Topological Materials with Complex Long-Range Order

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The objective of this research is to study exotic metallic behavior in frustrated quantum magnets. These materials are closely associated with quantum spin liquids, an exotic state of matter characterized by strong quantum entanglement. Such systems will in general form complex ordered ground states that involve multiple broken symmetries including time-reversal, inversion and translational symmetry. Metallic states that coexist in this complex magnetic background are thought to inherit some of the characteristics of these ground states, leading to novel transport phenomena that can be sensitively tuned by external stimuli such as applied magnetic, electric and strain fields. This works seeks to understand and manipulate the properties of these exotic materials.

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

Probing Ion Solvation and Charge Transfer at Electrochemical Interfaces Using Nonlinear Soft X Ray Spectroscopy

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Direct observation of ion solvation and charge transfer at electrode–electrolyte interfaces will provide important new understanding of the physical processes that determine the efficiency of electrochemical energy conversion and storage. This project will use 2-wave mixing of a soft x-ray pulse created by high harmonic generation (HHG) with an optical laser pulse to probe ion coordination geometry and charge transfer at working electrode surfaces. Soft x-ray sum frequency generation (SFG) will be applied to the study of ion solvation at biased electrode interfaces as well as metal oxide electrodes used as catalysts for water oxidation. Here, soft x-ray SFG will be used to determine the state-specific charge donor level in electrochemical catalysts that mediate the kinetics of hole transfer during the water oxidation reaction. In addition, soft x-ray SFG will be used to investigate the mechanism of ion de-solvation and adsorption at biased electrode surfaces. The ability to observe electrochemical interfaces directly with element specificity and chemical state resolution will provide new insight into the mechanisms of electrochemical catalysis and will inform the design of new materials for high efficiency applications.

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

Coherent Neutrino-Nucleus Scattering: A Tool to Search for New Physics

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At first blush, the fundamental particle that we call the neutrino does not interact with anything, does not weigh anything, and cannot be observed. Predicted in 1930 to explain the apparent violation in nuclear beta decay of the very basic physics precept of energy conservation, the neutrino eluded detection for over two decades. The "little neutral one," as Enrico Fermi named it, can be difficult to work with but has traditionally offered vistas to a better understanding of the physical world. The coherent scattering of neutrinos off nuclei is one such vista. Predicted over 40 years ago, it has long been one of the "hard" problems in neutrino physics. The daunting technological challenge and the dearth of suitable sources of neutrinos has so far stymied efforts to see this process. The situation is rapidly changing with new developments in detector technologies and with the construction of the Spallation Neutron Source (SNS) in Oak Ridge National Laboratory. The COHERENT collaboration has recently endeavored to measure this process for the first time at the SNS. A precision measurement of coherent neutrino scattering can test for extensions to current models of the weak force; it is a sensitive test for large neutrino magnetic moments which can arise in theories with large extra dimensions; it can investigate the dependence of the interaction of the neutrino on different types of quarks; and it is perhaps the most natural way to search for sterile neutrinos, a flavor of neutrino which may be even more weakly interacting than its cousins. An elegant and simple detector concept will be developed that incorporates numerous nuclear targets as swappable, low-threshold, kilogram-scale gas ionization detectors. The detectors provide for a robust, systematically clean and information rich suite of experiments. Coherent neutrino-nucleus scattering is a long awaited tool that will enable sensitive searches for fundamental particle physics beyond our current understanding.

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

Multiscale Dynamics of Reactive Fronts in the Subsurface

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Carbon dioxide (CO_2) sequestration is considered one of the potential carbon capture and storage technologies for controlling and stabilizing atmospheric carbon emissions by trapping CO_2 in geologic formations for thousands of years. Yet, geologic storage still poses great uncertainty in terms of quantifying and predicting future CO_2 migration and potential leakages. Such difficulty arises because subsurface flow and reactive transport take place in complex heterogeneous media and pervasively exhibit non-linear dynamics and lack of temporal and spatial scale separation. For example, acidification reactions at the pore-scale can dramatically modify permeability of the host rock at the field scale. The overreaching goals of the research are to develop a multi-scale physics-based framework to understand and predict permeability changes in host rocks due to CO_2 injection over a multiplicity of temporal and spatial scales. This will be achieved through a combination of analytical, computational and experimental tools, including homogenization techniques, multi-scale numerical methods and microfluidic experiments.

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

Leveraging the Higgs to Discover Physics Beyond the Standard Model

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The discovery of a Higgs boson at the Large Hadron Collider (LHC) heralds a new era in particle physics. The Higgs discovery not only marks the completion of the Standard Model framework but also offers numerous opportunities in the search for more fundamental physics underlying the Standard Model. For example, the Higgs boson raises a pressing theoretical problem known as the hierarchy problem: why is an elementary scalar particle so light when quantum corrections tie its mass to the highest energy scales? The Higgs also provides an unprecedented experimental opportunity as a bellwether of new physics: it may be merely the first of several Higgs bosons, while its production and decays may provide unique evidence for additional particles. This research program leverages the Higgs boson to explore new physics from both directions, developing novel approaches to solving the hierarchy problem posed by the Higgs boson and directly employing the Higgs as a new tool for discovery. Solutions to the hierarchy problem predict new particles around the same energy scale as the Higgs boson, but existing proposals are under increasing pressure from null results at the LHC and other experiments. This project pursues original solutions to the hierarchy problem wherein the new particles protecting the Higgs boson from quantum corrections are neutral under the Standard Model and present unique signatures at the LHC. These theories motivate the existence of new particles and interactions in additional hidden sectors that can be probed across the energy, intensity, and cosmic frontiers. In employing the Higgs as a tool for discovery, this work articulates a systematic approach to searching for additional Higgs bosons at the LHC. It also strengthens the search for new physics by using the recently-discovered Higgs as a direct probe of new physics processes; as an indirect probe through its couplings; as a portal to states neutral under the Standard Model; and as a source of exotic processes. By using the Higgs in diverse ways to explore the structure of physics beyond the Standard Model, this research aims to understand how the universe works at its most fundamental level.

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

Determining Astrophysical Reaction Rates for Classical Novae and X-ray Bursts via Indirect Methods

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Classical novae and Type I X-ray bursts are the most common stellar explosions in the Galaxy. Both occur in binary star systems where hydrogen-rich matter from a companion star is accreted onto the surface of a white dwarf or neutron star, respectively. As matter builds up on the surface, pressure and density increase, leading to a rise in temperature that triggers a thermonuclear runaway on the surface of the accreting star. During these thermonuclear explosions, proton-rich nuclei are synthesized via a series of charged-particle capture reactions, which are dominated by resonances. As many of these reactions involve unstable nuclei, the reaction rates can be difficult, if not impossible, to measure directly using current technology. Rates must therefore be calculated by indirect means using experimentally determined nuclear structure properties of these resonances. Specifically, the properties of resonances for some of the most uncertain reactions in novae and X-ray bursts, such as those involving ^{26}Al and ^{20}Na, will be measured through this research. The experimental work will rely on state-of-the-art techniques for nuclear spectroscopy using both stable and radioactive ion beams at the John D. Fox Accelerator Laboratory at Florida State University and the Argonne Tandem Linac Accelerator System facility at Argonne National Laboratory. Using these data, important reaction rates will be calculated accurately for the first time, eliminating key uncertainties in understanding classical novae and X-ray bursts.

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

Active Impurity Control For Maximum Fusion Performance

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Achieving the highest possible value of fusion power for a prolonged duration enhances the economic feasibility of a fusion power plant using magnetic confinement. Success of the ITER tokamak experiment and other future facilities relies on the attainment and sustainment of a long pulse, high confinement operating regime that also maximizes plasma purity and hence fusion power production. Controlling the accumulation of impurities in the core of a fusion plasma to maximize plasma purity is thus crucial for optimizing fusion power performance, especially in the presence of high-Z components in contact with the plasma. The development of an active feedback control system to minimize high-Z impurity content is pivotal to extending our experimental capabilities from our current experience with low-Z carbon walls, lithium coatings and short-lived boron films. The objective of this research is to develop an integrated real-time active control approach aimed at achieving long-pulse tokamak plasma discharges with reduced fuel dilution and lower radiative losses in the core while avoiding the formation of deleterious radiation induced instabilities. A unique soft x-ray detector with appropriate time, space and energy resolution will be assembled and deployed on the National Spherical Torus Experiment Upgrade (NSTX-U) to track impurity content. The output of the detector will be used to control various actuators to flush impurities from the hot plasma. Comprehensive impurity transport measurements and validated physical models describing plasma transport and instabilities in the core of fusion experiments will strengthen the physics basis of operation for ITER and beyond.

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

Resilience Design Patterns: A Structured Approach to Resilience at Extreme Scale

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Extreme-scale, high-performance computing (HPC) will significantly advance discovery in fundamental scientific processes by enabling multiscale simulations that range from the very small, on quantum and atomic scales, to the very large, on planetary and cosmological scales. Computing at scales in the hundreds of petaflops, exaflops, and beyond will also lend a competitive advantage to the US energy and industrial sectors by providing the computing power for rapid design and prototyping and big data analysis. Yet, to build and effectively operate extreme-scale HPC systems, the U.S. Department of Energy cites several key challenges, including resilience, defined as efficient and correct operation despite the occurrence of faults or defects in system components that can cause errors. These innovative systems require equally innovative components designed to communicate and compute at unprecedented rates, scales, and levels of complexity, increasing the probability for hardware and software faults. This research project offers a structured hardware and software design approach for improving resilience in extreme-scale HPC systems so that scientific applications running on these systems generate accurate solutions in a timely and efficient manner. Frequently used in computer engineering, design patterns identify problems and provide generalized solutions through reusable templates. Using a novel resilience design pattern concept, this project identifies and evaluates repeatedly occurring resilience problems and coordinates solutions throughout hardware and software components in HPC systems. This effort will create comprehensive methods and metrics by which system vendors and computing centers can establish mechanisms and interfaces to coordinate flexible fault management across hardware and software components and optimize the cost-benefit trade-offs among performance, resilience, and power consumption. Reusable programming templates of these patterns will offer resilience portability across different HPC system architectures and permit design space exploration and adaptation to different design trade-offs.

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

Nanostructured, Targeted Layered Metal Oxides as Active and Selective Heterogeneous Electrocatalysts for Oxygen Evolution

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A long-standing goal in heterogeneous catalysis is to develop catalysts with targeted surface functionality and high uniformity. Recent advances combining novel synthetic chemistry, advanced characterization techniques, and the predictive power of theoretical calculations have led to the development of metal-based heterogeneous catalysts with controlled surface structure and morphology that results in high activity and selectivity for chemical reactions. However, control over the structure and morphology of complex metal oxide-based heterogeneous catalysts (such as perovskites and nickelates) remains significantly more challenging. This project focuses on a promising class of complex layered oxide catalysts, known as nickelate oxides with high potential for efficiently catalyzing reactions involving oxygen, such as the oxygen evolution reaction (OER). OER is an important electrochemical reaction that governs the performance of technologically relevant energy processes such as electrochemical water splitting for hydrogen production. The objective of this research is to tune the geometric and chemical properties of layered nickelate oxides to obtain highly active and stable non-noble metal based electrocatalysts for OER. This will be achieved using insights from quantum density functional theory calculations to guide the selective synthesis of nickelate oxides with optimal activity and stability for OER. This work will facilitate the design of non-noble metal based catalysts for energy conversion and storage.

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

Assessing Subtle Variations in the Actinyl Oxo Reactivity through Characterization of Neptunyl Complexes

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The neptunyl cation, $[Np(V,VI)O2]^{n+}$ (n = 1,2), is a byproduct of the nuclear fuel cycle and has unique chemical properties not observed elsewhere on the periodic table. Interaction between the neptunyl cation and neighboring molecules in solution is a basic chemical process that impacts radiochemical separations, corrosion of spent fuel, and environmental transport. Currently this process is poorly understood; thus, there is a critical need to understand the overarching chemical components that influence actinyl oxo chemistry. The objective of this research is to determine the fundamental mechanisms that can influence the intermolecular interactions occurring between neptunyl cations and neighboring species. The overall hypothesis of the research is that these intermolecular attractions are primarily controlled by the electronic properties of the neptunyl cation but can be further influenced by the electron-donating properties of the equatorial ligands. Insights gained from these studies could lead to technological advances in separations and environmental remediation. This research will lead to an enhanced structural and spectroscopic understanding of the intermolecular interactions of the neptunyl cation thorugh the characterization of novel molecular complexes.

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

Functional Characterization and Regulatory Modeling of Lignocellulose Deconstruction in the Saprophytic Bacterium Cellvibrio Japonicus

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The degradation of plant biomass (lignocellulose) is a critical component of global carbon cycling and renewable energy production. Every year, microorganisms in the environment degrade one hundred billion tons of plant biomass. These microorganisms have found effective ways to completely break down plant biomass and use it for energy. This process is very efficient because the microorganisms in the environment produce large numbers of enzymes that can degrade lignocellulose. While some of the mechanisms of lignocellulose breakdown are understood, which enzymes are essential to plant biomass degradation and how their production is regulated is less known. There is little understanding of how plant biomass degradation is regulated in bacteria because it is not known how these microorganisms are able to detect plant biomass as a nutrient source. This project will use the plant biomass-degrading bacterium *Cellvibrio japonicus* to address these questions. Using next-generation DNA sequencing technologies, this research will determine what enzymes are highly produced when C. *japonicus* is degrading lignocellulose. This information will direct additional experiments to identify the essential enzymes for plant biomass degradation and will compare the enzymes that *C. japonicus* produces to those currently used for biofuel production. Finally, by understanding how *C. japonicus* is able to effectively degrade plant biomass, this project will create a model of how microorganisms in the environment are able to detect lignocellulose as a nutrient. The knowledge obtained from this research will help develop biotechnology strategies to enhance the economical production of biofuels.

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

Cross-Scale Land-Atmosphere Experiment (CSLAEX)

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It is now well recognized that land-atmosphere interactions play an important role in both weather and climate prediction. These interactions take place over a wide range of spatial and temporal scales. Most current formulations of surface turbulent exchange of momentum, heat and moisture are informed by observations with a limited temporal and spatial scale and hence may have limited applicability. The objective of this work is to improve the *multi-scale* representation of the *near-surface heat exchange* using observations based on *high-frequency fiber optic cables*. Our knowledge and predictive capacity in land-atmosphere coupling is limited by our ability to observe the full-scale spectrum in action. The first long-term *Cross-Scale Land-Atmosphere Experiment (CSLAEX)* will bridge this fundamental gap in observation capacity by measuring components of the surface energy balance at a spatial scale relevant to meteorological applications and remote sensing (~2 kilometers) along with recording observations of the nested subscale processes using fiber optic measurements based on novel *Distributed Temperature Sensors (DTS)* at 20-centimeter spatial resolution and 1-Hertz temporal frequency. The CSLAEX experiment will be deployed at the Department of Energy's (DOE) Atmospheric Radiation Measurement (ARM) Southern Great Plains (SGP) site near Lamont, Oklahoma. The data recorded from the Surface Energy Balance and simultaneous observations of the atmospheric state (boundary layer, cloud, convection) available at the DOE ARM SGP site will be used to frame and evaluate new transport laws and parameterizations for the boundary layer and the land surface that can then be implemented into the Weather and Research Forecasting (WRF) model and Community Atmospheric Model (CAM). The results of this study will impact multiple fields including meteorology, climate, hydrology and remote sensing.

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

Actinide Materials under Extreme Conditions

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Nearly 20% of the world's electricity today is generated by nuclear energy. However, the microscopic processes that control transport and thermodynamic behaviors in actinide materials used in power plants are not well understood. Key to understanding phonon, spin and charge transport in actinide materials is a knowledge of the coupling between lattice vibrations, spins and carriers and how the coupling of the low-energy excitations is represented in important physical properties. These interactions will be probed by extensive transport, thermodynamic, and spectroscopic measurements performed under extreme conditions such as high pressures, low temperatures and very high magnetic fields. The characteristic responses of these materials to extreme experimental conditions will help elucidate the underlying transport mechanisms and provide decisive data for theoretical models. This new information and the advances will also have broad implications across actinide materials science generally.

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

Photoconversion in Disordered Semiconductors: Spatial, Spectral, and Temporal Insights through Nonlinear Microscopy

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Solar energy transduction in the disordered compositions of organic and hybrid inorganic/organic solar cells emerges from the interplay of events in the nanoscale and mesoscale domains. It is therefore important to interrogate these power conversion systems at the local level, where structural and compositional heterogeneity can be correlated precisely with the variation in solar cell functionality. Utilizing ultrafast laser spectroscopy coupled together with optical microscopy, this project will examine how excited states and free charges evolve spatially and energetically on length scales between 10 nanometers and 10 microns and on timescales from 50 femtoseconds to 50 microseconds. Conversion of solar photons to useable energy in a photovoltaic system requires two processes to occur successfully. The initial photoexcited state must efficiently produce electrons that are free to move, and the electrons must be transported to electrical contacts before excess energy is lost as heat. The focus of this project examines the spatial and energetic dynamics of these two primary events of photoconversion in blended organic materials and organic-inorganic hybrids. The electronic properties of these systems are complex, involving defects, interfaces, and trap sites, and are strongly influenced by the cumulative interaction of local morphology and composition. Insights gained from measurements made on these characteristic length and time scales will provide an understanding of how nanoscale and mesoscale properties control the macroscopic performance of disordered photovoltaic systems.

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

Universality in Quantum Gravity

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Quantum mechanics and general relativity, two pillars of modern physics, have yet to be reconciled. Theoretical advances in string theory and related subjects over the last two decades indicate that this can be achieved if we abandon the assumption that space and time are fundamental. Instead, spacetime is an approximation that emerges only at long enough distances, and it must be replaced at short distances by a very large number of microscopic constituents. This idea, known as holography or emergent gravity, is supported by numerous calculations, but the underlying mechanism remains poorly understood. Furthermore, although emergent gravity is suspected to be a generic feature of a wide class of quantum theories, little is known about what defines this class of theories, or whether all such theories are string theories. The goals of this research are to understand how general relativity emerges at long distances and to identify the class of the quantum field theories that exhibit this phenomenon. New techniques will be developed to analyze quantum systems with many degrees of freedom, high energy density, and strong entanglement. These techniques will be applied to the dynamics of black holes and other gravitating systems. Progress in these areas would be a significant step toward resolving longstanding questions in quantum gravity, including Hawking's black hole information paradox, the uniqueness of string theory, and the connection between gravity and thermodynamics.

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

Hybrid Methods for Complex Particle Systems

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This project is focused on the development of hybrid, hierarchical, and multilevel algorithms for the simulation of complex many-particle systems. Such systems are key components in a variety of energy generation and energy storage devices. The proposed research is relevant to the computational study of gas-dynamics, plasmas, multiphase flows, and charge transport in materials. The computational complexity of particle system simulations stems from the large numbers of unknowns and the large variations in the spatial and temporal scales over which the systems evolve. This multiscale, multiphysics research challenge will be addressed by hybrid methods that leverage simplified or reduced models to increase the efficiency of simulations so that computational resources can be effectively applied to resolve important fine scale features. This effort relies on the central role played by mean-field models from kinetic theory, which can capture non-equilibrium behavior and also approximate detailed information about particle correlations stochastically via collision operators. The first goal of this project is to connect the fluid and kinetic descriptions in a single efficient algorithm for attacking multiscale problems. The second goal is to improve the efficiency of molecular dynamics solvers using the mean-field solution of the kinetic model as a first approximation.

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

Combined Capture and Conversion of CO_2

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Energy-efficient CO_2 capture from post-combustion exhaust streams is a formidable scientific challenge as current state-of-the-art technologies result in a 30% energy loss in coal-fired power plants. Tailored CO_2-capture solvents - such as switchable ionic liquids (SWILs) - hold the promise of significantly reducing this energy penalty. Sizable gaps exist, however, in the fundamental understanding of the CO_2 capture mechanisms in SWILs. The unusual kinetic/thermodynamic behavior, not seen in other CO_2-capture solvents, is likely related to changes in the SWIL's micro-domain solvent structure. The goals of this project are to use a combined experimental and theoretical approach to explore the structural changes found in SWILs and determine how this structure impacts the SWIL's ability to separate and convert CO_2 into energy carrier molecules. Building on past work with SWILs, this project will conduct a rigorous exploration of how to manipulate such molecular environments to enable energy-efficient CO_2 capture and its subsequent catalytic conversion into practical energy carriers. Two synergistic thrusts will be studied concurrently. The first will exploit combined experimental and theoretical studies to determine the mechanism of liquid carboxylation (formation of alkylcarbonates when CO_2 reacts with the ionic liquid). The molecular reorganization in the SWIL solutions provides a platform to study how the CO_2 dissolution and complexation mechanisms change as a function of CO_2 loading. Studies will characterize the molecular reorganization to learn how the solvent's environmental reconfiguration impacts the solvent characteristics that affect CO_2 uptake. The second thrust is an experimental study to determine the correlation between the electronic properties associated with mesoscopic SWIL structure and the reactivity of the alkylcarbonate versus catalyst location within the SWIL ionic domain.

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

Rheo-structural Spectroscopy: Fingerprinting the in situ Response of Fluids to Arbitrary Flow Fields

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Understanding how processing flows control nanoscale morphology is critical for designing soft materials with enhanced properties for energy production and conversion. However, experimental capabilities to directly measure and test such structure-processing relationships are currently limited to environments that produce pure shearing or elongational deformation. This research will develop a fluidic device and associated experimental methodologies that enable a completely new capability – *in situ* structural measurements using small angle neutron scattering (SANS) under arbitrarily variable deformation type. Leveraging recent advances in time-resolved neutron measurements, new capabilities will be devised to probe nanoscale fluid structure and dynamics in complex, time-varying flows that emulate those encountered in real processes. This new tool will be combined with detailed computational modeling to "fingerprint" a fluid's microstructural response to arbitrary changes in deformation, allowing its processing behavior and morphology to be directly predicted from its flow history. This new tool will be employed to study two important classes of materials: polymeric fluids and self-assembled liquid crystals. Specifically, this research will examine how molecular conformation and aggregate morphology are impacted by complex flows, and how these nanoscale phenomena underlie a number of commonly observed flow instabilities. Ultimately, the goal is to provide detailed guidelines for designing processing flows to obtain new or highly refined non-equilibrium structures of soft matter. The flow device developed in this work will be made available to the scientific community at national neutron scattering facilities in hopes that it will become a central tool in studying flow-structure coupling in a wide range of complex fluids.

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

CALORIE: A Constraint Language and Optimizing Runtime for Exascale Power Management

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Scientific discovery is reliant on computation for insight. The next generation of exascale supercomputers will place tremendous computational power in the hands of scientists. That power, however, comes at the cost of an unprecedented complexity of software development. This complexity arises from the need to schedule myriad low-level resources to meet high-level application requirements. Requiring scientists to be experts in both high-level application constraints and low-level computing resources creates an unrealistic burden, delaying scientific insight. The objective of this research is to create a new programming model that relieves this burden. In this model, scientific application developers will directly express high-level goals and constraints. System software will support this model by automatically tuning low-level computing resources to ensure that the goals and constraints will be met. Using this model, scientists will focus on their area of expertise while the burden of managing the complexity of exascale supercomputers will be automated, greatly increasing productivity and the rate of new scientific insights.

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

Unraveling Principles for Targeted Band Structure Design Using High-Throughput Computation with Application to Thermoelectrics Materials Discovery

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Many technological applications – including thermoelectrics, photovoltaics, solid state lighting, and transparent conductors – would attain significantly higher performance and lower cost if one could design materials that exhibit optimal electronic properties. For example, thermoelectric devices can convert waste heat from industry and automotive exhaust into usable energy but have traditionally been limited by low efficiency. This project will develop theoretical approaches based on density functional theory calculations to screen for high figure-of-merit thermoelectric materials on a large scale and in a multifaceted way. For the first time, band structure and electronic transport data on hundreds of thousands of potential new thermoelectric materials will be generated. This large dataset will be used to reverse-engineer the factors that produce good performance. Novel methods to encode chemical, structural, and electronic properties as meaningful structured data will feed into powerful machine-learning methods that uncover hidden structure-property relationships, and specific features in the band structure will be connected to details of atomic orbital interactions in the presence of secondary environments. In parallel, joint computational-experimental work will establish a framework for synthesis and optimization, resulting in lab-scale demonstration of a high figure-of-merit thermoelectric candidate. This data-driven paradigm of materials discovery will establish new strategies that make possible the design of materials possessing atypical band structure features (e.g., compounds possessing high mobility and high valley degeneracy) that are very difficult to predict or control by other methods. These principles would serve as a foundational capability that could in the future be applied towards the design of several types of semiconductor devices.

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

Mesoscale Fragments of Crystalline Silicon by Chemical Synthesis

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The semiconductor silicon has revolutionized life in the last century, from the development of computer chips to the discovery of solar cells that make telecommunication satellites possible. The frontier for silicon research and development is at the mesoscale. The incredible potential of mesoscale silicon arises from the properties it shares with bulk silicon – earth abundance and low precursor toxicity – and the distinctive optoelectronic properties that emerge at small sizes. Fully exploring and developing this essential energy-relevant material demands absolute control over material length in all dimensions. The goal of this research is to develop an innovative length-controlled synthetic strategy enabling the realization of structure-dependent optoelectronic properties in silicon-containing molecules and polymers. Reflecting bulk silicon's ubiquitous application, the materials that arise from these synthetic studies will be broadly relevant to the energy sciences with the potential to serve as functional components of solar cells, light-emitting devices, and energy storage materials.

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

Interactions between Surface Chemistry and Gas-Phase Combustion: New Optical Tools for Probing Flame-Wall Interactions and the Heterogeneous Chemistry of Soot Growth and Oxidation in Flames

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Some of the most stubborn and technologically critical problems in combustion are dominated by heterogeneous processes. While purely gas-phase combustion systems have been the subject of intense theoretical and experimental study, combustion phenomena occurring at interfaces are far less understood. This is partly caused by the lack of experimental approaches capable of probing locations very close to an interface, especially in the hostile environment of combustion. The aim of this project is to develop and use the needed optical diagnostic tools to study two classes of the most important combustion processes that are inherently entangled with surface-mediated chemistry. The first topic of study is that of soot particle growth and oxidation in flames. While many experimental techniques have been developed for studying soot particles collected from flames, these are nearly universally *ex-situ* analysis techniques. Nonlinear optical probes will be developed that are both noninvasive to the combustion process and capable of capturing the surface chemistry of soot growth and oxidation in the act. The second target of study utilizing the developed optical toolset is that of a combusting flow interacting with a metal wall- a ubiquitous situation for combustion devices and burners. Flame-wall interactions are a major source for pollutant emissions, such as unburned hydrocarbon and particulate emissions, as well as a major cause for combustion device ageing and failure. A new femtosecond/picosecond nonlinear sum-frequency generation vibrational spectroscopy scattering technique will also be developed and employed in the soot surface chemistry and flame-wall interaction studies. This optical diagnostic is selective to probing just the molecular monolayers near an interface. These methods will be combined with multidimensional coherent hyperspectral imaging to define the boundary conditions such as gas-phase temperature and species concentrations. Ultimately, the new insights into the chemical mechanisms of flame-wall interactions and soot growth and oxidation will inform combustion chemistry models that increase the fidelity of predictive numerical simulations of combustion devices, chemistry, and processes. In turn, this will lead to reduced pollutant formation, such as soot and unburned hydrocarbons, in practical devices.

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

Non-Collinear Magnetism and Dynamic Effects in Dzyaloshinskii-Moriya Magnets

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The objective of this project is to understand the effect of spin-orbit interactions in mesoscale and nanoscale magnetic systems. Spin-orbit interactions are usually described by the Dzyaloshinskii-Moriya (DM) interaction. These magnetic systems exhibit fascinating physics related to the formation of topological objects such as skyrmions, magnetization dynamics, and phase transitions. The objectives of this project are to: (1) understand effects of DM interactions on spin/energy transport phenomena and magnetic order dynamics in systems with and without magnetic textures such as domain walls, magnetic vortices, and skyrmions by developing a hydrodynamic description combined with diagrammatic and linear response approaches; (2) understand dynamic effects in the context of novel emergent phases in magnets with DM interactions; and (3) assess the feasibility of novel ultra-low-power spintronic devices that combine logic and memory functionalities by employing theoretical descriptions of spin and energy currents and their interplay with magnetic order dynamics. The project will combine analytic and numerical components to study the properties of various phases as well as the time dependent response to applied fields.

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

Elucidating Biological Energy Transduction from Ammonia

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While most organisms metabolize carbon-based chemical fuel, a select few organisms evolved to derive sufficient biological energy from the six-electron aerobic oxidation of ammonia to nitrite. This process, referred to as nitrification, involves two remarkable steps. The first is the hydroxylation of ammonia by the enzyme ammonia monooxygenase (AMO) to form hydroxylamine. AMO uses a copper cofactor to activate the strong N–H bond of ammonia using dioxygen as the oxidant. The second step involves the oxidation of hydroxylamine to nitrite by hydroxylamine oxidoreductase (HAO). The oxidation of hydroxylamine to nitrite by HAO is a four-electron process requiring proton management. HAO uses a heme cofactor, heme P460, which is unique in its ability to directly remove electrons from substrate bound to its iron center. Mastering the fundamental chemical principles underlying these reactions will fuel the development of novel catalysts for small molecule activation and selective, proton-coupled redox transformations. Moreover, mechanistic knowledge of AMO and HAO will spur the development of improved nitrification inhibitors that would alleviate economic and ecological burdens resulting from the nitrification of nitrogenous fertilizer. However, molecular level understanding of the mechanisms involved in nitrification has remained elusive. This is partly due to the difficulty of isolating sufficient quantities of AMO and HAO from nitrifying bacteria and archaea, which are slow-growing microbes that achieve low cell densities. This project describes the use of stopped-flow kinetics to study the reaction mechanisms underlying the step-wise oxidation of ammonia to nitrite. These experiments will be complemented by cutting-edge, synchrotron-based high-resolution X-ray spectroscopies that will be used to characterize the resting states and reactive intermediates of AMO and HAO. These studies will leverage our newly developed recombinant expression system for AMO that uses rapidly proliferating bacteria to produce active protein in quantities sufficient for biophysical characterization.

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

Precision Probes of the Strong Interaction

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At the heart of all ordinary matter lie the protons and neutrons (hadrons), dynamic conglomerates of quarks and gluons (partons) bound together by the strong interaction, described by the well-established theory of Quantum Chromodynamics. Yet there remain some basic puzzles to be explained. Among these are the detailed structure of the proton in terms of its partonic constituents and how the partons' angular momentum adds up to the total proton spin; the precise value of the strong coupling that sets the size of the strong interaction, for which a number of existing determinations are in tension; and the precise effect of nonperturbative hadronization (binding of partons) on strong interaction cross sections. This research will develop and apply the powerful tools of effective field theory aimed at high precision understanding of these phenomena. The project will focus especially on hadronic jet cross sections in electron-proton and proton-proton collisions that are sensitive to the strong coupling, to hadronization, and to the details of parton distributions inside protons. This work brings the power of the modern Soft Collinear Effective Theory (SCET) into the arena of medium-to-high-energy nuclear physics being pursued at the U.S. experimental frontier at facilities such as Fermilab, the Relativistic Heavy-Ion Collider, Jefferson Lab, and the planned Electron-Ion Collider as well as the Large Hadron Collider in Europe. SCET makes possible the factorization of physics at widely separated energy scales in hadronic cross sections, the resummation of perturbative predictions for them to high accuracy, and the identification of universal nonperturbative effects across different observables. Reaching new levels of accuracy and precision in these theoretical predictions will lead to new and more precise extractions of the strong coupling and parton distributions that reveal the inner structure of the proton.

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

Study of Heavy Flavor Mesons and Flavor-Tagged Jets with the CMS Detector

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In relativistic heavy ion collisions, a new form of matter consisting of liberated quarks and gluons, the Quark Gluon Plasma (QGP), is predicted by Quantum Chromodynamics (QCD) calculations. This strongly interacting matter, first discovered at the Relativistic Heavy Ion Collider (RHIC), was found to flow more freely than any other known fluid. One typical way to study a new medium of interest is to understand the passage of particles through it. However, studies of this kind are very difficult because the QGP created in the collider lasts for just yoctoseconds (10^{-24} seconds). To overcome this difficulty, one studies heavy ion collisions, which produce not only the QGP but also energetic gluons and quarks. Those high energy probes then lose energy by radiating gluons or by colliding with the other quarks and gluons as they traverse through the QGP medium. This sizable in-medium energy loss, observed as the suppression of high energy particles at RHIC or the attenuation of quark and gluon jets at the Large Hadron Collider (LHC), shows that the stopping power of the QGP is incredibly strong. Models based on QCD predict that the gluons, which carry larger color charge, lose more energy than quarks. At the same kinematic energy, the heavy quarks, which are moving more slowly than the light quarks, are expected to radiate less energy than the light quarks. Due to their smaller in-medium radiative energy loss, heavy quarks are ideal tools for the study of energy loss though elastic scatterings in the QGP. This research program will fully exploit the capability of the Compact Muon Solenoid detector at the LHC and utilize new means of selecting interesting events to collect high statistics data on heavy quarks in heavy ion collisions. The program of heavy quark data analysis will aim to provide important information on the elastic scattering power of the QGP to test theoretical calculations based on QCD and models connected to quantum gravity and string theory.

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

In Situ TEM Study of Branched Nanocrystal Growth Mechanisms: Understanding Non-Classical Processes Controlling Formation of Hierarchical Nanostructures

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The objective of this project is to develop an understanding of the formation mechanisms that determine nanocrystal size and morphology to enable the design of highly branched nanomaterials with controlled physical and chemical properties. The new morphologies and tailored properties enabled by that knowledge will accelerate the use of nanocrystalline materials in energy storage, photovoltaic, catalytic, and photonic applications. Branched nanowires are of great interest for these applications because their high surface areas, small dimensions, and complex geometries provide unique control over chemical reactivity, transport of electrons, and absorption of light. However, the ability to design and synthesize these materials is limited because no quantitative framework exists to describe the formation mechanisms, which are typically distinct from the well-described classical mechanisms responsible for bulk crystal growth. These "non-classical" processes are known to involve the assembly of molecular clusters, dense liquid droplets, and nanocrystals. Development of a predictive understanding of these mechanisms requires data on the dynamics of nanocrystal formation as it happens - rather than just information about the nanocrystals after they are formed. This work will employ *in situ* transmission electron microscopy and atomic force microscopy, which provide direct observation of atomic structure and its evolution under actual conditions of synthesis, to investigate the movement and assembly of the precursors that are key elements in the synthesis of these nanostructures. These phenomena will be correlated with the surface charge of the precursors as well as the orientation-dependent forces between them. This approach will be applied to TiO_2 and PbS branched nanowires, which are believed to form through two distinct but general classes of non-classical crystal growth processes. These studies will fill a void in our knowledge of the principles underlying these two fundamental processes that govern synthesis of a broad range of nanomaterials. Moreover, developing an understanding of the principles underlying formation of complex nanomaterials addresses the grand challenge of achieving atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties.

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

Understanding Topological Pseudospin Transport in van der Waals' Materials

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Because of symmetry, crystals often have degenerate valleys in the conduction or the valence band. This “valley” degree of freedom, similar to electronic charge and spin, has been proposed as an information carrier for new classes of electronic and optoelectronic devices. The basic requirement of information processing is to be able to create and manipulate a flow of valley pseudospin, i.e. valley pseudospin current. Valley pseudospin currents have been demonstrated in recent experiments in monolayer molybdenum disulfide and graphene on hexagonal boron nitride. However, the key fundamental questions regarding the nature of valley pseudospin transport remain open. This project will investigate the importance of Berry curvature effects in valley pseudospin transport and explore regimes for quantized valley Hall conductivity and pure valley pseudospin currents. The study will rely on combined optical and electrical transport techniques to create, manipulate and detect valley pseudospin currents in two-dimensional (2D) van der Waals’ materials of hexagonal structure. The insights provided by this research will deepen the understanding of valley pseudospin transport in 2D and help the development of novel valley-based technologies.

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

On the Interaction between Non-Thermal Plasmas and Small Metallic Particles: Plasmonic Plasmas

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Despite finding broad applications ranging from lighting to semiconductor processing, non-thermal plasmas remain far from being completely understood. In particular, there is a need for understanding the rich physics underlying dusty plasmas – discharges with small powder particles dispersed within the plasma volume. There is still a significant gap of knowledge with respect to how the presence of such small particles influences the plasma properties, a fact that can be largely attributed to the lack of a detailed experimental characterization of such systems. This project will establish an enabling approach that will advance the state-of-the-art in dusty plasmas by using small metallic particles in place of the most common semiconducting nanoparticles. Metallic particles will be injected in a low-pressure discharge using different approaches but with independent control over particle size and density in the plasma. This procedure will enable application of the Langmuir probe technique for the characterization of electron kinetics in dusty plasmas and exploration of new regimes in which there is a strong coupling between the optical emission from the discharge and the plasmonic response from the nanoparticles dispersed within the plasma volume. In addition, ultra-fast laser excitation of plasmonic particles dispersed within the plasma volume will be used as an additional novel tool to control basic plasma properties. A complementary theoretical investigation of the dusty plasma system under consideration will be performed by solving the Boltzmann transport equation while accounting for the presence of nanoparticles in the discharge in a self-consistent manner.

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

Biomolecular Assembly Processes in the Design of Novel Functional Materials

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The ability to design complex functional materials by harnessing DNA-mediated interactions between nano- and micron-sized particles holds exciting promise for revolutionizing energy-related material applications such as catalysis, molecular separations and sensing. This project seeks to develop a comprehensive computational strategy to seamlessly connect various scales involved in DNA-mediated particle assembly, ranging from interactions between both standard Watson-Crick and often ignored non-Watson-Crick base pairs to interactions between two complementary DNA-coated particles and then to multi-particle assembly into complex crystalline phases. Advanced computational methods will be used to identify candidate solid crystalline phases and the rates of transformation between these phases in order to isolate the effects of thermodynamic and kinetic variables. This project also aims to elucidate the role of shear as a potentially novel handle for overcoming some of the persistent stumbling blocks in DNA-mediated assembly of crystalline structures such as the narrow temperature window for crystallization and kinetic slowdown. This comprehensive strategy will enable elucidation of assembly mechanisms and their sensitivity to, and thereby identification of, key system parameters available for rationally designing and controlling DNA-mediated assembly. Ultimately, advances made in this research will improve the knowledgebase of multi-scale DNA-mediated particle interactions to a level enabling facile translation into sets of fundamentally rooted design rules. These will prove invaluable for guiding rational design and assembly of particulate structures of prescribed crystalline symmetry and lattice parameters as well as tailored complexity and function.

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

Exploiting Small Signatures: Quantifying Nanoscale Structure and Behavior

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In catalysis, biomineralization and drug delivery, fuel cell and battery chemistry, geological processes, and a host of functional phenomena at the nanoscale, unique properties and material characteristics are governed by intricate structural details eluding current characterization methods. This effort will encompass side-by-side development and application of neutron total scattering methods aimed at uncovering the links in nanostructure between surface chemistry, particle morphology, and "internal" crystal structure. The influence of surface absorbed species on the atomic distortions, structural stability, and growth pathways of titania nanocrystals will be explored, experimentally isolating and characterizing the fluid and atomic interface structures that impact polymorph formation in solvothermal and hydrothermal environments. The distinct effects of particle shape and surface termination on the properties and structural phase transitions of ferroelectric oxide nanocrystals will be pursued, investigating factors that stabilize polarization at smaller nanocrystal dimensions, across phase transitions, or under applied field. Concurrently, instrumentation, data collection, data reduction, and structure refinement methodologies will be advanced for *in situ* and stroboscopic neutron total scattering measurements. These investigations will set the stage for a broader approach to nanostructure and interface characterization that validates theory and simulation, evaluates synthesis and fabrication, and demonstrates enhanced performance in atomic- and nano-scale material processes.

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

Damage Mechanism Interactions at the Plasma-Materials Interface

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This research intends to improve the scientific basis for design of plasma-facing materials (PFMs) for fusion power by quantitatively characterizing the initiation of radiation-induced damage at the plasma-materials interface. New high performance PFMs capable of withstanding the harsh environment of magnetic fusion energy (MFE) are of crucial importance for achievement of commercially viable fusion power plants. The divertors in MFE concepts such as ITER will be simultaneously subjected to high temperatures and heat flux, high-dose neutron irradiation, and bombardment by high fluxes and fluences of helium and hydrogen isotopes. These multiple damage modes cause severe degradation that will put MFE operation at risk. Tungsten is the primary PFM candidate, but suitable strategies to mitigate degradation do not exist. There is a knowledge gap between computational materials science of PFMs under irradiation and the empirical understanding of the response of plasma-exposed materials in these environments. Bridging this gap requires experimentally confirmed knowledge of what processes and interactions occur between the atomistic-theory and phenomenological-observation ranges. This research intends to improve the science-based design of future PFM alloys by providing quantitative experimental measurements of nanometer-scale defect nucleation and early evolution under irradiation. This research will use ion irradiation, in-reactor neutron irradiation, and plasma exposures at tokamaks and linear devices and, through a combination of thermal desorption spectroscopy, positron annihilation spectroscopy, and electron microscopy, will quantify helium-induced defect nucleation and growth as functions of tungsten's starting structure and pre-irradiation condition. This information will be related to what is known from atomistic modeling and simulation and from experimental observations at more macroscopic levels. The work will support the Office of Fusion Energy Sciences (FES) mission and help provide a fusion nuclear science basis for ITER and beyond.

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

Three-dimensional Structure of the Nucleon

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Protons and neutrons, the building blocks of the atomic nucleus, are understood to be different quantum states of a single entity known as the nucleon. The nucleon is a bound state of three elementary particles known as quarks, confined in nucleons by the strong interaction. Owing to recent advances in experimental capability and theoretical understanding, it is now possible to map the nucleon's three-dimensional quark structure in both coordinate and momentum space through detailed studies of energetic electron-nucleon collisions. The recently completed 12 gigaelectronvolt (GeV) upgrade of Jefferson Lab's Continuous Electron Beam Accelerator Facility (CEBAF) nearly doubles the maximum beam energy for electron scattering experiments in the existing experimental Halls A, B and C. Combined with the unparalleled intensity and polarization of CEBAF's continuous beam, the 12 GeV upgrade enables a three-dimensional (3-D) nucleon imaging program of unprecedented breadth and precision. The major objective of this research is the execution of a family of experiments in Jefferson Lab's experimental Hall A known as the Super BigBite Spectrometer (SBS) program. The SBS is a novel magnetic spectrometer designed for the detection of forward-going, high-energy particles produced in electron-nucleon collisions at the highest achievable intensities of CEBAF. The planned physics program of SBS will dramatically improve the world's knowledge of two complementary aspects of nucleon structure. Measurements of proton and neutron form factors using SBS will determine the spatial distributions of the nucleon's electric charge and magnetism at distance scales approximately twenty times smaller than the charge radius of the proton. The SBS will also probe the neutron's three-dimensional spin structure with unprecedented precision. Planned measurements of spin asymmetries in electron scattering from polarized ^{3}He nuclei will provide critical input to the 3-D imaging in momentum space of the spin and orbital motion of quarks in the neutron.

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

Understanding Soil Microbial Sources of Nitrous Acid and their Effect on Carbon-Nitrogen Cycle Interactions

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Our current understanding of Earth's climate is based on predictive atmospheric models that have become necessarily complex as they are extended to answer global-scale questions. Unfortunately, current models are unable to accurately represent all of the important chemical components due to challenges in identifying details of biogeochemical processes occurring within the terrestrial environment that have a significant impact on the atmosphere above. This is especially true for soil microbial emissions of reactive nitrogen (e.g., nitrous acid, nitric oxide, and nitrogen dioxide), which directly and indirectly affect climate by controlling the oxidative capacity of the atmosphere, lifetime of greenhouse gases, and formation rate of aerosols. This project will provide an improved mechanistic understanding of the fate of reactive nitrogen in soil that will enable these processes to be more accurately scaled from the laboratory to the ecosystem and global scales. A unique multidisciplinary approach will be taken to examine how variability in land surfaces and soil properties impact reactive nitrogen emissions, and to link soil fluxes of these gases to their microbial sources using a combination of laboratory and field studies, isotopic analysis, and genomic techniques. In addition, this research will leverage DOE investments in instrumentation at the Environmental Molecular Sciences Laboratory (EMSL) to study the effect of biogenic emissions of reactive nitrogen on the oxidative capacity of the soil environment and to understand how this is then coupled to the combined land-atmosphere carbon cycle. Results will be parameterized and included in the Community Earth System Model (CESM), with the goal of improving representation of the land-atmosphere exchange of reactive nitrogen in global climate models. These outcomes will support the Biological & Environmental Research Program's goal of "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.

Doping Metallic Grain Boundaries to Control Atomic Structure and Damage Tolerance

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Grain boundaries and other interfaces often act as nucleation sites for cracks and voids that lead to failure during plastic deformation of metallic materials. While it is known that interface character and structural state can greatly influence this damage nucleation process, the current level of understanding and control over such details is relatively limited. The objective of this research is to obtain a fundamental understanding of how grain boundary structure can be controlled by locally and selectively adding other elements with the idea of inducing planned grain boundary phases or "complexions" for desired behavior. The effect of complexion structure on dislocation accommodation mechanisms will also be studied to improve the field's understanding of damage nucleation at interfaces and identify materials design strategies for extremely tough materials. This research will use a combination of cutting-edge computational, experimental, and characterization techniques to isolate and understand the importance of atomic grain boundary structure as well as interfacial chemistry. The fundamental insights provided by this research will enable the creation of advanced engineering metals with improved damage tolerance.

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

Hybrid Nanoscale X-ray Imaging: Direct and Computational Imaging with Advanced X-ray Diffractive Optics

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In the past decade, advances in x-ray photon science capabilities have paved the way for new scientific advances in areas such as energy-related materials characterization, nano-crystallography, and ultrafast chemical probing using synchrotrons and x-ray free electron lasers. Advances in nanofabrication of x-ray optics technology can greatly expand the existing capabilities through development of new ways to control and manipulate x-ray beams in space and time. The emphasis of the planned work is to advance scientific capabilities at synchrotrons and x-ray free electron laser facilities through the development and use of advanced diffractive optics and hybrid imaging techniques. New nanofabrication technology will be extended to produce high-efficiency nanoscale focusing optics for both synchrotrons and x-ray free electron lasers. Specialized x-ray diffractive optics will be used to extend hybrid x-ray imaging techniques and will address current limitations in sample throughput, radiation damage, and hardware.

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

Defining the Minimal Set of Microbial Genes Required for Valorization of Lignin Biomass

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As the world population surpasses seven billion, science and engineering are faced with the pressing challenge of creating technology to shift reliance on petroleum resources to renewable feedstocks for the production of liquid fuels and platform chemicals. A primary candidate feedstock is plant biomass, where most of current efforts have focused on converting cellulosic sugars to biofuels, replacement petrochemicals, and novel renewable materials. However, the other major fraction of plant biomass is lignin, a hydrocarbon-rich biopolymer left over after cellulose is used to make ethanol and other liquid biofuels. Lignin is the second most abundant biopolymer on earth and represents a critically underutilized renewable resource that could be a major feedstock for future biorefineries. Unfortunately, without sufficient tools to convert lignin into its simple aromatic components, we are unable to generate valuable compounds from this abundant biopolymer; instead, lignin is typically burned for thermal energy. This project will use a novel approach to identify the minimal set of microbial enzymes necessary for the synthesis of valuable chemicals from lignin as a byproduct of biofuel production from biomass. This research will examine two separate stages of lignin breakdown carried out by the microbes that do it best: (1) early breakdown of lignin into soluble fragments by wood-rotting fungi and (2) further conversion of those lignin fragments into useful chemicals performed by specific soil microbes. The initial goal of the project is the discovery and biochemical characterization of the enzymes required for lignin metabolism. The fungal and bacterial genes that code for those enzymes will be then used to engineer a microbial host that will efficiently convert lignin waste streams directly into valuable platform chemicals. This effort will leverage DOE investments in microbial genome analysis, and secure a critical channel for lignin biomass utilization that will also help to render lignocellulosic biomass a viable feedstock for the production of renewable liquid biofuels.

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

Crystal Growth, Nucleation, Structure and Dynamics at Metal-Organic Framework/Solution Interfaces

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Metal-organic frameworks (MOFs) are a hybrid materials made from metal cations bridged by molecular linking groups. These components assemble under synthetic conditions to generate three-dimensional crystalline solids. MOFs exhibit extremely high surface areas and, as such, have been employed for a wide variety of applications, including gas adsorption, separations, sensing, and catalysis. Yet synthesis of specific, targeted, MOF structure can be an elusive goal, requiring a delicate balance of reaction conditions, often discovered empirically by time consuming screenings over reaction conditions. In general, targeted MOF synthesis is currently hindered by the lack of a comprehensive and predictive model of the fundamental processes occurring at the MOF-solution interface under synthetically relevant conditions. This work addresses the need for a predictive model of MOF interfacial properties by using state-of-the-art simulation approaches to model MOF interfacial structure and stability, crystal growth, nucleation, and post-synthetic modification. This will provide crucial insights into how those processes can be influenced in terms of synthetically controllable parameters.

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

Plasma Material Interaction with Three-Dimensional Plasma Boundaries

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The quest to understand the interaction of a high temperature plasma and its surrounding material surfaces is one of the key challenges on the path to harness fusion power as a new, fundamental energy source. This challenge typically involves the goal of achieving high density, low temperature (detached) plasmas close to magnetic field divertor target plates as well as understanding the plasma material interactions (PMI) in this regime. This area of research involves studying physical processes at spatial scales from nanometers to meters in all states of matter and across a broad range of energies. New modeling capabilities, which help interpret data from current experiments and enable extrapolation to future devices, are required. This is particularly true for toroidal magnetic confinement devices with three-dimensional (3D) plasma boundaries such as tokamak devices when perturbing external magnetic fields are applied and for stellarators with an inherent 3D plasma configuration. The goal of this research is to examine and assess the impact of 3D plasma boundaries on PMI in combination with detached plasma regimes. A critical element will be to experimentally identify critical common and unique features of 3D boundaries as compared to axisymmetric edge plasmas. Establishing a numerical toolset to support the development of predictive capabilities for these regimes is the intended key outcome of the research project. The complexity of this scientific endeavor requires a broad approach, and this research effort will help establish a solid basis to advance understanding in this area.

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

In Situ Thermodynamics and Kinetics of Mixed-Valence Inorganic Crystal Formation

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Efficient synthesis of materials with tailored properties is a Grand Challenge in Basic Energy Sciences. This project will enable controlled access of new phases by establishing a toolkit of experimental and computational methods for probing reactions out of equilibrium. In particular, the phase formation of light-absorbing semiconductors will be studied. In these materials, new crystalline phases would offer unique routes to control the transport of electronic charge. Most traditional materials synthesis methods assume that the crystalline products are close to thermodynamic equilibrium. In those cases, the processes obey phase diagrams and the formation energy can be calculated in a straightforward way. On the contrary, the stepping stones between reactants and products are less well-behaved. They are often metastable materials that can be isolated and modified for technological gain. A central focus is charting the path of reactions *in situ* with X-ray diffraction. In addition to probing the reactions that create specific target materials, the thermodynamic and kinetic barriers to tailoring these materials will be explored by *in situ* gas flow. Reconciling experimental results with computational predictions will move this field toward a regime of design.

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

Confronting Dark Matter with the Multiwavelength Sky

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Dark matter comprises roughly eighty percent of the matter in the universe; its existence is a key clue to new fundamental physics. However, its nature remains an open question and a central focus of the High Energy Physics program of the Department of Energy. This research will develop the theoretical foundation for dark matter searches using light from both our Galaxy and the early universe. It will encompass data-driven methods to extract putative signals from complex astrophysical backgrounds, numerical modeling of the young cosmos, and novel particle theory techniques adapted from collider experiments. Furthermore, this research will explore a bright glow of high-energy light from the center of our Galaxy that has been identified as a possible product of colliding dark matter particles, seeking to delineate both its detailed properties and the implications if it indeed originates from new physics. Understanding this signal will either illuminate the hidden bulk of the universe's matter for the first time or point toward unexpected and striking astrophysical phenomena in the heart of the Milky Way.

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

New Studies of Short-Range Correlations and their Effects on Nuclei

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The nuclear force, which is responsible for holding the nucleus of an atom together, has been under investigation for more than a century. Over the last decade, tremendous progress has been made with the experimental evidence of a special configuration of protons and neutrons called short-range correlations. These short-range correlations consist of protons and neutrons so close to one another that they end up overlapping in the nuclear medium. Understanding their properties is not only important to elucidate where the nuclear force's missing strength is coming from but also has potential to clarify a forty-year-old-question about how the structure of protons and neutrons are modified inside the nucleus. Short-range correlation studies will also help in the area of astrophysics in modeling the cooling process of the neutron stars and also in the area of neutrino physics, where very precise nuclear models are needed to find the small signal created by neutrino oscillations. This project will conduct several approved experiments scheduled to run using the upgraded Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Laboratory in Newport News, VA. The results from these experiments will provide different insights into the manifestation of the nuclear force that have the potential to answer a many-decades-old-question related to the origin of the nuclear force and its effects on the substructure of protons and neutrons.

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

Tunable Oxygen Reduction Electrocatalysis by Phenazine-Modified Carbons

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The kinetically challenging reduction of oxygen to water is the efficiency-limiting chemistry underlying next generation energy conversion devices including fuel cells and metal-air batteries. Nitrogen-doped carbons are a promising class of low-cost, non-toxic, earth-abundant materials that are able to catalyze this difficult reaction. However, the active site structures responsible for catalysis on these materials remain elusive, preventing systematic improvement of catalyst activity, selectivity, and durability. This project targets the chemical modification of carbon surfaces to generate well-defined nitrogen environments that are active for oxygen reduction catalysis. In particular, the research will focus on developing bottom-up strategies for constructing tunable catalyst active sites by ligating polyfunctional organic molecules to carbon surfaces. By modifying the structure of the organic molecule, the project will systematically pursue modulation of the electronic structure, proton transfer environment, and metal-binding affinity of surface active sites and correlation of these changes with catalyst performance. The final aim is to uncover the design principles that underlie efficient heterogeneous oxygen reduction catalysis on nitrogen-containing carbon surfaces and, thereby, provide a roadmap for developing designer electrodes for next generation energy storage technologies.

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

Tracing Non-equilibrium Phenomena in Correlated Materials by Using Ultrafast Electron Probes

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The intimate coupling between the charge, spin, orbital and lattice degrees of freedom engenders many emergent properties in strongly correlated materials. However, it is challenging to unravel the complex interplay of these degrees of freedom by probing equilibrium states using time-averaged techniques, thus preventing a complete interpretation of their novel properties. This project aims to establish an understanding of the competing orders in these complex materials by investigating non-equilibrium phenomena. The project will be carried out using an existing ultrafast electron diffraction (UED) instrument at Brookhaven National Laboratory. Utilizing pump-probe techniques with MeV (megaelectronvolt) electrons as the probe, the UED system has demonstrated the potential for extraordinary sensitivity and high temporal resolution in detecting electronic structures far from equilibrium. During the course of the project, instrumentation modifications will be conducted to enhance the performance of the UED. Individual orders, such as charge order and orbital order, associated with optical excitations will be probed and analyzed separately in the ultrafast time-domain to distinguish their roles in structural relaxation. The characterization of the non-equilibrium electronic states will reflect universal rules that govern the behavior of materials while offering guidance towards designing new materials with ultimate property control.

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

Scaling Analytics for Image-Based Experimental Data

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Department of Energy (DOE) research across a myriad of science domains is increasingly reliant on image-based data from experiments; this project is aimed at helping scientists uncover relevant but hidden information in digital images. The project will deliver a new *modus operandi* for analyzing imaging results of experiments conducted at Lawrence Berkeley National Laboratory and other DOE facilities, providing insight to guide and optimize experiments in collaboration with colleagues in Basic Energy Sciences and Advanced Scientific Computing Research (ASCR). To better exploit the scientific value of high resolution, multidimensional image datasets, this multi-disciplinary work is designed around a coordinated research effort connecting (1) state-of-the-art data analysis methods based on pattern recognition and machine learning; (2) emerging algorithms for dealing with massive data sets; and (3) advances in evolving computer architectures to process the torrent of data. The result will be a set of data science models and new software infrastructure that provide tools that work "on the factory floor" as well as workhorse techniques for processing experimental data at ASCR supercomputing centers. These advances will accelerate the analysis of image-based recordings, scaling scientific procedures by reducing time between experiments, increasing efficiency, and opening more opportunities for more users of the imaging facilities.

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

Ultra-precise Electron Spectroscopy to Measure Neutrino Mass

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It is firmly established that neutrinos have a small but non-zero rest mass, contrary to the Standard Model prescription of exactly massless neutrinos. Neutrino mass could have broad consequences for physics, ranging from the microscopic details of quantum field theories for physics beyond the Standard Model to the understanding of large-scale structure in the universe. Evidence for neutrino mass follows from the observation of oscillations among the three Standard Model neutrino flavor eigenstates. Oscillation phenomena reveal the mass differences but do not depend on the absolute scale of neutrino mass. Furthermore, of the two independent mass differences, the sign is only determined for one, leading to an ambiguous hierarchical ordering of masses. The most auspicious way to measure the absolute neutrino mass scale is by the tritium endpoint method in which neutrino mass is revealed by its effects on the endpoint region of a precisely measured tritium beta-decay electron spectrum. This research will develop the recently demonstrated technique of cyclotron radiation emission spectroscopy (CRES) into a tritium endpoint experiment. The ultimate neutrino mass sensitivity of CRES has been estimated to be sensitive to neutrino masses typical of the so-called inverted mass hierarchy. An existing CRES instrument will continue to provide data for systematic studies and early tritium endpoint results. A new CRES instrument will be established with the goal to produce a neutrino mass limit comparable to existing upper limits from tritium endpoint experiments at Mainz (Germany) and Troitsk (Russia). These results will lay the foundation for the proposal of Project 8, the ultimate CRES tritium endpoint experiment to reach the neutrino mass scale of the inverted hierarchy.

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

Exploring Covalency in the Actinides Using Soft Donor-Based Ligands and Metal-Ligand Multiple Bonding

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The actinide elements are known to prefer oxygen and other hard Lewis bases. Curiously, the use of extractor ligands that contain sulfur, a soft Lewis base, has led to the selective sequestering of actinides over their lanthanide counterparts. Therefore, the coordination chemistry of energy production relevant actinides, specifically thorium, uranium, and neptunium, with soft Lewis bases (sulfur, selenium, phosphorous, arsenic) warrants further investigation. Additionally, compounds containing multiple bonds between the actinide and ligands coordinated to them will be explored to examine pi-bonding with 5f orbitals. The overall impact of this project will be the creation of new compounds that demonstrate the unique structure, bonding, and reactivity of these under studied elements while developing the underlying fundamental science involved in the separation of actinides. Furthermore, this research will support the dwindling nuclear workforce by training the next generation of students to characterize, manipulate, and safely handle radioactive elements.

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

Ensemble Simulation Techniques and Fast Randomized Algorithms

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This project develops novel ensemble simulation techniques and fast randomized algorithms for DOE-mission science problems. Applications include the determination of electronic ground states of chemical systems and efficient molecular dynamics simulation for drug design. For science problems involving the estimate of statistical averages, a conventional approach is to run multiple, non-communicating copies of the simulation and then to average the results. In contrast, the proposed ensemble simulation techniques intentionally introduce limited communication between the copies to achieve problem-specific goals, such as: incorporation of information from observed data; exploration of rare events of acute physical interest; or faster relaxation of a dynamical system to equilibrium. Such low-communication schemes are ideally suited for emerging, multi-core and many-core computational systems. The project also explores new directions in fast numerical linear algebra methods (as motivated by the ensemble simulation approach) and includes new low-cost iterative eigenvector solvers for large-scale computational physics and data analysis applications.

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

Muon g-2: Precision Determination of the Magnetic Field and Enhanced Trolley Features

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The muon is the heavier cousin of the electron and is used in a variety of particle physics experiments. A prominent example is the new Muon g-2 experiment currently being built at Fermi National Accelerator Laboratory to measure an intrinsic property of the muon called the anomalous magnetic moment (g-2), which is sensitive to many forms of new particles and physics. Currently, the most precise measurement of g-2 shows a slight deviation from the prediction of the standard model. The new Muon g-2 experiment will improve the current sensitivity by a factor of four, which will transform the currently measured value into a discovery of new physics and particles if the measured value remains the same. This improvement in the determination of g-2 requires a high-precision measurement of the magnetic field of a 14-meter diameter storage ring. The main component of this research is the establishment of a dedicated analysis center to determine the magnetic field and all of its associated measurement uncertainties. The analysis will incorporate over 400 magnetic field probes and a special trolley system to precisely map the field along the 45-meter circumference storage ring. Hardware upgrades to the trolley will reduce measurement uncertainties and improve the overall precision of the experiment, increasing its sensitivity to new physics. This research is essential for obtaining a precise measurement of g-2 and is therefore an important ingredient for the successful execution of the Muon g-2 experiment.

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

The Effect of Soil Moisture and Surface Heterogeneity on Clouds and Precipitation: Inferences from ARM Observations and Large-Eddy Simulations

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The goal of this project is to improve our scientific understanding of the processes through which soil moisture and surface heterogeneity affect the formation of clouds and the triggering of precipitation events. Large discrepancies exist in the representation of such processes in various global or regional climate models. The need to use observational data and cloud-scale models to understand the relevant physical mechanisms at the process level and thus constrain climate model development has become increasingly clear. This work will use observations from the DOE Atmospheric Radiation Measurement (ARM) Program's climate facility at the Southern Great Plains (SGP) site, which has a network of stations with long-term, continuous measurement of soil moisture, heat fluxes, clouds, and precipitation. The observational analysis will: 1) use the constrained variational analysis method to characterize regional moisture recycling and the land-atmosphere coupling strength for different convective regimes, e.g., locally versus non-locally generated, and over different land covers; 2) investigate the mechanisms by which soil moisture influences precipitation due to the effects of the soil moisture anomaly on atmospheric stability and humidity; and 3) explore the effect of mesoscale circulation induced by heterogeneities in soil moisture on the triggering and maintenance of convection. Large-eddy simulation coupled with land-surface models will resolve cloud and rain processes at their native physical scales and help explain the observational findings and develop insights into the responsible physical mechanisms. The work will also include diagnosis and testing of parameterizations of turbulence, convection, and land features in regional and global climate models run in weather-forecast mode based on relationships and mechanisms found in the observational studies and large-eddy simulation results. The process-level findings are critical for constraining climate-model parameterization development and for resolving discrepancies, thus reducing uncertainties in climate simulations. This work will bridge the gap between *in-situ* measurements made at DOE's ARM facility and the DOE-supported next generation of high-resolution regional and global climate models.

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