Laser Driven X-ray Sources for High Energy Density Science Experiments

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Understanding the relationships between temperature, pressure, and density in extreme environments is one of the grand challenges of high energy density (HED) plasma science. Lasers and x-ray free electron laser (XFEL) facilities are now capable of driving matter to extreme states of temperature and pressure. However, these HED plasmas are extremely difficult to probe because most of the time they are in a non-equilibrium state and are transient in nature. Hence, there is a critical need to configure and test new diagnostic tools to measure the properties and dynamics of HED plasmas. This project brings one of the most promising applications of laser-based plasma accelerators (betatron x-ray radiation) to probe HED plasmas with unprecedented sub-picosecond resolution. Our research will generate new data on sub-picosecond dynamics of electron-ion equilibration in warm dense matter, laser-driven shocks, and opacity in HED plasmas that cannot be measured by other existing methods. Our integrated experimental approach, combined with a host of theoretical models and tools, will allow us to probe radiation-matter interactions under extreme conditions to accelerate breakthroughs in frontier plasma science.

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

Ultrafast Dynamics of Molecules on Surfaces Studied with Time-Resolved XUV Photoelectron Spectroscopy

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The capture and storage of solar energy involves the separation and steering of electrons and holes created by the absorption of light. In dye-sensitized solar cells, electrons are injected from a photo-excited dye molecule into a semiconductor. In heterogeneous photo-catalysis, excitation of the electrons in a solid can cause reactions on the surface, storing the photon's energy in chemical bonds. In both cases, the dynamics of charge separation and subsequent reactions are complex and often involve multiple intermediate states. The objective of this work is to provide important fundamental insight into these dynamics using time-resolved photoelectron spectroscopy to track the motion of electrons, holes, and nuclei in prototypical systems. The experiments are enabled by a new light source, which uses frequency-comb methods and high-harmonic generation to deliver ultrashort pulses of tunable extreme ultraviolet (XUV) light at very high repetition rates. Probing with XUV light provides the highest surface sensitivity and allows access to all relevant energy levels of the molecules and the semiconductor being studied, and the high repetition rate of the instrument produces the high signal-to-noise ratio necessary for resolving subtle processes.

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

Tracking Photochemical and Photophysical Processes for Solar Energy Conversion via Multidimensional Electronic and Vibrational Spectroscopic Methods

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Photosystem I (PSI) is one of the two main pigment-protein complexes that catalyze oxygenic photosynthesis in plants, algae and cyanobacteria. This complex is also known to be the most efficient energy converter in nature with an internal quantum efficiency approaching ~100%. Understanding the molecular level parameters that lead to this high quantum efficiency may in turn lead to future developments of bio-inspired systems for solar energy conversion. The main objective of this research is to unravel the underlying photophysics and photochemistry that lead to the high quantum efficiency of PSI. This will be accomplished through applying mixed visible and mid-infrared multidimensional spectroscopies to wild-type and mutant PSI complexes isolated from different cyanobacteria. These investigations will lead to new insight into the mechanism of electronic energy transfer, the initial charge separation event, and protein-cofactor interactions of PSI complexes.

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

Transport Properties of Magnetized High-Energy-Density Plasma

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This project will develop and test a theory describing transport phenomena arising in magnetized high-energy-density plasmas (HEDP). Recent inertial confinement fusion (ICF) experiments have observed that extreme magnetic fields can be generated from either imposed or self-generated seed fields as a dense plasma compresses. These strong magnetic fields are sufficient to magnetize electrons and fusion products, even at high-density conditions. They may be utilized to lower the stringent compression ratio requirements encountered in ICF by providing thermal insulation and by confining energetic fusion products. Future design and analysis will rely on a detailed understanding of the microphysical processes giving rise to these macroscopic transport properties. Addressing the combination of strong magnetic fields and HEDP physics, including strong coupling of ions and degeneracy of electrons, challenges current theory. This project will develop a transport theory addressing this novel state of matter, focusing on properties relevant to the ICF effort: thermal conductivity, fast ion stopping power, mixing (diffusion) rates and electron-ion thermal equilibration rates. The theory will be cast in a form that is convenient to implement in the integrated magnetohydrodynamic design codes used to model the macroscopic behavior of these systems. Validation will be sought using a variety of molecular dynamics simulation techniques.

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

Visible Light Photo-Catalysis in Charged Micro-Droplets

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The objective of this research is to study photochemical reactions under the confined environment of charged micro-droplets that are capable of accelerating chemical reactions using only picomoles (10^{-12} mol) of reactants. A laser source will be coupled with a novel, contained-electrospray ionization mass spectrometry technique for direct and rapid screening of reaction conditions in ambient air. The ionic environment of the charged droplets exists at the interface of the solution phase and the gas phase, yielding information that is directly transferrable to large scale chemical synthesis. The hypothesis is that the effect of electric fields used during charged droplet generation, the effect of concentration achieved by solvent evaporation from the resultant charged droplets, and the effect of droplet exposure to a highly intense and coherent visible laser source will enable the production of unique, reactive photo-chemical species for novel pathways that might be difficult to access in traditional bulk, condensed-phase conditions.

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

Quantum Phenomena in Few-Layer Group IV Monochalcogenides: Interplay among Structural, Thermal, Optical, Spin, and Valley Properties in 2D

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Sulfur, selenium, and tellurium are known as chalcogens. Carbon, silicon, germanium, tin, and lead are group-IV elements. Similar to graphite, materials that contain a group-IV element and a chalcogen can form layered phases that have strong chemical bonds in two spatial directions and a weaker (van der Waals) bond along a third (perpendicular) direction. These materials, known as layered group-IV monochalcogenides, have been proposed as next-generation solar cells and also have shown great potential in thermoelectric applications due to a structural phase transition at finite temperature. This structural phase transition occurs in single-layer materials as well. The goals of this research are to understand the consequences of this phase transition on the material properties of thin (few-layer) monochalcogenides and to lay down a comprehensive route towards the use of these two-dimensional (2D) quantum materials in novel device paradigms at finite temperature for optoelectronic, spin, valley, and thermoelectric applications. Specific objectives of this project are: (1) determining the 2D order/disorder transition temperature in bulk layered monochalcogenides; (2) determining the effective electronic, spin, and valley properties of disordered monolayers; (3) assessing the interplay between a giant piezo-electric effect and the structural phase transition in layered monochalcogenides; (4) investigating the excitonic spectrum of monolayers; (5) determining the materials properties of stacks of monochalcogenides when combined with other 2D materials; (6) assessing the chemical degradation of few-layer monochalcogenides; (7) generalizing the discovery of 2D disorder relative to other puckered 2D materials beyond graphene; and (8) investigating new paradigms for thermoelectrics by design of layered materials with degenerate ground states. Due to the richness of this material platform, results from this research will help design new generations of thermoelectric, light-harvesting, valleytronic, and piezoelectric devices from materials with out-of-equilibrium structural ground states.

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

Non-Equilibrium Plasma-Interactions with Biomaterials, Biological Solutions and Tissues

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Cold atmospheric pressure plasma discharges offer an abundant source of reactivity at room temperature, enabling unique interactions with biomaterials, biological solutions and tissues. These interactions, particularly with biological tissues, present an exciting and important intellectual frontier in plasma science with promising potential applications in plasma biomedicine and advanced biomaterial processing. The lack of insight into the underlying mechanisms of the interaction of plasma with biomaterials gives rise to many interesting scientific questions and represents a bottleneck for further development of new technology. This project will develop a comprehensive model of the important interaction mechanisms of non-equilibrium atmospheric pressure plasmas with biomaterials, including a direct quantitative link between the plasma properties and their biological impact. Particular emphasis will be on the impact of charge at the plasma-biomaterial interface, the impact of species transfer across this interface and the fundamental limitations of plasma penetration in biomaterials. To achieve this goal, this project will strongly rely on advanced optical plasma diagnostics.

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

Using Verified Lifting to Optimize Legacy Stencil Codes

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Many modern image processing, physical simulation, and machine learning applications are expressed as stencil computations. In recent years, various high-performance domain-specific languages (DSLs) have been proposed to optimize stencil computations. Unfortunately, leveraging such DSLs often requires rewriting existing applications or developing custom compilers to transform the original applications to make use of the new DSLs, both of which are tedious and error-prone processes. This project will make use of program analysis, program synthesis, and theorem-proving techniques to automatically transform legacy stencil computations into DSLs. Our system will identify portions of the legacy application that can benefit from being rewritten into DSLs and translate them using the target DSLs. During translation, our system will generate a proof that guarantees that the rewritten code preserves the semantics of the original. The overall goal is to enable legacy applications to automatically leverage the latest developments in high-performance DSLs and domain-specific compilers without building new compilers or manually rewriting the code and verifying the soundness of the rewrite.

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

MAPSTER Microscopy: Multimodal Acquisition of Properties and Structure with Transmission Electron Reciprocal-space Microscopy

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This project will develop a new experimental capability called Multimodal Acquisition of Properties and Structure with Transmission Electron Reciprocal-space (MAPSTER) Microscopy to simultaneously map multiple material properties at the atomic scale using a new generation of high-speed detectors. MAPSTER Microscopy supersedes the conventional "image of atoms" approach of electron microscopy in favor of massive data analytics where one can effectively perform many virtual experiments from a single multidimensional dataset. Key algorithm and instrument developments will also turn this complex methodology into a user-accessible capability for the Molecular Foundry that directly outputs materials property maps at the nanoscale without burying scientists under hard drives full of data. Complex metal oxides offer an extensive array of applications in data storage, energy generation, microscopic motors, and power transmission enabled by strong couplings between properties such as strain, polarization, local distortion and electromagnetic fields. These coordinated features can be probed simultaneously in the MAPSTER paradigm to directly link the atomic structure, mesoscale properties, and overall performance of these materials. MAPSTER Microscopy will also enable mapping of structural domains in soft materials and high-throughput characterization of combinatorial nanoscale syntheses, supporting unique strengths of the Molecular Foundry. MAPSTER Microscopy is transformational in its ability to extract multiple simultaneous properties from a single dataset at the atomic scale to directly address the Department of Energy Office of Basic Energy Sciences Grand Challenge: "How do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents and how can we control these properties?"

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

The Core-collapse Supernova Sensitivity Machine

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Massive stars die in cataclysmic explosions called core-collapse supernovae. These supernovae are the most extreme laboratories for nuclear physics in the universe. Supernovae give birth to neutron stars and black holes and, in the process, synthesize most of the elements heavier than helium throughout the universe. The behavior of matter at extreme densities is crucial to the supernova mechanism. Fundamental nuclear interactions are crucial, too. Despite the key role supernovae play in many aspects of astrophysics and decades of research effort, we still do not understand the details of the physical mechanism that causes these explosions. This leaves us uncertain about the chemical evolution of the universe and makes it difficult to directly connect nuclear physics to observational data of supernovae. This project aims to increase our understanding of stellar death, the creation of the elements, and the role that nuclear physics plays in both through a comprehensive, end-to-end study of the explosions of massive stars. This research includes exploration of the role of turbulence in supernovae through cutting-edge simulations of stellar core collapse and explosion. New computational techniques will be explored that may point the way toward astrophysical simulations at the exascale. This project will make direct connections between observations of supernovae and nuclear physics through detailed parameter studies of stellar explosions with varied input physics. This resarch will lead to the development of a publicly available framework for carrying out controlled-parameter studies of the supernova mechanism. Through quantifying the sensitivity of key supernova observables to uncertain nuclear theory parameters, this project will provide guidance to experimental efforts at nuclear physics facilities.

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

Consequences of Plant Nutrient Uptake for Soil Carbon Stabilization

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Carbon storage in tropical forests is likely to respond to expected reductions in rainfall. Tropical forests are of particular importance in the global carbon cycle because they contain > 25% of carbon storage on land. However, this biome is poorly represented in large-scale models used to predict long-term changes in global carbon cycling. Belowground processes, in particular, present one of the largest sources of uncertainty inhibiting our ability to predict carbon cycle responses to climate change. This project examines how changes in rainfall in tropical forests alter the transfer of carbon from living plant roots into soil, where carbon can be stored for much longer time periods than in living plants. In addition to changes in rainfall, soil characteristics like nutrient availability can have a large effect on carbon transfer and storage. Root characteristics that can affect transfer of carbon into soils include root biomass, root death rates, exudates of carbon, tissue chemistry, and nutrient uptake rates, with each of these sensitive to changes in moisture and soil fertility. This project measures these root characteristics and soil carbon storage across a series of tropical forest sites in Panama. The sites include paired high- and low-fertility soils across a rainfall gradient, which allows the effects of rainfall to be distinguished from effects of soil fertility. The project also uses rainfall reduction structures to decrease rainfall by 50% at a subset of sites and a long-term nutrient addition experiment to assess the effects of drying and soil fertility on soil carbon storage in a controlled setting. Additionally, a greenhouse experiment uses isotopically labeled carbon dioxide to closely track how carbon moves into plant roots and the ways that this carbon then moves into soils or is lost back to the atmosphere. These cross-scale field and greenhouse measures are used in a plant-nutrient/soil-carbon model to scale up results and predict how tropical forest carbon storage will respond to reduced rainfall globally. This project undertakes fundamental research on tropical rainforest belowground dynamics and applies this research in modeling efforts to advance predictive understanding of complex environmental systems in the context of climate change. In particular, new information on drivers of long-term soil carbon storage in tropical forest soils may be used for more strategic atmospheric carbon dioxide mitigation efforts, which is necessary for a sustainable energy future and is central to the Department of Energy Office of Biological and Environmental Research mission.

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

Controlling Atomically Precise Ordering and Phase Transitions in Oxide Thin Films

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Transition metal oxides (TMOs) with ordered vacant lattice sites enable easy electron and ion intercalation reactions and thus have been extensively investigated for energy conversion and storage applications, particularly for use as mixed electronic/ionic conductors, electrocatalysts, and electrodes in batteries and fuel cells. However, phase transitions are often observed when intercalation reactions take place, causing drastic changes in physical properties and device performance. The objective of this research is to understand, predict, and ultimately control the phase transitions occurring in structurally ordered TMO thin films to enable the rational design, synthesis, and use of such materials. A broad toolset available at Pacific Northwest National Laboratory and U.S. Department of Energy synchrotron facilities will be used to establish well-defined structure-stability-function relationships. The combination of highly controlled synthesis by molecular beam epitaxy and *in situ/in operando* structural and chemical imaging by advanced transmission electron microscopies, with guidance from theoretical simulations, will allow us to reveal, verify, and eventually control the transport dynamics, intermediate states, phase transition trajectories, and reaction outcomes. This work meets two of the grand challenges identified by the Basic Energy Sciences Advisory Committee by seeking to "*characterize and control matter away from equilibrium*" and develop a better understanding of "*how remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents*" and will lead to the discovery and design of more robust functional materials.

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

Nuclear Data for Spallation Neutron Radioisotope Production

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Over 50 million nuclear medicine procedures are performed annually, leading to a multi-billion dollar market for radioisotope production. The demand for new medical and research isotopes continues to grow, and the Nuclear Science Advisory Committee (NSAC) has recently identified dozens of radioisotopes whose supply is insufficient. Most radioisotope production today utilizes charged particle or low-energy neutron irradiation of a target. Isotope production using neutrons with 10^{1-2} MeV incident energies is a relatively unexplored option. There is a tremendous opportunity associated with a growing number of suitable domestic and international facilities buttressed by hundred million dollar global investments (e.g., the Los Alamos and Brookhaven Isotope Production Facilities, the European Spallation Source in Lund, and the Korean Multi-purpose Accelerator Complex in Gyeongbuk). In part due to a lack of supporting nuclear data that would make modeling radioisotope yields and purities possible, these facilities do not utilize their high-energy neutron fluxes for isotope production. I propose to measure neutron reaction excitation functions relevant to the large-scale production of critical radioisotopes, enabling development of cost-efficient isotope production methods, contributing to the improvement of theoretical models, and enhancing the value of national isotope production facilities. Reactions that form ^{67}Cu, ^{32}Si, and alpha-emitting isotopes like ^{225}Ac are chosen for their consistent prioritization by NSAC panels, representation of diverse reaction mechanisms, fit to unique Los Alamos National Laboratory expertise, and relative lack of supporting nuclear data. Accurate measurement of these data is presently made using quasi-monoenergetic neutron beams, which are produced by bombarding thin lithium targets with protons at only a few laboratories in the world. These laboratories' experimental focus has not yet been brought to bear on the potential for fast neutron-induced radioisotope production. This work will establish valuable international collaborative relationships with the potential to create a sustained measurement program; characterize new medium-energy neutron-induced reactions relevant to radioisotope production, facility design, and the ongoing effort to improve nuclear codes' predictive power; and enable consideration of achievable yields and radioisotopic impurities likely formed in reactions of current interest to the Department of Energy's Isotope Program.

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

Formation of Superconducting Nb_3Sn Phase for Superconducting Radio Frequency (SRF) Cavities

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Superconducting cavities are an essential part of many energy-efficient particle accelerators around the world. The current material of choice for superconducting cavities is niobium, which is the material with the highest transition temperature among pure metals. Today's multi-cell structures reach accelerating gradients and quality factor values close to the intrinsic limits of niobium. Future improvements of superconducting cavities will require a different material with a higher transition temperature. In particular, superconductors with a critical temperature higher than that of niobium would enable equivalent operation at a higher temperature, thereby reducing the very significant cryogenic capital and operational costs. This research aims to understand and improve the present state-of-the-art Nb_3Sn coatings for accelerator applications. The project, being targeted at accelerating charged beams, will pursue both fundamental and practical aspects of Nb_3Sn coatings on cavity structures. At the same time, we will pursue understanding of the coating limitations via research using single-cell cavities and small samples. This project will expand our understanding of new materials for accelerator applications, which is a growing research area at Jefferson Lab. Successful coating of Nb_3Sn on cavities will result in quality factors and gradients higher than those presently available in niobium cavities. This will provide more efficient superconducting cavities, thereby potentially impacting any future accelerator project based on superconducting radio frequency technology.

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

Advanced Electronic Structure Theories for Strongly Correlated Ground and Excited States

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The collective behavior of strongly correlated electrons is responsible for several fascinating and still poorly understood phenomena in chemistry, physics, and materials science. The properties of these systems are intrinsically determined by the mutual interactions of many particles. Therefore, strongly correlated electrons cannot be described using conventional theories that build on an independent particle picture. The objective of this project is the development of new quantum chemical methods for strongly correlated electrons based on renormalization group ideas. These methods will be used to map a complex problem involving strongly and weakly interacting electrons onto a simpler one in which few electrons interact via modified interactions. This project will develop methods to accurately compute potential energy surfaces of molecules in their respective ground states. It will also produce theories for the description of excited states of large molecules. The methods and software developed in this research will provide new computational tools for studying problems relevant to basic energy science including combustion processes, transition metal catalysts for energy conversion, and the photochemistry of multi-electron excited states.

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

Exotic Kondo Phases: the Non-Kramers Doniach Phase Diagram

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A key goal of condensed matter physics research is realizing new macroscopic phases by designing materials with specific microscopic physics. Heavy fermion materials, where magnetic moments due to localized f-electrons coexist and interact with free and mobile conduction electrons, host a wide range of macroscopic phenomena. At low temperatures, these two types of electrons can hybridize via the Kondo effect, an antiferromagnetic interaction by which the conduction electrons screen the local moments, giving rise to a “heavy” Fermi liquid with effective masses up to one thousand times those of free electrons. Alternatively, the local moments can decouple from the conduction electrons to order magnetically. The competition between these two tendencies leads to novel quantum critical behavior and unconventional superconductivity and is captured in the *Doniach phase diagram*. However, the canonical Doniach phase diagram is only relevant to materials where the f-electron ions have an odd number of electrons, like cerium. These *Kramers ions* typically undergo single-channel Kondo physics. This research will address Kondo physics in *non-Kramers ions* – those with even numbers of f-electrons, like praseodymium. In non-Kramers ions, the Kondo effect is always a two-channel Kondo effect, where conduction electrons with two different symmetries compete to screen the same local moment. Non-Kramers materials realize a new set of phases in quantum materials, including a symmetry-breaking heavy Fermi liquid with a spinorial order parameter, called *hastatic order*; a novel type of superconductivity, where two electrons screen the same local moment to form a composite pair; and non-Fermi liquid phases. This research project will explore these novel phases in real quantum materials by including the relevant band structure and spin-orbit coupled hybridization terms to develop a comprehensive theoretical understanding of the nature of the different possible non-Kramers Kondo phases and how they compete or cooperate based on realistic materials models. In addition to the analytical work, this project will involve close collaborations with experimental groups to grow and characterize new non-Kramers doublet materials and with computational physicists to examine numerical models that can capture effects beyond mean-field theory. Specific objectives include: (1) exploring simple two-channel Kondo phase diagrams, collective modes and topological defects to learn how to tune hastatic order with a wide variety of handles; (2) developing material-specific models to explore how to detect hastatic order; (3) studying how superconductivity manifests in non-Kramers doublet materials, with a focus on how it changes with materials details; and (4) examining non-Fermi liquid physics by implementing large-scale numerical simulations, including developing a Hubbard model with a non-Kramers doublet ground state to enable quantum Monte Carlo studies. This research will broaden our understanding of how Kondo physics develops in non-Kramers doublet materials, which will span emergent phenomena from exotic nematic phases to unconventional superconductors to novel topological defects.

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

Bio-inspired Catalysts Featuring Earth Abundant Metals and Secondary Coordination Sphere Interactions for the Reduction of Oxyanions

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The overall goal of this research program is to catalytically reduce oxyanions to their more benign counterparts using a sustainable earth abundant catalyst featuring a bio-inspired support. These supports have been modeled after nature, which has demonstrated the ability to effectively reduce these oxyanions. A major component of this research is to gain fundamental insights into what dictates the reactivity, catalysis and method by which these catalysts operate for continued improvement and enhancement.

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

Mass Measurements and Decay Spectroscopy of the Heaviest Elements

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What is the heaviest nucleus that can exist? Is there an island of stability with 'long-lived' superheavy (SHE) elements beyond uranium? These questions have been at the center of nuclear physics for nearly half a century. They remain some of the most fascinating and elusive open problems in nuclear physics and ones that test our fundamental understanding of nuclei. Over the past 15 years, six new elements with proton numbers Z=113-118 have been discovered, and much progress has been made towards determining whether an island of stability exists for superheavy nuclei beyond uranium (92 protons). Most strikingly, these new elements can currently be produced at the rate of atoms-per-week (Z=112-113,116-118) or even atoms-per-day (Z=114, 115). However, very little is known about these nuclei other than their average lifetimes and that they mainly decay through the emission of α-particles or spontaneous fission. Even the atomic numbers and mass assignments of SHEs remain unconfirmed. The goals of this project are to initiate a new program of experiments aimed at determining the masses and atomic numbers of SHE and then to delve further into understanding the nuclear properties of these superheavy nuclei by obtaining detailed information on their nuclear structure.

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

Dark Matter and Track Triggering with the CMS Experiment

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Remarkably little is known about the substance that comprises 85% of the matter content of the universe. Although gravitational observations provide indirect evidence for the existence of this "Dark Matter" (DM), direct approaches to DM detection have not yet established its particle nature. This research uses the European Center for Nuclear Research (CERN) Large Hadron Collider (LHC) to provide a powerful and complementary means of DM discovery and characterization. Data from the Compact Muon Solenoid (CMS) experiment are used to search for the production of DM particles in LHC collisions. The search focuses on DM produced in association with top quarks, a process that is enhanced in many new physics scenarios. Results of the top-associated DM search are combined with those of related DM searches to maximize overall sensitivity to DM production at the LHC. This work involves the development of new techniques for reconstructing the particles produced in LHC collisions and the design of novel statistical tools to extract potential DM signals. The ultimate discovery potential of the LHC will be achieved in the era of high luminosity (HL-LHC). CMS data rates will grow significantly, providing unprecedented sensitivity to rare DM processes and other new phenomena. The key enabler of CMS physics goals at the HL-LHC is a cutting-edge, hardware-based data filter (a "trigger") that can reconstruct the trajectories of charged particles ("tracks") within microseconds. A second objective of this research is to tackle the crucial challenges of data distribution and track reconstruction in the development and construction of the CMS track trigger. Hardware algorithms that leverage the newly available tracking information are developed to improve the acceptance of DM signal, greatly extending the CMS reach for DM discovery at the HL-LHC.

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

Molecular Interactions of the Plant-Soil-Microbe Continuum of Bioenergy Ecosystems

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The accumulation and stabilization of organic matter in soil is important for the global carbon cycle because it contributes to soil fertility and helps reduce the release of the greenhouse gas carbon dioxide into the atmosphere. A better understanding of the processes related to soil carbon accumulation is critical for designing strategies to increase soil carbon storage. Emerging experimental and theoretical evidence suggests that the residues of dead soil microbes play an important role in increasing the stabilization and long-term storage of carbon in soil. This project will study the deposition of dead microbial cells on different mineral surfaces and its effects on long-term carbon stabilization in soils used for both annual and perennial bioenergy crops. This research will identify the metabolic pathways and chemical components of microbes that contribute to soil carbon accumulation under controlled laboratory conditions. Field experiments will also be conducted to characterize the accumulation of microbial cells in response to crop selection and soil characteristics. The experimental data will be used to develop models of carbon cycling in bioenergy cropping systems under different soil conditions. These models will generate new knowledge on beneficial plant-microbe-soil interactions that increase carbon storage in biofuel agroecosystems. As new marginal lands are cleared and greater quantities of biomass are harvested, this project will provide the basic science needed to develop sustainable biofuel feedstocks to ensure healthy soils and promote a low-carbon economy outcome.

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

Nanoscale Ferroelectric Control of Novel Electronic States in Layered Two-Dimensional Materials

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The ability to locally control the charge degree of freedom in nanoscale and low dimensional materials can often lead to new electronic behaviors and novel quantum phenomena. The goal of this project is to leverage the built-in, nonvolatile, switchable polarization field of a ferroelectric gate to impose quantum confinements and band structure designs in layered two-dimensional (2D) materials, including graphene and 2D transition metal dichalcogenides. Conducting atomic force microscopy and piezo-response force microscopy will be employed to create nanoscale domain patterns in the ferroelectric gate, which will induce local potential confinement and carrier density modulation in the neighboring 2D electron channel via the electric field effect. Various artificial nanostructures, including homojunctions, nanoribbons and superlattices, will be defined electrostatically without introducing additional chemical or structural disorders in the material platform. The electronic, magnetic, and optoelectronic properties will be correlated with the geometric design and the edge configuration of the nanostructures. These studies will advance the fundamental understanding and rational design of the ferroelectric and 2D material hybrid systems and facilitate the development of van der Waals materials based nanoelectronic and optoelectronic applications with programmable functionalities.

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

Search for Dark Matter using mono-Higgs and the ATLAS Pixel Detector

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A large component of the mass-energy of the universe is composed of dark matter (DM), whose properties and interactions with known particles are not yet understood. Searches for DM at the Large Hadron Collider (LHC) provide important information, complementary to direct and indirect detection experiments, that is necessary to determine whether an observed signal indeed stems from DM. Furthermore, the discovery of the Higgs boson provides a unique avenue to search for DM because the potential interaction of the Higgs with DM would lead to the unique signature of a Higgs boson recoiling against DM. This process is typically referred to as mono-Higgs because DM does not interact strongly with most known particles and will therefore pass unseen through the detector, leading to a single detected Higgs boson and a large imbalance of momentum. Due to the strength of the interactions of the Higgs with Standard Model particles, it is unlikely for a Higgs boson to be radiated from initial state quarks. Therefore, the observation of this process would provide direct insight into the mechanism by which DM couples to known particles. The objective of this research program is to search for the dark matter particles produced in association with a Higgs boson at the LHC using the ATLAS (A Toroidal LHC Apparatus) detector, specifically when the Higgs boson decays to two bottom quarks. This research will benefit greatly from the development of innovative identification techniques of boosted Higgs bosons. The program includes the upgrade of the ATLAS Pixel readout system which is critical to maintain high performance of tracking, vertexing, and boosted Higgs tagging in the planned higher luminosity run of the LHC.

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

Accelerating Applications of High-Performance Computing with Quantum Processing Units

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High-performance computing (HPC) is an important part of the Department of Energy mission to advance scientific discovery. As persistent demand for computing continues to grow, barriers to increased power and performance loom on the horizon for existing technologies. New computing paradigms that offer breakthrough solutions are needed to overcome these barriers. Quantum computing promises new approaches for solving hard computations by using the quantum physical processes found in atoms and molecules, but it is not yet clear how these newfound capabilities can translate into the large-scale computing systems required by DOE stakeholders. Dr. Humble's research investigates how emerging quantum computing platforms can be leveraged to support scientific computing at DOE HPC facilities. This research assesses the potential for quantum computing to accelerate scientific applications in computational chemistry, materials science, and data analytics as well as many other domains. The project translates scientific software into a representation that can run on computer systems that host both conventional and quantum processing units. This model of hybrid computation requires the development of novel run-time and system execution models to manage and process quantum programs. New methods for simulating these hybrid systems are also needed to analyze the behavior and performance of hybrid scientific applications. Constraints on programming, communication, and energy that arise within the context of large-scale HPC environments must also be included to provide realistic estimates of time-to-solution, scaling, and power consumption. Developing expectations for future quantum processing units allows HPC stakeholders to evaluate the merits of quantum computing when planning next generation systems. These early insights are also critical for supporting the broader development of algorithms, programming languages, and software tools needed by next-generation HPC systems.

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

Resilient and Robust High Performance Computing Platforms for Scientific Computing Integrity

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As technology advances, computer systems are subject to increasingly sophisticated cyber-attacks that compromise both their security and integrity. Recent research has highlighted that high performance computing platforms are vulnerable to these attacks. This situation is made worse by a lack of fundamental security solutions that both perform well and are effective at preventing threats. High performance computing platforms used in commercial and scientific applications involving sensitive, or even classified, data are frequently targeted by powerful adversaries. Current security solutions fail to address the threat landscape or ensure the integrity of sensitive data. As challenges grow in this area, both private and public sectors are expressing the need for robust technologies to protect computing infrastructure. Novel solutions hardening high performance computing platforms without loss of performance or energy efficiency are being developed by Dr. Jin and his research group at the University of Central Florida. Advancing the state-of-the-art in high performance computing research, Dr. Jin is developing fine-grained memory protection that is scalable, adaptive, and lightweight to enhance intrusion detection and is addressing the threat landscape facing high performance computing environments. Dr. Jin's work offers optimized, secure, and efficient solutions that will keep pace with security and user demands for both current and future platforms. Dr. Jin's research helps the Department of Energy achieve its mission of providing secure exascale computing platforms to the scientific community.

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

Characterizing the Dynamic Response of Surfaces to Plasma Exposure

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The science of plasma-material interactions is fundamental to the realization of magnetic fusion as a viable clean energy source. However, predicting how materials behave in the extreme environments characteristic of fusion devices remains among the most daunting technical challenges in materials science. This research focuses on one of the most difficult aspects of the problem: *how the intense bombardment of low-energy hydrogen and helium dynamically modify the structure of solid materials*. Emphasis is placed on experiments that reveal the underlying mechanisms of defect creation and growth, hydrogen and helium transport, and subsequent stresses induced in the materials during plasma exposure. Photon-based analytical tools, along with medium-energy ion beam analysis, will be applied to diagnose the surface during plasma exposure. These results will be benchmarked through analyses of materials exposed using high-flux plasma simulators at the University of California, San Diego. In parallel with testing practical material systems, this research aims to break down the complexity of plasma-material interactions into basic atomic-scale processes using low energy ion beam experiments performed in a well-controlled high-vacuum environment. An envisioned outcome of this research is a comprehensive physical picture of hydrogen and helium behavior in the near-surface that will enable accurate predictions of surface composition and structure evolution during plasma exposure. Going forward, this scientific basis for understanding dynamic effects in the near-surface will have an essential role in guiding the development of new plasma-facing materials for future magnetic fusion experiments.

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

Physics-Based Real-time Analysis and Control to Achieve Transient-Free Operations for the ITER Era

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This effort involves a dedicated research program to develop the physics and technical basis of real-time disruption avoidance and feedback control for the ITER tokamak using the DIII-D National Fusion Facility. Rapidly growing instabilities may lead to disruptions in a future fusion reactor in which the heat and particles are released from the confined plasma onto the vessel wall in a very short timescale, potentially damaging the reactor. This research program will develop a real-time system to avoid disruptions on the DIII-D tokamak with the aim of applying these techniques to ITER and beyond. A system to provide high quality plasma equilibria in real time will be established at DIII-D using information from the motional Stark effect, Thomson scattering, and charge exchange recombination spectroscopy diagnostics. These equilibria will be analyzed to determine the plasma stability thresholds and to obtain plasma response models. These calculations will be used to understand the underlying physics of the disruptions in ITER-relevant scenarios on DIII-D and to develop disruption avoidance methods. The enhanced situational awareness and physics insight will be used in advanced real-time feedback control of pedestal and core structures and allow the pursuit and sustainment of high performance tokamak plasma regimes.

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

Dynamic, Robust, Radiation-Resistant Ceramics: Harnessing Thermodynamic and Kinetic Driving Forces

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Porosity or void evolution within nuclear ceramics–fuels, cladding or waste containment schemes–has remained difficult to characterize and control, making it just one of many deleterious consequences of the extreme thermal, mechanical and irradiative conditions. Yet, there are many applications that capitalize on the relative stability of porous structures in ceramics at elevated temperatures, ranging from catalysis to filtration, bone scaffolding, and thermal barrier coatings. Inspired by these examples, the overarching objective of this research is to establish a class of structural ceramics that leverage dynamic porosity evolution to enhance radiation tolerance. Specifically, this research aims to clarify synergistic mechanisms that exist between radiation-induced defects, inherent thermal gradients, and local thermodynamic driving forces in the presence of free surfaces. This insight will provide the baseline necessary for the integration of engineered ceramics into the fuel cycle by allowing the development of more accurate models and efficient materials processing routes.

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

2D IR Microscopy--Technology for Visualizing Chemical Dynamics in Heterogeneous Environments Forces

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Energy technologies, with examples ranging from battery and fuel cell technologies to subsurface technologies (such as enhanced oil recovery), rely upon chemistries occurring in heterogeneous environments. Understanding and predicting chemical dynamics, such as solvent-solute interactions, adsorption processes, and transport processes, requires the ability to probe these environments directly. Therefore, imaging modalities that are capable of reporting chemical dynamics at ultrashort timescales while connecting the observed dynamics to macroscopic observables, such as flow patterns in pore structures, are extremely attractive. This project will leverage new mid-infrared laser technology to reduce the acquisition time of two-dimensional infrared (2D IR) spectra drastically and will interface a microscope with a high-speed 2D IR spectrometer, making it possible to probe environments with scales extending from molecular-scale interactions to mesoscale phenomena.

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

New Methods Enabling a Precise First-Principles Computation of the Muon Anomalous Magnetic Moment

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The anomalous magnetic moment (g-2) of a fundamental particle, such as the electron or its heavier version, the muon, encodes how quantum phenomena affect its interactions with a magnetic field. In particular, the muon g-2 is very sensitive to possible effects from very short distances (at least a thousand times smaller than a proton) that are mediated by new particles, potentially beyond the direct reach of high-energy experiments at the Large Hadron Collider. Interestingly, there is a long-standing and non-negligible disagreement between the prediction of the standard model of particle physics for muon g-2 and its most precise experimental determination to date. For this reason, the measurement of this quantity is now one of the main targets of the U.S. high energy physics experimental program, and the Fermilab E989 experiment aims to reduce the current uncertainty of its measured value by a factor of four. A similar reduction in uncertainty of the standard model prediction is needed to match the experimental improvement. The current standard model precision is limited by the lack of precise knowledge of how quantum effects from hadronic states such as pions, which are governed by the strong nuclear interaction, affect the muon's interaction with the magnetic field. This research uses new methods, developed over the last two years, based on supercomputer simulations of the strong interaction on a four-dimensional space-time lattice that have made it possible to compute the required hadronic contributions from first principles and at the necessary precision. The results of these simulations are essential for maximizing the scientific impact of the more precise muon g-2 measurement at Fermilab.

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

A Comprehensive Framework for Modeling Emissions from Tropical Soils and Wetlands

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Tropical wetlands and wetlands soils account for over 2/3 of the global wetland methane (CH_4) emissions. Tropical wetlands are also important contributors to other greenhouse gases such as carbon dioxide (CO_2) and nitrous oxide (N_2O). Emissions from soils and wetlands, however, are neglected in the existing Climate and Environmental Sciences Division (CESD) programs. Gas emissions in soils and wetlands are complicated and are affected by fluctuations in water levels and oxygen (O_2) availability. Most models lack the ability to transition between these conditions and therefore the ability to predict gas emissions. Further, emissions are strongly affected by soil microbes and available sources of energy such as nutrients and minerals. The objective of this project is to develop a modeling framework that represents microbial functions, energy sources, and soil moisture. Fieldwork will be conducted along transects from valleys to ridgetops in a wet tropical forest in Puerto Rico and at a peat bog in Panama. Long-term, continuous measurements of CO_2, CH_4, and N_2O from soils will be made at each site. Lab experiments will measure emissions of CO_2, CH_4, and O_2 from soils under specific water content, nutrient additions, and O_2 concentrations. Microbial functions (or traits) will be identified using advanced genomic techniques as well as by measuring enzyme activity and metaproteomics. The influence of soil minerals and nutrient status will also be measured. Variation in gas emissions will be related to microbial traits; water and O_2 content; and soil characteristics at each field location using modeling. This model will be rich in details, and it will be appropriate for spatial scales ranging from millimeters to decimeters. A simplified modeling approach will also be developed for applications from meters to kilometers. Finally, information about the exact locations and extent of tropical wetlands is lacking, so data from the new Soil Moisture Active Passive satellite will be used to make a new global inventory of tropical wetlands. This project relates microbial traits, soil characteristics, soil water content, and soil O_2 concentrations and uses the information to build models to improve predictions of soil gas emissions in wet tropical soils and wetlands.

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

Tropical Forest Response to a Drier Future: Turnover Times of Soil Organic Matter, Roots, Respired CO_2, and CH_4 across Moisture Gradients in Time and Space

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Globally, tropical forests account for over half of the carbon sequestered on land each year and nearly 30% of the carbon stored in soil, but belowground carbon feedbacks to climate change are unknown. Recent research suggests moisture may be particularly important in driving soil carbon storage and emissions in the tropics but that the role of moisture is underrepresented in current models. Data on belowground carbon cycling in the tropics are sparse, making extrapolation from field experiments to the tropics as a whole uncertain and limiting our ability to test and improve model performance. The objectives of this research are to 1) investigate how moisture regime and seasonality shape belowground carbon age and transit time in tropical forests and 2) identify specific areas for improvement in tropical land carbon modeling by Earth System Models. In this research, natural amounts of radiocarbon (^{14}C) will be used to trace carbon as it moves into, within, and out of belowground carbon pools to investigate how moisture regime and seasonality shape belowground carbon cycling in tropical forests with differing moisture regimes. Field data will be compared to belowground carbon variables modeled for study sites with DOE's new Earth System Model, the Accelerated Climate Model for Energy (ACME). Finally, for each field site, different soil carbon model structures, environmental drivers, and soil characteristics will be assessed to identify the critical next steps in model development. This is the first cross-site field study on belowground carbon dynamics spanning the entire range of moisture regimes experienced by tropical forests. This work will inform future research and drastically improve models of carbon cycling in the tropics, reducing uncertainty in tropical forest carbon feedbacks to climate.

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

Compensation of Nonlinear Space Charge Effects for Intense Beams in Accelerator Lattices

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Intense charged-particle beams are used for applications in high-energy physics, spallation neutron sources, and nuclear energy. For example, the U.S. High Energy Physics Program is investing in world-class experiments that use intense beams of protons in high-energy accelerators to study the properties of the neutrino. In intense beams, the repulsive force between particles (the space charge effect) can damage the beam's quality, limiting the accelerator performance. Highly original accelerator designs have been proposed to control the effects of space charge. However, to predict how beams will behave in these new accelerators, one needs numerical models with extraordinarily high resolution. This is needed to avoid numerical noise and to resolve low-density regions of the beam. This research will use high-performance parallel codes that are uniquely capable of modeling intense beams at high resolution using several billion simulation particles. These tools will be used to evaluate whether the proposed strategies for controlling space charge can provide the required beam quality and accelerator performance. Alternative strategies for controlling space charge will also be explored.

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

Spatially Resolved Rhizosphere Function: Elucidating Key Controls on Nutrient Interactions

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Microbes play a key role in providing nutrients to plants. A better understanding of plant-microbe interactions is thus important for ensuring sustainable biofuel production from plant feedstocks in the face of a changing climate. Plants acquire their nutrients from the soil around their roots (the rhizosphere) through a process controlled by a dynamic suite of biogeochemical cycles. These cycles facilitate nutrient exchange between the soil, microbes, and plant roots through the rhizosphere interface. There is spatial heterogeneity in both microbial activity and nutrient accessibility throughout this interface. This project will improve our understanding of the spatial controls on rhizosphere nutrient exchange, identify key microbial functions involved in nutrient exchange, and test whether nutrient amendments to the soil can be used to stimulate plant-microbe interactions in spots of high activity (hotspots) within the rhizosphere to increase plant biomass productivity. Central to this study is the use of a series of spatially resolved techniques to pinpoint specific locations within the rhizosphere where enhanced nutrient exchange between roots and soil organisms occurs. How these nutrient exchange hotspots are generated will be characterized through elemental and functional analyses of the rhizosphere. Fundamental understanding of these crossroads of nutrient exchange at the spatial scale of the rhizosphere will form a knowledge framework for directed manipulations of these complex, yet vitally important, nutrient conduits. Ultimately, effective management of rhizosphere processes will enable enhanced plant nutrient acquisition from marginal lands, thereby contributing to improved biofuel feedstock productivity with lower chemical inputs.

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

Host-Microbial Genetic Features Mediating Symbiotic Interactions in the Bioenergy Crop Salix

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Many microbes present in the soil surrounding plant roots (the rhizosphere) can be beneficial for the plant, promoting growth and the incorporation of carbon dioxide into the plant biomass. Yet, only 10% of the microbes in the rhizosphere are able to establish a beneficial interaction with plant hosts due to defense mechanisms that evolved in plants to protect them from microbial infections. Those defense mechanisms pose a fundamental challenge in the utilization of symbiotic microbes to enhance sequestration of carbon dioxide, a potent greenhouse gas, and its fixation into economically valuable plant feedstocks. In compatible plant-microbe interactions, biomass increases of up to 200% have been achieved in perennial feedstocks inoculated with growth-promoting symbiotic microbes. However, compatible interactions are largely host specific, thereby limiting application across diverse plant species. Using willow, a widely used biofuel feedstock and pioneer species with increasing presence in the warming arctic region, this project will identify and characterize unique host-derived genetic factors that allow select microbes to successfully evade defense mechanisms and establish a functional presence inside the plant with no adverse effects. The plant cell surface contains proteins called membrane-bound pattern recognition receptors (PRRs) whose function is to recognize microbes with high fidelity through their microbe-associated molecular patterns (MAMPs). Upon recognition of MAMPs, PRRs trigger a signaling cascade that results in the suppression of host defense mechanisms and facilitates plant colonization by the microbe. Understanding these molecular dynamics presents a unique opportunity to couple new growth-promoting microbes with willow to increase carbon sequestration in the vulnerable arctic region. This project will advance toward DOE's mission in energy and the environment by increasing plant biomass yields for the sustainable production of cellulosic biofuels.

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

Electronic Structure, Bonding and Reactivity in f-Element Chemistry

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Detailed insight into electronic structure and bonding in heavy element chemistry remains poorly developed despite the critical role of actinide and lanthanide compounds in environmental, non-proliferation and energy issues. Furthermore, such insight into electronic structure in heavy element systems is critical in order to define the origins of their unique chemical properties as well as to broaden our understanding of fundamental quantum chemistry. The objective of this research is to develop and apply advanced inorganic spectroscopic methods to actinide chemistry, including well-defined compounds, *in-situ* generated complexes, and transient species, in order to advance our understanding of electronic structure, bonding, and reactivity in heavy element systems up to the level currently available for transition metals such as iron and palladium. Towards this goal, we will develop and apply **C**-term magnetic circular dichroism spectroscopy to well-defined heavy element complexes with an emphasis on actinide compounds to elucidate electronic structure, including ground and excited states; determine polarizations of electronic transitions; and, importantly, obtain insight into spin-orbit coupling effects. In addition, we will develop and utilize freeze-trapped spectroscopic methods to study unstable and transient species and gain detailed molecular level insight into the reaction pathways of actinide complexes. Importantly, freeze-trapped spectroscopic methods can be applied across the breadth of actinide molecular chemistry, including for the determination of electronic structure, bonding, and reactivity of low stability actinide organometallic complexes; identification of transient species in redox reactions; and identification of intermediates in reactions to form actinide-ligand bonds. Combined with additional studies focused on the development and application of ^{237}Np Mössbauer spectroscopy, these physical-inorganic methods will enable a deeper understanding of electronic structure and bonding in actinide complexes as well as detailed insight into the reactivity of these species.

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

Informed Materials Design Principles from Local Structures and Dynamics In Hybrid Inorganic-Organic Perovskite Halides

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Hybrid inorganic-organic perovskite halides have the potential to shift the paradigm by which we use functional semiconducting materials for energy-conversion technologies, as the structure/property relationships of hybrid perovskites seem to follow a distinct set of rules. The presence of disordered organic dipoles in the crystalline perovskite lattice challenges our conventional wisdom that disorder in materials localizes electronic carriers and disrupts efficient energy conversion and transport. In this project, we will elucidate the materials design principles behind if and how organic dipoles and disorder correlate with the paradigm-shifting electronic properties in hybrid inorganic-organic perovskite halides. The potential for transformative properties of these materials (e.g., high photovoltaic energy conversion efficiencies, radiation detectors, thermoelectrics) suggests that new materials design principles are needed to produce materials with tailored properties that will enable the next generation of energy-relevant technologies.

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

Magnetic Imaging of Topological Phases of Matter

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Topological phases of matter are predicted to exhibit a wealth of fundamentally new electronic phenomena, such as the quantum anomalous Hall effect, topological magnetoelectric effects, electric field-induced magnetic monopoles, and emergent axion electrodynamics. Although the quantum anomalous Hall effect has recently been realized, opening the door to an exciting array of experiments and potential applications, many aspects of the effect remain unclear, largely due to a lack of detailed understanding of the materials involved. This project seeks to advance our understanding of the relevant materials and to explore new materials predicted to exhibit topological order. The experimental approach combines local and non-invasive magnetic scanning probes with low-noise transport and high-frequency excitations to image, probe, and manipulate the properties of relevant materials. The insights provided by this research may lead to the realization of new electronic phenomena based on topological phases of matter and help the development of materials for spintronics-based low-power electronic devices.

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

Does Mycorrhizal Symbiosis Determine the Climate Niche for *Populus* as a Bioenergy Feedstock?

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Microbes are found in virtually every environment on Earth and many of them play beneficial roles, maintaining the health of plants and animals. Perhaps the most ubiquitous form of beneficial interaction in terrestrial ecosystems occurs between fungi and plant roots. In these fungus-root (or "mycorrhizal") symbioses, the plant provides sugars that feed the fungus, which in return supplies the plant with critical nutrients such as nitrogen and phosphorous. Most plants are associated with a diverse variety of mycorrhizal fungi. However, the ecological factors that control the distribution and abundance of mycorrhizal symbioses are still poorly understood. To advance toward understanding the role of climate, soil environment, and mycorrhizal interactions in determining growth and competition in plant communities, this project will focus on *Populus*, a native North American tree and a potential biofuel feedstock, and the mycorrhizal fungi associated with it. Using a global forest database, the distribution of different *Populus*-mycorrhizal associations will be mapped and modeled across different regions and climates. Based on those models, laboratory experiments will be conducted to measure the precise ways in which beneficial plant-mycorrhizal interactions determine the distribution of *Populus* in its natural habitat and how these interactions affect competition with other tree species. Finally, the flow of carbon from *Populus* to mycorrhizal fungi and other soil microbes will be studied in different environmental conditions using stable isotope labeling. These experiments will not only provide fundamental insights into the way beneficial interactions shape the natural world, but they will also allow us to predict how carbon flow is affected by climate change. The knowledge gained in this project will have a direct impact on predicting the suitability of different environments for bioenergy crops.

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

Developing the Next Generation of Superconducting RF Cavities with Nb_3Sn

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To probe the fundamental laws of physics at the highest energy scales, scientists collide beams of particles in kilometer-scale accelerators. In state-of-the-art facilities, acceleration is achieved by passing beams through superconducting radiofrequency cavities, hollow structures that contain intense electromagnetic fields. The cavities transfer energy to the particle beams, preparing them for high energy physics experiments. Traditionally, these cavities are made of niobium, which is relatively easy to work with and has good superconducting properties. However, after years of developing this material, researchers are reaching fundamental limits of its capabilities, while the requirements of accelerators continue to increase. To make frontier research accessible, accelerator scientists are looking to alternatives to niobium. One candidate material with great potential is Nb_3Sn, an alloy of niobium and tin, that is predicted to have an ultimate limiting field twice as high as niobium and—in recent proof-of-principle experiments—is demonstrated to operate efficiently at significantly higher temperatures. These advantages would substantially reduce infrastructure and operating costs for accelerator facilities. The objective of this research is to develop Nb_3Sn cavities from proof-of-principle to a demonstrated accelerator technology. Capitalizing on knowledge gained in previous research, novel approaches will be used to push performance and to scale up to production-scale cavities. If this research is successful, Nb_3Sn cavities would dramatically increase the reach of powerful large-scale accelerators and enable new small-scale industrial applications, including those in medicine, border security, and flue gas and wastewater treatment.

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

Coming in from the Cold: A High-Pressure Gaseous Argon Time Projection Chamber as an Option for the DUNE Near Detector

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The mystery of why our universe is dominated by matter instead of being composed of equal amounts of matter and antimatter may be solved in part by understanding if there are asymmetries in the behavior of neutrinos and antineutrinos. An international collaboration has been formed to build the flagship Deep Underground Neutrino Experiment (DUNE), aiming for transformative discoveries about the origins and evolution of the universe, starting with the questions of the violation of the symmetry under the combined charge conjugation and parity inversion or CP violation (differences in behavior of neutrinos and antineutrinos) and neutrino mass hierarchy (which type of neutrino is heaviest). The experiment will send a high-intensity beam of neutrinos from Fermi National Accelerator Laboratory (FNAL) in Batavia, IL, to the Sanford Underground Research Facility (SURF) in Lead, SD, a baseline of 1300 km from the neutrino source. It will have a detector near the neutrino source to measure the neutrinos before their journey to South Dakota and a detector located at the far site to observe the changes that occur during their travel. These so-called "long baseline" neutrino experiments benefit from having the same neutrino target material at both the near and far detectors so that systematic uncertainties related to the neutrino interaction target cancel in analyses involving both detectors. DUNE will have a liquid argon time projection chamber as its far detector; the project funded by this award will build and operate a small, high-pressure gaseous argon time projection chamber (HP-GArTPC) to test its feasibility as an option for the DUNE near detector. The prototype HP-GArTPC detector performance will be characterized in a dedicated charged particle test beam comprised primarily of pions, muons, and electrons with energies in the energy range that is directly relevant to DUNE. It will then also be placed in a well-understood neutrino beam at Fermilab to further probe neutrino interaction mechanisms, making measurements that will refine the input to neutrino interaction simulations. This project will explore new techniques to achieve improvement in the uncertainties associated with final state interactions in neutrino experiments while also building experience and understanding of HP-GArTPCs that will inform and influence the design of the DUNE near detector.

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

Discoveries in Blast-Wave-Driven Turbulence of Astrophysical Relevance

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The present research is an integrated experiment and simulation program to discover the fundamental physics associated with blast-wave driven hydrodynamic instabilities in configurations (two-dimensional and three-dimensional diverging system) and regimes (large density contrast and near compressible regime) that have not yet been explored. In interstellar and intergalactic media, shock and blast waves associated with relativistic jets, supernovae, interstellar winds, and spiral density waves interact with gaseous media of variable thermodynamic quantities, resulting in significant disruption to the evolution of interstellar and intergalactic media. It has been hypothesized that the blast-wave driven hydrodynamic instabilities play a key role in supernovae evolution from the explosion to the remnant phase. The project aims to determine the role of initial conditions and flow geometry on the late time evolution of the turbulent flow field in these environments, providing high resolution data from three-dimensional simulations validated with our well diagnosed experiments and designing High-energy-density (HED) diverging blast-wave experiments to connect the low energy hydrodynamics to strong shock HED hydrodynamics.

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

High-precision Penning trap Measurements of β-decay Q-values for Neutrino Physics

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The discovery of neutrino flavor oscillations has shown that neutrinos have non-zero masses. This result has led to modifications of the Standard Model and has wide-ranging implications in fields from particle physics to cosmology. However, important fundamental questions remain: *What is the absolute neutrino mass scale? Is the neutrino a Majorana or a Dirac particle?* To address these questions, several large-scale neutrino experiments are now underway, and more are being planned. These include both direct neutrino mass measurements and searches for neutrinoless double beta-decay. Planning these experiments and interpreting their results will require accurate determinations of the relevant beta-decay “Q-values.” The Q-value is essentially the mass difference between the initial (parent) and final (daughter) nuclides in the decay. The goal of this research is to provide, using Penning Trap Mass Spectrometry (PTMS), high-precision Q-values for the beta decays of the isotopes under consideration for neutrino experiments. A new PTMS facility will be constructed at Central Michigan University to determine the Q-values of ^{187}Re and ^{163}Ho to a fractional precision of about 10 parts per trillion, which is the accuracy required for direct neutrino mass measurements. In addition, existing PTMS facilities at the National Superconducting Cyclotron Laboratory and Argonne National Laboratory will be used to search for ultra-low Q-values (less than 1 keV) in beta decays of certain initial isotopes to excited-state daughter nuclei. In many *a priori* possible candidate beta decays, the masses of the parent and daughter nuclides are not yet known with sufficient accuracy to determine whether the decay is actually allowed. If a beta decay with an ultra-low Q-value is identified, it may prove useful in motivating future direct neutrino mass measurements. We will also carry out PTMS measurements that determine double beta-decay and double-electron-capture Q-values as well as Q-values for other rare weak decays, which may prove useful for other current and future experiments.

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

Constraining Dark Energy with Galaxy Clusters and Baryon Acoustic Oscillations

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Gravity pulls. Therefore, the expansion of the Universe must slow down. Alas, somebody forgot to tell the Universe. Rather than slowing down, we now know the Universe is expanding at an ever increasing rate! This observation has staggering physical consequences: either the Universe is full of a previously unknown form of energy - the so-called dark energy - or our understanding of gravity is incorrect. Either solution will overturn one of the pillars of physics, be it the standard model of particle physics or general relativity. This research seeks to distinguish between these two possibilities by using galaxies and galaxy clusters found in the Dark Energy Survey (DES), our Nation's current premier astronomical survey. DES galaxies will be used to search for the "echo" of the Big Bang in their distribution in the sky, enabling measurements of the expansion of the Universe, while DES galaxy clusters will constrain how quickly gravity forms these structures across cosmic time. Together, these measurements will help us understand the biggest puzzle in cosmology today: why is the Universe accelerating?

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

Resilient Hydrogels from the Nanoscale to the Macroscale

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Biological systems illustrate how a material composed of fragile molecular components can be highly resilient. While the average protein, cell or even tissue may not last more than a few weeks, many animals and plants have lifetimes of a century or more. Continual component regeneration and multiple systems to resist mechanical and chemical damage together make this capacity possible. The goal of this project is to develop biomimetic methods to enable a material, specifically a DNA-crosslinked hydrogel, to resist damage to different features and across multiple scales using distinct, modular damage protection mechanisms. Because hydrogels share many features with biological tissues, they are an ideal substrate for exploring biomimetic strategies for designing resilience and self-repair. In DNA-crosslinked hydrogels, assembly is controlled by how single DNA strands link together, making it possible to use new tools from dynamic DNA nanotechnology to control the gel's structure and behavior. To develop methods to allow such materials to heal or resist damage at the nanoscale, gels will be designed in which embedded molecular sensors detect and actively resist strain that could cause damage. Other features will be incorporated that actively reform gel regions that are punctured or severed before greater damage can occur. The ability to design resilient materials capable of self-repair could have important implications for materials engineering. Instead of designing a material to withstand the worst stresses it may encounter, we could instead design a material to survive under average conditions but to self-repair or reconfigure to resist impending damage. Resilient, self-repairing hydrogels will also have diverse applications such as sensors or actuators.

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Overcoming Charge Transport Limitations in Thin Film Semiconductor Photoelectrodes

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The capture of solar energy and its direct conversion to chemical fuel in artificial photosystems provides a promising route to sustainably meet global energy demands and overcome the current reliance on fossil fuels. Development of practical systems for using sunlight to synthesize fuel requires light-absorbing elements that are simultaneously efficient, durable, and inexpensive. Emerging thin film transition metal oxides, nitrides, and oxynitrides offer potential to meet these requirements. However, practical deviation of achieved efficiency from the theoretical limit is ubiquitous in these systems. Indeed, a significant challenge lies in reliably transporting charge through real semiconductors and across real interfaces to drive desired catalytic transformations while minimizing recombination loss and catastrophic corrosion side reactions. Dominant efficiency limiting processes in semiconductors are associated with disorder, common sources of which include: (i) point defects, which can contribute either beneficially or detrimentally to transport, (ii) polarons, in which self-trapping of photogenerated charge induces lattice relaxation, resulting in photo-induced disorder and low carrier mobilities, and (iii) interfaces, both internal at grain boundaries and external at phase boundaries, where translational symmetry is broken and complex physical and chemical interactions govern function. The objective of this research is to determine how the landscape of disorder impacts macroscopic transport properties by probing the structure of charge localization and analyzing its impact on the life cycles of photogenerated charge carriers. Knowledge gained from measurement will be used to develop strategies for promoting desired chemical transformations by overcoming intrinsic and extrinsic transport limitations. This will be accomplished by controlling defect incorporation and passivation, creating novel hierarchical structures for directing charge transport, and exploring infrared spectrum utilization to stimulate transport.

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The Dynamics and Stratigraphy of Distributary Channel Networks

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On river deltas, the transport of water and sediment self-organize to form complex distributary channel networks. In the subsurface, ancient distributary channels are a fundamental architectural element of delta deposits, forming high-permeability pathways for fluid flow. The dynamics controlling channel spacing, bifurcation, and growth trajectories are poorly understood, limiting prediction of subsurface heterogeneity. This research seeks to leverage recent advances in tributary network dynamics to further understand distributary networks. Preliminary data show that the characteristic bifurcation angle in experimental and field-scale distributary networks is identical to the confluence angle found in tributary networks, suggesting that the processes governing bifurcation in each network are similar. Whether the network is accumulating or dispersing flow appears to be insignificant to the bifurcation process. This provides an exciting new context in which models of distributary network dynamics can be built and tested. The central hypotheses are that distributary network dynamics are dictated by (1) flow patterns outside the channel network and (2) the flow and sediment transport conditions along the channel network boundary. Flow outside tributary networks fed by groundwater seepage can be described by the the Laplace equation near the channel network boundary, reducing the complexity of flow pattern calculations. It is expected that distributary networks will also exhibit Laplacian flow near network boundaries. The tributary network boundary occurs where surface flow becomes sufficient to transport sediment. It is expected that the distributary network boundary will occur where the suspension of bed material ceases.. Theory will be developed by using simple models of fluid flow around distributary channels and by modeling the emergent channel network as a classic moving boundary problem. Predictions of network evolution, flow patterns, and sedimentology will be tested on a modern delta with a rapidly evolving channel network using repeat surveys of channel bathymetry and *in situ* flow and sediment transport measurements. The moving boundary model of network growth will be compared to engineering-grade numerical simulations to confirm the validity of the simple model where long-term network evolution is resolved. Finally, ancient channel networks resolved in seismic volumes will be used to test model predictions of subsurface geometry. This work will develop tools that can quantitatively predict network morphology and connectivity in subsurface strata where information is incomplete, illuminating structural heterogeneities in deltaic strata from the channel scale (0.1 km) to the delta scale (100 km).

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Harnessing Order Parameter in Ternary II-IV-V_2 Semiconductors

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Recent advances in semiconductor growth, characterization, and theory have enabled a new understanding that controlled disorder can be used to deterministically modify materials. In particular, the use of cation disorder as a new free parameter to enable tailored properties in optoelectronic semiconductors is now possible. In the present work, we will develop a systematic understanding of the control of cation order parameter and its impact on properties in II-IV-V_2 semi-conductors, a class of compounds with structure and properties similar to III-Vs but with a doubled conventional unit cell size due to the substitution of group II and IV elements for group III cations. Building off a foundation of work on III-V ordering, we will introduce a new set of materials for optoelectronics with performance similar to that of III-Vs but with wider tunability though chemical complexity. We will address two transformative opportunities for energy science recently identifed by the Basic Energy Sciences Advisory Committee: *Mastering Hierarchical Architectures and Beyond-Equilibrium Matter* and *Beyond Ideal Materials and Systems: Understanding the Critical Roles of Heterogeneity, Interfaces, and Disorder*. We will study phosphide and nitride materials, representing the two different structure types available in II-IV-V_2 materials. These materials can be readily integrated with III-Vs as well as silicon, enabling applications ranging from optoelectronics spanning the visible spectrum to extremely efficient yet inexpensive photovoltaics to platforms for improved lasers and optical computing. This work will have profound implications, moving semiconductor optoelectronics into a new phase space of available materials both for traditional devices and exploration of new physics in optical structures.

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A Compact Laser-Plasma-Accelerator-Based FEL for Ultra-Fast Hyper-Spectral Experiments

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This research aims to develop the technology that will lay the foundation for a new generation of light sources. Laser plasma accelerators (LPAs) have already enabled the availability of high-quality GeV (gigaelectronvolt) electron beams at compact facilities. A compact, LPA-driven free-electron laser (FEL) will be developed, delivering high-peak-power coherent soft X-ray pulses synchronized with ultra-short radiation from THz (terahertz) to gamma rays. Such a source would enable novel experiments in the biological, chemical, and physical sciences. This light source benefits from the key advantages of LPAs, including (1) the hyper-spectral nature of the source (electrons, X-rays, gamma rays, THz radiation, laser), (2) ultra-short durations (~10 femtosecond or fs), (3) intrinsic small timing jitter (few fs or less), (4) high peak-current e-beams (>1 kiloamp), and (5) a small facility footprint (single-room scale). Several key technologies will be implemented such as the operation of stable high-quality LPAs with advanced targets, transport of LPA electron beams with recently developed active plasma lenses, and electron beam manipulation with a chicane. The high-intensity X-rays will enable experiments based on X-ray-pump/X-ray-probe and other hyper-spectral non-linear X-ray configurations. Because of the compactness of this novel source (at a fraction of the cost of conventional FELs), small- to mid-scale laboratories worldwide would be enabled to pursue non-linear X-ray science.

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Mathematical Methods for Optimal Polynomial Recovery of High-Dimensional Systems from Noisy Data

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This project is focused on the development of polynomial approximation methods for data from physical experiments and numerical simulations. The need for efficient approximations naturally arises in many important energy and materials science applications, where constructing the high-dimensional solution map requires repeated measurements from time-consuming experiments or an ensemble of high-dimensional, parameterized numerical simulations. Parameters for the deterministic variables may correspond to spatial position or velocity, and the stochastic variables characterize uncertainty in experimental or input data. The research pursues advances in constructive approximation theory, convex and constrained optimization, sparse models, data reduction, and high-dimensional sampling strategies. Innovative methods that exploit sparsity and compression will be developed for inexpensive and accurate approximations that can be used in understanding and analyzing problems arising in plasma physics, molecular electronic structures, turbulent flows, and other DOE-mission applications.

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

Understanding Mesoscale Nonequilibrium Heterogeneity by Multimodal X-ray Imaging

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Heterogeneous materials are by nature comprised of separate yet connected regions with distinctive properties. In condensed matter physics, the heterogeneity of interest is often on the order of nanometer to micrometer length scales and exhibited by different structural, charge and magnetic states. The strong interaction between such mesoscopic heterogeneities is intimately tied to a number of fundamental phenomena such as metal-to-insulator transitions, high-temperature superconductivity, and colossal magnetoresistance. However, the experimental characterization of these heterogeneities has been limited primarily to states in thermal equilibrium. The non-equilibrium transformation of heterogeneity under external stimuli holds a key to understanding the correlated nature of important physical phenomena and has only just begun to be explored. This project is targeted at understanding and controlling mesoscale heterogeneity in order to bridge the knowledge gap from atomistic to macroscopic length scales as a material evolves in time. This project will achieve this goal by developing a novel *in-situ*, multimodal, spatiotemporally resolved imaging system at the Advanced Photon Source using suitable ultrafast terahertz, optical and x-ray radiation. Snapshots of localized material properties with distinct structural, electronic, magnetic and optical characteristics will be captured simultaneously and correlated unambiguously. Quantitative correlation of heterogeneous properties in both space and time will provide crucial information with which to understand and subsequently harness the mesoscale properties of materials with new and enhanced functionalities. The developed methodology and instrumentation will be generalizable for use at other large scale synchrotron x-ray facilities and free electron lasers.

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

Non-Empirical and Self-Interaction Corrections for DFTB: Towards Accurate Quantum Simulations for Large Mesoscale Systems

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This project will develop, analyze, and introduce non-empirical quantum-mechanical corrections to the density functional tight binding (DFTB) formalism for probing the electron dynamics of large mesoscale systems. Specifically, this transformative approach will utilize two different (but complementary) approaches for improving the accuracy of DFTB: (1) non-empirically tuned range-separated exchange-correlation kernels, and (2) computationally-efficient self-interaction corrections (SICs) constructed via unitary transformations on the DFTB density matrix. Implementing both of these methods provides a comprehensive approach for improving the accuracy in DFTB for treating large mesoscale systems. Within the broader computational objectives of DOE-BES, the DFTB enhancements proposed in this project will also lay the theoretical and computational groundwork for addressing recent BES interests in mesoscale materials and processes. In conjunction with these new non-empirical corrections, high-performance GPUs will be utilized in the DFTB approach to enable an efficient and detailed assessment of the importance of quantum effects in mesoscale processes, creating an exciting opportunity for BES leadership in these large, complex systems.

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Critical Thermonuclear Reactions in Classical Novae and Type I X-ray Bursts

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This research will experimentally constrain the thermonuclear rates of the $^{30}P(p,\gamma)^{31}S$ and $^{15}O(\alpha,\gamma)^{19}Ne$ reactions, which strongly influence nucleosynthesis and energy generation in simulations of classical novae and type I x-ray bursts, respectively. To accomplish this, a micro pattern gas amplifier detector will be constructed at the National Superconducting Cyclotron Laboratory on the campus of Michigan State University to measure the low energy proton and α-particle emissions following the β decays of ^{31}Cl and ^{20}Mg, respectively. The experimental results will be used as input to state-of-the-art computer simulations of these astrophysical events in order to predict the composition of nova ejecta and the shapes of x-ray burst light curves. Comparing the simulations to observation will help to identify pre-solar nova grains in primitive meteorites, determine peak nova temperatures, and use x-ray bursts as a window on the extreme nature of neutron stars.

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