms of transition metal oxides (TMOs) for use in supercapacitors. This project will focus on the fundamental structure-property relationship of faceted spinel TMO nanoparticles, including simple spinel (e.g., Co_3O_4 and Mn_3O_4) and binary spinel (e.g., $Co_{1-x}Mn_{2-x}O_4$ and $Fe_{1-x}Mn_{2-x}O_4$). The hypotheses to be investigated are (1) nanosized TMOs will have high specific surface area for ionic conductance; (2) faceted spinel nanoparticles with higher percentages of reactive and/or stable surfaces will facilitate the fast charge-transfer reaction and long cycle life. Through the interplay between novel material syntheses, structural and functional characterizations, and synchrotron-, neutron-based in situ measurements, the ultimate goal of the proposed research is to provide fundamental understanding of electrode materials for supercapacitors that can store more energy while maintaining a stable electrode/electrolyte interface. The outcome of the proposed research will support directly the nation's effort to diversify its energy supply portfolio, and help to reduce the global carbon footprint.

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

Residue Specific Characterization of Electrostatics, Conformational Heterogeneity, and Dynamics of Electron Transfer Proteins with Linear and Nonlinear Infrared Spectroscopy

Dr. Megan C. Thielges, Assistant Professor
Department of Chemistry
Indiana University
Bloomington, IN 47405

The goal of this project is to further the understanding of photosynthetic electron transfer by studying proteins and their motion with high spatial and temporal detail. Biological electron transfer occurs between sites embedded within the proteins from which water is excluded, creating an environment that is very different from that found in normal bulk liquids. Further, the electron transfer reactions are very fast – typically occurring within tiny fractions of a second – and thus involve short-lived binding interactions between the donor and acceptor. These factors, combined with the structural complexity inherent to such large macromolecules, make the experimental study of these systems very challenging. This project will adapt, combine and develop new spectroscopic approaches to measure the motions of molecules after labeling specific parts of the proteins, which will enable a deeper understanding of the local sites where electron transfer occurs. The insights provided by this research will deepen the understanding of electron transfer in photosynthesis and should greatly aid efforts to create artificial systems for solar energy capture and storage.

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

Imaging Interfacial Electric Fields on Ultrafast Timescales

Dr. William A. Tisdale, Assistant Professor
Department of Chemical Engineering
Massachusetts Institute of Technology
Cambridge, MA 02139

The objective of this research is to explore a novel methodology for visualization of ultrafast electronic processes at interfaces. The method, which is based on optical stimulation, builds upon previous success using spontaneous surface nonlinear optical probes to track the temporal evolution of interfacial electric fields resulting from charge separation across an interface. A goal is to speed signal acquisition by up to seven orders of magnitude so that laser scanning ultrafast microscopy becomes feasible. The ultimate aim is to generate movies of interfacial electronic phenomena occurring on femtosecond timescales and submicron length scales, thereby informing our understanding of disorder, heterogeneity, and morphology, and how these factors affect ensemble behavior in photovoltaic, electrochemical, and optoelectronic systems.

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

Exploring the Fundamental Origin of Cosmic Acceleration

Dr. Andrew J. Tolley, Assistant Professor
Department of Physics
Case Western Reserve University
Cleveland, OH 44106

The central goal of the proposed research program is devoted to exploring a compelling set of descriptions for the fundamental physics responsible for the dynamics of cosmic acceleration, both in the late and early universe. In particular, it shall capitalize on the significant recent progress in the development of two new classes of infrared modified theories of gravity: Massive Gravity and related Galileon theories. The general aims of this program will: (1) determine if Massive Gravity models are viable alternatives to the standard cosmological paradigm for the dark sector - a cosmological constant and cold dark matter; (2) explore their predictions for gravitational tests via post-Newtonian corrections and gravitational radiation; (3) understand the nature of black hole thermodynamics and holography in the models; and (4) develop a consistent picture and numerical procedure for quantum corrections. In parallel, this research program will explore the implications of analogous dynamical models that rely of nonlinearly realized symmetries for early-time cosmic acceleration, with a particular focus on the influence of fluctuations of heavy fields, the breaking of global symmetries from gravity, and their predictions for primordial non- Gaussianities. The potential observations of the latter in current probes of the Cosmic Microwave Background (CMB) would provide an exceptional window into fundamental physics, and the initial conditions of the universe.

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

Beyond the Black Box: Combining System and Model Dynamics to Learn About Climate Uncertainties

Dr. Nathan M. Urban, Energy Security Fellow
Computational Physics and Methods Group
Computer, Computational, and Statistical Sciences Division
Theory, Simulation, and Computation Directorate
Los Alamos National Laboratory
Los Alamos, NM 87545

Changes in climate due to greenhouse gases and other warming or cooling agents have large uncertainties because internal changes to the climate system, known as “climate feedbacks,” are poorly known. Climate feedbacks can amplify or suppress greenhouse warming, for example by melting snow to expose dark soil that absorbs more sunlight, thereby accelerating warming. Climate models include these feedbacks, but the formulations and magnitudes of the feedbacks differ among models. This project will address this challenge, developing a new approach for climate projection using a statistical method to quantify the uncertainty in individual climate system feedbacks, such as changes to snow, ice, or clouds. It will combine information contained in a multi-model ensemble of numerical climate simulations with the observational climate record. The statistical method centers on the development of a simple and flexible statistical-physical climate model, whose behavior can be adjusted to reproduce the feedbacks and other dynamics seen in complex physical simulations and observational data. This method will permit a wider and much more rapid exploration of possible Earth system behaviors than seen in individual climate models. It will improve upon existing "black box" statistical methods that average together model predictions without knowledge of the physical dynamics underlying different components of the Earth system. The new statistical method will be applied to improve the probabilistic prediction of trends, spatial patterns, and variability in the future climate by more fully exploiting information about climate dynamics contained in both physical theory and data. Once developed, an exploratory study will be conducted to discern the rate at which particular continued observations of the Earth system may be expected to reduce our uncertainty about the future climate. The method may also be used to quantify the respective roles of human impacts and natural climate variability, and as a predictive decision support tool for integrated climate-economic-impacts modeling and assessment.

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

Plasmon-Mediated Electrochemical Reactions: The Influence of Nanoparticle Structure

Dr. Katherine A. Willets, Assistant Professor
Department of Chemistry and Biochemistry
University of Texas at Austin
Austin, TX 78712

Noble metal nanoparticles interact with light through the excitation of plasmons, which are light-driven collective oscillations of the conduction electrons at the nanoparticle surface. This project will use noble metal nanoparticles as electrodes for electrochemical reactions to determine whether excitation of plasmons in these electrodes can affect the redox potentials and rate of electron transfer of molecules on the nanoparticle surface. Surface-enhanced Raman scattering and fluorescence will be used as optical readouts for the redox state of the molecule, with a change in the optical signal occurring as the molecule transitions between the oxidized and reduced forms. The role of nanoparticle structure will be investigated at both the single particle length scale (10-100 nanometers) and at the single molecule length scale (1-10 nanometers) in order to determine how different nanoparticle shapes and nanoscale features impact the redox potentials and electron transfer rates of the molecules on the surface. This project will generate insight into how light can be used to lower energy barriers in electrochemical reactions, making them more energetically favorable.

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

Gluonic Excitations in Mesons

Dr. Michael Williams, Assistant Professor
Department of Physics
Massachusetts Institute of Technology
Cambridge, MA 02139

At the most profound level, the principal goal of research in physics is to learn about the fundamental laws that govern our universe. Two ways to accomplish this are searching for new phenomena and performing stringent tests of accepted theories. The Gluonic Excitation Experiment (GlueX) experiment, currently being built at Jefferson Lab in Newport News, VA, will do both. In the standard model of particle physics, interactions between quarks and gluons are described by the theory of quantum chromodynamics (QCD). While the equations of QCD have been known for decades, solutions to these equations have yet to be found at energy scales that are relevant for describing protons, neutrons and nuclei. In recent years, much progress has been made towards obtaining numerical solutions to QCD using supercomputers and a technique called lattice QCD. Recent lattice QCD calculations predict the existence of states of matter with quantum numbers that have not yet been observed in nature. GlueX will confirm or deny the existence of these states, thereby providing a quantitative test of the theory of QCD. This project will contribute to enhancing the performance of the GlueX detector and to analyzing the data that it collects. Work will be done to allow the experiment to collect data at higher rates. Advanced analysis techniques will be developed and applied to the data collected by GlueX. The work funded by this proposal will greatly increase the potential for GlueX to advance our understanding of interactions between quarks and gluons.

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

Generation of Tunable Fully Coherent Stable Terawatt-Level Hard X-ray Free Electron Laser Pulses with Femtosecond Duration

Dr. Juhao Wu, Staff Scientist
Free Electron Laser and Beam Physics Department
Accelerator Research Division
Accelerator Directorate
SLAC National Accelerator Laboratory
Menlo Park, CA 94025

Terawatt (TW) peak power x-ray pulses from a Free Electron Laser (FEL) will make it possible to image single molecules and study structures at the subnanometer scale. This project will study the feasibility of generating such pulses from a hard x-ray FEL. The pulses would have more than 10^{13} photons in a pulse with a 10 femtoseconds duration and a very narrow bandwidth, much narrower than can be produced by an unseeded FEL. Such pulses will have more than an order of magnitude higher peak power than can be currently provided by existing hard x-ray FEL facilities like the Linac Coherent Light Source (LCLS). These high power FEL pulses will be generated with a seeded photon beam passing through a highly tapered undulator. The seed must be predominantly coherent with stable intensity and a large signal-to-noise ratio for efficient response. A technique called improved Self-Amplified Spontaneous Emission (iSASE) will be studied to generate such a tunable coherent seed. Other seeding techniques, such as self-seeding, will also be studied and compared to the iSASE scheme. The amplification of the coherent seed in a tapered undulator to reach TW peak power requires a multi-dimensional optimization. The studies will include theoretical modeling, numerical simulations, hardware prototyping, and experimental verification. This project will develop a path to generate TW x-ray pulses and will prototype hardware for upgrades of the LCLS and LCLS-II.

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

A Laboratory Astrophysical Jet to Study Canonical Flux Tubes

Dr. Setthivoine You, Assistant Professor
Department of Aeronautics and Astronautics
University of Washington
Seattle, WA 98195

This project aims to simulate a magnetically-driven jet launched by an accretion disk in the laboratory to improve the understanding of plasma shear flows interacting with magnetic fields. The experiment replaces an accretion disk that would rotate in the vacuum chamber at impractical speeds with three independent concentric annular electrodes. In combination with a background magnetic field, the radial electric field can therefore be set up to approximate the rotation profile of an accretion disk, to produce a magnetized plasma jet with axial and azimuthal shear flows. An advanced diagnostic capable of reconstructing 3D flow fields will track the complex flow patterns, using Doppler tomography techniques similar to those used in medical imaging. The apparatus will thus be able to study the fundamental role of canonical flux tubes (magnetic flux tubes with strong mass flows), and see whether intuitions about twist, writhe and link transformations in these tubes are subject to a remarkably simple conservation rule. With this theory of canonical flux tubes and the well-diagnosed experiment, the research program intends to improve the theoretical understanding of how astrophysical jets are highly collimated, often very straight and extremely long. The fundamental role of canonical flux tubes is directly relevant to magnetized plasmas undergoing reconnection, the origin of magnetic fields in dynamo problems, and improved performance in magnetically-confined fusion plasmas and advanced space propulsion.

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

Accurate Ab Initio Methods for Correlated Surface Problems

Dr. Dominika Zgid, Assistant Professor
Department of Chemistry
University of Michigan
Ann Arbor, MI 48109

Transition metal surfaces are widely used in heterogeneous catalysis; however, modeling of catalytic processes on such surfaces remains very challenging due to the difficulty in describing accurately the electronic correlation in the d-orbitals of the transition metals for bulk problems containing thousands of atoms. The objective of this project is to develop new theoretical techniques to address the challenge of correlated surfaces and to properly describe different correlations present between the localized, strongly correlated d-orbitals and the delocalized, weakly correlated s- and p-orbitals in a systematically improvable, ab-initio manner. In this project, methods from both condensed matter physics and quantum chemistry will be employed to build a computationally feasible embedding approach that tackles the size of the problem. This newly developed approach will be used to study the complex interactions between molecule and surface, to model directly measurable experimental quantities such as the photoelectron spectra and to enable a systematic search for new classes of catalytic materials.

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