

## **Establishing Defect-Property Relationships for 2D-Nanomaterials**

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In recent years, studies of new families of two-dimensional nanomaterials (2DNMs) established that they have unique properties that don't conform to the behavior rules of their bulk counterparts. Therefore, there are important questions that still need to be answered: how tolerant are 2DNMs to extreme photon and particle fluxes and what are the mechanisms governing their radiation response? It has been recently pointed out that graphene is not as representative of other 2DNMs as previously believed. But why graphene's response differs from other 2DNMs and what causes this behavior is not clear. This project seeks to understand the physical processes occurring at multiple length scales in transition metal dichalcogenides (TMDs) and determine the structural stability and property evolution in TMDs in conditions far away from equilibrium. These goals will be accomplished through an experimental effort investigating the similarities and differences between various types of 2DNMs and the fundamental mechanisms governing their radiation response. In-situ and ex-situ ion and electron irradiation will be used to directly control the structure and properties of TMDs. To complement the experimental work, density functional theory calculations, analytic solutions to diffusion, and kinetic Monte Carlo simulations will be employed to elucidate the mechanisms of defect formation and evolution in these 2DNMs. The long-term goals of the project are to 1) establish defect formation and evolution mechanisms in 2DNMs subjected to irradiation, 2) quantify radiation tolerance of 2DNMs, and 3) develop the requisite fundamental knowledge base needed to understand defect-property relationship in this unique class of materials.

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**Genome-scale *in vivo* determination of Gibbs free energies ( $\Delta G$ ) in metabolic networks**

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Recent breakthroughs in genome editing and metabolic engineering are expected to expand the range of microorganisms and synthesis routes that may be used to produce biofuels and valuable bioproducts from renewable biomass resources. Thus, there is an increasing need for new tools to characterize the metabolic capabilities of nascent industrial organisms and improve the efficiency of their production pathways. Thermodynamic analysis can help us understand how energy is transferred and transformed within metabolic networks and has emerged as a powerful tool for pathway design and metabolic engineering. This project will integrate thermodynamic analysis with advanced mass spectrometry, computational modeling, and metabolic engineering to develop an approach for *in vivo* determination of Gibbs free energies ( $\Delta G$ ) in metabolic networks. This project will also investigate how the thermodynamics of biosynthetic pathways in microbial biofuel producers change dynamically as substrates are depleted or products accumulate. This research will result in the construction of computational models that quantitatively define trade-offs between energy efficiency of biosynthetic pathways and their overall catalytic rates. The approach developed in this project will be useful for identifying thermodynamic bottlenecks in native and synthetic pathways and pinpoint the enzymes whose expression levels will have the largest effect on production rates and final product yields. It will be suitable for high-throughput analysis of a wide range of organisms and aid the design of new and more efficient metabolic routes for advanced biofuel production.

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## **Exploring the Lifetime Frontier with New Detectors and New Searches**

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Reconstructing remnants of elementary particle interactions at high energy collider experiments traditionally relies on measurements of particles' energy and position using calorimeters and tracking detectors. While performing such measurements, the one remaining component of the particle's coordinates, its time, has generally not been utilized to its full potential. This research program aims to exploit this last dimension by developing novel detectors with precise timing and position information for the High-Luminosity Large Hadron Collider (HL-LHC) upgrade of the Compact Muon Solenoid (CMS) detector at the European Organization for Nuclear Research (CERN) in Switzerland, and by performing searches for new particles with long lifetimes using the data collected by CMS. Such an analysis will provide a sensitive test of theories that predict particles with measureable flight paths. High-precision timing detectors would effectively remove contamination from multiple concurrent proton-proton interactions at the LHC, resulting in an increase in data usable for analysis, improved performance, and corresponding cost savings. Additionally, these detectors will enable unique new capabilities in searches for new phenomena, significantly enhancing the reach in searches for long-lived particles. The techniques developed through this research will help advance particle detection and instrumentation beyond those used at the HL-LHC, paving the way for 4-dimensional space and time track reconstruction in collider experiments at future particle accelerators.

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## **Understanding and Controlling the Fundamental Photochemistry of Protonic Solar Energy Conversion**

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All major fuel-forming redox reactions are driven through changes in the concentrations of electrons, holes, protons, and/or hydroxides. While traditional solar-energy conversion processes use light to directly perturb the concentrations of electrons and/or holes, few works have used light to perturb the concentration of only protons. This process is of particular interest because it is unique to photochemistry in that it does not (yet) have a productive analog in solid-state physics. Therefore, the planned research will interrogate the fundamental photochemistry of photoacid-dye-sensitized polymer membranes, where solely light-driven proton release will be used to drive solar photochemical reactions. The planned research will leverage photophysical and solid-state physics theories, techniques, and design strategies previously developed for the study of traditional solar-energy conversion processes. The project will use several photoacid dyes, commercial polymers, and polymer syntheses that are available from prior work. Understanding the basic science of these membranes and their photochemical mechanisms is of use to the DOE-relevant processes of solar photochemical fuel formation, solar photodialytic desalination, and solar cells. These functional materials may have broad-reaching importance to many fields and may provide the foundation for a completely new, inexpensive, and flexible energy technology that provides added benefit to society.

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

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### **Scalable Data-Efficient Learning for Scientific Domains**

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Extracting knowledge from scientific data—produced from observation, experiment, or computation—presents a significant hurdle for scientific discovery. As the U.S. Department of Energy (DOE) has moved toward data-driven scientific discovery, machine learning—in particular, deep learning—has emerged as a critical driver for data-intensive scientific discovery. Deep learning methods have been especially successful in dealing with regular data, such as images, where there is an underlying Euclidean structure. In many DOE applications, however, data come from non-Euclidean domains such as unstructured and irregular grids. Directly applying to the non-Euclidean domain deep learning methods that had been developed for Euclidean data results in a loss of learning efficiency and poor prediction accuracy. The overarching goal of this research is to develop scalable, non-Euclidean deep learning approaches that can learn in complex DOE scientific domains with limited training data. We will conduct research in four connected areas: (1) geometric deep learning; (2) data-efficient, few-shot learning that integrates physical models and domain constraints; (3) neural architecture and hyperparameter searches; and (4) scalability on DOE leadership-class systems.

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

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## **Reaction Mechanism and Kinetics for Electrochemical Hydrogenation and Hydrogenolysis of Biomass-Derived Species**

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Chemical conversion of biomass platform chemicals into more stable and desirable compounds at the biorefinery is important for making these biomass-derived compounds viable for transport and use, however, traditional chemical transformations require extensive infrastructure at large scales to be economical. Small, on-site upgrading of products from biomass conversion, known as Biomass Upgrading Depots (BUDs) have been proposed. By electrochemically converting biomass, modular units that do not require significant infrastructure or the same scale as traditional chemical processing facilities, can be utilized in these BUDs. Reduction and oxidation reactions can be performed electrochemically to obtain valuable chemicals and intermediates on-site. When paired with excess renewable electricity (from sunny or windy days), the process has promise to be economical and sustainable, all while addressing the energy storage problem associated with renewable electricity generation. Electrochemical hydrogenation and hydrogenolysis (ECH) are reduction reactions that can be used in these BUD systems. ECH offers additional benefits over traditional chemical reactions because they can run at ambient conditions and do not require externally-supplied hydrogen gas (which can be challenging to provide in large quantities at remote locations where biorefineries are located). For ECH to become a viable method for chemical upgrading at the biomass refinery, the underlying phenomena controlling ECH must be understood. The research will investigate the ECH reactions involving furfural and 5-(hydroxymethyl)furfural (HMF), both considered biomass platform chemicals, as reactants. Products of ECH from the reactions of both furfural and HMF include fine chemical intermediates, polymerization agents, and biofuels. The reaction kinetics, side reactions, and reaction mechanisms will be investigated. The experimental work will be completed using electrochemical, chemical and spectroscopic techniques. The understanding gained through this research will allow for better catalysts and reactors to be developed. Additionally, the findings will provide valuable experimental results that could be fed back into future computational studies, further enhancing the understanding of these systems.

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**Revealing Collective Spin Dynamics Under Device-Operating Conditions  
to Enhance Tomorrow's Electronics**

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The technological revolution of the past decades stemmed from the ability to control the motion of charges in semiconductors and to manufacture semiconductor-based devices of ever-decreasing size for information processing and storage. However, these gains are diminishing as semiconductor technology is starting to reach physical limits for storage density and speed, for reasons mostly due to heat dissipation. Collective spin excitations in quantum materials provide a revolutionary alternative for devices with improved performances and energy efficiency as they permit the transfer of information without requiring any movement of charge, thus eliminating the dominant source of energy dissipation. Understanding how to manipulate these collective spin excitations would provide a foundation for the next generation of energy-efficient electronics. This research will undertake the first study of the microscopic spin dynamics in technologically-relevant quantum materials under device-operating conditions. It will use soft X-ray Resonant Inelastic X-ray Scattering (RIXS) at the world-leading RIXS spectrometer at the National Synchrotron Light Source II – the only instrument capable of providing the required energy resolution for this study – and develop a unique sample environment, called *Opera*, to realize device working conditions. The combined use of *Opera* and RIXS will provide an unprecedented insight into the material properties and the behavior of the collective spin excitations when subject to device-relevant perturbations of current, electric-field, magnetic-field, temperature gradient, and strain. These results will be used to develop strategies towards optimizing the materials and their parameters in order to improve the generation, propagation, and manipulation of collective spin excitations in quantum materials in the form of spin waves, topological spin arrangements like skyrmions, or spin supercurrents. This is a key-enabling step towards designing devices with enhanced spin-signal propagation performance and spin-control possibilities, in response to the need for a new era of energy-efficient technologies.

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## Uranyl Capture and Activation with Lewis Acids and Macrocyclic Hosts

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Nuclear power is attractive for meeting the current and future energy needs of society, in that it does not release carbon dioxide or other pollutants into the atmosphere during routine use. However, preparation of nuclear fuel, recovery of useful components from used fuel, and handling of waste materials remain significant impediments to further deployment of important nuclear technologies. In part, these problems arise from limited availability of chemical reactions that can reliably interconvert forms of uranium and other heavy elements during preparation and processing. For example, harsh and expensive chemicals are often required for making and breaking chemical bonds to uranium, and the reactions involved are inefficient. The overall objective of this research is to harness knowledge of chemical structure and bonding to develop a useful and predictive understanding of the fundamental parameters that govern bond activation at the most common form of uranium, the unique uranyl ion ( $\text{UO}_2^{2+}$ ). Quantitative control of these parameters is to be pursued using assembly of molecular structures containing multiple metal ions, a strategy inspired by metal-containing cofactors found in nature that engage in bond making and breaking with high efficiency. Electron- and group-transfer reactions involving uranium will be studied in this work, including detailed electrochemical studies of multimetallic species dissolved in solutions as well as analogues immobilized on electrode surfaces. Outcomes from this research are anticipated to include new knowledge of design rules for chemical reagents that could be used for uranium processing, as well as a quantitative understanding of the interaction between uranium and redox-inactive Lewis acidic ions.

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## **Microwave Single-Photon Sensors for Dark Matter Searches and Precision Neutrino Measurements**

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The new and growing field of quantum information science (QIS) gives us tools and technologies that enable cutting-edge particle physics research. This program will use superconducting, solid-state qubits as low-noise photon counters to search for dark matter. The axion is a well-motivated dark matter candidate particle, whose existence would also help solve the so-called "strong CP problem" and explain the neutron's anomalous electric dipole moment. In the presence of a strong magnetic field, axions convert into photons and these photons can be detected using equipment that is common in accelerator and particle physics. However, the signal power from axion-to-photon conversion is expected to be less than  $1e-23$  watts. At that level, even amplifiers operating at the quantum limit, such as DC SQUIDS, can be too noisy for experimental requirements. We will apply quantum nondemolition measurement techniques, adapted from QIS, to reduce detector error rates and improve axion signal sensitivity. Quantum nondemolition may be thought of as an extreme case of state-squeezing, in which the phase of a photon state is randomized at every measurement so that amplitude (i.e. photon number) can be measured repeatedly and with high precision. This technique, enabled through qubits provided to us by partners at the University of Chicago, has the potential to enhance axion search speeds by four orders of magnitude while enabling sensitivity to weak axion-photon coupling models. The goal of this research program is to adapt quantum nondemolition measurement techniques for use in an axion search. It would form the basis for a next-generation axion experiment.

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## **Enabling Predictive Metabolic Modeling of Diurnal Growth Using a Multi-Scale Multi-Paradigm Approach**

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Although photosynthetic microorganisms such as algae and cyanobacteria have great potential as renewable sources of energy and valuable chemicals, a lack of genetic engineering tools has prevented their use as biofactories. Furthermore, most research on these organisms is conducted with cells grown in constant light, which does not replicate the conditions of outdoor ponds with natural day/night cycles. By integrating a variety of mathematical modeling techniques and experimental data, this research will develop an advanced predictive model of growth and productivity in photosynthetic organisms, capturing the changes in metabolism during day/night cycles, interactions between cells, and the availability of nutrients and light in the environment. The project will focus on the emerging model green algae *Chromochloris zofingiensis*, which accumulates large amounts of lipids that can be used to synthesize biodiesel and other high-value added products. The performance of the model will be tested using data collected from large-scale outdoor algal growth studies. The model generated in this project will not only allow more predictive computer simulations of algal physiology, but it will also enable advanced and safe engineering of photosynthetic microorganisms for optimal growth in outdoor ponds. The model will be easily adaptable for other organisms as well as more complex microbial consortia, supporting BER's mission in energy and the environment.

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## **Multi-Hadron Systems via Lattice Quantum Chromodynamics**

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The vast majority of the states of Quantum Chromodynamics (QCD) are composed of more than one hadron. These manifest themselves as very short lived resonances or as stable bound states (light nuclei). The goal of this research is to use lattice QCD to develop and implement a universal framework for studying these systems directly from QCD. This framework will open up new classes of physical observables, presently out of reach of theoretical studies but crucial to guiding, confirming, and complementing experimental efforts to understand the QCD spectrum at the Jefferson National Accelerator Laboratory and beyond. Two major milestones are expected to be reached by this research. The first includes developing and implementing techniques for a first study of three-hadron states, allowing for the determination of three-nucleon forces and QCD excitations that couple to multi-hadron states as in the so-called Roper resonance. The second milestone entails studies of the structural composition of resonant and non-resonant few-hadron systems. Combined, these two goals will give access to unexplored sectors of QCD states and allow for construction of an image of their intrinsic character.

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**Building a comprehensive understanding of ice nuclei sources from the ground up: Establishing the impact of sea spray and agricultural soils**

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Prediction of ice crystal concentrations in clouds is an outstanding problem in atmospheric sciences. Among the obstacles to achieving this predictive understanding is the challenge of predicting atmospheric ice-nucleating particles (INPs) across a range of atmospheric conditions. INPs play a critical role in initiating freezing in clouds, impacting cloud radiative properties, and the location and timing of precipitation. Despite their importance, our understanding of the emission, removal, and atmospheric transformation processes controlling the atmospheric abundance of INPs is still in its infancy. Immersion-freezing INPs active at warmer temperatures ( $> \text{ca. } -25^{\circ}\text{C}$ ) are especially critical to mixed-phase clouds, i.e., those that contain both liquid droplets and ice crystals. Their abundance is often controlled by biogenic particles (e.g., organic matter in soils and sea spray), which are challenging to distinguish observationally and to represent in models. This project will transform predictive understanding of the sources of ice-nucleating particles to the atmosphere by advancing understanding of how two less-studied but important particle types contribute to determining real-world INP concentrations, and tackling the grand challenge of predicting INP concentration from the observed characteristics and sources of atmospheric particles. This project will use unique field campaign data from the Atmospheric Radiation Measurement (ARM) user facility and measurement capabilities from DOE's Environmental and Molecular Sciences Laboratory (EMSL) to take on the grand challenge of predicting INP abundance, with a focus on two less well studied classes of immersion-freezing nuclei active at  $T > -25^{\circ}\text{C}$ —sea spray and agricultural soils. The improved process-level understanding developed in this project can ultimately be incorporated into atmospheric models, increasing their process realism and their utility as a tool for understanding complex surface-atmosphere-cloud interactions in the Earth System.

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## **Local Site Magnetic Susceptibility for Quantum Materials by Polarized Neutron Diffraction**

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Discovery and development of new quantum materials will be key to drive future computation, information storage, sensor devices, and other energy relevant technologies. Understanding the interactions leading to magnetic quantum phenomena in a wide range of quantum materials is extremely important for developing such materials. Quantifying these interactions in materials that potentially exhibit exotic states such as quantum spin liquids, topological insulators, and Weyl semimetals, are currently being limited by a range of challenges. These include the lack of sizable high-quality crystals for inelastic neutron scattering, limited high pressure capabilities, and the ability to disentangle the intrinsic quantum phenomena versus effects from defects and site-disorder. To overcome these challenges, magnetic interaction characterization on a small crystal is highly desirable. This project will develop Local Site Magnetic Susceptibility methods based on polarized neutron diffraction, both under ambient and high pressure conditions, to understand the balance of subtle magnetic interactions in quantum materials that lead to the key quantum states. The methods use high resolution spin densities reconstructed from polarized neutron diffraction data to visualize spin/orbital distributions and magnetic interactions, and use deduced site magnetic susceptibility tensors to extract magnetic anisotropy and interactions through spin Hamiltonian modeling and density functional theory calculations. The project will provide the opportunity to investigate structures, magnetic states, magnetic interactions, and other bulk properties on the same crystal and enable high pressure and field tuning of quantum states of a material. The project will complement the bigger ORNL plan of studying and predicting quantum materials using the premier high-performance computing facilities available at the lab. The proposal will take advantage of ORNL's strong neutron scattering user facilities and build off the expertise in the Basic Energy Sciences (BES) Materials Sciences and Engineering program.

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## Probing Attosecond Bound Electron Dynamics Driven by Strong-Field Light Transients

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The measurement and control of ultrafast dynamics in electronically-excited states of molecular systems have opened new frontiers in the study of internal energy conversion, charge transfer, and coupling of electronic and nuclear degrees of freedom. Recently, such control has been extended to the attosecond (1 attosecond =  $10^{-18}$  seconds) regime, owing to the development of carrier-envelope phase-stabilized few-cycle lasers and isolated attosecond extreme ultraviolet (XUV) pulses. This project applies innovative laser techniques to reconstruct the time-dependent quantum mechanical wave packets initiated by strong-field excitation in bound electronic states of gas-phase atoms and molecules, and to control their dynamic evolution on attosecond to few-femtosecond (1 femtosecond =  $10^{-15}$  seconds) timescales. These dynamics have largely been hidden from previous experiments due to the lack of suitable spectroscopic techniques to probe attosecond electronic motion in bound electronic and vibrational states. Time-dependent electronic and vibrational wave packets initiated by intense, single-cycle laser field transients will be reconstructed through all-optical measurements of the coherent XUV polarization emission, allowing time-domain characterization of the build-up and decay of wave packet coherence under different excitation conditions. The research will provide new perspectives on strong-field coherent control of intramolecular energy transfer and chemical reactions, and will enable new tests of theoretical models of strong-field interactions in multi-electron atoms and complex molecular systems.

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**Discovering the Mechanisms and Properties of  
Electrochemical Reactions at Solid/Liquid Interfaces**

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Interfaces between solids, liquids, and gases play a pivotal role in how energy is stored, transferred, and converted. Such electrochemical processes include the conversion of chemical energy to electrical energy in a fuel cell, the storage of electrical energy in a battery, and the conversion of gases such as carbon dioxide into useful chemical fuels using an electrolyzer. To improve these electrochemical reactions, more selective, stable, and efficient interfaces are needed, which requires a better understanding of complex molecular interactions at solid/liquid electrochemical interfaces under realistic conditions. This research will clarify these interactions by synergistically combining experimental techniques, advanced modeling, and computation. Specifically, the approach will leverage a suite of advanced spectroscopy and microscopy techniques at Lawrence Berkeley National Laboratory's Advanced Light Source, including ambient-pressure X-ray photoelectron spectroscopy (APXPS). APXPS can probe, under operating conditions, the reaction environment and products at electrified interfaces, providing comprehensive and fundamental insight into the interactions between electrodes and electrolytes. The knowledge gained through this work will enable future electrochemically based innovations and will extend across scientific fields, including environmental, geological, chemical, materials, and biological sciences.

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## **Parallel-in-Layer Methods for Extreme-Scale Machine Learning**

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The goal of this project is to transform how domain experts integrate experimental data and simulation by using machine learning and deep neural networks (DNN). Commercial applications such as image classification have been revolutionized by the use of DNNs. The proposed research aims to speed the adoption of DNNs in DOE science and security mission spaces. One research thrust focuses on developing a key “parallel-in-layers” technology for the scalable training of DNNs on high-performance computing architectures. Another research thrust aims to broaden the range and predictive capability of DNNs. The third research thrust focuses on applications to the prediction of sea ice thickness, inversion in plasma modeling, and other DOE mission-relevant challenges. This scientific machine learning technology will integrate DOE software frameworks (e.g., Trilinos, HYPRE, PETSc) with cutting-edge machine learning tools under development such as TensorFlow and Caffe.

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**Gluon Saturation Search in the Deep Small Bjorken-x Region using the Large Hadron Collider Beauty Experiment (LHCb)**

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High-energy collisions, such as the ones produced at Relativistic Heavy Ion Collider (RHIC) in Brookhaven/NY and at the Large Hadron Collider (LHC) at CERN/Switzerland, can produce matter with high gluon densities. Gluons are the particle mediators responsible for the strong nuclear interactions. At high density gluons can start to fuse and form condensates, similar to cold atom experiments where discoveries have been awarded four Nobel prizes in the last 20 years. These condensates show particles with interesting collective behavior. This research aims for the unambiguous observation of gluon condensates in collisions produced at the LHC using the LHC Beauty experiment (LHCb), which has a unique detector coverage to observe saturated gluons. This study will include development of improved techniques to select events with isolated photons, improve tracking of particles and analysis directed at demonstrating the existence of the predicted gluon condensate. The results of this work will have implications in the current understanding of particle production in proton and nucleus collisions and the quantum behavior of the strong forces.

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**Structure of the Cyanobacterial NAD(P)H Dehydrogenase Complex (NDH-1) and Its Role in Cyclic Electron Flow and Carbon Dioxide Hydration**

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Photosynthesis is a vital source of energy for nearly all living organisms on earth. Using energy from the sun, plants, most algae, and cyanobacteria combine water and carbon dioxide (CO<sub>2</sub>) to make sugar. The process of photosynthesis is divided into two steps: the light reactions and the dark reactions. The light reactions use the sun's energy to split water and generate the cellular energy molecules adenosine triphosphate (ATP) and nicotinamide adenine dinucleotide phosphate (NADPH). The dark reactions use both of these energy molecules to produce sugar from CO<sub>2</sub>. The ratio of ATP:NADPH produced and consumed by photosynthesis needs to be precisely controlled. This is achieved in the light reactions via two pathways: the first, called linear electron flow, produces ATP and NADPH at a ratio of 1:2.5, the second, called cyclic electron-flow, produces only ATP. Although the first pathway is well studied, very little is known about the molecular mechanism of the cyclic pathway. The research will close this knowledge gap by performing a series of structural and functional experiments on a protein complex called NADPH dehydrogenase. NADPH dehydrogenase is thought to be a key component of cyclic electron flow and is the last of the large photosynthetic protein complexes to be understood at a mechanistic level. Once the process of cyclic electron flow is understood, better manipulation of the light reactions of photosynthesis to generate the correct ratio of cellular energy, required for bio-engineering applications, will be possible, thereby improving the yield of bio-products.

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## **Exploring New Diamond Surfaces with Precision Chemistry and Quantum Spectroscopy**

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Diamond is a superlative material, and has been explored as a potential material platform for a wide range of future technologies, including high power electronics, electrochemical cells in harsh conditions, implantable biomedical devices, quantum sensors, and quantum networks. However, these applications have been hindered by a lack of control over the diamond surface. Uncontrolled surfaces can lead to electronic defects, magnetic noise, and changes in material properties that can affect even bulk devices. New methods will be developed to understand and control the surface of diamond. This is a challenging project because diamond is an inert material, making it difficult to alter chemically, and also because it is the hardest material, making it difficult to polish and process. To address these challenges, the research will use high precision chemistry, surface spectroscopy, and quantum spectroscopy techniques in a home built instrument operated under ultrahigh vacuum in order to study the reactivity of the diamond surface and to prepare novel surfaces that are inaccessible by conventional methods. In addition, new forms of solution-based chemistry at diamond surfaces will be studied, leveraging the novel surfaces created with ultrahigh vacuum surface chemistry. This foundational study will enable the development of diamond as a platform for a large number of classical and quantum applications, and will also contribute to the fundamental understanding of surface reactivity and surface spectroscopy.

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

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## **Project 8 at Penn State: Developing the Ultimate Neutrino Mass Experiment**

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The neutrino mass is one of the most important unknown quantities in physics. The most sensitive direct searches for the neutrino mass rely on the beta decay method: nuclei undergoing beta decay emit an electron and a neutrino. Thanks to energy conservation, one can determine the mass of the neutrino from the shape of the electron spectrum near its endpoint, that is, the maximum energy of the emitted electrons. The Project 8 experiment has developed a novel technique called Cyclotron Radiation Emission Spectroscopy (CRES) to precisely measure the beta decay spectrum in tritium, and thus obtain a neutrino mass measurement with sensitivity surpassing that of existing experiments. An electron trapped in a uniform magnetic field will emit cyclotron radiation with frequency that depends on its kinetic energy, so that a measurement of the radiation provides a nondestructive electron energy measurement. The Project 8 collaboration has already demonstrated the viability of this technique using a small-scale ( $\sim 10 \text{ cm}^3$ ) prototype. However, an attempt at measuring the neutrino mass will require a vast increase in the number of tritium decays, which can be accomplished through an increase in detector volume to 10-100  $\text{m}^3$ . One crucial feature of such a detector is the ability to identify single electrons in a large cavity instrumented with a multi-channel antenna array, which will present unique challenges for the acquisition and reconstruction of signals. This project will develop the signal reconstruction techniques and electronics needed to take CRES to the next level, such as the use of digital beam-forming for single electron detection and tracking in large volumes. This research project will include the simulation of the expected electron signal in software and hardware; building of test chambers instrumented with multiple prototype antennas and electronics; development of signal reconstruction algorithms; and the construction and operation of the Project 8 detector, with a focus on signal acquisition, electronics, and data analysis. The successful completion of this project will extend the functionality of the CRES technique to large scales, providing essential tools and support that will allow Project 8 to move into the next phases of its experimental program, and lead to the ultimate neutrino mass experiment.

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## **Controlling Interfacial Charge Separation Energetics and Kinetics**

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Charge separation at interfaces is critical to many energy related technologies including solar powered photovoltaics and photoelectrochemical cells. A better understanding of how to control the potential energy of charge separation and the duration of photoinduced charge separations at interfaces is needed for solar-to-electric and solar-to-fuel systems. The lack of a set of design principles for photoactive components in large potential energy charge separation systems is currently limiting the development of many solar-to-electric and solar-to-fuel systems. Basic understanding of large potential energy photoinduced charge separations across interfaces is needed for the full potential energy use of the highest energy photons provided by sunlight. This project seeks to address the fundamental knowledge required to enable solar-to-electric and solar-to-fuel systems access to efficient use of sunlight. Research will focus on synthesizing tailored molecules specifically to generate large potential energy charge separations at organic-inorganic material interfaces. Rational molecular design principles will be put forward through this research that could enable the rapid design of next generation solar conversion systems.

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**Understanding Impurity Transport in Magnetically Confined Fusion using Interpretive Modeling and High-Sensitivity Material Characterization Techniques**

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Control of the plasma-material interface represents a significant challenge to sustained operation of a fusion device, both in terms of how the plasma facing components (PFCs) will withstand the intense particle and heat fluxes generated by the fusion plasma and how the plasma responds to the influx of impurities produced by the gradual degradation of the PFCs. The presence of impurities in the plasma can result in prohibitively high radiative power losses that drain heat from the plasma that is needed to maintain the high temperatures required for fusion. These losses become increasingly more severe for higher mass (high atomic number, or high-Z) elements. Many of the leading candidates for PFCs are high-Z materials such as tungsten and molybdenum due in part to their relatively high melting temperature and low erosion rate. The purpose of this research is to confront the challenge of controlling contamination of the core plasma (highest temperature region) by high-Z impurities. This will be accomplished through global impurity transport studies and a directed focus on the transport of high-Z impurities in the plasma edge (near the PFCs) and the ability of the edge plasma to screen impurities from the core plasma. This work will contribute to upcoming research campaigns on several fusion experiments focused on the effects of high-Z PFCs. Experiments will be designed to determine the operating conditions that can best benchmark global impurity transport models, and *ex-situ* analysis of PFCs will be performed after the research campaigns to integrate the diagnostic data into advanced interpretive models. The advanced modeling and characterization tools will be used to determine how properties of impurity transport are affected, and may be actively modified, by the plasma operating configuration. This research will make an invaluable contribution to the fusion community's effort to address the challenge of impurity driven radiative power losses in fusion devices.

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

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**Chemical Organization, Structure and Dynamics at Complex Liquid-Liquid Interfaces: Mechanistic Insight into Selective Solvent Extraction and Self-Assembly**

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A major challenge in separating a mixture of molecules or ions from one another is understanding and controlling the chemical processes that occur at a liquid-liquid interface, such as oil and water. The interface between two liquid phases is a hotspot for molecular self-assembly and anomalous chemical processes that ultimately dictate how species can move from one phase to another. Despite the widespread use of liquid-liquid extraction methods, the chemical events governing selectivity and efficiency are not well understood, which limits the ability to rationally design new separations schemes to meet the demands of the next generation of clean energy technology. A key barrier to obtaining this insight is the current inability to directly probe the structure and dynamics of the molecularly thin interface using conventional spectroscopic methods while not being overwhelmed by the signals originating from the bulk phases. Thus, to understand the events at the interface, one must develop an approach that is uniquely capable of providing chemical insight into the interfacial chemical composition, organization, and dynamics. The overarching goal of this work is to develop a unified understanding of the molecular structure and dynamics governing the mechanisms of chemical separations at liquid-liquid interfaces using surface-specific spectroscopies, such as vibrational and electronic sum frequency generation, in conjunction with neutron scattering methods to advance the design of selective and efficient chemical separations. To address this goal, the proposed work will pursue three specific aims to address the following thematic questions: (1) What are the differences in local chemical environment and molecular ordering that mediate selectivity at liquid-liquid interfaces? (2) How does curvature at liquid-liquid interfaces impact self-assembly and selectivity? and (3) How are ultrafast molecular dynamics of interfacial recognition complexes manifested in chemical selectivity? This novel approach using a tailored set of complimentary nonlinear spectroscopic measurement techniques developed at Oak Ridge National Laboratory is poised to address these long-standing questions underlying selective and efficient chemical separations for the first time by probing different aspects of the same chemical phenomena on characteristic time and length scales. The new insight gained from this work will accelerate the design of selective and efficient next generation separation schemes by providing missing mechanistic insight into the phenomena taking place at the liquid-liquid interface during extraction. Through understanding the mechanisms by which extractions operate, new more efficient and selective separations targeting complex, or undesirable supply streams, such as nuclear waste and rare-earth waste streams, can be developed. This underpins the DOE Grand Challenge Science questions in understanding and controlling matter at the molecular level to ultimately produce efficient energy technologies.

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

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## **Improving Neutrino Detection in DUNE with Pixel Sensors**

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Do neutrinos and antineutrinos behave identically? Is the mass of the third neutrino state much heavier or much lighter than the other two states? The Deep Underground Neutrino Experiment (DUNE) intends to answer these questions by looking for subtle differences in neutrino versus antineutrino propagation over ~1300 km to large cryogenic liquid argon time-projection chamber (LArTPC) detectors. The capability of this experiment will depend significantly on precise knowledge of the neutrino beams produced by the particle accelerator at Fermi National Accelerator Laboratory. Characterization using another LArTPC located near the origin of the neutrino beam has distinct advantages, but is hindered by an intense neutrino flux. The intensity will result in multiple simultaneous neutrino interactions, which would be difficult to disentangle when using standard projective readout techniques. I aim to establish the techniques for operation of a LArTPC detector in a high-rate environment, including the development of a true three-dimensional (3D) micro-power charge readout system and related feature recognition algorithms. Not only will these developments enhance the expected sensitivity the DUNE measurement of neutrino oscillation, but should also enable high-statistics searches for new phenomena in intense neutrino beams. These techniques have additional potential for use in the DUNE far detector, where they would enhance discrimination of signal from background, as well as in future dark matter searches and nuclear security applications.

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

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## **New perspectives on QFT and gravity from quantum entanglement**

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The objective of this research is to study fundamental aspects of quantum field theory (QFT) and the nature of space-time and gravity via the patterns of quantum entanglement present in these theories. These patterns will be harnessed to find new constraints on the dynamics of QFT and quantum gravity. These topics find a natural home within the holographic duality, a deep mathematical correspondence discovered in string theory where a gravitational system can be described by a quantum system without gravity. By studying the spatial distribution of quantum correlation in various quantum systems one goal is to directly observe the holographic emergence of quantum gravity within this setting and to characterize the space-time structure that emerges along with it. In achieving these aims this research will shed light on the thermodynamic nature of gravity and explore the implications of this paradigm for our understanding of the unification of gravity with quantum mechanics. Additionally, this project aims to develop new tools for studying the structure of quantum entanglement in QFT and in so doing, use powerful constraints satisfied by entanglement and its generalizations to place bounds on the basic data of the QFT. In turn these bounds will be related to causality constraints and quantum energy conditions, which are local and non-local bounds on the energy density for arbitrary out of equilibrium states of the QFT.

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

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## **Integrated Predictive Modeling of ELM Suppression and Mitigation**

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A magnetic fusion reactor must successfully maintain plasma at 100 million degrees Celsius, while simultaneously limiting the temperature of plasma-facing components of the reactor to a small fraction of that. In tokamaks, instabilities known as Edge Localized Modes (ELMs) intermittently eject significant energy from the plasma edge, potentially melting or eroding plasma-facing components in reactor-scale tokamaks. It has been found that applying 3D magnetic perturbations—often called “Resonant Magnetic Perturbations” (RMPs)—can successfully mitigate or suppress ELMs under some conditions. However, the physical process underlying RMP ELM suppression is not well understood, and we do not have a model that can successfully predict the conditions required for suppression. Recent experimental results suggest that RMPs create localized thermal and particle transport that suppress thermal gradients below the ELM stability threshold, but modeling this process has been challenging due to the complex interplay between the 3D magnetic field geometry generated by the RMPs and the heat and particle transport properties of that magnetic field configuration. We propose to address this challenge by integrating our best models of 3D plasma magnetic equilibrium with models of transport in 3D fields. In doing so, we will quantify the expected changes to the transport properties of a tokamak plasma that occur when RMPs are applied. By applying this integrated model to a database of discharges from various tokamaks in which RMPs were applied, we will determine which transport mechanisms are dominant, and which correlate with the observation of ELM suppression. Ultimately we hope to provide both an improved understanding of the physics of RMP ELM suppression and a validated, predictive model that can be used to design and optimize future tokamaks with confidence.

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

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## **Weak Interactions in Nuclei and Nuclear Matter**

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The goal of this project is to develop a comprehensive understanding of the structure and electroweak processes in nuclei and nucleonic matter that are critical to present and future experiments at rare isotope facilities, high-energy accelerators, and to astrophysical observations. Neutrino interactions with nuclei and dense matter, in particular the theory support to future double beta-decay experiments, have been identified as one of the most important scientific questions in nuclear physics in the most recent Nuclear Science Advisory Committee long-range plan. These properties are critical to an understanding of finite nuclei, how they interact with high-energy electrons and neutrinos produced at accelerators, and also to astrophysical environments like neutron stars and supernovae. In order to solve for these problems, sophisticated computational techniques are required. In this project we use numerical methods based on Monte Carlo integrations. These methods can efficiently exploit the largest available supercomputers, and our codes are developed to efficiently use the largest available high-performance machines. The main input for these calculations are i) the interactions describing how nucleons interact within nuclei, and ii) the interactions of nucleons with external probes like electrons and neutrinos. We use numerical methods to calculate nuclear properties with the goal of validating our models for i) and ii) by comparing our calculations with available precise data on beta decays and electron scattering in nuclei, and then make predictions for neutrino scattering, neutrino propagation in neutron stars and supernovae, and relevant matrix elements for double beta-decay experiments.

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

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## **Time-Resolved Imaging of Non-Equilibrium Electron Dynamics with Novel X-ray Holographic Approaches**

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The ability to follow transient structural changes is essential for understanding and controlling non-equilibrium phenomena such as catalytic reactions, ultrafast phase transitions, and energy transfer from light to matter. These processes often evolve from a complex interplay between rapid electronic and nuclear motions at the nanoscale, which are hardly accessible with conventional microscopic methods. State-of-the-art imaging tools often require long exposure times to achieve high spatial resolution and thus, their sensitivity to short-lived phenomena is limited. Ultrafast spectroscopic methods can provide valuable information about transient states, but the signal ambiguity often increases with the complexity and heterogeneity of the sample. The capabilities offered by current and next-generation X-ray laser facilities, such as the Linac Coherent Light Source (LCLS) and its successor, LCLS II, offer the potential to directly visualize ultrafast dynamics with high spatial and temporal resolutions. This research program will develop and apply novel ultrafast X-ray diffraction imaging approaches that exploit these cutting-edge X-ray sources to advance the fundamental understanding of non-equilibrium processes in complex nanoscale systems.

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

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**Dynamic Multinuclear Active Sites Formed from Mobilized Single Atoms on Heterogeneous Supports  
for Selective Oxidation Catalysis**

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The nation's energy future has been changed irrevocably by the advent of domestic shale gas resources, which are cheap and abundant enough to meet energy demands for the next one hundred years. Shale resources are distributed across a vast geographical footprint and often in remote locations, which incurs high transportation costs for collection at centralized chemical plants, refineries, or export terminals. The largest component of shale gas is methane, familiar as the main hydrocarbon in natural gas. Methane can be converted into energy through combustion to form water and carbon dioxide. Converting methane to methanol, however, would form a liquid compound that can be transported more easily and subsequently converted into a variety of chemicals and fuels. The challenging task of oxidizing methane selectively to form methanol may be made possible with a catalyst: a material that contains active sites, which are geometric arrangements of specific atoms that are proficient at changing the chemical identity of reacting molecules by trading electrons and rearranging their chemical bonds. This research will address methane conversion by applying a new concept in catalyst design: dynamic multinuclear active site formation, which describes how single metal atoms located within carefully chosen porous structures and in the presence of a solvating environment can form ionic metal complexes. These metal complexes become mobilized and can interact with other metal complexes in a reversible manner to form multinuclear active sites. The objective of this research is to understand the structure and function of dynamic multinuclear active sites in order to design catalysts that react with molecular oxygen ( $O_2$ ) to oxidize hydrocarbons. The knowledge gained from this research has the potential to develop new technologies for continuous methane oxidation to methanol, and to diversify the strategies available to use the nation's abundant hydrocarbon resources.

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

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## **Emergent Phenomena at Mott Interfaces – a Time- and Depth-Resolved Approach**

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Rational design and efficient ultrafast control of new electronic and magnetic phases of matter at oxide interfaces is considered to be one of the most promising avenues toward realizing new generations of energy-efficient devices. The key requirement for the realization of such groundbreaking technology is a clear understanding of how new phases of matter arise and evolve far from equilibrium in both time- and space domains. In order to gain such understanding, this program will use intense THz electric-field pulses generated by a femtosecond laser to directly modify the electronic structure and magnetic states at the atomically-abrupt interfaces between ultrathin oxide layers (calcium manganite and lanthanum nickelate). The objective is to disentangle, understand, and harness control over the intricate competing interactions responsible for tunable emergent magnetism at the layer interface. In order to effectively investigate such interfacial phenomena both statically and in the time domain, this program will marry the x-ray standing-wave method with the ultrafast polarization-dependent x-ray scattering and imaging techniques enabled by the most recent technological advances at the DOE's x-ray free-electron laser (XFEL) and synchrotron facilities. This will result in the development of a powerful new experimental platform that can be used to study electronic and magnetic systems driven out of equilibrium with time and depth resolution. The new depth-resolved ultrafast x-ray scattering techniques and instrumentation developed in the course of this program will be generalizable for immediate use at the DOE's synchrotron and XFEL facilities.

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

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## **Kinetic effects on self-organization in low-temperature magnetized plasmas**

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Self-organized patterns and structures occur in many systems, including a wide variety of space and laboratory plasmas. Laboratory plasmas with crossed electric and magnetic fields, such as magnetron discharges and Hall-effect thrusters, can exhibit well-arranged, coherent structures but the processes for such structure formation in plasma are not well understood. The physics of partially-ionized, low-temperature magnetized plasmas is complex because collisionless instabilities can affect collisional phenomena, such as ionization and transport, and vice versa, and the presence of materials, such as sheath and electron injection, can influence the properties of the plasma. The aim of this research is to advance the fundamental understanding of low-temperature magnetized plasmas, particularly the nonlinear coupling between small-scale kinetic phenomena and large-scale self-organizing structures. Self-consistent particle-based kinetic models will be developed in canonical and realistic configurations of a cross-field discharge. This project also involves development of massively-parallel numerical algorithms using high performance computing capabilities for feasible multiscale simulations of low-temperature magnetized plasmas. Understanding the interplay of small-scale kinetic phenomena and large-scale self-organizing structures is crucial for improving the controllability of plasma flows and reactions.

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

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## **Geophysical Signatures of Crack Network Coalescence in Rocks at Multiple Length Scales**

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Subsurface discontinuities, ranging in scale from micro-cracks (micrometer) to fractures (millimeters to meters) to faults (10s of meters to kilometers), control subsurface rock integrity and permeability. Processes involving the organization of small cracks into larger fractures occur quickly and at multiple spatial and temporal scales, creating immense challenges in understanding the underlying causes of crack network coalescence and in predicting fracture network evolution over a range of subsurface stress perturbations. The goal of this research is to identify key geophysical signatures of crack coalescence in rocks under realistic stress conditions through a novel laboratory design allowing, for the first time, concurrent recording of optical, acoustic emission, and ultrasound images. These data will provide new insight needed to interpret stresses and fracture evolution from micro-seismic events in the subsurface.

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

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## **Implications of Aerosol Physicochemical Properties Including Ice Nucleation at ARM Mega Sites for Improved Understanding of Microphysical Atmospheric Cloud Processes**

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A specific subset of atmospheric particles can act as ice-nucleating particles (INPs) in mixed-phase clouds and, ultimately, influence precipitation and the Earth's radiative energy balance. Despite the importance of INPs, current ambient INP data derived from field measurements are not well interpreted with detailed aerosol and cloud properties, except for a few short-term field studies. This project will fill this gap by using long-term measurements from DOE's Atmospheric Radiation Measurement (ARM) sites, complemented with robust and well-characterized INP measurements that will be archived in the ARM database. Detailed ARM observational data of aerosol chemical composition speciation, abundance, cloud condensation nuclei activity, and hygroscopicity are of the utmost importance for better understanding of INP mixing states, as well as their implication in cloud, precipitation, and regional weather patterns. The proposed new INP measurements will experimentally characterize abundance and physicochemical properties of ambient INPs at the ARM Southern Great Plains (SGP), Eastern North Atlantic (ENA), and North Slope of Alaska (NSA) atmospheric observatories. A combination of a new *in situ* expansion chamber and the offline droplet freezing assay technique for INP measurement, as well as microspectroscopic characterization techniques, will be used to elucidate abundance and physicochemical properties of ambient INPs at the above-mentioned ARM observational sites. Different INP episodes (agricultural, marine biogenic, and Arctic at SGP, ENA, and NSA, respectively) will be assessed and evaluated to help understand convective and mixed-phase cloud systems typically observed in these regions. The proposed research will generate data to understand how particle chemical composition and mixing state influence ambient ice nucleation propensity at the ARM sites. Such datasets have long been a missing piece in the study of cloud microphysics and atmospheric chemistry, and are of importance to improve atmospheric models of cloud feedback and to determine their impact on the global radiative energy budget. Currently, ice formation processes are very poorly represented in weather and earth system models, including DOE's Energy Exascale Earth System Model (E3SM), and this study will support the DOE mission by providing INP parameterizations representative of the ARM sites. To constrain E3SM, this project will produce a variety of INP parameterizations, such as ice nucleation active surface site density, cumulative number concentration of INPs per volume of air, and water activity-based freezing descriptions.

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

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## **O-Acetylation and methylation engineering of plant cell walls for enhanced biofuel production**

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Polysaccharides are major components of plant cell walls that can be converted into fuels by microbial fermentation, making plant biomass an important bioenergy resource. However, a substantial fraction of plant cell wall polysaccharides is chemically modified with methyl and acetyl groups that reduce yield of microbial fermentation. Although little is known about the biochemical and physiological functions of those cell wall modifications, it has been shown that their volatile intermediates (methanol and acetic acid) are tightly associated with plant growth, stress, and senescence processes but are not captured by traditional metabolomics analysis, representing an important gap in our knowledge of cell wall metabolism. This project will study the metabolism of those cell wall modifications and volatile intermediates as well as their role in central physiological processes in the emerging biofuel tree species California poplar (*Populus trichocarpa*) using field settings and controlled environmental conditions. The main goal of this research is to modify the expression of key genes involved in cell wall metabolism in order to reduce the amount of methyl and acetyl groups present on cell walls. These genetic modifications will be evaluated for potential impacts on important plant hydraulic and physiological processes including proper functioning of vascular tissues to support transpiration, leaf water potential and stomatal regulation, net photosynthesis, and high temperature/drought stress responses. Understanding and manipulating the metabolism of cell wall modifications will not only provide important knowledge on the physiology and ecology of plants but will also allow the generation of engineered bioenergy crops such as poplar for sustainable production of biofuels and bioproducts, addressing BER's goal of developing renewable bioenergy resources.

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

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**Development of Coherent Surface Scattering Imaging with Nanometer Resolution for Revealing 3D Mesoscaled Structures**

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At sub-microscopic length scales, structurally heterogeneous planar surfaces and interfaces provide many of the functional properties of technologically relevant advanced materials. The objective of this project is to determine the exact near-surface structure of such materials by developing a three-dimensional X-ray imaging technique that combines surface-sensitive grazing incidence X-ray measurements with phase inversion techniques that rely on the coherence properties of X-rays. This new capability will enable non-destructive imaging of sub-micron inhomogeneities and non-periodic structures on and within opaque, planar materials allowing the exact structure to be correlated with device performance. Application areas for this new method include layered or hetero-structured energy-related devices, hierarchically structured meta-materials for photonics and defect analysis in nano-patterned integrated circuits. This project will also deepen the understanding of X-ray scattering at surfaces using coherent radiation and will advance the development of wave-propagation simulation methods and software tools to further the application of reflective optics especially at coherent X-ray sources.

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

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## Single Molecule Fluorescence Imaging for a Background-Free Neutrinoless Double Beta Decay Search

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The nature of the neutrino and its mass are fundamental unknowns in nuclear and particle physics, with consequences for cosmological mysteries including the matter / antimatter asymmetry of the Universe, and the existence of new physics at very high energy scales. The only known way to establish experimentally that the neutrino is a Majorana particle (meaning that it is its own anti-particle) is through observation of the ultra-rare and still unobserved process of neutrinoless double beta decay. All experiments that have searched for this process to date have been plagued by backgrounds from ambient radioactivity in detector materials. To meet the target sensitivity of next-generation searches, ultra-low background techniques leading to contamination of less than 0.1 counts per ton per year in the signal region of interest are required. No such technology has yet been demonstrated to achieve this goal. This work involves R&D toward a novel method of achieving a background free search for neutrinoless double beta decay in xenon-136: barium tagging using single molecule fluorescent imaging, coupled to high pressure xenon gas time projection chambers. This mixes advances from biochemistry, microscopy, nuclear and particle physics to yield a technology that may be paradigm shifting for the field, enabling a new class of highly sensitive, background-free neutrinoless double beta decay searches.

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

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**Early Career - Exploring the Higgs Sector at the Energy Frontier with Bottom Quarks, Machine Learning, and the Upgraded ATLAS Pixel Detector**

Dr. Michael Kagan, Panofsky Fellow  
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The Higgs boson, recently discovered at the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN) located in Switzerland, remains among the least understood particles in the Standard Model (SM) of particle physics that describes the fundamental constituents of matter in the universe and their interactions. Deep mysteries of the Higgs boson still remain unanswered, such as how its self-interaction shapes the Higgs potential energy that is central in the process of Electroweak Symmetry Breaking (EWSB) or how new physics beyond the SM may alter its interactions. This research program plans to use data from the ATLAS (A Toroidal LHC ApparatuS) experiment at the LHC to explore such questions through searches and measurements of key Higgs boson interactions. More specifically, the analysis of high transverse momentum Higgs boson production, in order to study the high energy behavior of Higgs interactions, and double Higgs boson production, to study the nature of the self-interaction and its role in EWSB, will be pursued. Fundamental analysis challenges, including identifying decays of the Higgs to bottom quarks and discriminating against extremely large backgrounds, will be addressed by developing innovative analysis methods and bottom quark identification techniques. Many of these advancements will be built upon modern machine learning computational techniques. To ensure long-term efficacy, development of the inner barrel pixel system of the ATLAS Inner Tracker upgrade for the future High-Luminosity LHC (HL-LHC) era will be pursued. The tracking system will be vital for providing high performance bottom quark identification at the HL-LHC, further enabling detailed studies that probe the characteristics of the Higgs boson.

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

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## Quantum Control and Tuning of Magnetic Two-Dimensional van der Waals Heterostructures

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Two-dimensional (2D) quantum materials offer potential novel applications in energy-efficient, nanoscale information storage and computing. To accelerate the design and optimization for desirable electronic and magnetic properties, this project will develop cutting-edge, highly-efficient computational methods to predict and control such properties in these quantum materials. This project permits complex designs to be quickly tested for timely guidance to experiment for validation, and, in turn, also provides direct verification of the theoretical results. This project will focus on magnetic van der Waals layered materials, which are ideal platforms for 2D magnetism. Beyond accelerating the discovery of novel magnetic materials, this project will also advance the fundamental understanding of quantum effects in nanostructures for the design of transformative technologies.

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

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## **Tetravalent Actinide Speciation: Template Directed Assembly, Speciation, and Reactivity**

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Developing an enhanced understanding of actinide chemical behavior is of great strategic and scientific importance to areas ranging from nuclear waste management to radiochemical separations chemistries. In comparison to the other elements of the periodic table, the chemical and physical properties of the actinide elements are uniquely complex and the behavior of these elements is often difficult to control and predict. Speciation (i.e. the complexes that form under a given set of conditions) is critical to describing the behavior of these metal ions. For the actinides, speciation depends largely on oxidation state, and our knowledge of the structural and energetic properties of tetravalent actinide (thorium, uranium, neptunium, and plutonium) complexes is quite limited. Particularly the speciation of Np and Pu, has posed significant challenges in the ability to predict actinide behavior under chemically complex conditions. To fill this knowledge gap, this research will systematically address the effects of (1) complexing ligands, (2) non-bonding interactions, and (3) functionalized surfaces on actinide speciation. These effects will be examined through the molecular-level structural characterization of tetravalent actinide phases formed in solution and the solid state using a suite of synthetic, spectroscopic, X-ray diffraction and scattering techniques. Through this multi-faceted experimental approach, in combination with complementary computational efforts, trends that govern speciation and reactivity in the early actinides will be identified, thus opening the door to greater control and predictive ability of the solution behavior of these elements. Fundamental insights into the factors that govern the speciation and reactivity of various structural units could lead to technological advances in separations, process chemistry, and the ability to predict the migration of these radionuclides in complex chemical systems. Compounds isolated as part of this work may also serve as a basis for theoretical studies focused on the electronic properties of the actinides and changes that occur with successive filling of the  $5f$  orbitals, which may be critical to understanding how the electronic configuration of the metal ion affects the chemical and physical properties of these elements.

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

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## Exploration of Energetic Particle Confinement in Stellarators

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This research plan will explore the physics of energetic particle confinement in stellarators using data collected from the Wendelstein 7-X (W7-X) experimental facility. In a magnetically confined fusion power plant, alpha particles ( $\text{He}^{+2}$  ions) produced by the fusion of deuterium and tritium must remain confined in the plasma long enough to transfer their kinetic energy to the plasma. This process is fundamental to achieving a burning plasma state, sustaining the plasma temperature. These particles are considered energetic, as their kinetic energy is much greater than that of the thermal energy of the deuterium and tritium plasma from which they are born. In optimized stellarators such as W7-X, the three dimensional shape of magnetic fields is tailored to provide beneficial confinement to non-energetic particles. The neutral beam and radio frequency heating systems on W7-X provide sources of energetic particles, which mimic the characteristics of alpha particles in a larger reactor. The presence of these particles enables the study of how stellarator three dimensional magnetic fields affect energetic particle motion. Numerical simulations of these particles will be compared to experimental measurements, providing validation of the simulations. Validated simulations are then used to optimize the three dimensional shape of magnetic fields for improved energetic particle confinement. Additionally, these simulations will help determine the optimum location for diagnostics that are key to measuring energetic particle confinement in W7-X. The successful demonstration of such an optimization capability will allow the development of transient-free, steady-state power plants based on the stellarator design.

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

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## **Exploiting Synergies Between Lensing and BAO Surveys for Improved Cosmological Constraints**

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Pinning down the nature of dark energy is one of the most pressing questions in modern physics. There are multiple large missions underway, or that will begin in the next 5 years, that will address the question of dark energy. Among these efforts are the Dark Energy Spectroscopic Survey (DESI), the Hyper Suprime-Cam (HSC) survey, and the Large Synoptic Survey Telescope (LSST). DESI will measure the distances to tens of millions of galaxies. LSST and HSC as “imaging surveys” (large maps of the sky that reveal millions of galaxies) are designed to measure the “gravitational lensing” effect (distortion of galaxy shapes due to the bending of space-time by intervening dark matter). These missions aim to measure the properties of dark energy in different but complementary ways. The objectives of this research are to take advantage of the synergies between these different approaches and data-sets in order to increase their scientific payoff. This research will advance our understanding of dark energy as well as the theory of gravity, and will provide robust constraints on the parameters of the standard Lambda Cold Dark Matter (LCDM) cosmological model.

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

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## **Analyzing Multifaceted Scientific Data with Topological Analytics**

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This project will develop a new class of techniques suitable for analyzing the massive, complex datasets currently generated with high-performance computing resources. Specifically, the major challenge with these data is not just that they are massive in scale, but that they are multifaceted as well. Multifaceted data represent multiple values of interest simultaneously. For example, a typical, Earth system model might seek to understand the connections between (a) arctic sea ice, (b) the currents and temperature of the ocean, (c) surface temperature models, (d) atmospheric behavior that affects the surface, ocean, and ice, and (e) solar radiation's effect on the atmosphere. These values may be data from multiple sources, may encode variability or uncertainty across parameters, or may be the result of multiple physical models being computed simultaneously. Analyzing multifaceted data presents new challenges in that we seek not just to understand each facet of data, but rather we also want to understand the interactions and relationships among facets. The proposed solution develops a new field of analysis techniques called topological analytics, which couple machine learning—techniques for building statistical relationships—with topological analysis—techniques for analyzing the features of a single facet of data—to develop new analyses for multifaceted data.

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

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## **Probing Coherence in Nanoscale Energy Transport with High Spatial-Temporal Resolution**

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The phase coherence of microscopic energy carriers, such as electrons, phonons and photons, as well as their collective excitations could serve as a valuable resource for energy transport and conversion. From a thermodynamic point of view, lower entropy content is associated with higher phase coherence, indicating the potential for a higher energy conversion efficiency. Moreover, coherent energy carriers, e.g. lattice vibrations (phonons), can dynamically modulate the physical properties of the host material, producing non-equilibrium states with tunable energy transport properties. Therefore, fundamental understanding of coherent phenomena in nanoscale energy transport not only provides new opportunities to improve the efficiency of energy conversion systems, but also holds the promise of controlling energy transport with coherent excitations. One major challenge for directly probing coherent transport processes is the short coherence time and length associated with microscopic energy carriers, limiting most previous studies to cryogenic temperatures and atom-perfect samples. This research will apply a unique and newly developed scanning ultrafast electron microscope (SUEM), a photon-pump-electron-probe technique that combines the nanometer spatial resolution of scanning electron microscopes with the femtosecond temporal resolution of ultrafast pulsed lasers, to probe coherent energy transport and coherent modulation of energy transport in materials relevant to energy applications. Specifically, time-resolved secondary electron imaging and electron diffraction will be combined, as implemented in SUEM, to directly visualize the coherent coupling of photo-excited electron-hole plasma with coherent phonon modes, analyze the decoherence process of coherent phonons through phonon-phonon interaction and understand the associated entropy generation, and demonstrate dynamic control of electron transport properties via coherent phonon excitations. The expected outcomes will bring fundamental advancements in basic scientific understanding of coherent interaction processes of microscopic energy carriers beyond the familiar incoherent and instantaneous "scattering" picture (e.g. electron-phonon and phonon-phonon scatterings) and serve as a cornerstone for future developments of coherent solar/thermal energy harvesters, coherent phonon lasers and ultrafast electronic devices dynamically tunable by coherent phonons. The research will also establish the newly-developed SUEM as a mature, quantitative and versatile platform to characterize ultrafast dynamics in condensed matter systems, accompanied by a suite of multiscale simulation tools.

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

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## **Understanding and Controlling Water-Organic Co-Transport in Amorphous Microporous Materials**

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Achieving revolutionary reductions in upstream and downstream industrial separations, energy intensity has been identified as a promising approach for improving the sustainability of critical hydrocarbon processing infrastructure. Realizing these reductions requires a “step change” in separation technology from heat-based techniques (e.g., distillation) to molecular size- and shape-based techniques. Molecular sieving membranes have shown promise for separating molecules based on subtle differences in molecular size and shape; however, this sieving ability often occurs at ideal conditions far away from what might be encountered in the field. Indeed, a critical scientific challenge is the development of relationships between membrane microstructure and the transport of competing guest molecules (i.e., water molecules and organic molecules) under realistic operating conditions. To address this challenge, this research project aims to create disordered carbonaceous molecular sieve membranes and challenge these membranes with water-organic mixtures found in real-world settings (e.g., produced water). More specifically, the experimental campaign conducted in this project will result in (i) the creation of a test set of molecular sieve membranes with a variety of micropore sizes and structures, (ii) the development of relationships between the membrane pore size/structure and the adsorption and diffusion of water-organic mixtures within the membrane material, and (iii) the capability to predict permeation of complex water-organic mixtures in disordered microporous membranes. The experiments and analysis conducted in this research project will lay the foundation for new membrane technology capable of displacing existing energy-intensive separations techniques, which would achieve the “step change” necessary for more sustainable hydrocarbon processing industries.

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

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## **Multi-ps Short-Pulse Laser-Driven Particle Acceleration for Novel HED and ICF Applications**

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Today's large-scale laser facilities have the unprecedented ability to compress and heat matter to energy densities similar to those at the center of stars, allowing for the laboratory investigation of extreme states of matter. However, measurements of fundamental material properties – such as the equation of state and opacity – continue to be challenging due to the need that the plasma be in a single-temperature, single-density state. Constant volume isochoric heating using energetic particle beams serves as one of the most promising methods to achieve such conditions. Thus, there is a necessity to develop and optimize laser-driven particle acceleration for new short-pulse Kilojoule-Petawatt laser facilities that have recently come online such as GEKKO-LFEX (Japan), LMJ-PETAL (France), and NIF-ARC (USA), which reside in a novel regime of very high energy (kilojoule) and relatively long (multi-picosecond (ps)) pulse lengths. This work will explore the scaling physics of electron, proton, and light ion generation in this unique parameter space, and utilize both demonstrated techniques for particle acceleration as well as innovative ideas to achieve unprecedented particle beam brilliance and energies. Using an integrated experimental and modeling approach, the fundamental physics of particle acceleration with multi-ps high intensity laser pulses will be investigated, optimized, and applied to create and study HED matter.

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

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## **Optimal Design of Radio Frequency Algorithms and Models for Next Generation Accelerators**

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Modern particle accelerators have a broad range of significant applications in a number of scientific fields. Advances in accelerator science lead not only to discoveries in the field of physics, but also fuel fundamental research in a wide range of scientific and technological fields. Innovative developments in a broad range of subfields of accelerator physics and technology are required to achieve the beam specifications for the next generation of particle colliders and photon sources. This work is focused on the accelerating field, which is provided by the Radio Frequency (RF) system. This project will support the design, simulation, and analysis, of robust algorithms to configure, optimize, and control RF systems and their feedback loops (Low Level RF) for several modern accelerator systems. The optimal configuration and operation of the upgraded Super-Proton Synchrotron (SPS) RF system will be investigated, considering maximum impedance reduction, hardware limitations, and noise issues. Algorithms will be developed to configure multiple stations at the Linac Coherent Light Source II (LCLS-II). A feedback system will be designed to achieve the specifications of the Compact Linear Collider (CLIC) and the system performance will be estimated in terms of bunch position and power requirements using simulations. Algorithms will be developed to match the gap transients for the US Electron-Ion Collider (EIC) project. These algorithms will automatically adjust to beam intensity and pattern. Studies will be conducted to narrow the High Luminosity LHC (HL-LHC) crab-cavity LLRF design parameters. Control algorithms will be developed and the system performance will be estimated. This project also has a strong educational component. At least six undergraduate students will participate in this project each year. The students will actively engage in cutting-edge accelerator physics research.

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

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## **Constraining Neutron Star Structure with Indirect Nuclear Reaction Studies**

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How matter behaves at the highest densities achieved by nature is an open question. Studies of neutron stars, ultradense remnants from stellar explosions, provide unique windows into the behavior of matter existing at densities beyond that of an atomic nucleus and at temperatures low enough for quantum phenomena to emerge at macroscopic scales. Such studies often rely on comparisons between astrophysics model calculations and astronomical observations. However, these model calculation results sensitively depend on largely uncertain nuclear physics input. Of particular interest are the nuclear reactions responsible for energy generation and element creation in Type I X-ray bursts, thermonuclear explosions on the surface of a neutron star accreting material from a companion star. The objective of this project is to remove or reduce the most significant nuclear physics uncertainties for these bursts using indirect nuclear reaction measurements at the Edwards Accelerator Laboratory at Ohio University and the National Superconducting Cyclotron Laboratory at Michigan State University. To assess their impact, measurement results will be included in state-of-the-art astrophysics model calculations of observable phenomena from accreting neutron stars. The overall outcome of this work will be substantial improvement in our understanding of the outer structure of accreting neutron stars and, thereby, of high-density low-temperature matter.

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

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**Quantification of the Crack Evolution Process by Extracting Relevant Signal Components from Wave Propagation and Diffusive Transport Front Measurements**

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The dynamical behavior of fractures in the earth's subsurface influences key processes that govern the extraction of energy resources and isolation of energy wastes in the shallow crust. Fracture evolution depends on complex interactions involving mineralogy, pore structure, rock fabric, effective mechanical moduli, fluid saturation, and pre-existing microcracks in the rock, and also on the strain rate and the thermal, chemical, and stress history. Such complexities and heterogeneities are subject to substantial uncertainties, often precluding the direct translation of fracture evolution into reductionist physical models. This project will use new geophysical signals and develop new machine learning/deep learning algorithms that produce fresh mathematical/statistical frameworks describing crack evolution and that create and inform improved micromechanical models that can be used to understand and predict how fracture networks respond to external perturbations, such as those resulting from fluid injection or extraction, under shallow crustal conditions.

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

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## **Molecular Photochemistry and Photocatalysis in Confinement**

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The goal of this research is to understand the fundamental physical, chemical, and electronic properties governing molecular photochemistry and photocatalysis in confinement. A central challenge encountered in the development of molecular architectures to enable light-driven chemical transformations is the inability to overcome typical diffusion-limited charge transfer kinetics in solution. Another obstacle commonly faced in molecular photocatalysis is the lack of control over the molecular interactions beyond the binding site, and understanding how the environment far beyond the first coordination sphere influences the primary charge and energy transfer processes, and ultimately reactivity and selectivity. In this research, these challenges will be addressed by confining modular molecular and supramolecular architectures within nanoporous membranes and systematically investigating the effects of confinement on photo-induced electron transfer between molecular electron donors and acceptors, as well as electron transfer across tailored interfacial chemistry. The light-responsive and redox-active confined molecular architectures will be probed by a variety of high-resolution, steady-state and time-resolved optical and synchrotron X-ray characterization techniques to capture the important features of both their ground and excited states. The research will enable the development of sophisticated molecular architectures confined within surface-specific porous nanostructures to: 1) control the kinetics of interfacial electron transfer to drive chemical transformations and 2) tune the environment surrounding catalyst modules to provide control over substrate binding and selectivity, reaction kinetics, and nanoscale separations.

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

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## State-to-State Molecular Reactions in the Ultracold Regime

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Chemical reactions contribute to almost all aspects of our lives, yet at the most fundamental level, a tractable quantum-mechanical treatment of complex reactions does not exist. In fact, only after many decades of work has the quantum description of the simplest atom exchange reaction,  $AB + C \rightarrow A + BC$ , been solved for light atoms. Reactions involving 4 atoms,  $AB + CD \rightarrow AC + BD$  for example, are a new frontier to extend the exact quantum understanding. The objective of this proposal is to gain state-to-state experimental data for both the  $AB + CD$  and  $AB + C$  types of reactions that can be compared to advanced theoretical calculations and elucidate the role of quantum mechanics in the processes of bond breakage and formation. Specific examples of the potassium-rubidium metathesis reaction  $KRb + KRb \rightarrow K_2 + Rb_2$  and the atom exchange reaction  $K + KRb \rightarrow K_2 + Rb$  are chosen because the technology of quantum internal and motional state control of these types of molecules is ripe. This experiment will operate at ultracold temperatures (1 mK) such that quantum effects of translational motion are an important factor. At first glance, studying reactions at ultracold temperatures may seem counter-intuitive. However, certain reactions become surprisingly efficient due to the wave-like nature of atoms and molecules. At the lowest temperatures, non-classical effects such as wavefunction delocalization and tunneling through barriers can dominate the reaction rate. Reactions in this regime will serve as a sensitive probe to compare to high accuracy *ab initio* potentials and quantum scattering calculations. Pushing theoretical frameworks to describe the 3-atom and 4-atom system studied in this proposal will ultimately provide insight for more complex problems in chemistry and energy production.

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

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## **Dynamical Aspects of the Quark Gluon Plasma**

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Shortly after the Big Bang the entire universe was filled with a nearly perfect fluid, known as the Quark Gluon Plasma. Relativistic heavy ion collisions can now reproduce this fluid in the laboratory. The Quark Gluon Plasma exhibits a rapid, but smooth cross-over phase transition into hadrons at vanishing net-baryon densities. Recent experiments plan to explore finite baryon densities, where a critical point is expected. If found, this would mark the first discovery of a critical point in a relativistic system described by a fundamental theory of nature, which would have far-reaching consequences for high-energy nuclear physics and nuclear astrophysics (such as in neutron star mergers). Characteristic temperatures of equilibrium (e.g., the inflection point of the entropy density) and transport coefficients (e.g., the minimum of the shear viscosity over entropy density) vary widely at a cross-over phase transition, but converge at a critical point. Extracting the behavior of these characteristic temperatures is a major focal point of this research. Specifically, the interplay between strange and light hadrons is exploited to study the flavor hierarchy in the cross-over region. To investigate this, a viscous relativistic hydrodynamics framework with two conserved charges is being developed into a new open-source code, along with initial conditions that contain baryon number and strangeness. Flow observables sensitive to the equation of state and transport coefficients are calculated across beam energies. New techniques are developed to study this flavor hierarchy from first principles and to extract the characteristic temperatures from experimental data. Through the new dynamical framework, this project provides essential guidance to the Beam Energy Scan II runs at the Relativistic Heavy-Ion Collider and the future Facility for Antiproton and Ion Research in Germany in the search for the Quantum Chromodynamics critical point and subsequent investigation of the baryon-rich Quark Gluon Plasma.

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

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## **Imaging Beyond the Shot Noise Limit with Quantum Electron Microscopy**

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Transmission Electron Microscopy (TEM) is used in materials science and biology to image structures at very small length scales, down to individual atoms. One of the primary challenges in TEM imaging is that using too many electrons can damage the sample. However, using too few electrons produces very noisy images. This restriction, called the “shot noise limit,” affects all classical measurements. The emerging field of Quantum Metrology provides a way around this limit. New quantum mechanical imaging methods can increase TEM signal-to-noise without increasing the number of electrons needed to get good images. The objective of this project is to use these concepts to produce instrument designs for Quantum Electron Microscopy (QEM). A prototype instrument will be built to prove the QEM concept. Development of future QEM instruments at Nanoscale Science Research Centers will allow researchers to image more sensitive samples with higher resolution and clarity than ever before.

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

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**Probabilistic data fusion and physics-informed machine learning: A new paradigm for modeling under uncertainty, and its application to accelerating the discovery of new materials**

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The analysis and optimization of complex physical systems from first principles requires an agile arsenal of techniques in stochastic modeling, high-performance computing, and probabilistic machine learning. The proposed research focuses on scalable probabilistic machine learning for scientific data analysis. This research will enable advances in the seamless synthesis of numerical simulations with physical experiments of variable fidelity. New research capabilities also include the discovery of governing equations and the prediction of complex dynamics from incomplete models and incomplete data. Taken together, these developments target the effective and judicious exploration of high-dimensional decision spaces for identifying optimal design configurations under uncertainty. The cross-cutting nature of the proposed tools will benefit a wide range of science domains, including applications in materials discovery and optimization, subsurface transport, and earth system modeling.

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

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## **Chemo-Mechanically Driven In Situ Hierarchical Structure Formation in Mixed Conductors**

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Essential materials for energy technologies tend to exhibit “hierarchical” functions – they perform multiple, inter-related tasks at different locations, across disparate length and time scales. To best support this heterogeneous function, there is a fundamental need to understand and direct formation of corresponding tailored hierarchical architectures. In particular, a wide variety of applications, from energy conversion and storage to sensing and gas separation, rely on oxide mixed ionic and electronic conductors (MIECs). These critical ceramic materials catalyze reactions at their surfaces and transport ionic and electronic species. Ideally, MIECs should adopt hierarchical structures with 1) high surface areas, 2) surface compositions exhibiting high catalytic activity, and 3) microstructural connectivity in the direction needed for fast charge transport. In practice, however, MIECs are typically fabricated at elevated temperatures, leading to coarse, non-directional structures with poisoned (chemically segregated) surfaces. This work therefore applies a new approach, applying stimulated chemo-mechanical actuation to non-equilibrium films, to transform homogeneous MIECs into ideal hierarchical structures in situ. Key questions to be addressed, leveraging DOE user facilities and a novel contact-free high throughput optical approach, include: 1) how/why does the structure change across multiple length scales during transformation, 2) how/why do different process variables direct hierarchical structure evolution, and 3) how/why do the ionic/electronic transport and surface reactivity change during transformation? The new hierarchical structures demonstrate high surface catalytic activity with potential for improved device performance. Moreover, they serve as a platform to develop a fundamental understanding of MIEC processing-structure-property relationships, leading to rational design for energy applications.

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

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## **Templating Lattice-Confined Catalysts for Selective Hydrocarbon Upgrading**

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Hydraulic fracturing (“fracking”) has substantially increased the domestic supply of natural gas. Insufficient processing infrastructure coupled with the implicit challenge of long-range transportation of gaseous hydrocarbons, however, has prevented efficient utilization of these resources. To avoid direct atmospheric release of light hydrocarbons, which are more potent greenhouse gases than carbon dioxide (CO<sub>2</sub>), these resources are often burned in extraction-site flares. The development of chemistry to convert light hydrocarbons to more valuable chemical feedstocks and fuels has been a long-standing goal of catalysis. The relative carbon–hydrogen (C–H) bond strengths of hydrocarbons and the product derived from C–H oxidation render selective hydrocarbon oxidation a serious chemical challenge. This project will develop new synthetic methods to provide atomistic control over the active sites in porous heterogeneous catalysts and will develop new analytical tools to characterize the reactive intermediates involved in hydrocarbon functionalization. These investigations will provide new tools to 1) identify catalyst materials for hydrocarbon oxidation, 2) understand the activity of the developed catalysts, and 3) tune catalyst activity to achieve selective C–H functionalization.

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

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## **Elucidating Processes Controlling Arctic Atmospheric Aerosol Sources, Aging, and Mixing States**

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The objective of this project is to determine aerosol chemical composition, sources, mixing states, and aging processes across the entire annual cycle in the high Arctic, and in the Alaskan Arctic during fall – winter, to address the most significant gaps in Arctic aerosol observational data. The proposed project is based on the rapid sea ice loss across the entire Arctic, as well as the major delays in sea ice freeze-up in the Chukchi Sea, off the North Slope of Alaska (NSA). The project will: 1) identify the sources of Arctic aerosols as a function of season, 2) determine the mixing states and aging extents of Arctic aerosols as a function of season, and 3) ascertain the most important factors (e.g., sea ice extent, radiation, meteorology) modulating the sources, chemical composition, mixing states, and aging processes of Arctic aerosols. The proposed study will focus on analysis and interpretation of Atmospheric Radiation Measurement (ARM) field campaign samples and data collected during late fall/early winter at Utqiagvik, AK and during the year-long international Multidisciplinary drifting Observatory for the Study of Arctic Climate (MOSAIC) in the high Arctic. The project will use state of the art measurement techniques including real-time aerosol time of-flight mass spectrometry (ATOFMS), on-line aerosol sizing, and off-line computer-controlled scanning electron microscopy with energy-dispersive X-ray (CCSEM-EDX) spectroscopy. The project will provide an unparalleled opportunity to study seasonal changes in aerosol processes in the high Arctic. Size-resolved number fractions of observed individual particle sources will be determined for each month, with quantitation of locally emitted vs. long-range transported aerosols. Number fractions of aerosols internally mixed with various secondary species will be determined, and aerosol mixing state indices will be calculated. Sea ice extent and fracturing impacts on sea spray aerosol will be examined. For predictions of Arctic atmospheric composition and feedbacks, knowledge of aerosol sources, mixing states, and aging processes is critical and is a significant current gap in our understanding of Arctic aerosols. The proposed project will provide unprecedented and critical knowledge of Arctic aerosol mixing states and processes. The overarching impact of the project will be the generation of Arctic aerosol observational data and improved understanding of Arctic aerosol processes to inform and evaluate future simulations of Arctic atmospheric composition and climate.

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

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## Non-Equilibrium Effects in Quantum Magnets

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Our daily lives revolve around the use of solid state materials in non-equilibrium settings. For instance, the electronic switching of silicon-based transistors has transformed energy and information applications in the 20<sup>th</sup> century. Over the past few decades, *quantum materials* have emerged as promising candidates for components of future technologies that could produce paradigm shifts in these areas. Yet, the non-equilibrium properties of quantum materials (e.g. how they respond to fast switching, or how information can propagate through such materials) are just beginning to be explored both experimentally and theoretically. Theoretical progress is quickly being made within a class of models based on interacting “spin” degrees of freedom known as *quantum magnets*, the simplest example being the transverse field Ising model. This project will make use of neutron scattering to study material realizations of this model after they are driven out of equilibrium by fast field pulses from resistive pulsed magnets, i.e., “quantum quenches”. This project will provide direct connections and guidance to theories of non-equilibrium phenomena in bulk quantum materials, as well as advances in the neutron scattering methods used to probe non-equilibrium phenomena. These advances will fuel future discoveries in quantum materials that may be used in next-generation technologies.

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

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## Particle Dark Matter Across Scales

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Dark matter is about five times more abundant in the Universe than ordinary matter. It plays a key role in forming galaxies like our own Milky Way. However, while dark matter is well understood on large astrophysical scales, the identity of the microscopic dark matter particles themselves remains a mystery. This research investigates the particle nature of dark matter. Understanding the composition of dark matter is a key science goal of the Department of Energy High Energy Physics program. Many of the leading particle dark matter models predict that dark matter should produce small amounts of light in astrophysical systems and precision laboratory experiments. This research will explore possible signatures of dark matter in astrophysical and laboratory photon data across a range of frequencies ranging from the radio band to the gamma-ray band. The work will investigate the relationship of the possible photon signals to the underlying theoretical dark matter models and to the spatial distribution of dark matter in astrophysical objects like galaxies and cluster of galaxies. As an example, the research will explore anomalous bright glows of light in the gamma-ray and X-ray bands, which have been observed arising from the center of the Milky Way and other nearby astrophysical systems. The aim of this investigation is to deduce whether these anomalies are due to particle dark matter interactions. If evidence of particle dark matter is found, this evidence would shed light on the nature and composition of dark matter, while giving greater context to how ordinary matter is embedded within the fundamental laws of nature.

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

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## **Physics-reinforced Machine Learning Algorithms for Multiscale Closure Model Discovery**

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Advances in artificial intelligence have led to a renaissance in learning and extracting patterns from complex data. Despite successes in other areas, applying machine learning techniques in the field of fluid mechanics is relatively new. Most efforts are primarily focused on finding parameters for existing turbulence models. This project explores a big data approach that learns from physical constraints without assuming any heuristics for underlying turbulence physics. Our overall research program will develop novel physics-reinforced data-driven approaches for geophysical turbulence. The research will also involve deep learning approaches that can discover closure models for complex multiscale systems. Research insights will facilitate the building of improved numerical weather prediction models and better parameterization strategies for DOE mission-relevant challenges.

*This research was selected for funding by the Office of Advanced Scientific Computing Research and the DOE Established Program to Stimulate Competitive Research.*

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**Optimal and robust reconstruction of BAO, redshift-space distortions and the Alcock-Paczynski effect**

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The goal of this project is to optimally reconstruct cosmological information that has been lost from large-scale clustering of galaxies due to cosmic structure growth. The outcome of our research will be used to improve dark energy and other cosmological constraints from the ongoing extended Baryon Oscillation Spectroscopic Survey (eBOSS) and the upcoming Dark Energy Spectroscopic Instrument (DESI). The large-scale galaxy clustering data contain two important features: the Baryon Acoustic Oscillations (BAO) and the overall shape from small to large scales. The latter feature has potential to improve dark energy constraints as well as the structure growth rate (therefore the nature of Gravity) and neutrino mass constraints. Such a feature is, however, very susceptible to various nonlinearities caused by structure growth and/or peculiar velocities of galaxies. While the current BAO reconstruction scheme has been successful for reducing such nonlinear effects from the BAO feature, thereby substantially improving dark energy constraints, its performance in reducing nonlinearities from the overall shape has not been fully investigated. This research plans to extend the success of the BAO reconstruction technique further, and in new directions, by developing an optimal method to recover cosmological information that has been lost from the overall shape of galaxy clustering. This research will be conducted by using the perturbation theories and cosmological N-body simulations, and applying the resulting method to current/future galaxy redshift survey data. The outcome will increase the overall science return of current and future dark energy missions with little extra cost. Naturally, this will contribute to the infrastructure of such missions.

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

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**Finding missing links associated with aerosol-cloud interactions: Aqueous and cloud-phase secondary organic aerosol formation**

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Interactions between clouds and aerosols play a major role in Earth's energy budget and are among the largest uncertainties in projections of future Earth-system changes. Cloud-aerosol interactions are manifestations of many nonlinear processes governing the number, size, and chemical composition of aerosols that serve as cloud condensation nuclei. Aqueous- and cloud-chemistry pathways that lead to the formation of secondary organic aerosol (SOA) are some of the least understood of these processes but could be associated with significant regional-scale heterogeneities in Earth's aerosol, cloud, and radiation fields. To date, representations of aqueous- and cloud-phase organic chemistry in Earth-system models have been overly simplistic, making it difficult to diagnose how variations in the cloud, chemistry, and meteorological regimes in the atmosphere affect aerosol-cloud interactions and radiation. Although recent field campaigns and laboratory experiments provide a wealth of measurements, there is a persistent gap in terms of coherently connecting these measurements to advance our understanding of aqueous- and cloud chemistry pathways of SOA. The vision of this U.S. Department of Energy (DOE) Office of Biological and Environmental Research (BER) Early Career Project is to advance the fundamental understanding of SOA formed within aqueous aerosols and cloud droplets, thus providing a complete description of coupling between cloud-aerosol interactions and chemistry. This will be achieved through a multipronged approach that integrates 1) analyses of laboratory measurements and multiple field measurements of aerosols, clouds, radiation, and the dynamic and thermodynamic structure of the atmosphere and 2) observationally constrained high-resolution modeling approaches, which will be used as analytical tools to assess processes governing the formation of SOA through aqueous- and cloud-chemistry. Many of the measurements used in this research come from BER's Atmospheric Radiation Measurement (ARM) user facility and complementary data sets from both the Amazon and the Southern Great Plains (SGP) sites. The proposed data analyses will elucidate new aqueous SOA processes, determine the role of aqueous chemistry in the formation and growth of nanoparticles in the atmosphere, and establish parameters needed to improve the predictive ability of models. Aqueous SOA processes determined from analyses of field and laboratory measurements will be incorporated in a high-resolution regional model to investigate how these processes are manifested in the chemical and dynamic evolution of SOA in the atmosphere. Additionally, large eddy simulations will be conducted to investigate how subgrid-scale aqueous SOA chemistry processes and cloud-aerosol cycling affect aerosol-cloud interactions. This work will lead to groundbreaking new insights and discoveries that can be used to improve large-scale, Earth-system models and inform further research on aqueous- and cloud-phase SOA formation. A solid understanding of the coupling between atmospheric aqueous SOA chemistry and clouds is critical to advance our understanding of Earth's energy budget and to address some of the most critical scientific questions facing the nation and DOE.

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

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## **Portable Parallel Algorithms and Frameworks for Exascale Graph Analytics**

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Graphs are used to model the interactions among various entities in a wide variety of fields including biology, chemistry, and cyber-security. Analyzing the structure and properties of graphs is an important component of the scientific discovery process for many applications. With the explosion in the volume of data, graphs have become very large and can contain more than hundreds of billions of vertices and trillions of edges. Analyzing these graphs efficiently is a significant hurdle. This project will make large-scale graph analytics more efficient and accessible to scientists, thereby improving the efficiency of scientific data analysis in critical DOE mission areas. First, this project will design parallel graph algorithms that are efficient both in theory and in practice so that they can perform well under all possible inputs and across many machine parameters, and scale gracefully to larger data sets. Using these algorithms, scientists will be able to perform analytics on massive graphs on exascale platforms much more efficiently than before, and confidently predict the performance of the algorithms due to their theoretical guarantees. Second, this project will develop a domain specific language for graph computations to reduce the programming effort required by scientists and ensure that the analysis codes run efficiently on a variety of different platforms.

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

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## **Bio-inspired Polymer Membranes for Resilience of Electrochemical Energy Devices**

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Electrochemical energy storage and conversion devices such as batteries and fuel cells function by creating a difference in electrical potential across two electrodes that drive electron flow through a circuit to power devices. The polymer membrane that separates these electrodes is critical for controlling ion transport and must be mechanically robust. The objectives of this planned research are to discover the fundamental physical mechanisms for self-regulation of synthetic polymers and gels under electric fields. Biological membranes are constantly assessing evolving conditions such as electric field and optimizing their function by dynamically adjusting their properties. In contrast the current generation of polymer membranes are static and unable to readily adjust to changing operating conditions making them less durable and vulnerable to performance degradation. This in turn has adverse consequences for device operation and sometimes even for safe use. Membrane performance and durability can be dramatically improved by imbuing the polymer membrane with the ability to sense and adapt to the local electrochemical environment, similar to what is possible in biological membranes. Enabled by the emerging approaches for tailoring polymers through modulating the mechanical strength of particular bonds, this unexplored concept will be pursued computationally through simulations that explicitly represent the atomic structure of the material and development of theories that describe the overall material behavior. The findings will then be experimentally proven by making and characterizing polymers with mechanical and self-healing properties that should be dynamically tunable by electric fields. This work will open up a new concept in design of polymer membranes that predictably self-regulate internal bonding dynamics and interactions in response to changes in external electrical fields to tune instantaneous mechanical properties such as stiffness and strength, paving the way for safer and more durable electrochemical energy devices.

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

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## **Precision Computations in Strongly Coupled Conformal Field Theories**

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Quantum field theory (QFT) is a universal language for theoretical physics, describing everything from particle physics to exotic materials to magnets and boiling water. However, precise computations in QFT are often extremely difficult. Tools for studying the simplest (so-called "weakly-coupled") QFTs were developed in the 20th century. However, many of the most important QFTs are "strongly-coupled" and cannot be studied with these tools. The goal of this research is to develop new tools for precise computations in strongly-coupled QFTs. The work will focus on conformal field theories (CFTs), which describe phase-transitions (for example, water turning into vapor), and are basic building blocks of general QFTs. The special mathematical structure of CFTs can lead to powerful predictions that work even in strongly-coupled theories. This research will explore this structure using a combination of pen-and-paper and computer-based techniques.

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

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## **Towards a Next Generation Search for Time-Reversal Violation Using Optically Addressable Nuclei in Cryogenic Solids**

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Certain rare pear-shaped nuclei have unmatched sensitivity to new kinds of forces between subatomic particles that are not the same when the arrow of time is reversed. Such forces are believed to be responsible for the near absence of antimatter in the observable Universe. These rare isotopes, some for the first time, will be produced in large numbers at the Facility for Rare Isotope Beams currently under construction at Michigan State University providing an unprecedented opportunity to probe for new physics. In anticipation, we will use abundant isotopes to develop new techniques to manipulate nuclei embedded inside an optically transparent solid at cryogenic temperatures. Implantation into a solid, such as neon and argon, is potentially an effective way to both efficiently capture and repeatedly probe the small number of rare nuclei, such as radium and protactinium. An optically transparent host medium at cryogenic temperatures would allow for the laser manipulation of the nuclei in a thermally quiet and stable environment for a wide variety of guest species such as polar molecules. In such systems, the nuclei are exposed to extraordinarily large electric fields and magnetic field gradients, which significantly amplifies the measurability of certain time-reversal violating effects. The potential sensitivity of this new approach could be at least a few hundred times greater than the current leading experiment which uses mercury atoms.

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

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## **Rational Sub-Nanometer Manipulation of Polymer Morphology for Efficient Chemical Separations**

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Molecules are almost always found in impure mixtures, but to be useful, they need to be separated and purified into their individual components. In many cases, the most challenging separations are for small molecules that differ by less than an Angstrom (0.1 nm) in size, a dimension that is approximately equivalent to only one millionth the thickness of a strand of human hair. These challenging separations are often accomplished by processes like distillation, which require energy-intensive phase changes, or absorption, which require the use of environmentally harmful solvents. An energy efficient and environmentally friendly alternative to these traditional processes is membrane-based separations. Today, nearly all gas separation membranes are formed from entropically disordered yet easily processable polymers, which can be formed at scale into selective thin films of only 100 nm thick. Unfortunately, the disordered nature of these state-of-the-art polymers precludes using them for some of the most energy-intensive and environmentally relevant separations that are practiced today. This research program envisions a strategic shift in materials design to template ordered free volume elements into otherwise entropically disordered polymers. Free volume elements describe the nanoscopic spacing devoid of electron density that allows molecules to diffuse in polymer films. To create isoporous free volume elements with molecular precision, processable polymers are synthesized with chemical moieties of the exact shape and size of small molecules that need to be separated. By tethering these moieties to a polymer backbone by weak chemical bonds, selective thin films can be formed using traditional approaches. However, after forming the films, these bonds can be selectively and quantitatively broken. Through careful experimental design, these moieties decompose into small molecules and can be removed from the polymer matrix, leaving behind isoporous free volume elements designed for a specific separation. Various chemical moieties can be incorporated to leverage the versatility of this approach for a variety of separation applications. In addition to the potential benefits in separation performance, this strategy also permits access to creating polymers that have identical chemical composition but unique packing structures, which can enable a fundamental decoupling of materials performance from processing considerations. To target these opportunities, advanced strategies in design, synthesis, and characterization will be coupled with theory to create new membrane materials capable of separating complex chemical mixtures into pure molecules with Angstrom-level resolution.

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

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**Development of high throughput techniques for superconducting microfabrication, assembly and deployment for future high energy physics experiments**

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How did the universe begin? What is the universe composed of? How did the universe evolve over time? These are some of the most fundamental questions about the universe that fascinate many of us. Advancements in technologies have been a key element that has ushered in the era of precision cosmology to answer these questions. Among many technological advances, microfabrication processes made it possible to produce high performance detectors with its ability to realize fine resolution features and access to exotic materials. This project is intended to establish high-performance microfabrication capabilities for ultrasensitive, superconducting detectors and readout electronics components with commercial foundries, and to boost manufacturing throughput while improving quality and lowering cost. The developed processes could be used for cosmological experiments such as those that seek to improve measurements of tiny fluctuations in the universe's oldest light, the Cosmic Microwave Background radiation, or that seek to find low-mass dark matter particles, and they could also benefit quantum computing.

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

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## **Elucidating the Morphological Instability Mechanisms during Electroplating of Active Metals**

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The objective of this research is to understand how a group of metals relevant to batteries develop unstable growth morphology during the electrodeposition or electroplating process, a process important for the function of batteries. These metals include alkali metals (e.g. lithium, sodium and potassium) and zinc that have large atomic mobility and high reactivity with the electrolytes used during the battery process. They are very attractive electrode candidates for the next-generation rechargeable batteries that promise several times higher energy density at lower cost. However, the prevalent formation of highly non-uniform morphologies, represented by the growth of filament-like and moss-like structures, presents a major barrier to their successful application since it causes rapid capacity fading and even internal shorting of the batteries. This research focuses on an important question that has received little attention so far: Does plating-induced residual stress play a critical role in inducing the morphological instability of the electroplated active metals? Using zinc as the main model system, this question will be investigated through three integrated tasks: (1) quantification of the correlation between plating stress and morphology, (2) three-dimensional imaging of the microstructure and chemical distribution of the mossy structure at nanoscale, and (3) the development of stress-aware electroplating models across length scales to interpret experimental observations and provide further predictions. The outcome of this work will close a fundamental knowledge gap in the electrodeposition of active metals and potentially establish the scientific basis for developing stress-based methods to overcome a key failure mode of advanced batteries.

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

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## **Splitting Photons: Singlet Fission in Nanocrystal-Molecule Hybrid Structures**

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The goal of this research is to enable all the energy contained in sunlight to be harvested by making full use of the blue and green wavelengths of light. Current systems are unable to extract all of the energy available from photons in this wavelength range due to rapid relaxation processes that dissipate a considerable fraction of the energy as heat. In this work, inexpensive earth-abundant components capable of supporting multi-excitonic processes involving more than one tightly bound excited state are investigated as a way to exceed the Shockley-Queisser limit of solar cells. The research will examine hybrid organic-inorganic nanostructures capable of singlet fission, a process by which one high-energy spin-singlet state is converted into two lower-energy spin-triplet states, and subsequent triplet exciton transfer. Specifically, the organic molecules diphenylhexatriene and tetracene that maximally absorb blue light and are known to exhibit singlet fission will be bound to lead chalcogenide nanocrystals. A variety of steady-state and time-resolved spectroscopic techniques will be used to study energy transfer from the spin-triplet excitons created in the organic molecules to the nanoparticle acceptors. The hybrid nanostructures will be fully characterized both in solution or thin film via electronic absorption and photoluminescence spectroscopy, nuclear magnetic resonance spectroscopy, high-resolution mass spectrometry, transmission electron microscopy, photoelectron spectroscopy, time correlated single photon counting and transient absorption experiments. The effect of molecular and nanocrystal structure on the electronic coupling between the hybrid components will be examined to establish fundamental relationships between structure and triplet energy transfer efficiency. The findings will be applicable to a potential tetracene-silicon platform that may ultimately enhance the power conversion efficiency of silicon solar cells.

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

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## **GPU/FPGA Accelerated Deep Learning Technique Development for Discovering Physics in Liquid Argon Time Projection Chambers**

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The experimental observation of neutrino oscillations, a physics phenomenon that proves neutrinos have mass, is one of the most intriguing and active developments in physics beyond the Standard Model during the last decades. Detector technologies that allow high precision measurement of neutrino interactions are needed more than ever. The liquid argon time projection chamber (LArTPC) is an imaging detector that can record charged particle trajectories at sub-millimeter spatial resolution with detailed calorimetric (energy deposit) information, making it the detector of choice for current and future accelerator neutrino experiments. The Short Baseline Neutrino (SBN) program employs three  $\approx 100$  ton LArTPC detectors at a short distance ( $\approx 1$ km) to investigate the electron neutrino excess observed in MiniBooNE experiment, which could be an indication of new types of neutrinos. The Deep Underground Neutrino Experiment (DUNE) employs four 10 kiloton LArTPCs to search for proton decays and measure neutrino oscillations at a long distance ( $\approx 1300$ km) which may shed light to one of remaining questions in physics, the asymmetry in the presence of matters and anti-matter in the current universe. Despite the potential of this novel detector technology, data reconstruction and analysis techniques for large scale LArTPC detectors remain challenging after many years of software development effort. This project brings modern machine learning algorithms from the field of computer vision and artificial intelligence to develop a high quality data reconstruction chain that enables physics measurements in SBN and DUNE experiments. The core of this research is R&D of innovative software algorithms as well as the hardware acceleration using graphical processing units (GPUs) and field programmable gate arrays (FPGAs). These developments will target near term physics measurements in the SBN program to benchmark the developed reconstruction algorithms. The outcome of this research project will allow us to use the full potential of LArTPC detectors to discover new physics and answer the fundamental questions of the universe.

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

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## **Towards table-top neutrino detectors: A 10 kg Skipper-CCD experiment**

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The Skipper Charge-Coupled Device (CCD) is a ground breaking technology that is opening unprecedented windows to the universe through the detection of single photons and electrons. Fundamentally, a CCD is an integrated circuit etched onto a silicon surface forming sensitive elements called pixels. When light or other particles interact with the silicon they produce an ionization charge that is collected in the pixels. On standard CCDs this charge is discarded after it is measured as part of the readout process. In contrast, the Skipper-CCD is able to make multiple non-destructive measurements of the pixel's charge and uses this additional information to reduce the readout noise to a negligible level. The first gram-scale instrument using the Skipper-CCD technology was produced in 2016 at the Fermi National Accelerator Laboratory in collaboration with the Lawrence Berkeley MicroSystems Lab. This prototype system was able, for the first time, to unambiguously and reliably detect single electrons over millions of pixels reaching the theoretical limit of silicon ionization sensors. The overarching goal of this project is to explore the potential of the Skipper-CCD technology to scale up to particle detectors with thousands of sensors and tens of kilograms of active mass. This technological leap will open a new path for the next generation of short baseline neutrino oscillation experiments and dark matter searches. Furthermore, it will provide a novel nuclear reactor monitoring option for Non-Proliferation Treaty Verification. Skipper-CCD sensors also have natural and immediate applications to imaging and spectroscopic instruments for astronomical, quantum physics and biomedical research. This project will develop the tools to enable the adoption of the Skipper-CCD technology for a wide range of future high-sensitivity instruments.

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

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## **Interaction and Transport Effects in Driven Magnetic and Topological Materials**

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Quantum materials, when driven by light into highly non-equilibrium conditions, can exhibit novel and non-trivial properties not available in equilibrium. Understanding driven quantum matter could enable efficient photovoltaic applications and powerful quantum information technology. An important class of quantum materials is comprised of van der Waals crystals (e.g. graphene), which are characterized by their atomically thin structure and bonding through the van der Waals force. While there has been much progress in the investigation of van der Waals crystals and heterostructures due to their novel magnetic and topological properties, their non-equilibrium behavior is not fully understood. Bridging the two fields of van der Waals materials and non-equilibrium matter, the planned research aims to firmly understand and demonstrate the possibility to control van der Waals materials under strongly non-equilibrium conditions. This project will involve studies of three key interwoven topics: (1) exploring the effects of strong electromagnetic fields on magnetic van der Waals trilayer structures; (2) understanding the effects of electronic interaction in strongly driven van der Waals systems; (3) investigating nonlinear transport properties in strongly driven van der Waals systems. Developments in these three key areas are expected to bring significant progress in finding novel strategies to control the magnetic, interaction, and transport properties in non-equilibrium quantum materials.

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

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## **Fluctuations in Quantum Materials**

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This research will study fluctuations in charge, spin, or orbital order that underlie collective dynamics in quantum materials. A new method developed for accessing these fluctuations at low energies and on their natural timescales is key to understanding the relationship between fluctuations and the range of phases and transitions in these types of complex solids. These fluctuations are relevant to properties such as magnetism, poor metallic conductivity, charge ordering, and superconductivity. The main focus of this work will be to unravel unconventional superconductivity and its relationship to other electronic phases by studying the fluctuations involved. The tool for this research, called X-ray quanta fluctuation scattering or XQFS, has initially been used to investigate magnetic materials at SLAC's X-ray free-electron laser. Early results show tremendous potential for providing important new insight into how the materials respond to internal fluctuations near phase transitions. By harnessing coherent X-rays, XQFS directly measures spin or charge fluctuations on a timescale that was previously unavailable. This work focuses on further developing this method as well as using it to study superconductivity in quantum materials. The research will provide a fresh perspective on fundamental interactions and how multiple connecting aspects of electron behavior give rise to novel phases of matter.

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

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**Next Generation Superconducting Radio Frequency (SRF) Cavities with Optimized RF Performance via Energetic Condensation Thin Film Technology**

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A key to future generations of particle accelerators is to sustain the highest possible acceleration kick with minimum construction and operation costs. Bulk niobium (Nb) is currently the standard material used in superconducting radio-frequency (SRF) accelerating cavities. Current techniques are approaching the fundamental limit of this material. The greatest potential for new performance capabilities and cost reduction lies with methods and materials that directly engineer the sub-micron-thick critical surface layer of superconducting material inside cavities. Recent strides in the development of novel deposition techniques (energetic ion vacuum deposition) open the door to the production of engineered SRF surfaces either as a single layer superconductor, such as niobium on copper (Nb/Cu), or multilayered superconductor-insulator-superconductor structures. This innovation promises to extend the performance of SRF Nb cavities beyond the current material limits. While conventional deposition techniques rely on thermally induced growth processes, which limit the deposition quality of refractory materials such as Nb and its compounds on low temperature substrates (Cu), energetic ion deposition techniques allow film growth processes to be manipulated, to produce high quality crystalline materials with excellent adhesion to the substrate and sharp, clean transitions between layers. The increased flexibility and control of the deposition processes lead to films with improved characteristics. This research focuses on the development of SRF cavities coated with (1) vanguard-quality Nb films and (2) nanometric Nb<sub>3</sub>Sn-based multilayered structures. Ultimately, both thin film technologies will be integrated to produce fully engineered SRF surfaces useful at different frequencies, and at possibly higher temperatures. These highly performing thin film SRF cavities will also simplify the accelerating system, dramatically changing the cost framework of SRF accelerators. The final integrated concept will provide significantly improved RF performance, higher efficiency and quality control for accelerating structures relevant to next generation research accelerators for science and other societal and commercial applications.

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

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## **Quantum Criticality and Topology in Non-Equilibrium Systems**

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A key goal of condensed matter physics research is to identify new phases of matter, and to understand the universal features of the phase transitions between them. In the past decade, physicists have uncovered a wealth of new phases with interesting surface properties, exemplified by the theoretical prediction and subsequent experimental discovery of topological insulators and superconductors. Traditional condensed matter systems are usually in a thermal equilibrium state and typically at very low temperatures. Very recently, experimental advances have sparked interest in the non-equilibrium setting. Non-equilibrium systems can host new phases and phenomena with no equilibrium counterpart, and could also enable robust ways to build quantum memory devices to store and manipulate quantum information in a coherent manner. These phases and phenomena are inherently 'dynamical': they are described not by changes in the arrangement or structure of the constituent particles, but instead marked by sharp distinctions in how the particles move and exchange energy or quantum information. The discovery of robust non-equilibrium phases raises many fundamental questions: Can a systematic theory of states of matter and of dynamical transitions between such states be developed? How can such states be realized and probed experimentally? This research will explore the emergence of topological phases and quantum criticality (two cornerstones of modern condensed matter physics in equilibrium) in such non-equilibrium quantum systems. Specific goals include (1) using tensor networks to efficiently represent non-equilibrium states of matter and their phase transitions; (2) studying and designing new probes for periodically driven systems; and (3) developing analytic and numerical tools to analyze non-equilibrium topological phase transitions. Advances in these directions will be achieved using novel techniques appropriate to study the non-equilibrium dynamics in many-body quantum systems combining strong interactions and randomness. This research will lead to a new conceptual framework for understanding the emergence of quantum critical and topological properties in quantum systems far from thermal equilibrium.

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

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**Novel Experimental Probes of Quantum Chromodynamics in Semi-Inclusive Deep-Inelastic Scattering and  $e^+e^-$  Annihilation**

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The mass of most visible matter in the universe is due to the dynamics of the interaction of quarks and gluon inside nucleons. While the theory of quantum chromodynamics (QCD) provides an accurate description of the fundamental laws governing strong interactions, a comprehensive description of the dynamics that give rise to the observed properties of the nucleon still eludes us. We aim to develop experimental and analysis techniques that make full use of the unprecedented statistical power provided by the datasets to be collected at the upgraded electron scattering facility at the Jefferson National Accelerator Laboratory (JLab). In particular, we plan to utilize correlations in the angular distributions of particles produced from quarks when nucleons are broken up in hard scattering events and their polarizations. These methods will have broad applications in the exploration of QCD. With the first datasets collected at the upgraded JLab we can for example gain insight into the force that the gluon fields inside the nucleon exert on the quarks as they move through the field as well as elucidate the role of spin in the formation of bound quark states. Combining these results with an independent measurement in  $e^+e^-$  annihilation, using data from the new SuperKEKB facility in Japan, will allow us to disentangle the effects of interactions of the quark inside the nucleon from those the quark underwent after the breakup of the nucleon.

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

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**Understanding the Optoelectronic Properties of Doped 2D Organic-Inorganic Halide Perovskite  
Quantum Wells: Towards Efficient Ultrafast Quantum Well IR Photodetectors**

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The detection of low-energy photons is important for numerous applications such as defense (navigation, night vision, and weapons detection), remote sensing, cryogenic wind tunnels, optical communication (aerospace and terrestrial), infrared cameras, and biomedical and thermal imaging. The fabrication of efficient and low-cost, large-area infrared (IR) photodetectors comprising defect-tolerant materials is still a challenge since the only way of growing these materials is by using laborious and expensive vacuum deposition techniques. Recently, quantum well IR photodetectors have emerged as an alternative choice due to their low cost, high reproducibility and uniformity, and ease of fabrication when compared with traditional silicon bulk IR photodetectors. This research will develop two-dimensional (2D) organic-inorganic hybrid perovskite (OIHP) multiple quantum wells having strong spin-orbit coupling, high carrier mobility, and tunable quantum well structures. The studies will shed light on new breakthroughs in both materials design and modulation of fundamental physical phenomena by carefully elucidating the role of dopants, sample heterogeneity, orientation, structure, and bias stress effects on the performance of 2D OIHP IR photodetectors. The research efforts also involve the use of in situ and in operando characterization tools to generate a mechanistic understanding of the degradation processes and/or phase transformations occurring in 2D OIHP quantum well IR photodetectors under working conditions. The research, when brought to fruition, will significantly impact the development of 2D OIHPs for IR photodetectors while being simultaneously cost-competitive and solution processable. Moreover, these 2D OIHP –when optimized in thin films– will perhaps be one of the few doped materials available for ultrafast short-to-mid wavelength IR photodetection.

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

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## **Mesoscale Defect Interaction Mechanisms in Structural Alloys**

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Materials in radiation environments such as nuclear reactors develop microstructural damage over time through the accumulation of defects created by the radiation. The defect interaction and evolution control microstructural changes during irradiation processes and determine materials' properties and performance. The defect interaction and evolution process is multiscale in time (from femtoseconds to decades) and length (from angstroms to meters) and has been extensively studied experimentally at macroscales and at atomistic scale through modeling and simulation. However, there exists a significant gap in understanding these phenomena at mesoscales (intermediate time and length scales). Mesoscale interactions are critically important for understanding how defects lead to changes in materials' properties and performance as they represent the transition from local atomistic events to macroscopic effects. This research aims to develop a mesoscale mechanistic understanding of radiation-induced defect interaction and evolution in pure metals and metal alloys, using a recently co-developed approach called "SEAKMC" that is ideal for the research at the mesoscale where these interactions are less understood. The understanding developed will provide the basis for extending the operating life of structural materials in existing nuclear reactors and the development of next-generation structural materials for use in future nuclear energy systems. This project will also advance computational capabilities at the mesoscale, which will be widely applicable to other fields of materials science, physics, and chemistry.

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

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## **Non-volatile Active Control of Spin Transport Using Interfaces with Molecular Ferroelectrics**

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Spintronics (spin electronics), which studies both spin and charge degrees of freedom of electrons and their couplings, already demonstrated important applications such as in the read head of hard disks, based on the effect of magnetic field on the electric current flowing through magnet/nonmagnet interfaces. Presently, the spintronics research focuses on elucidating the mechanism for variation of the spin degree of freedom (spin current), as a foundation for the next-generation information storage, computing, and energy conversion applications. In the past decades, significant advancement in the generation and detection of spin current have being made, using magnet/nonmagnet interfaces and using non-magnetic materials with strong coupling between the spin and charge degrees of freedom (spin-orbit coupling). In contrast, the manipulation of spin current has been much less studied. This project studies the non-volatile active control of spin current using interfaces with molecular ferroelectrics, crystalline materials that exhibit spontaneous electrical dipoles switchable by an external electric field. The results of the project will not only deepen understanding of the effect of interfacial arrangement of atoms and electrons on the spin current through the magnet/nonmagnet interfaces, but also will shed light on the mechanism of charge and spin current in crystalline organic semiconductors. In addition, it will provide insight on the tunability of charge/spin current conversion in spin-orbit coupled materials by adjusting their subtle arrangement of electrons. The success of this project is anticipated to open new routes in non-volatile control of spin current, which is an important step toward spin-based electronic circuits.

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

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## Probing New Physics with Tau Leptons using the CMS Detector

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The Standard Model (SM) of particle physics is a thoroughly well-tested theory of all electroweak scale phenomena to date, the most recent test being the discovery of the long-predicted Higgs boson particle. However, much evidence exists to suggest that the model is incomplete. On the formal side, the mass of the Higgs particle itself is perplexingly small. On the experimental side, among other things, the SM lacks a candidate to account for dark matter, which is now known to play an indispensable role in astrophysical large scale structure formations. Many theories that address such fundamental puzzles of the SM predict the existence of multiple Higgs bosons, including a very light boson that couples preferentially to third-generation fermions. Observation of a new light boson would therefore provide a distinctive sign of new dynamics in nature. As the world's most energetic particle accelerator complex, the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN) in Switzerland is an ideal laboratory for producing and studying a light Higgs state that may provide the missing piece in the SM puzzle. This research program plans to use the large and growing dataset collected by the Compact Muon Solenoid (CMS) detector at the LHC to explore boosted signatures of tau leptons decaying from a new light boson to efficiently reconstruct tau final states. To this end, a supporting aim of the program is to refurbish and recommission the CMS innermost silicon pixel tracking system by replacing power converters in order to sustain high radiation levels and increased data rates foreseen during future CMS operations, and thereby, increase the overall availability of the tracker for improved tau identification and momentum measurements. Going forward, the associated High-Luminosity LHC detector upgrade of CMS will take advantage of a high granularity calorimeter that will allow unprecedented imaging of boosted taus arising from the production of light bosons. Overall, the search for new particles and their interactions coupled with a technologically advanced detector will aim to provide unique insights into our understanding of nature.

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

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**Building Artificial Layered Solids from the Bottom-up: Materials by Design to Enable New Energy Technologies**

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Synthetic nanostructured inorganic solids are emerging as promising building blocks for a broad range of applications from electronics, optoelectronics, to energy and environmental technologies, given that their chemical and physical properties can be controlled and optimized by tunable parameters such as size, morphology, crystal structure, chemical composition and surface/interface. As dimensionality is one of the defining parameters in nanoscience, the same chemical compound may exhibit drastically different properties depending on how the atoms are structurally arranged in dimension. The objectives of this research are to develop a suite of structurally controlled artificial two-dimensional (2D) layered solids from the bottom-up (Lego-like piece-by-piece), and to enable new synthetic tools for functional nanosheet materials beyond graphene. Combined with computational simulations to guide design, rational synthesis of inorganic 2D crystals will be integrated with their self-assembly and predictable organization of molecular assemblies to form artificial layered solids. This research will expand fundamental knowledge on how nanoscale synthesis and self-assembly can encode properties and functionality into materials in a predictable manner. The new materials by design platform of artificial layered solids with exceptional catalytic/transport properties will have direct implications for advanced energy science and technologies.

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

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**The Emergent Photophysics and Photochemistry of Molecular Polaritons: A Theoretical and Computational Investigation**

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When molecules are placed between closely spaced mirrors, they interact strongly with the photons that are trapped between them, generating new quantum states that are no longer exclusively material nor photonic alone, but rather, coherent superpositions of both. These hybrid states are known as molecular polaritons, given that they arise from the strong interaction of the electric field of light and the electrical polarization of the molecules. Recent experimental advances in fabrication of molecular polariton architectures have successfully demonstrated the feasibility to control the rate and outcome of a certain class of chemical reactions in condensed phases. Importantly, these reactions proceed in strongly dissipative environments such as liquid solvents and lossy mirrors that allow for photons to escape from their confinement. The purpose of this research is to formulate quantum mechanical theories and computational tools that can elucidate the origin of these intriguing phenomena and simultaneously predict capabilities that this new generation of molecular materials affords. Attention is placed on harnessing polaritons to carry out photophysics and photochemistry that challenge existing paradigms, such as the optimization of energy conversion processes in organic solar cell or light-emitting devices, or unconventional phenomena such as long-range excitation energy transfer, remote control of chemical reactions, and a new quantum mechanical regime of chemical reactivity resulting from wavefunction overlaps among a large number of molecular polaritons (Bose condensation). This research explores a frontier of chemistry and physics where electrons, vibrations, and photons interact strongly with each other to generate emergent behavior that can be creatively exploited to address contemporary challenges in Basic Energy Sciences.

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

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**Improved Biofuel Production through Discovery and Engineering of Terpene Metabolism in Switchgrass**

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Plants employ complex and often species-specific networks of small molecules to cope with environmental challenges as well as to communicate with other organisms. In many major crops, a diverse group of metabolites, called terpenes, function as key biochemical mechanisms to respond to different stresses and are essential to agricultural productivity. As terpenes are also used as precursors for renewable biodiesel and aviation fuels, a better understanding of their biochemical networks can be used to generate stress-tolerant crops with enhanced potential for biofuel production. This project will investigate and harness terpene-mediated stress defense mechanisms in switchgrass (*Panicum virgatum*), which is a valuable bioenergy crop due to its high net energy efficiency. Genetic, genomic, biochemical, and protein structural analyses will be used to gain detailed knowledge of the biosynthetic machinery controlling the switchgrass terpene network. Plant-microbe interactions will also be studied to better understand the role of terpenes in the plant's response to stresses such as drought. The knowledge thus obtained on the biological function of terpenes will be applied to carry out advanced genome engineering of switchgrass and develop varieties with improved stress resilience and tailored terpene blends for advanced biofuel production on marginal land, advancing BER's objective of developing sustainable and renewable bioenergy resources that do not compete with food agriculture.

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

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## **Studying Nuclear Astrophysics with Inertial Fusion Implosions**

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Throughout the universe, nuclear reactions play a critical role in the dynamics of stars and the formation of the elements. They are responsible for the production of all elements other than hydrogen, through processes including big-bang nucleosynthesis, stellar nucleosynthesis, and production of heavy elements in explosive scenarios such as supernovae and neutron-star mergers. Fusion reactions are the primary energy source of the stars, determining their physical properties and lifetime. In the universe these processes occur in a plasma environment that is fundamentally different from accelerators, where nuclear physics is typically studied. Laser-fusion facilities in the United States, notably the National Ignition Facility and Omega, can generate plasmas at extreme conditions, with temperatures up to hundreds of millions of degrees, densities many times higher than lead, and pressures exceeding 100 billion atmospheres. These plasma conditions are comparable to many astrophysical systems, including the universe a few minutes after the big bang and the core of our sun, and can include neutron fluxes comparable to supernovae and neutron-star mergers, unlike any other laboratory source. This project will use these plasmas to study several aspects of nucleosynthesis in the laboratory, including the production of elements in stars, during the big bang, and in supernovae or neutron star mergers, and do so in conditions directly analogous to astrophysics. These data will fundamentally improve our understanding of how the elements were produced.

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