Harnessing f-Orbital Bonding through Precision Antenna Ligand Design for Actinide Complexation

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Controlling the selectivity of ligands to bind actinides (such as uranium and plutonium) in environmentally and industrially relevant environments necessitates the ability to understand and predict the fundamental coordination properties of actinide-specific ligands. The objective of this work is to enable the selective tuning of spectroscopic and thermodynamic properties of specific actinide complexes through precision ligand design and molecular recognition. A library of ligands with molecular structures built around a variety of chemical functions will be designed and prepared, resulting in compounds that exhibit specific actinide-binding properties and spectroscopic features. A particular feature that will guide the ligand selection is their efficiency at sensitizing actinide luminescence through the so-called antenna effect. Some chemical functionalities appended to the ligands can act as chromophores that absorb visible light by exciting an electron from the ground state of the ligand into an excited state followed by subsequent excitation of the actinide that ultimately results in luminescence decay. Such energy transfer processes are finely modulated by the different contributions to ligand binding from each of the actinide electronic orbitals. Systematic and iterative characterization of the designed species will therefore be used to harness the contribution of the actinide *f*-orbitals and *d*-orbitals on ligand-bond formation and to characterize the influence of these orbitals on the differences in actinide complex energetic and coordination features, including kinetic, thermodynamic and optical properties. Understanding the fundamental bonding interactions of selective actinide ligands presents a rich set of scientific challenges and is critical to the development of highly efficient separation reagents. The approach taken in this project paves the way to fulfill this difficult task by combining the precision ligand design, sensitive luminescence characterization, and theoretical modeling. The information gained from this effort will not only provide "molecular signatures" for the designed actinide coordination systems, it will yield fundamental knowledge of the role of *f*-electrons in actinide bonding and spectroscopic properties and will lay the foundations for further spectroscopic and synthetic work and discovery related to nuclear energy applications such as separation and waste storage processes.

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

Interface-Driven Chiral Magnetism in Ultrathin Metallic Ferromagnets: Towards Skyrmion Spintronics

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Magnetic skyrmions are localized chiral magnetic textures in the form of nanoscale vortices or bubbles that are topologically protected from being 'unwound'. Their topological nature gives rise to rich behaviors including ordered lattice formation, emergent electrodynamics and robust current-driven displacement at remarkably low current densities. However, magnetic skyrmions have so far been restricted to just a few materials and observed only at low temperatures, limiting the experimental accessibility and technological application of these unique topological objects. This project aims to realize magnetic skyrmions at room temperature in a new class of engineered chiral ferromagnets that exploit broken mirror symmetry at interfaces to generate helical magnetic order. Ultrathin magnetic heterostructures will be engineered and patterned into laterally-confined nanostructures in which skyrmions can be stabilized, manipulated, and detected for the first time under ambient conditions. Static and dynamic properties will be examined using advanced x-ray imaging and nanoscale electrical probes to provide a fundamental understanding of topological magnetic phases. The interactions between magnetic skyrmions and electron charge and spin currents will be studied to identify fundamental new physics and enable device applications. These experimental studies, supported by detailed modeling, will help launch a new subfield of skyrmion-based spintronics in which individual skyrmions can be used to encode, store, and transport information in high-performance, low power memory and logic devices.

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

Actinide N-Donor Thermodynamics: Expanding the f-Element Covalency Dialogue

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Unraveling the fundamental chemistry of the heaviest elements remains a scientific grand challenge. The challenges of studying the heaviest elements stem from their unique chemistry, radiological hazards, and lack of availability. Understanding this chemistry will only become more important as nations worldwide consider and develop peaceful nuclear technology to meet future energy demands. To address current knowledge gaps, this research will study the chemistry of the actinide elements uranium, neptunium, plutonium, americium, curium, berkelium, californium, and einsteinium. While most of the elements to be studied have reasonable availability, the berkelium and einsteinium isotopes will be produced using U.S. Geological Survey's TRIGA® Reactor located at the Denver Federal Center. The thermodynamics of the interactions of these elements with nitrogen donor complexants (nitrogen complexants that donate electrons) will be investigated to gain insight into how these elements share electrons with other elements or materials. The interaction of actinides with these complexants is particularly interesting as nitrogen has demonstrated some ability to share electrons (bind covalently) with actinides. Resolving this chemistry will allow for improved management of used nuclear fuel and provide the United States with key fundamental knowledge in this important area of technology. The data that will be gathered at the extreme edge of the periodic table will elucidate uncertain and suspected periodic trends.

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

High Performance Equilibrium Solvers for Integrated Magnetic Fusion Simulations

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In tokamaks, conditions routinely reach the high temperature and pressure required for self-sustained fusion reactions. However, the rate of heat transport from the hot core to the colder edge is high, so external heating must be applied to maintain these conditions. A key to making fusion an attractive option for electricity generation is to understand heat loss mechanisms in tokamaks and to design devices that better confine heat and reduce external heating requirements. Experimental and theoretical evidence suggests that the turbulent behavior of hot plasmas is responsible for the observed level of heat transport. Understanding the interplay between turbulence and heat loss is a formidable challenge because the mechanisms are highly nonlinear and involve dynamics at vastly separate temporal and spatial scales. Multi-scale numerical solvers have recently been developed to address this challenge. They compute the turbulence on a fine space-time grid and use the results to evolve the macroscopic properties of the plasma on a coarser grid. These promising solvers are currently limited in their ability to model experiments because they do not include the effect of turbulence on the confining magnetic field. Our project seeks to solve this issue by coupling the solvers with equilibrium solvers that update the magnetic configuration. We will develop equilibrium codes specifically for this purpose, with accuracy and speed requirements beyond existing capabilities. The codes have to be fast so that the computational time is mostly spent on the costly turbulence calculations; they have to be accurate to minimize uncertainties associated with error propagation. We will implement advanced numerical methods based on integral equation formulations and algorithms for fast summation to satisfy these performance requirements.

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

Quantifying Global Structural Errors in Predictive Scientific Simulations

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Computational simulations of complex systems, such as climate and power grid applications, are needed to understand physical phenomena and design efficient systems. In this context, making accurate predictions is critical to DOE's mission. A major difficulty in predictive modeling is correctly capturing the physics and component interactions across vastly different temporal and spatial scales. “Structural” errors quantify what is present in the real system but not represented by the model, due to an incomplete phenomenological understanding or misrepresentation across scales. Typically, the model captures only a subset of the physics and component interactions, leading to structural errors in model predictions that can result in inefficient operation or system overdesign. To address this problem, this project will develop mathematically rigorous and robust numerical strategies for quantifying and modeling global structural errors in complex simulations. This work constitutes a novel direction in the way uncertainty is represented in dynamical simulations and will provide rigorous uncertainty prediction bounds in many engineering and science applications important to the DOE mission.

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

A Scintillating Xenon Bubble Chamber for Dark Matter Detection

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The nature of dark matter is one of the great mysteries of modern physics. Originally hypothesized as a simple way to increase gravity at large scales, dark matter is now a central element of cosmology, making up 27% of the energy density in the universe (five times the density of normal matter). Despite this abundance, cosmological requirements that dark matter be non-baryonic, non-relativistic, long-lived and electrically neutral indicate that dark matter must lie outside the standard model of particle physics. The leading candidate for dark matter is an as-yet undiscovered weakly interacting massive particle (WIMP). The PICO Collaboration (formerly PICASSO or Project in Canada to Search for Supersymmetric Objects and COUPP or Chicagoland Observatory for Underground Particle Physics) is one of several groups working to unambiguously detect WIMPs from our local halo in terrestrial detectors. The bubble chamber technique employed by PICO has the unique feature that it is not restricted to a particular target material – any superheated fluid can serve as a dark matter target. This award will support a key exploitation of this versatility, the construction and operation of a prototype scintillating xenon bubble chamber. The motivation for this technology is twofold. It will allow a direct comparison between bubble chambers and the xenon time projection chambers that currently lead the dark matter detection field, critical for both present calibration and future characterization of any dark matter signal. The xenon bubble chamber should also prove to be a superior detection technology in its own right, combining the extreme (10^{-10}) gamma- and beta-insensitivity, easy 3-D position reconstruction, high efficiency and inexpensive instrumentation of the bubble chamber with the energy resolution and chemical stability of a xenon scintillation detector. The work supported here will pave the way for a future large-scale scintillating xenon bubble chamber for dark matter detection.

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

Probing the Magnetic Excitations in Complex Oxide Interfaces and Heterostructures

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When atomically thin layers of transition metal oxides are sandwiched together, they exhibit numerous novel electronic properties. Our understanding of these interface phenomena, however, is limited by our lack of tools for probing the details of the magnetic interactions in atomically thin layers. This program exploits a revolution in inelastic x-ray scattering techniques to measure the magnetic excitations at these interfaces. These magnetic excitations encode the parameters that describe magnetic interactions in these thin layers of transition metal oxide materials. A systematic study of the various interfacial effects will be carried out, first at existing synchrotron sources and ultimately at the National Synchrotron Light Source II where the world-leading brightness translates into a factor of 10 improvement in resolution for such measurements. The goal of the program is to obtain a detailed understanding of the role of interfacial effects in determining magnetic interactions. This is a vital step towards exploiting these effects to obtain the desired properties for next generation functional devices.

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

Quasiparticle Couplings in Transport of Heat, Charge, and Spin for Novel Energy Materials

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Understanding the microscopic processes involved in the transport and conversion of energy from the atomic-scale to the meso-scale is critical for the development of next-generation materials for energy sustainability. The goal of this project is to understand heat, spin and charge transport in novel energy materials by elucidating the couplings among microscopic degrees-of-freedom of atomic vibrations, spins, and electrons. At a microscopic level, these couplings result from interactions of phonons (atomic vibrations) with other phonons, resulting in lattice thermal resistivity, or interaction of phonons with electrons, causing electrical resistivity in metals. An additional and exciting dimension to these interactions has arisen from the realization of the importance of the interaction of phonons with magnons (spin oscillations) in materials for novel spin-caloritronic applications. This project will systematically investigate these quasi-particle interactions using state-of-the-art neutron and x-ray scattering techniques, optical spectroscopy, synthesis and transport measurements, and first-principles computer simulations. This new information and understanding about the interactions among quasiparticles will rationalize the interplay of thermal transport and spintronic properties for applications in novel devices.

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

Competing Orders in Correlated Materials: Impact of Disorder and Non-Equilibrium Perturbations

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Correlated materials provide unique access to the microscopic behavior of interacting electrons, unveiling fundamental properties of the quantum world while serving as cornerstones for exciting technological applications. A hallmark of correlated materials is the existence of multiple competing ordered states such as unconventional superconductivity, magnetism, and charge order. Controlling and understanding these competing electronic phases is a fundamental problem of contemporary condensed matter physics not only because this competition, for example, suppresses high-temperature superconductivity but also because it can give rise to novel emergent states in which electrons self-organize in inhomogeneous patterns. This project will employ a multifaceted theoretical approach to tackle this problem, focusing on the copper-based and iron-based high-temperature superconductors. It will combine phenomenological models and quantum many-body techniques and consider a variety of experimental probes. Realistic features of these correlated materials – such as disorder – will be investigated, and new directions will be explored, such as the use of non-equilibrium perturbations to probe and control phases that compete with superconductivity. The goal of this project is a deeper understanding of the role of competing phases in correlated materials and the discovery of novel ways of tuning and exploring them with potential implications for applications and new technologies.

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

High Repetition Rate Ultra-Fast Electron Diffraction Development

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Combined information on structure and dynamics of atoms and molecules in matter is an essential requisite for understanding the laws of nature to the level that would enable control and mimicking. Natural time scales of structural changes expand well below the picosecond with characteristic lengths of the order of Angstroms, calling for instruments with unprecedented resolution in the four dimensions. This research project aims at the development of an innovative tool for ultra-fast science that will provide access to four-dimensional visualization of atomic and molecular dynamics. A high-brightness, high-repetition rate electron source will be used to produce relativistic femtosecond pulses with high peak and average flux. An electron diffraction beamline will deliver electron pulses to the sample for pump-probe experiments at high repetition rate (up to MHz). Ultra-short pulses will provide direct access to femtosecond dynamics, and the high electron flux will enhance the spatial accuracy, enabling dynamical studies of complex molecules in gas and liquid phase. The instrument will combine high accelerating fields, relativistic energies, and high repetition rate to tackle most of the issues limiting the resolution of ultra-short electron probes such as pump-probe velocity mismatch, time and pointing jitters, and low signal-to-noise ratio. The blending of time resolution and high dose rate at the sample will have an enormous impact on many different fields of science, unveiling the connections between the structure and the function of biological systems, enhancing our understanding of chemical and biochemical reactions, and following transformation pathways that could ultimately lead us to more efficient energy storage and clean energy production.

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

Time-Resolved Electrical, Optical, and Thermal Probes of Topological Spin Textures in Magnetic Nanostructures

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Efforts to understand and control magnetic states on nanometer length scales have revealed new fundamental science and enabled the development of new technology. The objective of this project is to investigate the dynamical motion of recently discovered topological spin textures confined in nanoscale magnetic channels. These magnetic spin textures, known as magnetic skyrmions, have a nanoscale magnetic configuration that is topologically distinct from ordinary magnetic states, giving them "particle-like" properties and potentially providing a measure of protection from defects. In addition, they move under extremely small applied currents, making them interesting for ultra-low power control of information at the nanoscale. Experimental progress in understanding the motion of individual skyrmions has been limited because of skyrmions' nanoscale size and because existing measurements with single skyrmion sensitivity lack time resolution. To overcome these barriers, this research will combine a variety of techniques, including advanced nanofabrication, high-frequency electrical measurements, Lorentz transmission electron microscopy, and magneto-optical/magneto-thermal microscopy. With this hybrid approach, this project will examine how skyrmions move in response to electrical, thermal, and magnetic stimuli. The fundamental insights into magnetic skyrmion motion may lead to new approaches for storing and manipulating information at the nanoscale using topologically protected magnetic states.

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

Statistical Methods for Exascale Performance Modeling

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Large computer simulations are critical for a broad range of scientific disciplines. Despite this need, adapting a scientific simulation code to run efficiently on a new supercomputer is tedious and time consuming. For the most complex applications, the process can take six months or more. Predictive mathematical models of performance and power consumption could accelerate this process, but the behavior of modern adaptive codes can change, depending on the input data. This makes existing modeling techniques difficult to apply. This project will develop statistical models of applications that can represent adaptive, data-dependent behavior in a scalable manner. The project will also develop techniques to reduce the complexity of application models so that they are easily understood by application developers. These models will provide simulation developers with insights that allow them to quickly optimize the performance of their code, ensuring that applications can take full advantage of the performance of future exascale machines.

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

Strongly-Driven Attosecond Electron-Dynamics in Periodic Media

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This project uses intense laser pulses to create extremely fast electron oscillations in crystalline materials. The oscillations occur on time scales measured in attoseconds, or billionths of a billionth of a second. The objective of this research is to initiate, control, and measure this attosecond electron motion using specially crafted laser pulses. The strong electric fields associated with these pulses interact with the periodic structure of the crystal to create a nonlinear electrical current. This, in turn, causes the crystal to emit attosecond bursts of light that are precisely synchronized with the driving laser field. This research will lead to a fundamental understanding of high-intensity laser matter interactions of relevance to novel material processing and information technology. Controlling electrical currents in materials on an attosecond time scale may lead to the development of devices that are a million times faster than those possible with conventional methods.

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

Unifying Principles for Catalytic Hydrotreating Processes

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Fast pyrolysis of biomass, a renewable and sustainable resource, is a promising low-cost technology that produces bio-oil suitable for use as transportation fuel after an appropriate upgrade step. The upgrade can be achieved by reducing the high oxygen content of up to 35 – 40 wt.% through hydrotreatment over heterogeneous catalysts, but the complexity of bio-oils with ca. 400 different oxygenated compounds and the fact that this technology has only recently gained interest are both responsible for the lack of fundamental knowledge in this field. In contrast, the petroleum industry has been using hydrotreating reactors with cobalt and nickel promoted molybdenum sulfide based catalysts for the removal of sulfur impurities for decades, and the catalyst structure, nature of the active site, and elementary reaction steps are largely understood. This project builds on the hypothesis that the hydrotreating processes for the removal of oxygen and sulfur are fundamentally similar at the atomic-scale and existing knowledge from the treatment of petroleum derived feedstock can be leveraged for the design of novel catalysts for the upgrade of bio-oil. Electronic structure simulations on high performance computing infrastructure and kinetic modeling will be used to improve our mechanistic understanding of bio-oil hydrotreatment and to derive characteristic catalyst properties that are responsible for high activity and selectivity. From the resulting structure-function relationships we can extract common features of hydrotreating catalysts and develop unifying principles that lead to the accelerated design of novel materials for bio-oil upgrade.

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

New Searches for Ultralight Particles

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There are many lines of evidence indicating physics beyond the Standard Model of Particle Physics and Cosmology. In particular, the observational evidence for dark matter proves there must be new physics beyond what is known. There are many searches for new particles, for example at the Large Hadron Collider or in dark matter direct detection experiments. However, almost all of these searches are designed to detect new heavy particles that deposit significant energy in a detector through single, hard particle scatterings. There are few searches for new light fields such as the axion or dark photon, which also make good dark matter candidates. This project will improve the ability to detect such light particles through the invention of novel experimental techniques. In particular, there is the possibility of searching for the dark photon through the coupling it will induce between two resonant microwave cavities. If electromagnetically shielded from each other, such cavities will only couple through a new light field such as a dark photon. The calculations in this project will greatly increase the reach of previous experiments and motivate novel proposals. This work may be extended to make a novel detector for dark photon dark matter using a high-Q resonator inside electromagnetic shielding. This experiment would extend the reach for dark photon dark matter by many orders of magnitude in both cross section and mass. Further, extensions of previous proposals for axion detection using nuclear magnetic resonance and spin precession technology will allow for novel types of dark matter detectors searching for dark matter coupled to nucleon or electron spins. Such technology may even allow a novel type of neutrino detector that measures total neutrino flux instead of energy deposition. By proposing such new experiments this project will improve the ability to detect many new types of dark matter.

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

Impurity Doping of Niobium for Ultra-Efficient Superconducting RF Cavities

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Improving the performance of superconducting radio frequency (SRF) cavities is a critical task on the way to realizing future goals in accelerator technology at the energy and intensity frontiers as well as at the cutting edge of low and medium energy nuclear physics or for accelerators for industrial applications and medical purposes. The objective of this research is to develop SRF accelerating cavities performing consistently with higher quality factors than can be currently achieved with the-state-of-the-art cavity surface processing. Increasing the efficiency of niobium SRF cavities is of great importance for nearly all SRF accelerators, especially those where a substantial part of capital and operating costs is dominated by the cavity cryogenic losses. It was recently demonstrated at Fermilab that introducing a small amount of impurities like nitrogen at the surface drastically modifies the behavior of the niobium cavity surface resistance, resulting in cavity quality factors two to three times higher. The results so far indicate that doping the cavity surface with a certain (above typical) concentration of impurities modifies beneficially the RF surface resistance. The goal of this research is therefore to improve upon these recent findings by finding the ideal concentration and dopant to achieve the highest possible quality factor at different gradients. This research will also study whether higher than typical accelerating gradients can be achieved via doping. The final outcome of this work will be to have different optimized and consolidated surface processing recipes for quality factor maximization for SRF structures operating at different frequencies and gradients.

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

Exploration of Main-Ion Properties at the Boundary of Fusion Reactors

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ITER ("the way" in Latin) will be the world's largest fusion experiment and is currently being constructed by an international team to demonstrate the scientific and technical feasibility of fusion energy. Success of the ITER mission relies on the achievement and sustainment of high-confinement (H-mode) plasmas that operate stably and with high performance. The core reactor performance is closely linked to the ion temperature and velocity near the plasma edge, and a primary focus of modern tokamak plasma physics is to develop models able to predict the edge parameters and transport processes to extrapolate to ITER and beyond. Currently, the physics basis for a prediction of the edge pressure, ion temperature and plasma rotational velocity remains elusive. At the edge of an H-mode plasma the main-ion properties are known to deviate significantly from the more commonly measured impurity ion properties, and therefore a critical research need is to validate current state-of-the-art simulations of the tokamak H-mode pedestal with a diagnostic that measures the properties of the main-ion fusion fuel, deuterium. This research combines diagnostic development with model validation. A new diagnostic system will determine the deuterium plasma temperature, velocity and density at the plasma edge for a range of experimental configurations and establish the scaling of these parameters with external actuators such as plasma current, shape and heating. Key dependencies identified by these new measurements will be compared to impurity ion measurements and to transport theories in the edge. Comprehensive main-ion measurements and validated physical models of the plasma edge will strengthen the physics basis of H-mode operation for ITER and future fusion reactors.

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

Non-Equilibrium Atomic Physics in High Energy Density Material

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The objective of this project is to develop a coherent modeling framework for non-equilibrium atomic physics in extreme material environments. Today's high-energy-density physics facilities are exploring new regimes of matter at extreme conditions, compressing megajoules (MJ) of energy into microscale targets over nano- or femto-second timescales to produce radiation-dominated, highly magnetized, and extremely transient non-equilibrium plasmas. Currently, atomic-scale models used to design and diagnose these experiments almost universally assume full or partial equilibrium. This project will systematically remove equilibrium constraints from the existing fully quantum mechanical self-consistent-field model, calculating the response of electronic wavefunctions to high fields and time-varying non-thermal photon, electron, and ion distributions. These wavefunctions will be used to generate predictions of observable quantities for comparison to experiments including transport coefficients and the detailed emission and scattering spectra that reveal the electronic and ionic structure of matter. The code developed will be made openly accessible to other researchers in the high-energy-density physics community.

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

Search for New Phenomena at the 13 TeV LHC: Fast Start and Strong Finish

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The Large Hadron Collider (LHC) at the European Center for Nuclear Research (CERN) in Geneva, Switzerland will increase its center-of-mass energy from 8 TeV to 13 TeV in 2015, thereby providing one of the greatest single extensions of direct sensitivity to new physics over the next two decades. The Compact Muon Solenoid (CMS) experiment must be poised to efficiently analyze the first data at this energy for evidence of physics beyond the standard model (BSM) and to collect large samples of high quality data in order to fully characterize a discovery or to continue BSM searches in the longer term. Motivated by these requirements, the objectives of this research program are two-fold. First, the research involves searches for supersymmetry (SUSY), a leading candidate for BSM physics, which provides an explanation for dark matter hypothesized in astronomy and which helps solve theoretical problems related to the stability associated with the recently observed Higgs boson. In particular, searches for SUSY particles decaying to hadronic final states will be performed with the first 2015 data. Subsequently, as more data are collected at the LHC, these searches will evolve towards challenging signatures with low missing energy associated with undetected SUSY particles. In addition, the project aims to upgrade the CMS calorimeter subsystem to allow longer term operations in the high radiation environments foreseen at the LHC with a focus on the development of next generation readout electronics and new active materials with enhanced radiation tolerances.

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

Kinetics of Particles with Short-Range Interactions

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Nano- and micro-scale particles provide a promising set of building blocks for many new energy-applicable technologies, such as materials for energy storage or meta-materials. Designing particles so they assemble spontaneously into a desired structure is critical for making these technologies efficiently, but performing this optimization is a challenge because the timescales of the short inter-particle attractions are typically much faster than the long, diffusive timescales of assembly. This project will develop a set of conceptual and computational tools to analyze the kinetics of assembly for systems dominated by short-range interactions and to optimize over the set of possible parameters to design building blocks that assemble efficiently.

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

In-situ Thermodynamics Measurements at Metal Oxides-Solution Interfaces Using Flow Adsorption Microcalorimetry

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The overarching goal of this project is to complete a systematic study of the thermodynamic properties of ion exchange, ligand sorption and surface charge reactions occurring at four metal oxides surfaces: goethite, gibbsite, rutile and quartz. Metal oxides/solution interfaces are critical for our environmental and energy future. In Earth-surface environment, metal oxides are ubiquitous in nature, existing as relatively pure minerals such as gibbsite and goethite, and as poorly crystalized hydrous oxyhydroxide phases, such as ferrihydrite, that bind and coat other soil components. They are arguably the most important components controlling the solubility and mobility of anthropogenic pollutants in the environment. In technological settings, metal oxides such as rutile and quartz are critical for our energy future as catalysts for the synthesis of chemicals and for the production of fuel cells, solar fuel photocatalysts, and solid reactants. The work will be accomplished primarily through the construction and application of novel flow adsorption microcalorimetry instrumentation and techniques. These unique and specialized flow microcalorimeters will operate at various temperatures and solution chemical compositions, most notably absent CO_2. In addition to key thermodynamic parameters (enthalpies), calorimetric measurements provide a wealth of mechanistic information about reaction energetics and kinetics, surface charge characteristics, and structure-reactivity or selectivity relationships, all obtained in situ and in real-time. Determining thermodynamic properties for contrasting metal oxide sizes, different ligand properties, various solution chemical compositions, and across temperature ranges will help us understand the relationship between a metal oxide surface structure and its reactivity well enough to predict its behavior and performance under a suite of variable conditions. Considering the centrality of the studied elementary chemical reactions in geochemical, environmental, biological and technological applications, the project will generate data and produce new analytical capabilities of value to scientists across a spectrum of disciplines and specializations. Integrating key thermodynamic data with the advances and sophistication other theoretical, experimental and computational methods have achieved maps out the blueprints of the next-generation understanding of metal oxides surfaces and interfaces.

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

Characterization of Backgrounds for EXO

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Neutrinoless double beta decay could occur if an atomic nucleus decays radioactively by emitting only two electrons, in contrast to the ordinary double beta decay in which two neutrinos emerge as well. Observation of this exotic decay mode would provide evidence that neutrinos are their own anti-particles, and that the symmetry of lepton number conservation is violated. Its observation would also provide strong experimental guidance for theories that go beyond the Standard Model, yielding insights into the origin of neutrino mass and the unexplained excess of matter over antimatter in the observable universe. The goal of this research is to search for neutrinoless double beta decay in the context of the Enriched Xenon Observatory experiment both in its current form (EXO-200), as well as in its next phase (nEXO or “next EXO”). One of the most important aspects of the design and data analysis of this experiment is to identify backgrounds that might obscure an observation of this extremely rare process. The main aims of this research are characterization of experimental background due to interactions of ambient neutrons with xenon and analysis of the EXO-200 data to develop techniques for removing this source of background for the planned nEXO experiment. Using xenon as the target material also provides a unique opportunity to directly tag the barium ions that are products of the decay, thus eliminating backgrounds from all other sources. A laboratory at Indiana University is being developed to study the mobility of single barium ions in the liquid xenon in order to achieve a barium-tagging capability in a second phase of nEXO.

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

Exploring Novel QCD Matter in Proton-Proton and Proton-Nucleus Collisions at the LHC

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In relativistic heavy-ion collisions, a new state of hot and dense matter with quarks and gluons freed from the protons and neutrons into which they are normally bound is created as predicted by the theory of Quantum Chromodynamics (QCD). The most striking feature of this quark-gluon plasma (QGP) matter is the evident flow of particles out of the collisions, which resembles a liquid of strongly coupled particles with nearly zero frictional resistance to the flow or viscosity. It was previously thought that the formation of the QGP fluid is only feasible in heavy nucleus-nucleus collisions where the system size is sufficiently large for a temperature to be established. However, the correlation of detected particles seen as evidence of the flow from the QGP created in the heavy ion collisions have unexpectedly been discovered recently in high-multiplicity (large number of final-state particles) proton-proton (pp) and proton-lead (pPb) collisions at the Large Hadron Collider (LHC). This finding suggests the possibility of creating a QGP droplet in a system that is 10 times smaller than a nucleus-nucleus collision. The proposed research will explore the properties of this novel correlation of particles in pp and pPb collisions in detail. Since very high-multiplicity pp and pPb events only occur on an extremely rare basis, this research will utilize a new online trigger strategy with the Compact Muon Solenoid (CMS) experiment to improve detection and data collection of these events for future LHC runs. The comprehensive program of data analysis proposed will aim to pin down the origin of the particle correlations, and shed light on novel properties of QCD in high-density pp and pPb collisions.

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

Search for New Physics with Top Quarks and Upgrade to the ATLAS Liquid Argon Calorimeter

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The recent successful discovery of the Higgs boson at the Large Hadron Collider (LHC) at the European Center for Nuclear Research (CERN) in Geneva, Switzerland provides a long sought-after key to the Standard Model of particle physics. However, the existence (and mass) of this fundamental scalar does not resolve the tension between the electroweak and Planck scales, hinting at the possibility of new physics that may be accessible at the LHC. The objective of this research is to search for signs of such new physics, in particular for the existence of a supersymmetric partner to the top quark, using the ATLAS (A Toroidal LHC ApparatuS) detector at the LHC to reconstruct signatures of top quarks and missing energy from corresponding undetected particles. Furthermore, in order to ensure that the full potential of the LHC is harnessed in future searches for new physics, the project also entails the upgrade of the ATLAS Liquid Argon Calorimeter read-out electronics, thereby improving the performance of boosted objects, jets, and missing energy triggers for planned higher luminosity running conditions.

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

Exploring Superconductivity at the Edge of Magnetic or Structural Instabilities

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This project aims at understanding the interplay among structural, magnetic and electronic degrees of freedom in unconventional superconductors, a class of materials in one of the most challenging and interesting areas of condensed matter physics. Compared with conventional superconductors, unconventional superconductors cannot be explained by current theories and typically exhibit high critical temperatures (Tc's), meaning they can conduct electricity with low losses, some of them able to do this at or above liquid nitrogen temperatures. This property makes them of particular use for applications in energy generation and electrical energy transmission. These materials are also of fundamental scientific interest because the existence of structural, magnetic, orbital/charge and superconducting orders provide a platform in understanding and ultimately manipulating these interactions. Therefore, the objective of this research project is to design, fabricate and characterize new superconducting materials, including the iron-based superconductors that lie at the edge of structural/magnetic instability, using solid state reaction, crystal-growth methods, electrical transport and thermodynamic measurements with and without magnetic field. The goals of this research project are to help understand the relationship among different orders in these materials, to examine the structure-property relationship, and to shed light on the electron-electron interactions responsible for the superconducting phase transition.

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

Understanding Microbial Carbon Cycling in Soils Using Novel Metabolomics Approaches

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To predict and mitigate the adverse effects of climate change, we urgently need to improve our understanding of carbon cycling in soils. Carbon is accumulated in soils as decayed plant matter and chemically transformed by the metabolism of microorganisms that live in the ground. The products (metabolites) of these transformations carried out by microbes make up a large fraction of the soil carbon. While very little is known about the metabolite composition of soils, much is known about the types of microorganisms found in soils. This is a result of significant efforts to study soil microbes using DNA sequencing technologies. Unfortunately, we lack vital data that will enable scientists to link this sequence information to the microbial metabolic transformations that govern carbon cycling in soils. This project will help bridge this gap by resolving the current 'black box' of soil metabolites and develop approaches to understand how specific microorganisms produce and transform the soil metabolite pools. This will be achieved by pioneering analytical technologies to identify and quantify soil metabolites. We will use this technology to characterize the cascades of microbial activities that follow wetting of dry soils to correlate soil metabolite composition and microorganisms' activities. We will then develop detailed methods to determine the uptake and release of specific soil metabolites by key soil bacteria to make and test predictions of carbon cycling based on DNA sequence data. This program will provide an urgently needed complement to DNA sequencing that will enable the understanding and mathematical modeling of soil carbon cycling, ultimately improving our ability to predict and mitigate the effects of climate change.

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

Elucidating the Determinants of Alkali Ionic Conductivity in Oxide and Sulfide Frameworks

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The facile conduction of alkali ions in oxide and sulfide host structures is of critical importance in energy storage. Today, the dominant form of energy storage in consumer electronics and increasingly in large scale applications such as electric vehicles is the rechargeable alkali-ion battery, a device that functions entirely on the basis of the reversible transport of alkali ions. The Li^{+}/Na^{+} conductivity of a cathode (typically a transition metal oxide) has a direct influence on the rate capability of a Li/Na-ion rechargeable battery. Alkali ion conductivity is arguably of even greater importance in the solid oxide and sulfide electrolytes currently being investigated for high safety, all-solid-state batteries, where the diffusion length scales are significantly larger than in the electrodes. This project will elucidate the structural and chemical factors determining alkali ion conductivity in oxide and sulfide frameworks using large-scale first principles calculations and topological analysis. We will approach this problem through a series of detailed investigations into prototypical structures and chemistries as well as through a broader study carried out over a large number of materials using data mining techniques. The ambition of this project is to go beyond mere screening of materials and to acquire the insights necessary to achieve true "reverse design" capability to build high alkali ion conductivity structures from constituent anion frameworks, cation chemistry, and topology design.

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

Microbial Carbon Tranformations in Wet Tropical Soils: The Importance of Redox Fluctuations

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Tropical forest soils store more carbon (C) -in the form of plant litter and decomposed organic matter- than any other terrestrial ecosystem and play a critical role in the production of greenhouse gases (methane, nitrous oxide, carbon dioxide) that affect both atmospheric chemistry and climate. Humid tropical forests also exchange vast amounts of carbon, water, and energy with the atmosphere and can lose large amounts of dissolved carbon via runoff and leaching. The rapid carbon cycling characteristic of wet tropical ecosystems is driven in part by high rainfall and warm temperatures. This combination of environmental conditions causes tropical soils to alternate between oxygenated and anaerobic conditions and affects the behavior of tropical soil microorganisms that regulate many aspects of the belowground carbon cycle. In the coming half century, tropical forests are predicted to see a 2-5 degree Celsius temperature increase and substantial differences in the amount and timing of rainfall. Although the importance of tropical soils to the global C cycle is clear, we have a surprisingly poor understanding of how soil carbon cycling in wet tropical forests will respond to climate change. This makes predicting future climate impacts extremely difficult. Our ability to forecast how new moisture and temperature patterns will shape tropical microbial activity is also a gap in knowledge because so little is known about the fundamental abilities and chemical preferences of tropical soil microorganisms. If wet tropical forests experience shifts in rainfall patterns, becoming generally drier and more aerated, microbially-mediated processes that produce greenhouse gases or help store soil carbon will likely be affected. Only a few studies of microbial diversity have been conducted in wet tropical soils, and only a handful of them have evaluated microbial function with modern DNA sequencing technologies. This project will examine the genomic content and potential of tropical soil microorganisms as they experience shifts in soil temperature, moisture, and oxygen availability. By also tracking the degradation and fate of organic carbon compounds, this work will increase the accuracy of predictions about how microbial processes affect whether organic carbon is retained or lost from tropical systems. The mechanistic understanding produced by this research will directly benefit attempts to improve the predictive capacity of mathematical models that forecast future tropical soil carbon balance.

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

Understanding the Roles of Cloud Microphysics and Land Surface Coupling Feedbacks in Multi-Scale Predictions of Central US Summer Hydroclimate

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The climate sensitivities of the water cycle on regional scales are highly uncertain. Inspired by recent advances in solving the zeroth order problem of explicitly representing rainfall by organized summer storm systems in global climate models, this project seeks to understand next-order uncertainties linked to microphysics and land surface interactions. The primary analysis tool is the next-generation “Super-Parameterized” Community Earth System Model (SPCESM), which naturally bridges the meso-synoptic atmospheric scale gap by explicitly resolving two atmospheric scale regimes (planetary and cloud-resolving) through a heterogeneous multiscale grid. Superparameterized hindcast simulations of the Midlatitude Continental Convective Clouds Experiment (MC3E) field campaign (April-May 2011) will be used to investigate two issues, validated against high quality data from the Atmospheric Radiation Measurement (ARM) Facility's Southern Great Plains (SGP) site and against MC3E aircraft data. The first goal is to understand how uncertain assumptions about microphysics affect the propagation and structure of Central US storms in superparameterized global simulations. Applying field and ARM validation data will help optimize uncertain microphysical parameters in SPCESM. Sensitivity tests will probe questions such as the following: What is the role of buffering by non-local feedbacks on the microphysical sensitivities of explicitly simulated midlatitude convective systems? Do higher-order microphysics improve the partitioning between suspended/falling liquid/ice condensate? Does evaporative cooling of condensate linked to mesoscale storm organization play a critical role in enabling long-range propagating mid-latitude storms or is advection of potential vorticity the dominant controlling factor? The second problem is to understand the effects of explicitly resolved deep convection on land surface coupling energetics in superparameterized simulations. Results will be validated against soil moisture and surface flux observations from the ARM sites. Sensitivity tests will deconstruct the nonlinear complexities in land-atmosphere coupling feedbacks to address the following questions: How exotic is a negative soil-moisture-rainfall feedback when convection is explicitly resolved? How critical is explicitly resolved land heterogeneity for realistically representing mesoscale land-convection interactions in the context of regional and global hydrology? Are proposed irrigation-driven feedbacks on the Southwest Monsoon robust to a realistic representation of the mechanisms that drive convective precipitation in the Central US?

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

Detector Development towards Precision Measurements of Neutrino Mixing

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The mission of Department of Energy (DOE) Office of High Energy Physics (HEP) is to understand how our universe works at its most fundamental level through discovery and study of the most elementary constituents of matter and energy. One such constituent is the neutrino, a ubiquitous yet elusive particle that requires vast and sensitive detectors to observe. This research project focuses on detector development for precision experiments to measure neutrino properties, such as the Long-Baseline Neutrino Experiment (LBNE), a flagship HEP experiment for which data collection is planned to start in 2025. More specifically, this project seeks to improve the performance of large (many kilo tons) liquid argon (LAr) Time Projection Chambers (TPC). The team will refine our understanding of the most important scientific and technical requirements for LArTPC detectors to achieve high accuracy measurements of neutrino parameters, develop improved argon purification procedures, optimize detector designs, and analyze data from existing LArTPC detectors to verify expected performance. Supported by the extensive detector development experience and resources at Brookhaven National Laboratory, this project will strengthen the technical capability and overall physics potential of large LArTPCs and LBNE.

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

Incorporating the Hydrological Controls on Carbon Cycling in Floodplain Ecosystems into Earth System Models (ESMs)

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Floodplains are a critical missing component of Earth System Models (ESMs). Seasonally inundated regions are the dominant natural source of global methane (CH_4) emissions, and floodplains comprise the single largest terrestrial sink for carbon shed from the land to terrestrial waters. The annual burial of carbon in continental sediments exceeds that buried in ocean sediments by an order of magnitude. To close the terrestrial carbon budget and accurately predict land fluxes to oceans, the lateral exchange of carbon between rivers and floodplain systems must be incorporated into ESM representations of the land surface. This research will develop a new representation of the physical dynamics of floodplains within the vegetated land unit of the Community Land Model (CLM). Unique to this land representation will be the capability to model the exchange of sediment, carbon, and other particulate constituents, between floodplains and rivers. River and floodplain physical dynamics will be directly coupled, allowing for the eventual modeling of biogeochemical (BGC) feedbacks between floodplains and rivers. The development of this model will use geomorphic scaling laws to correlate dynamic landscape processes to measurable and/or predictable land surface properties. In the second half of this project, field work and high resolution process-resolving models will be used to quantify sensitivities of floodplain BGC cycling to both scaling simplifications used to parameterize floodplains in ESMs and to system heterogeneities not resolvable in global-scale ESMs.

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

Scalable and Energy-Efficient Methods for Interactive Exploration of Scientific Data

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This project will investigate novel methods and algorithms for interactive exploration of scientific data. Interactive exploration of scientific data obtained from experimental measurements or generated in simulations is a hard problem because the size of the data is extremely large, making even the execution of a single query time-consuming; the structure of the data varies across scientific applications; and data analysis algorithms are complex and continuously evolving. Three directions will be explored: parallel in-situ data processing methods with speculative loading and overlapped query execution that allow for data to be analyzed in place, multi-query processing strategies that allow complete data access sharing across the entire evaluation while maximizing the number of queries that can be executed in parallel, and parallel processing architectures that overlap normal query execution and randomized estimation in order to identify and eliminate non-informative queries early in the evaluation. The final goal of the project is to design and implement a system that integrates these research directions and makes interactive exploration a reality, even for the largest scientific datasets generated in many DOE projects, while providing considerable energy savings by minimizing data movement.

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

Development of a Comprehensive Description of High-Energy Nuclear Collisions at RHIC and LHC and Electron-Ion Collisions at a Future Electron-Ion-Collider

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Most of the visible matter in our universe is located in the nuclei of atoms. Our goal is to gain deeper understanding of nuclear matter and its interactions governed by the theory of quantum chromo-dynamics (QCD). Nuclear collisions performed at the Relativistic Heavy Ion Collider (RHIC) and the Large Hadron Collider (LHC) can probe the structure of nuclei and create a novel state of matter, the Quark-Gluon-Plasma (QGP). Its properties include almost perfect fluidity, opaqueness to highly energetic jets, and long-range correlations between produced particles. A detailed physical understanding of these fascinating properties and extraction of quantitative information from experimental data requires a complete theoretical description of the produced system and its space-time evolution. We will develop a multi-component numerical framework, which is required by the complexity of nuclear collisions, to provide this theoretical description. It will include QCD based computations of the gluon distribution in a highly energetic nucleus, including quantum evolution, classical field dynamics of the early time after a collision, viscous fluid dynamics to describe the later stages, and the interaction of high momentum probes with the fluid based on perturbative QCD. We will be able to determine how perfect the produced fluid is, extract limits on how small the smallest droplet of fluid can be, and gain deeper insight into the structure of nuclei at high energy, including gluon saturation phenomena. This research will benefit the physics programs for heavy-ion collisions at RHIC and LHC as well as a future Electron-Ion-Collider (EIC).

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

Advanced Methods for Immersed Domain Multi-Physics Computations

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Multi-physics problems have become dominant in the computational sciences. Among the many relevant applications at the Department of Energy, fluid/structure interaction is a prominent example in wind energy and nuclear reactor systems. A key feature of such systems is the geometric complexity of computational domains, which often makes standard mesh generation techniques impractical and, in turn, poses severe challenges to grid-based numerical methods for partial differential equations. These complex fluid/structure interaction problems will be attacked by means of new immersed boundary and embedded discontinuity methods, in which the fluid and solid domains are discretized using non-matching grids. Specifically, the variational structure of the finite element methods for discontinuous approximations will be used to design new embedded discontinuity methods of enhanced accuracy and robustness. At the same time, connections between finite element methods and modern finite volume or finite difference methods will be exploited to obtain more general computational strategies. This research aims at developing a framework for large-scale computations in complex geometry and ultimately delivering a new class of exascale-ready computational algorithms.

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

Probing Coherent States of Light and Matter in Two-Dimensional Semiconductors

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Hybrid quantum systems integrating light with matter offer a highly-controllable landscape for understanding the interface between disparate physical entities. The ability to enhance light-matter interactions using engineered optical environments is well-established in micro- and nano-photonics, but this capability has not yet been exploited for coherent phenomena in emerging two-dimensional semiconductor materials despite their rich correlations between spin, momentum, and light. The goal of this research is to explore quasi-particles of light and matter in monolayer semiconductors by harnessing their intrinsic helicity sensitivity. Combining optical and electrical techniques originating in several disciplines, the work will extend probes of coherent phenomena in two-dimensional materials to provide insights into low-dimensional confinement, material synthesis, and superpositions of degenerate valley excitations. These achievements will be important first steps toward manipulating coherent excitations in low-dimensional materials, which may prove critical for new capabilities in quantum photonic technologies that exploit the valley degree of freedom.

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

Testing the Standard Model and Fundamental Symmetries in Nuclear Physics with Lattice QCD and Effective Field Theory

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The matter in the Universe is made almost entirely of protons, neutrons and the atomic nuclei they form. These strongly interacting particles are described by Quantum Chromodynamics (QCD), the fundamental theory of nuclear interactions that comprises a cornerstone of the Standard Model of Particle Physics. This theory describes our terrestrial experiments with remarkable accuracy, yet there is very compelling evidence it is not complete: for example, the matter in the Universe, described by the Standard Model, makes up a mere 4% of the energy budget of the Universe. The studies supported by this award will provide basic input aimed at supporting potentially high-impact nuclear physics experiments probing the limits of the Standard Model and its fundamental symmetries as realized in nuclear systems. This will be accomplished by combining lattice QCD calculations, from which one can compute low-energy properties of protons, neutrons and light nuclei, resulting from the Standard Model and its possible extensions, with effective field theory, which is both necessary to interpret some of the lattice calculations and also helps build a connection between the lattice QCD results and more complex nuclear physics observables. This work will provide input for the interpretation of the following: (A) the manifestation of parity violation in nuclear and hadronic systems: Parity is a conserved symmetry of all the interactions in the Standard Model except for the elusive weak interactions. The fundamental parity violating (neutral) weak current will be probed by ever more sensitive experiments at the Spallation Neutron Source at Oak Ridge National Laboratory. (B) the elastic scattering of dark matter particles off nuclei in large underground detectors: Dark Matter comprises about 85% of the mass of the Universe (~25% of its energy budget) as determined through observations of the cosmos, yet we know very little about it. In order to constrain these direct experimental searches, we must understand how potential dark matter particles will interact with nucleons and nuclei. (C) future searches for permanent electric dipole moments of nucleons and nuclei: An observation of a permanent electric dipole moment will help us understand the observed matter-antimatter asymmetry; why is the Universe made of only matter? Searches for electric dipole moments remain one of the most powerful methods for constraining physics beyond the Standard Model.

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

Visualizing and Controlling Energy Excitation and Transport in Mesoscale Organic and Inorganic Material Composites

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The processes of creating energy from light in matter have been investigated since the advent of quantum mechanics. However, a lack of spatial resolution has limited any study of the propagation of excitons - electron/hole pairs that enable energy transport through matter. The energy efficiency of future devices relies on the understanding of this transport of energy from its point of origin at the molecular level to mesoscopic, microscopic and macroscopic distances where it can be harnessed. The objective of this research is to visualize, understand and control the transport processes of excitons through novel nano building block composites with molecular precision. Unique, state-of-the-art near-field optical microscopy and Localized Exciton Diffusion Microscopy were developed to map exciton transport at the native length scale through organic and inorganic semiconducting nano building block assemblies. Fundamental insight into energy propagation has profound implications for next generation light harvesting and emitting materials, artificial photosynthesis, and the creation of novel optoelectronic material functionalities.

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

Design of Efficient Molecular Electrocatalysts for Water and Carbon Dioxide Reduction Using Predictive Models of Thermodynamic Properties

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The proposed research focuses on developing catalysts that can perform the reduction of water to hydrogen and of carbon dioxide to formate using an electrochemical potential. Both products can be used directly as an energy carrier in fuel cells or to generate more saturated chemical fuels. Formate is also an intermediate in the sequential reduction of carbon dioxide to methanol, another useful chemical fuel. Molecular inorganic complexes provide an opportunity to use electronic and steric ligand effects to optimize the critical thermodynamic parameters in catalytic intermediates. These parameters will be systematically measured for a series of abundant metal complexes to form predictive models for metal and ligand electronic effects. This principle will be applied to the design of aqueous homogeneous catalysts for the reduction of water and carbon dioxide optimized to function at specific pH ranges. The thermodynamic properties measured will also be broadly applicable to other reductive reactions for the production and utilization of chemical fuels.

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