Ensuring Bunch Stability in Multi-MW Beams

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Successful delivery of intensity frontier science at Fermilab requires Mega-Watt (MW) class particle beams. For these beams to be delivered reliably and with minimal losses, it is essential that the particle bunches remain stable. The transverse mode coupling instability (TMCI) is known to be one of the main intensity limitations for bunch stability in circular machines. For many years, space charge (the repulsive forces between particles inside a bunch) was thought to have a stabilizing effect on TMCI raising the instability threshold to higher intensities. However, recent advances in the theoretical understanding of beam stability in the presence of strong space charge, has suggested a new class of instabilities known as convective instabilities. It is paramount that these instabilities are understood to ensure bunch stability in multi-MW beams. To tackle this problem, the research will involve an experimental program making use of Fermilab's existing accelerator complex, along with a set of complementary simulations. The research will characterize these instabilities in the presence of varying space charge and wake amplitudes. Usually, the wake amplitudes which drive instabilities are machine dependent and are determined by the impedance of the components installed within the machine. A novel approach to control instabilities will be to install a `waker' system, a dedicated wake-building feedback system. Once the instabilities are excited, they will be observed and measured using an intra-bunch motion monitor (IBM). The IBM will be able to resolve the transverse motion within the bunch and measure the growth rates and amplification factors of instabilities.

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

Discovery Science with New Multi-modal Pixel-based Noble Element Time Projection Chambers

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High Energy Physics (HEP) has long been a tool-driven field with discoveries enabled by breakthroughs in instrumentation. Large scale noble element time projection chambers (TPCs) play a central role in many HEP experiments and offer an opportunity to perform discovery level measurements through the enhancement of their capabilities. Detectors using noble elements, such as liquid and gaseous argon and xenon, have risen to become a prime technology used to: i) pursue the physics associated with neutrino mass, ii) search for new physics of dark matter, and iii) explore the unknown in searches for new particles and interactions. In a noble element TPC, particles interact with the medium and deposit their energy into three main channels: heat, charge, and light. Depending on the physics of interest, noble element detectors attempt to exploit one or more of these signal components. The objective of this research is to transform the physics reach of these instruments and develop new detection strategies to expand their capabilities to previously inaccessible regimes. To realize this challenge requires unambiguous 3D readout of the charge, maximum sensitivity to the full spectrum of light produced, and ideally having these capabilities integrated into a single sensor. This research undertakes this endeavor to realize such a detector through the exploration of low power pixel-based charge readout and research into novel light detection techniques utilizing various new materials. The penultimate outcome of this work is the integration of these two lines of research into an integrated readout device capable of detecting both the light and charge produced in noble element TPCs. If realized the outcome of this research, to quote Galileo, will be to ''measure what is measurable, and make measurable what is not so'' with the full capabilities of noble element TPCs.

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

Gold Catalyzed Polymerization Reactions of Unsaturated Substrates: Towards New Functional, Recyclable, and Upcycled Aromatic Polymers

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Aromatic polymers constitute a ubiquitous class of commodity and specialty "plastics" given that aromatic and pseudo-aromatic rings in the polymer backbone impart robust mechanical, chemical, and thermal properties. There remains a pressing need to create new technologies that cannot be accommodated within the scope of traditional polymerization reactions, that revolutionize the lifecycle of plastics, utilize unusable industrial and consumer waste, and which reduce environmental impacts. This proposal describes a research program with the goal of developing new patterns of catalytic reactivity and methods for the synthesis of aromatic polymers using Homogeneous Gold (Au) Catalysis (HGC). Synthetic strategies will be developed to polymerize monomers based on unsaturated precursors and access novel polymeric materials through the extension of Au catalyzed intermolecular processes. Specific objectives of this research include: (1) to extend Au catalyzed intermolecular reactions to bifunctional monomers; (2) to gain fundamental mechanistic insight into Au-catalyzed polymerizations; (3) to apply these reactions to the synthesis of new classes of aromatic polymers that can be readily and/or selectively deconstructed; and (4) to apply these chemistries to the upcycling of post-industrial plastics and post-consumer waste. These results will provide many of the first examples of HGC in the field of polymer science and provide the foundational knowledge needed to design new chemical reactions, catalysts, processes, and materials. In turn, this will enable efficient chemical syntheses from commercial feedstocks which are currently unusable, new depolymerization approaches for circular processing, and chemical upcycling strategies.

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

Transport of Complex Mixtures in Ion-Containing Polymer Membranes

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This research aims to improve the understanding of multi-solute transport behavior within ion-containing polymer membranes. Permselective ion-containing membranes are integral to many energy applications from water treatment, fuel cells, and solar fuels devices where the selective transport of molecules and ions is desired. In solar fuels devices, for example, ion-containing polymer membranes are responsible for permitting selective transport of ions between electrodes to maintain overall charge neutrality, yet limit transport of reaction products produced at the electrodes. While the transport of single solutes through such membranes has been well described, binary and multicomponent transport is poorly understood due to the myriad of interactions that occur in these systems (i.e. between co-permeants and between permeants and the membrane). This is just one of many cases where understanding the transport of multiple simultaneous species is critically important to limiting product crossover that reduces performance.

This experimental project includes the synthesis of ion exchange membranes with varied incorporation of comonomers (ionic and neutral moieties) in order to investigate fundamental relationships between membrane structure, membrane physiochemical properties, and transport behavior of solutes and complex solute mixtures through dense, hydrated membranes. The project leverages an in situ spectroscopic methodology to perform multi-component diffusion cell experiments with high fidelity which greatly reduces the experimental burden and complexity compared to traditional multicomponent experiments. The impact of the physicochemical properties of the synthesized polymer membranes on the multicomponent, emergent transport properties are evaluated. This investigation elucidates key structure-property relationships and hence advances the development of robust membranes with desired transport behavior. A key research focus is on the interplay of membrane chemistry and complex mixture chemistry on emergent transport behavior. Experimental tasks in this project are expected to result in (1) fabrication of a diverse set of ion exchange membranes with a variety of chemical composition, water uptake, and ionic conductivity, (2) experimental characterization of the transport behavior of solutes and their complex mixtures, and (3) new understanding of the relationships between membrane chemistry and transport behavior of solutes and their complex mixtures. This has the potential to impact the future design of ion containing polymer membranes for a range of applications including energy devices, water purification, and the separation of other complex mixtures.

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

Manipulating Interfacial Reactivity with Atomically Layered Heterostructures

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Tailoring chemical reactions at electrified solid–liquid interfaces requires surfaces that are both well-defined and highly tunable. The key basic science challenge entails control over the density and structure of participating electronic states in the solid, as well as the alignment of this electronic band with molecular energies of reactant species. Unlike traditional bulk materials in which the chemically active surface represents only some fraction of the total material, individual layers of atomically thin, so-called "two-dimensional" materials are essentially all surface. As a result, their physical properties are exceptionally tunable by marginal structural and electrostatic perturbations. Drawing on emerging insights for manipulating the physics of these quantum materials, this research aims to develop the fundamental knowledge and materials required to control the interfacial chemistry of electrochemical reactions at a molecular level. The advances that emerge from this program will establish a new design framework for the interconversion of electrical energy and chemical energy. These principles hold promise for next-generation energy technologies, particularly the electrically-driven transformation of abundant, low energy materials into important high energy chemicals and fuels.

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

A Neutral-atom Quantum Simulator for Nuclear Physics

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Quantum devices are poised to have a transformational impact on nuclear physics because they present an opportunity to solve significant problems that are intractable for classical computers. Such problems lie at the heart of nuclear physics: to fundamentally understand how properties of nucleons and nuclei emerge from the underlying theory of quantum chromodynamics (QCD). While general purpose quantum computers have demonstrated rapid progress in recent years, they are still many years away from addressing these challenges. To accelerate the impact of quantum information science on nuclear physics, this research will develop a quantum simulator that is tailored to address specific challenges in this field. In contrast to a quantum computer, which maps each problem to a set of standard operations on quantum bits, a quantum simulator manipulates an experimental apparatus to behave like the system under investigation. Quantum simulators can be extremely powerful tools for discovery when they efficiently reproduce key characteristics from the system of interest. This research will leverage neutral ytterbium atoms trapped in reconfigurable optical tweezer arrays to simulate quark-level effective theories for QCD. This experimental platform offers resource-efficient simulations of a simplified but rich theoretical framework, which will enable more rapid progress toward simulations of poorly understood phenomena in nuclear physics and inform future simulations of more complex theories as quantum devices improve.

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

Structural and Mechanistic Studies of O_2-dependent and O_2-independent Enzymes in Chlorophyll Biosynthesis

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With a growing population to sustain and increasing demands for food and energy, it is vital that we determine ways to accommodate an increasing infrastructure without sacrificing our environment. The ability of photosynthetic organisms to efficiently extract energy from sunlight and transform CO_2 into sugars and/or evolve hydrogen shows promise for both enhancing our food supply and decreasing our reliance on non-renewable fossil fuels. However, several limitations exist towards realizing the potential of photosynthetic organisms in these applications or emulating them in man-made technologies. Namely, there is a large fundamental knowledge gap regarding how photosynthetic organisms naturally survive in habitats that receive different amounts of light and O_2, both of which profoundly affect their growth and survival. Therefore, this research will detail fundamental biochemical mechanisms that photosynthetic organisms use to produce the essential photosynthetic pigments, chlorophyll and bacteriochlorophyll, under variable amounts of light and O_2. Towards these goals, the research will (i) resolve clear mechanistic deficits about how photosynthetic pigments are built and tailored in the presence and absence of O_2, (ii) describe how pigment biosynthetic enzymes coordinate with one another to maintain pigment production, and (iii) investigate evolutionary changes that have occurred in photosynthetic pigment-producing enzymes in response to changing environmental conditions.

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

Theory-informed Artificial Intelligence for Accelerating Materials Characterization

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Improvements in the capability to capture, convert, and store energy hinge heavily on the understanding and control of existing materials to inform the design of new ones. Such understanding depends on precise knowledge of the atomic and electronic structures of materials during synthesis and operation. At DOE Scientific User Facilities, multi-modal x-ray, electron, laser, and scanning probes, as well as computational modeling tools, have now become indispensable in providing complementary atomic-scale information. However, determining where the atoms are from scattering, microscopy, spectroscopy, or computational modeling data remains a substantial challenge. The goal of this project is to use a theory-informed artificial intelligence and machine learning (AI/ML) framework to allow researchers to determine atomic positions in real-time from experimental characterization data, via a user-friendly toolkit titled FANTASTX (Fully Automated Nanoscale To Atomistic Structure from Theory and eXperiment). Implementing the FANTASTX framework involves developing and connecting approaches for the simulation of x-ray, electron, laser, and scanning probe data; adopting and applying pattern recognition and computer vision algorithms for the matching of spectra and images; and constructing and training ML models for the relationship between spectroscopic data and the local atomic environment. FANTASTX incorporates physics into AI/ML by using theory to provide physical constraints towards the sampling of the infinitely large space of atomic arrangements. FANTASTX will allow the real-time determination of atomic-scale structural information during experimentation, which will in turn enable and accelerate nanoscale materials understanding and design.

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

Modeling the Nucleosynthetic Imprint of Stellar Merger Phenomena

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It is now accepted that the majority of stars - especially massive stars - in the Milky Way galaxy are in binary systems. The evolution of such systems is much more complex than the evolution of single stars due to the interactions occurring between the stars in the binary that is capable of altering their overall properties (such as their size, composition and rotation rate). In extreme cases, many of these systems will be unstable and will in-spiral and dynamically merge. These stellar mergers are associated by a burst of electromagnetic radiation - a "mergeburst" - accompanied by the ejection of some material while leaving behind a post-merger remnant star with potentially unusual chemical composition, high rotation and, in some cases, enhanced magnetism. This - likely more massive - remnant will eventually end its life as a supernova explosion within a complex circumstellar environment produced by the past merger, leading to an interaction between the supernova ejecta and the circumstellar material and, potentially, to a very luminous transient. In tandem, the merger-induced nuclear burning that will occur may significantly affect the surface chemical properties of these stars as compared to stars that did not suffer a merger. This first-ever complete numerical simulation campaign spans all the phases associated with stellar merger phenomena: the pre-merger evolution of the binary, the dynamical binary merger and mergeburst transient and the short and long-term nuclear processes in the merger and the remnant star via the use of large supercomputers. The resulting simulations will elucidate observations taken with some of the most powerful telescopes and will enable a more complete understanding of an important class of astrophysical transient events as well as the nuclear astrophysics associated with them.

This research was selected for funding by the Office of Nuclear Physics and the DOE Established Program to Stimulate Competitive Research.

Expanding Capabilities to Unlock the Mysteries of Complex Warm Dense Matter

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Understanding the properties of Warm Dense Matter—the elusive state of matter between hot solids and strongly correlated cold plasmas—is one of the grand challenges of High Energy Density science. Extreme densities and temperatures induce dramatic changes in the physical and chemical properties of materials in this regime, including structural and electronic phase transformations and the emergence of new states of matter. The advances in ultra-fast laser-driven compression techniques and the development of dynamic compression platforms at x-ray user facilities worldwide (X-ray Free Electron Lasers and synchrotron sources) is a revolution that now enables a new class of experiments to investigate the physics of matter at extreme conditions with unprecedented precision. This research will focus on unraveling the mixing properties of complex compounds with an emphasis on understanding the behavior of planetary constituent materials. This project will expand the current experimental capabilities pulling together ultra-fast X-Ray Diffraction and Extended X-ray Absorption Fine Structure combined with optical diagnostics to unravel the complex transformations happening at extreme conditions of pressure, temperature and timescale. This project will also investigate the atomistic pathways to structural phase transitions, elucidating kinetic and metastability effects arising at ultra-fast compression. This research will present opportunities for discoveries with transformational impact on a range of fields from High Energy Density to planetary science.

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

Atomic View of Molecular Photocatalysis using X-Ray Lasers

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Molecular photocatalysts have the potential to deliver an alternative sustainable method to produce fuels or other value-added chemicals using solar energy. Identifying the molecular properties that influence their reactivity is a critical first step to creating new and efficient photocatalysts. This research program aims to pinpoint and control the electronic excited state reaction pathways of transition metal complex photocatalysts. Nickel-based hydrogen-evolving catalysts with 'non-innocent' ligands, known to actively participate in the electron and proton transfer reactions of the catalyst, will serve as platforms to identify how catalyst charge distribution influences the excited state character and reaction mechanism. Achieving the ultimate goal of controlling photocatalytic reactivity first requires the ability to identify and manipulate the excited state charge distribution, relaxation mechanism, and geometry of the reaction site, which may involve metal or ligand atoms. These requirements inform the technical approach of this research, which exploits the atomic specificity and ultrafast time-resolution of X-ray spectroscopy at the Linac Coherent Light Source (LCLS) X-ray free electron laser. Ultrafast X-ray spectroscopy probing metal and ligand atomic sites will be used to map the excited state charge distributions, determine the transient catalyst structures, and differentiate the mechanistic roles of metal vs. ligand reactive sites. Through these experiments, this research will establish 1) how catalyst excited states initiate electron and proton transfer reactions, 2) the specific role of metal vs. ligand atom reactive sites, and 3) how to use ligand composition to influence critical excited state properties and reactivity. This novel approach using ultrafast X-ray methods to identify excited state reaction pathways and inform catalyst design will lead to new classes of molecular photocatalysts that efficiently convert solar energy to high value chemicals.

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

Probing lanmodulin's Mechanisms of Rare-Earth Selectivity for Protein-Based Bioseparations

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This project addresses the challenge of separating rare earth elements (REEs) from one another and from other ions, using Nature's solutions to this problem as guides. REEs are ubiquitous components of current technologies from permanent magnets and lasers to medical imaging agents. Separations of REEs from more abundant metals and from each other in mining and recycling applications is currently a laborious, energy- and resource-intensive process using relatively low-selectivity ligands. Increasing efficiency of these separations has the potential to lower costs, decrease waste, and allow usage of feedstocks with lower REE concentrations.

The recent discovery and characterization of lanmodulin (LanM), a highly selective REE-binding protein, forms the basis of this research. LanM has an intriguing framework in which to understand the fundamentals of the biological coordination chemistry of lanthanide ions; preliminary data also indicate that it is a protein with remarkable stability properties that enable it to quantitatively extract total REEs from industrially relevant feedstocks even under harsh experimental conditions. Although LanM displays exceedingly high selectivity for REEs versus non-REEs, its selectivity within the REEs is rather low. The present research program will utilize a multidisciplinary approach to develop LanM variants with higher intra-REE selectivities for REE separations. Whereas small molecules, materials, and whole cells have been explored for separations, effective macromolecular approaches are conspicuously absent. The promising performance, stability, affinity, and selectivity of LanM suggest that this protein and its derivatives may serve as guides for new and efficient approaches to REE separations.

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

Coupled Effects of Stress and Hydrogen on Stress Corrosion Cracking of Fe-based Alloys

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Hydrogen is the most abundant and the simplest element in the Universe. Yet, it exhibits complex behaviors because of its ability to donate all of its electrons or to double their number, depending on the environment. The rich variety of H-induced processes is responsible for catastrophic failures of structural materials through hydrogen-assisted cracking, even in high-strength steels. When steel is subjected simultaneously to an applied tensile stress and a corrosive, high-temperature aqueous medium, interplay of hydrogen and oxygen interactions with the alloy microstructure are thought to lead to intergranular stress corrosion cracking (SCC). Due to the low atomic mass and fast diffusivity of hydrogen in metals, the hydrogen concentration and distribution, as well as its effect on local oxidation and stress-induced deformation, are extremely challenging to analyze in a quantitative, spatially resolved manner at the atomic scale. The overarching goal of this research is to develop a predictive mechanistic understanding of how hydrogen, coupled with applied stress and intergranular oxidation, drives propagation of SCC in Fe-based alloys. This project will use a broad range of tools available at Pacific Northwest National Laboratory and U.S. Department of Energy synchrotron facilities. A combination of cryogenic-transfer atom probe tomography, in situ electron microscopy, synchrotron X-ray methods, and atomistic to continuum simulations will be used to obtain mechanistic insight into how individual diffusion and oxidation events underpin mesoscale SCC behavior. This work will provide the scientific basis for tailoring the microstructure of metallic alloys used in nuclear and automotive applications to control the impact of coupled extreme environments of corrosion, stress, and temperature.

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

Real-Time Artificial Intelligence for Particle Reconstruction and Higgs Physics

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With the discovery of the Higgs boson at the Large Hadron Collider (LHC), the world's highest-energy particle accelerator complex, at the European Organization for Nuclear Research (CERN) in Switzerland, scientists have acquired an important tool to study the fundamental building blocks of the universe. Precision measurements of Higgs bosons produced with large momentum allow for unique insights into the structure of the interactions of the Higgs boson with other particles that may shed light on physics beyond the Standard Model. While experimentally challenging, exploring such interactions with novel artificial intelligence (AI) methods can advance our understanding of the Higgs sector, including the Higgs boson's self-interaction. Moreover, today the LHC is undergoing a major upgrade to further increase its particle collision rate and thereby operate for an additional decade. The experimental detectors at the upgraded facility must process at least a factor of ten more data at rates of hundreds of terabytes per second all under challenging conditions. New AI techniques are required to reconstruct and select, or trigger on, the most physics-sensitive events in real-time to handle the resulting avalanche of data. The proposed research will achieve the goals of the LHC program at the Compact Muon Solenoid (CMS) experiment by developing a sub-microsecond event reconstruction system using real-time AI algorithms that employ field-programmable gate array technologies. By harnessing sophisticated AI techniques, this research focuses on measuring the production of Higgs bosons at large momentum while enhancing particle reconstruction methods in the trigger. Overall, the proposed research has broader implications for the use of AI in resource-constrained, low-latency embedded applications across all fields of science.

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

A Rapid Membrane-based Approach for Medical Isotope Purification

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Radiopharmaceuticals are widely used in diagnostic medical imaging and have great potential in other medical applications such as localized radiotherapy and theranostics (simultaneous therapy and diagnostic imaging); however, wide-spread use of these nontraditional radiotherapies has been restricted by their availability. The *overall goal* of the proposed research is to increase the availability of medical isotopes for fundamental research and clinical trials which requires *transformative* change from current production and purification methods. Resin-based chromatography is the current state of the art purification scheme and is known to suffer from diffusion limitations resulting in long-purification times and large column volumes to achieve sufficient product recovery. Current resins are prepared by physisorbing extractive ligands into a polyacrylic ester resin. Ligands can leach from these unstable resins overtime and contaminate the final product. Membrane chromatography is a promising alternative to resin-based chromatography because it is not diffusion limited and membranes are synthesized with covalently bound polymeric ligands. Practically, membranes are a chemically stable alternative to resins in which product recovery is not a function of flowrate. In this work, we propose the fundamental studies necessary to understand how to design membrane adsorber architecture and surface chemistry in order to (1) reduce radioisotope purification time from hours to seconds; (2) minimize elution volumes; and (3) provide a chemically pure product. Ultimately, the fundamental knowledge generated as a result of this proposal will lay the foundation for new radiochromatography processes that will increase the US supply of medical isotopes.

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

Infective Viruses and Inert Virions: Illuminating Abundant Unknowns in Terrestrial Biogeochemical Cycles

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Soil viruses have been recognized as highly abundant but virtually unknown members of the soil microbiome. By infecting soil microbes, viruses likely have substantial, as-yet unknown impacts on terrestrial biogeochemical processes under their hosts' control. Viral particles (virions) may also play more direct roles in soil biogeochemical cycling as packets of carbon, nitrogen, and phosphorous, but the time scales and environmental conditions that determine virion infectivity, transport, and/or sorption to soil particles are unknown. This project will use a combination of laboratory and computational approaches to distinguish between infective and degraded virions and assess their respective contributions to soil biogeochemical cycling. Using a multi-omics approach, this research will establish spatiotemporal patterns in soil viral community composition and virus-host dynamics in forests, chaparrals, grasslands, and wetlands. In order to identify feedbacks between soil viruses and carbon dynamics in additional, changing environments, planned research includes field experiments after a high-temperature prescribed forest fire as well as in a boreal forest ecosystem, leveraging the US Department of Energy's Spruce and Peatland Responses Under Changing Environments (SPRUCE) experiment. By integrating the knowledge gained in the analysis of these different environmental conditions over time, this project will expand our understanding of the global soil virosphere and its influence on global biogeochemical cycles.

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

Probing Ultrafast XUV/X-ray Induced Electron Correlation in the Molecular Frame

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Electron-electron correlation is ubiquitous in many natural and artificial processes. The consequent energy and angular momentum exchanges among multiple electrons initiate chemical processes and play a determining role in photochemical reactions. Being an essential interaction mechanism in many-body systems, electron correlation determines much of the structure and dynamics of molecules and composes one of the main themes in quantum chemistry. This group behavior of multiple electrons, critical to macroscopic material properties as well, occurs at the microscopic level within an extremely short period of time – attoseconds (1 attosecond = 10^{-18} second). With recent advances in attosecond laser technologies, the dynamics of electron correlation can now be probed directly in the time-domain, unveiling how the multielectron interaction evolves and can be possibly controlled. This project investigates the dynamics of electron correlation in molecules in their natural coordinates – the molecular frame. It also investigates the correlation between the multielectron interaction and the subsequent ion dynamics and the influence of molecular intrinsic properties and laser parameters on electron correlation. Extreme ultraviolet (XUV)/x-ray attosecond pulses and techniques of transient molecular alignment and electron-ion coincidence measurement will be applied to induce electron correlation and to time-resolve the dynamics with complete kinematic information. Data gathered in these studies will unambiguously reveal the dependence on the electronic structure of molecules, on the angle of the molecular axis with respect to the polarization of the external electromagnetic field, and on externally controllable laser parameters. This research will provide the fundamental basis for structural, geometrical, and photo-control of multielectron interactions.

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

Precipitate Stability and Helium Trapping in Advanced Steels

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It is estimated that over 10,000 tons of steel will be used in the construction of a civilian fusion energy device. The continued safe operation and utility of a fusion energy device will, in part, rely on the structural integrity of the steel-manufactured components used within its design. These components could see unique operating conditions, including a damaging flux of neutrons that alter the structure and chemistry of the steel components. The neutron flux creates both atomic displacements and helium via a transmutation reaction in the steels. The aim of this research is to understand how various regimes of the neutron flux will impact the response of advanced steels with innovative nanometric particle (e.g. precipitate) additions within its matrix. Specifically, the influence of the precipitate-matrix stability under a damaging energetic particle flux on the helium migration, coalescence, and trapping will be evaluated. The approach will use dual beam ion irradiations to experimentally simulate the various neutron damage and transmutation conditions in a model advanced steel developed using computational thermodynamics and printed using additive manufacturing. Post irradiation, the changes in structure and chemistry will be assessed using an extensive characterization campaign using electron-microscopy based techniques. The experimental efforts will be coupled with advanced computer analysis algorithms and theoretical models to elucidate the underlying mechanisms that control precipitate stability and helium trapping in advanced steels. The work will provide the additional fundamental insights needed to optimize the design and manufacturing of advanced steels for fusion energy systems.

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

Precision Neutrino Fluxes for LBNF/DUNE

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The Long-Baseline Neutrino Facility (LBNF) will include the world's most intense neutrino beam, creating hundreds of billions of neutrinos per second and sending them through the earth to the Deep Underground Neutrino Experiment (DUNE) in South Dakota. The neutrino beam will be created by colliding a high-energy beam of protons with a solid carbon target, creating many charged particles. These particles will be focused using large magnets known as focusing horns before they decay to neutrinos. The number of neutrinos in the LBNF neutrino beam is not precisely understood, primarily because of the complex nuclear physics that governs the creation of charged particles in the target. The goal of this research program is to provide an extremely precise measurement of the number of neutrinos in the LBNF neutrino beam. This will be done using two experiments designed to measure charged particles created when generating neutrino beams: the NA61/SHINE experiment at CERN and the EMPHATIC experiment at Fermilab. NA61/SHINE will make measurements of charged particles created in the target using replicas of the LBNF target. EMPHATIC will be used in combination with a replica setup of a neutrino beam target and focusing horn for the first precise measurement of particles exiting a neutrino beam focusing horn. Combined, these measurements will provide an unprecedented picture of accelerator-based neutrino beams and expand the possibilities for new physics discoveries at DUNE.

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

Probing Short-Range Structure and Magnetism in Next-Generation Energy Conversion Materials

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Next-generation materials will play a crucial role in transformative technologies that can address critical societal issues, such as the need to harness, store, and convert energy in a sustainable way. Many candidate materials for technological application derive their exceptional properties from the complex interplay between their atomic and magnetic structures on short, nanometer length scales. However, probing structural features on such a short length scale has historically been a difficult undertaking because conventional methods lack the required sensitivity. This project overcomes that challenge by using advanced neutron scattering methods and other complementary techniques to study three classes of materials with significant technological potential: (1) Magnetic thermoelectrics, in which magnetic properties can enhance the ability to convert thermal gradients into electrical energy via the thermoelectric effect; (2) magnetocalorics, which enable magnetic control of thermal energy; and (3) multiferroics, characterized by the ability to control electrical properties by magnetic means and vice versa. Experiments will be done at Department of Energy user facilities to reveal the connection between the observed properties and the short-range atomic and magnetic correlations in these materials, with the aim of transforming our understanding of the origin of the functional properties and guiding future materials discovery and optimization efforts. As a natural byproduct, the research will also aid in the development of cutting-edge neutron scattering techniques. The project features prominent involvement of undergraduate and graduate students, who will go on to fill important needs in the national STEM workforce.

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

Laser Spectroscopy of Exotic Atoms and Molecules Containing Octupole-Deformed Nuclei

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Atomic nuclei with certain numbers of protons and neutrons can exhibit large variations in their nuclear density distributions. The region of actinide nuclei – those having more than 88 protons (Z > 88) - is especially interesting, as it is expected to exhibit unique pear-like nuclear shapes (octupole deformation). This exotic deformation causes a large enhancement of their symmetry-violating nuclear properties. Measurements of these nuclear properties can provide answers to some of the most pressing questions of modern physics, such as the origin of the matter-antimatter asymmetry of our universe, and the properties of dark matter. Hence, these nuclei offer distinct laboratories to investigate the emergence of nuclear phenomena, to study the fundamental symmetries of nature, and to search for new physics beyond the Standard Model of particle physics. Despite their importance, our experimental knowledge of these nuclei is severely lacking. These exotic forms of matter belong to a frontier of the nuclear chart that has been particularly challenging to produce and to study with necessary detail. This proposal aims to perform precision laser spectroscopy measurements of atoms and molecules containing short-lived exotic actinide nuclei, which will be uniquely produced at the new Facility for Rare Isotope Beams (FRIB) in the US. Precision measurements of atoms containing exotic actinide nuclei will provide their nuclear electromagnetic properties. These properties are critical to understand the microscopic and collective structure of octupole deformed nuclei, and will establish important benchmarks for the development of theoretical models. A complementary part of this project will be focused on the study of molecules containing exotic isotopes of Th (Z=90) and Pa (Z=91). These molecules are of particular interest for the study of fundamental symmetries, as their octupole-deformed nuclei produce an enhancement of more than three orders of magnitude for their parity- and time-reversal violating properties. This nuclear enhancement is further amplified by the exceptionally high sensitivity of molecular systems to these effects, providing ideal laboratories to explore the violation of fundamental symmetries.

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

Experimental Study of Turbulent Impurity Transport in 3D Magnetic Fields

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Detailed understanding and control of impurity transport is essential for the success of magnetic
fusion as an energy source. Impurities dilute the D-T fuel and degrade the energy confinement of high temperature plasmas via intense line radiation, such that the accumulation of these charged particles needs to be avoided. The impurity transport can be described by neoclassical and turbulent contributions. While turbulent transport is mainly diffusive, neoclassical transport
has a strong convective term. In particular, for stellarators, this is challenging as neoclassical transport in these 3D devices is typically inwards directed. Therefore, a certain level of diffusive transport from turbulence might be required for stable plasma operation. However, it is not clear whether the required level of turbulence would overly degrade the energy confinement via enhanced heat transport.

This project will investigate turbulent impurity transport on the Helically Symmetric eXperiment (HSX) in Madison, WI and at the Wendelstein 7-X (W7-X) stellarator in Greifswald, Germany. The two experiments feature different 3D magnetic field topologies and allow transport studies from different perspectives. Existing laser ablation systems on both experiments will be equipped with optimized and calibrated glass targets that will allow active impurity injections with a well-controlled amount of particles. Moreover, a high-speed charge exchange recombination spectroscopy system will be installed to monitor characteristic line radiation emitted by the injected impurities. The spectroscopy measurements will provide absolutely calibrated impurity densities with excellent spatial resolution and will resolve the inwards movement of impurities toward the plasma core following the injections. Combined with further improvements of the analysis and modelling tools, details on the diffusive and convective impurity transport can thus be obtained. Resulting transport profiles will then be compared with neoclassical expectations. Moreover, trends of the remaining turbulence-induced (anomalous) transport will be compared with results from linear and non-linear gyrokinetic simulations. In addition, the observed levels of impurity transport will be compared with experimental heat diffusivities. This will permit the identification of conditions with good energy confinement and a well controllable impurity behavior.

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

Exotic Uses of Neutrons an X-rays as Probes for Chiral Magnets

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Computational architectures based on magnetism, termed spintronics, offer opportunities for low-power, miniaturized, highly-portable technologies. For most magnetic materials, the spins align parallel or antiparallel, but an alternative paradigm exists in-which the spins form twisted, chiral structures, e.g. helices, cycloids, and skyrmions. Magnetic skyrmions have a particularly exotic structure characterized by the spins continuously wrapping into a closed loop. The distinction between linear and chiral magnets can be appreciated by considering wind flowing in a continuous, linear path compared to vortex flow, like a tornado or hurricane. Chiral magnetic structures are also of interest due to their unique fundamental qualities which arise out of their non-trivial topology. Topology, in this context, means that chiral structures can be continuously distorted, but an energy barrier exists to their creation or destruction which lends stability and particle-like properties to the structure. Neutron and X-ray scattering play a critical role in the investigation of these structures due to their ability to resolve small features with only magnetic contrast. By leveraging recent advances in neutron and X-ray instrumentation, and applying creative experimental and sample environment design, it is possible to gain unparalleled insight into chiral magnets. In one research focus, measuring the small angle scattering from chiral magnets allows the three-dimensional structure to be determined; since the topology is defined by the geometry, it is critical to have a detailed understanding of the structure. In another research direction, time-resolved scattering can be used to capture the evolution of these structures in response to changing magnetic fields. In a third focus area, inelastic scattering can be used to measure the in-situ motion and structure of the chiral spin textures as they are dynamically excited. Understanding derived from this research will improve the ability to manipulate and control these unique structures for low-power spintronic technologies.

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

Thermodynamics and Transport Models of Strongly Coupled Dusty Plasmas

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Complex dusty plasmas are multi-species systems that consist of electrons, ions, neutral species, and charged micro/nanometer-sized grains interacting with each other predominantly through electrical forces. When the number of electric charges on each dust grain reaches ~10^2-10^4 electron charges, the electrostatic potential energy of the grains is either comparable or much higher than their kinetic energy. In this case the dust grains become strongly coupled due to strong electrostatic forces between them. Standard kinetic theories, used to describe dilute gases or weakly coupled dusty plasmas, are no longer valid to describe strongly coupled dusty plasmas because they ignore the interaction potential energy of the constituent grains. This theoretical investigation will quantify the effect of grain-grain, grain-plasma and grain-neutral gas interactions on the thermodynamic and transport properties of the grain phase. The central hypothesis to this effort is that the grain positions and velocity time series measured in dusty plasma experiments contain the information needed to calculate the evolution of the grain position and velocity distribution functions over time, without tedious numerical methods. Using methods of statistical mechanics, grain trajectories from a combination of experiments and computer simulations will be used to construct accurate equilibrium (thermodynamic equations of state) and non-equilibrium (transport coefficients) models of strongly coupled dusty plasmas. The basic aspects of correlated grain motion of relevance to strongly coupled plasmas and dense granular systems will be quantified as thermodynamic and transport models to fortify the prediction capabilities of hydrodynamic/fluid simulation approaches in order to accurately describe dust grain dynamics: (1) near the walls of thermonuclear fusion reactors where material ablation leads to the formation of highly charged nano or microparticles, (2) in planet and asteroid formation processes via accretion of charged grains and particles, and (3) of intentional or unintentional gas-to-particle conversion in plasma-based semiconductor manufacturing processes or plasma-based nanomaterial synthetic routes.

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

Optical Control of Spin-polarization in Quantum Materials

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The goal of this project is to enable the development of robust solid-state qubits as building blocks for applications in quantum sensing, quantum communication, and quantum computing. A central challenge encountered in the design of quantum materials is the identification and characterization of stable point defects with robust spin properties that dictate the light-activated quantum functionality. This limits ground-breaking discoveries with the potential to transform computing technologies or generate a new class of nanoscale sensors with enhanced sensitivity. One obstacle that needs to be overcome is a lack of control over the local environment of the defect, in addition to understanding how this influences the optical cycle of spin-polarization, and ultimately the quantum operativity. This project will develop the numerical tools needed to understand how to obtain defects with desired functionalities by controlling their local environments and will unravel the influence of external conditions. New computational capabilities will be developed in order to model light-activated mechanisms in spin-defects, and to systematically investigate the role of temperature, local structure, and quantum confinement. This research will leverage current pre-exascale modeling capabilities based on many-body perturbation theory and use a hierarchical modeling approach that harnesses artificial intelligence and quantum computing. The program will deliberately utilize Argonne's expertise and world-class user facilities, providing insight into optical control of the spin-polarization of color centers.

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

Probing the Flavor Dependence of Higgs Couplings with Charm Tagging

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The discovery of the Higgs boson in 2012 at the Large Hadron Collider (LHC), the world's most energetic particle accelerator complex, at the European Organization for Nuclear Research (CERN) in Switzerland, was the final piece to complete the Standard Model (SM) of particle physics, which describes all known elementary particles in the universe and their interactions. Despite the rapid progress made in recent years to understand the characteristic properties of the Higgs boson, many questions still remain. In particular, the direct interaction between the Higgs boson and the quarks was first measured only two years ago at the LHC by observing the Higgs produced in association with top quarks. The strength of the interactions or couplings between the Higgs boson and the quarks varies between the generations, and currently only faint experimental prospects exist to probe Higgs couplings to quarks outside of the third generation top and bottom quarks. This research program plans to develop an innovative computational algorithm to identify jets of particles containing second generation charm quarks at the ATLAS (A Toroidal LHC ApparatuS) experiment to measure SM physics processes containing charm and the Higgs coupling to charm using data acquired from the current LHC and the future High-Luminosity LHC runs. The charm-driven program promises to advance our knowledge of the strange quark content of the proton, which, in turn, will impact other precision analyses at the LHC such as the W boson mass measurement. An analysis strategy exploiting the discriminating power of the charm-tagging algorithm is expected to result in the combination of the full suite of Higgs-charm analyses reaching the SM sensitivity by the end of the High-Luminosity LHC era. The research can be expected to shed new light on the SM flavor puzzle by ascertaining if the Higgs mechanism is responsible for the masses of second generation quarks, and to determine if the Higgs-charm coupling strength is consistent with the predictions from the Standard Model.

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

Deformation of Nano-Metallic Glasses Made using Colloidal Synthesis

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Despite decades of intensive research, the deformation mechanisms that govern the mechanical behavior of metallic glasses remain mysterious. This prevents the use of metallic glasses as strong and hard structural materials and coatings. To solve this problem in metallic glasses, it is necessary to understand the influence of their disordered atomistic structure on strength, ductility and fracture, through controlled synthesis and high-resolution characterization. It has been challenging to accomplish this using conventional cast or sputtered metallic glasses because of a lack of control over metallic glass structure. In this work, colloidal synthesis will be used to fabricate metallic glass nanoparticles with tunable atomistic structure and composition, which can be consolidated into bulk nano-glasses. Advanced electron microscopy, X-ray measurements and nano-mechanical testing will be used to evaluate structure and mechanical performance. This project will 1) investigate the high ductility of colloidal metallic glass nanoparticles, 2) evaluate the mechanical behavior of nanoparticles modified using high pressure, and 3) determine the role of the interfaces within bulk nano-glasses. This work is focused on fundamental understanding of deformation mechanisms and is therefore well aligned with the BES mission.

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

Creating a Sea-Level-Enabled E3SM: A Critical Capability for Predicting Coastal Impacts

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Sea level change will be the most fundamental factor driving coastal change along the U.S. – and global – coastline in the coming decades and centuries, with profound disruption and displacement of infrastructure and communities. However, sea level does not change uniformly, due to interactions between the ocean, ice sheets, and solid earth. Regional sea level rise can be significantly larger or smaller (by 50% or more) than the global average, with the U.S. coast disproportionately impacted by these variations. This project fills a critical gap in the application of the Energy Exascale Earth System Model (E3SM) to coastal impacts by creating a regional sea level modeling capability within E3SM. This unique tool will be used to quantify the role of regional sea level in future storm surge along the U.S. coast. These first fully consistent regional sea level projections from an Earth system model will be used to investigate the accuracy of existing methods that rely on adding disparate, non-interacting contributions to sea level. The sea-level-enabled E3SM provides a critical missing link required for making actionable projections of coastal impacts with E3SM. The project provides the Department of Energy with a tool for predicting regional sea level targeted to agency needs.

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

Bidirectional Manipulation of Phase Transitions by Laser Excitation of Optical Phonons

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Dynamical manipulation of quantum materials by a femtosecond laser pulse is an emerging technique relevant to a wide range of applications including high-temperature superconductivity, ultrafast information processing, and quantum computation. Strong-field laser pulses tuned to specific infrared-active lattice vibrational modes can directly modify structural parameters, which are crucial to the physical properties of quantum materials. This research aims at bidirectional switching of ordered phases in quantum materials using laser excitation of optical phonons. The focus will be on laser manipulation to change the phase in either direction. The goal is to steer materials towards desirable states on demand, which will advance the understanding of phase transitions and competing interactions in quantum materials. The main objectives include: (1) Dynamical bidirectional tuning of nematicity in complex oxides and high-temperature superconductors and (2) Ultrafast bidirectional switching of ferroelectric polarization in ferroelectrics. If successful, the ultrafast light source developed in this project can be adapted to femtosecond x-rays or ultrafast electron diffraction, to investigate intertwined orders in quantum materials. It can also be integrated with time-resolved scanning probe microscopies for ultrafast imaging of spatial inhomogeneity in quantum materials, which is the basis of various novel electronic and magnetic properties.

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

Toward a Technology-Inclusive Whole Device Model

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Computational modeling and simulation play a critical role in the development and deployment of any complex engineering system—fusion energy is no exception. The Fusion Energy Sciences (FES) program supports research such as "Whole Device Modeling," which seeks to assemble numerous physics models to create an integrated simulation of the plasma. One of the grand engineering challenges on the path to fusion energy is the successful production and recovery of tritium in a breeding blanket. This work seeks to extend the domain of "Whole Device Modeling" by leveraging high-performance computing capabilities and the Multiphysics Object-Oriented Simulation Environment (MOOSE) to develop fundamentally informed simulation tools for the complex multiphysics environment of the blanket. The focus is on tritium transport in two blanket concepts identified as potentially transformative enabling capabilities for fusion energy: The Dual Coolant Lead Lithium (DCLL) and Cellular Ceramic Breeder. Hierarchical multi-scale modeling of the DCLL and the Cellular Ceramic Breeder will explore the influence of high magnetic fields and material structure on tritium transport. The MOOSE framework will facilitate coupling to other (e.g. neutronic) physics models and plant-scale thermal hydraulic and tritium transport simulation tools. The suite of tools developed will critically inform blanket concept down-selection, component design, and safety evaluations necessary for the realization of fusion energy.

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

Next-Generation Beam Cooling and Control with Optical Stochastic Cooling

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The ability to non-invasively detect the state and dynamics of charged particles and then actively manipulate those particles with feedback systems is a core conceptual and technological element underlying most accelerator-based science. This fundamental area advances through improvements in the granularity and rapidity with which beams can be sensed and manipulated, and one of the next frontiers is the use of each particle's incoherent optical synchrotron radiation (SR) to control its dynamics in a coherent fashion. The central purpose of this program is a multiple order-of-magnitude advance in the state of the art for particle-beam cooling and control. This will be accomplished at Fermilab's Integrable Optics Test Accelerator (IOTA) through the development and demonstration of an operational optical stochastic cooling (OSC) system with >1000x optical-power gain and an additional 60x increase in the density of transverse sensing and feedback. The flexibility and performance of this system will be used in concert with machine-learning techniques, such as online reinforcement learning, to modulate the OSC force and realize a new state of the art in active phase-space control. This program will also explore the development of specialized diffractive optics for OSC, which may open the way to fundamentally new capabilities and opportunities based on OSC physics and technology. Lastly, the results of this research will be applied to the design and optimization of operational architectures for near-term applications in beam cooling, radiation generation and phase-space sensing. Such applications include high-bandwidth cooling of high-energy hadron beams (~0.25 TeV to 6 TeV), electron-ring coolers for medium-energy hadrons, enhanced SR-damping systems for electron storage rings, platforms for quantum-science experiments using one or more relativistic electrons, and the development of novel beam-imaging diagnostics and advanced phase-space-control systems.

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

Realization of Full Neutron Polarization Control:
Next Generation Spherical Neutron Polarimetry for Neutron Scattering

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Quantum materials play a significant role in today's science and have the potential to revolutionize energy-related technologies and other fields. In particular, understanding magnetism lies at the forefront of basic research of many technologically relevant quantum materials. Advances in quantum spin liquids, skyrmion lattices, spin-orbit and spin-lattice couplings, and superconductivity all require a deeper understanding of magnetism in quantum materials. The fact that the neutron has no net charge and possesses a magnetic moment makes neutron scattering an ideal tool for studying magnetism. Moreover, like using a small probe magnet to measure magnetic field distribution, the ability to polarize neutrons makes neutron scattering even more sensitive to magnetism in materials. The goal of this project is to enable neutron scattering studies of complex noncollinear magnetic structures and investigations of hybrid correlation functions coupling different degrees of freedom (spin-lattice, spin-orbit, spin-chirality) using full polarization analysis. This will be accomplished by developing next-generation Spherical Neutron Polarimetry (SNP) capabilities to be deployed across multiple neutron instruments at the High Flux Isotope Reactor (HFIR) and the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL). The new SNP capability will deliver the most advanced tool in the world for the study of magnetism using neutrons and help resolve questions that are otherwise intractable or cannot be unambiguously determined using traditional methods. The technical development will place ORNL at the forefront of polarized neutron scattering capabilities world-wide, and its implementation will be game-changing across a range of science themes and will also lay the groundwork for its future application on instruments at the Second Target Station (STS).

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

Lattice Calculation of the QED Corrections to Meson Leptonic Decay

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The Cabibbo-Kobayashi-Maskawa (CKM) matrix elements, as the basic parameters in particle physics, describe how quark decays into other types of quark. Its precise measurement provides a rigorous test for particle physics' standard model. Determining the light quark-related CKM matrix element requires both experimental measurement and theoretical calculations of the corresponding hadron decay process. At present, accuracy is limited by theoretical calculations. In this research, high-precision lattice field theory calculations will be performed for the K meson (semi-)leptonic decay process to improve the accuracy of the corresponding CKM matrix element. The calculation will pay special attention to the effects of electromagnetic interaction, which is necessary to achieve the required accuracy. This research will mainly use two techniques to include electromagnetic effects. The first is to make full use of the parsed photon propagators in lattice calculations to improve accuracy. This method is very effective in the lattice field theory calculation of the contribution to the strong interaction of the muon magnetic moment. The second is to use the recently developed infinite volume reconstruction method. This method will effectively deal with the finite volume error and infrared divergence caused by the long-range electromagnetic interaction. The lattice field theory calculations performed in this study will also improve the determination of the light quark mass, determine the electromagnetic correction of the neutron decay, and provide theoretical limitations for the cross-section of neutrino nucleon scattering.

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

High Brightness Photocathodes in Photoinjectors

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The performance of existing and future ultrafast science instruments like X-ray Free Electron Lasers (XFELs), Ultrafast Electron Diffraction (UED), and Ultrafast Electron Microscopy (UEM) is limited by the brightness of electron beams produced from photocathodes in photoinjectors. Generation of brighter electron beams from photoinjectors requires the development of photocathodes capable of emitting electrons with the smallest possible mean transverse energy (MTE), or equivalently, the smallest possible intrinsic emittance. With the goal of improving the performance of the above applications, over the last decade, a significant effort has gone into understanding the process of photoemission and reducing the MTE of electrons emitted from cathodes. As a result, several ways of achieving low MTEs of 20-30 meV have been developed and MTE as low as 5 meV has been demonstrated. Despite these large improvements in MTE, photoinjectors still use cathodes with a large (~500 meV) MTE.

This research aims to identify and resolve the issues involved in using these low-MTE cathodes in photoinjectors and develop cathodes for low-MTE (sub-25 meV) operation in new photoinjectors, resulting in nearly 25 times brighter electron beams. The ultimate goal of the research is to demonstrate low-MTE (and thus high-brightness) operation in the existing and new photoinjectors being developed to power future XFEL and UED/UEM facilities. The proposed increase in brightness will result in a dramatically increased X-ray pulse energy in existing XFELs maximizing their potential to study atomic and electronic structural dynamics in quantum materials, electronic and nuclear coupling in biological and chemical processes and energy materials in situ. It is also critical for the development of compact XFELs to make them widely accessible. For UED/UEM applications, the proposed increase in beam brightness implies an increase in the spatio-temporal resolution greatly increasing the scientific reach of these ultrafast electron scattering techniques. Thus, this work will transform the capabilities of various existing and upcoming DOE facilities, opening new frontiers in ultrafast studies of quantum materials, energy technologies, and critical biological processes.

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

Extreme Drought, Heat and Wildfire Impacts on Future Coastal Water Relations

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Ecosystem water use plays a large role in determining surface water availability, and thus streamflow, and societies water resources. Water use and streamflow are highly sensitive to multiple climate extremes, many of which are co-occurring and compounding events. It is the co-occurrence of extremes that poses the biggest risk to ecosystems and society, as co-occurring climate extremes amplify impacts due to multiple nonlinear interactions. Coastal regions of the western US exhibit strong spatial gradients in water resources and provide an excellent testbed to understand the influence of compound and sequential extreme events on ecosystem water use and the resulting effects on streamflow and water relations. In tandem, dense observation networks such as AmeriFlux and the USGS stream gage network provide an opportunity to examine the impact of extremes on coastal water resources, as we move to no-analogue environments in the coastal regions of the future. This project will examine the impact of extreme drought, heat and wildfire on water relations of the coastal western US, integrating machine learning, Earth System Models, and emulators with distributed sensor networks to do so. The strategic combination of novel observationally-informed techniques within a model benchmarking framework, combining both the water and carbon cycles along with associated uncertainties, will greatly improve our understanding of the relationship between coastal ecosystem function and current and future water resources.

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

The Non-Equilibrium Quantum Frontier

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A central goal of condensed matter physics is to study universal emergent properties – those that characterize the collectivity but not the individual constituents – of macroscopic quantum systems with large numbers of interacting particles. In the traditional approach, a major conceptual simplification is afforded by studying many-body systems close to (thermal) *equilibrium* at long distances and low temperatures – a wildly successful enterprise that has led to the discovery of many novel phases of matter ranging from exotic superconductors to topological insulators. More recently, a confluence of theoretical and experimental advances across a range of subfields in physics has opened up a vast new territory of studying many-body phenomena in completely novel regimes: highly excited, quantum coherent, and *far from equilibrium*. In these settings, most well-established methods in quantum many body theory do not apply. Our understanding of even fundamental questions of quantum statistical mechanics, such as whether or how isolated quantum systems can bring themselves to thermal equilibrium under their own dynamics - or fail to do so - is still nascent. From the perspective of condensed matter physics, an exciting new opportunity entails understanding the new kinds of emergent universal many-body phenomena that can arise once the strictures of equilibrium thermodynamics are relaxed. A paradigmatic example is the recent discovery of *time-crystals* – a phase of matter disallowed in thermal equilibrium – in the intrinsically out-of-equilibrium setting of a periodically driven, many-body localized system.

This research spans three broad research thrusts: (i) formulating and understanding the full range of `dynamical universality classes', and the novel phase transitions between these; (ii) exploring new kinds of phenomena that may be realized out-of-equilibrium; and (iii) formulating new information theoretic approaches for studying many-body quantum dynamics. In all, this wide-ranging research plan aims to push the exciting and interdisciplinary non-equilibrium quantum frontier using a variety of analytic, numerical and information theoretic approaches.

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

Illuminating the Molecular Pathways of Trace Element Incorporation During Crystal Growth

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Natural aqueous fluids contain complex mixtures of dissolved constituents, so mineral growth in the environment leads to incorporation of impurities. These impurities impact the structure and stability of the precipitated minerals. Understanding impurity uptake is complicated by the fact that crystals can form by classical addition of individual ions such as Ca^{2+} or CO_3^{2-}, or by more complex, non-classical processes involving pairs or larger clusters of ions up to small nanometer-sized precursor crystallites. Our lack of understanding of how the different growth processes affect the uptake of trace elements undermines our ability to capture rare or energy-important elements from geologic or anthropogenic water sources and also to interpret Earth history through diagnostic trace element signatures present in the minerals in rock formations that record this history. This project aims to identify the molecular pathways of trace element incorporation for two important classes of minerals, carbonates and phosphates, which are known to form by classical and non-classical pathways. The core hypothesis informing this work is that the relative rates of monomer dehydration and growth unit attachment regulate the preferred incorporation pathway for a given species regardless of the product phase. A multimodal study is proposed to identify dominant molecular building blocks using time-resolved X-Ray scattering and spectroscopy and to trace the evolution of growth unit structure and composition during trace element incorporation using atomic-resolution imaging coupled with molecular simulations of the different types of growth processes. This work will inform the development of kinetic models that predict impurity uptake in multicomponent aqueous solutions with broad applicability to ionic crystals. These discoveries will impact the design of novel crystallization technologies to isolate valuable elements from complex feedstocks and to immobilize and secure toxic and radioactive species

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

The BeEST: A Search for keV-Scale Sterile Neutrinos using Superconducting Quantum Sensors

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The search for sterile neutrinos is perhaps the brightest possibilities in our quest for understanding the microscopic nature of the observed dark matter (DM) in our Universe. Sterile neutrinos – unlike the active neutrinos in the Standard Model – do not interact with normal matter as they move through space, and are thus best observed using their mass signature. In this work, complete momentum reconstruction of electron-capture (EC) nuclear decay is employed to perform a search for sterile neutrinos in the keV mass range that is 10,000 times more sensitive than previous experiments. This is achieved using the EC decay of radioactive beryllium-7 atoms implanted into sensitive superconducting tunnel junctions (STJs) - an experiment nicknamed the BeEST ("beast") for *Be*ryllium *E*lectron capture in *ST*Js. A discovery signature in the BeEST experiment would be a small fraction of these decays where the daughter (lithium-7) atomic recoil peaks are shifted to lower energies from momentum conservation with these new, heavy sterile neutrinos. This approach is a uniquely powerful experimental method since it relies only on the well-motivated existence of this new type of neutrino, and not on how they might hypothetically interact with normal matter.

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

HydroX: Using Hydrogen Doped in Liquid Xenon to Search for Dark Matter

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The nature of dark matter is one of the biggest mysteries in physics today. Experimental efforts searching for dark matter particles over the last few decades have ruled out many candidates, and the new generation of tonne-scale liquid xenon detectors like the LUX-Zeplin (LZ) experiment will cover two more orders of magnitude in sensitivity. Recent theoretical work suggests that dark matter might be lighter than the optimal search range of experiments like LZ, and this research aims to enable LZ to search for an order of magnitude lighter dark matter masses by adding hydrogen to the liquid xenon, in an upgrade called HydroX. Being the lightest element, hydrogen is a much better target than xenon for searching for light dark matter because it is easier to transfer momentum between objects of similar mass, much like a ping pong ball cannot impart energy to a bowling ball. Considerations of the nature of signal generation in liquid xenon argue that the signal produced by a dark matter-hydrogen interaction will be significantly larger as well, further increasing the sensitivity to the lightest particles. By putting hydrogen into the existing LZ detector, this research capitalizes on the significant investment already made in LZ construction, taking advantage of the most radioactively quiet place on earth. The first priority of this research is to measure the response of liquid xenon to hydrogen and determine the ultimate sensitivity of HydroX. The work will observe how much hydrogen can be readily dissolved in liquid xenon, and then expose that mixture to very low energy neutron sources to mimic dark matter particles. The second part of the research will focus on the thermodynamics of hydrogen-doped liquid xenon. In LZ, 10 tonnes of liquid xenon are circulated through a purifier every 2.5 days, and major effort is needed to understand how to introduce hydrogen on that scale without upsetting the balance required to keep the liquid xenon cold. The final result of HydroX will be a fully characterized upgrade to LZ that will increase the sensitivity by more than an order of magnitude towards lower dark matter masses and hopefully to understand the mysterious nature of dark matter.

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

A Unified Picture of Long- and Short-range Dynamics of Atomic Nuclei

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Atomic nuclei are self-bound systems of fermions that display emergent quantum-mechanical phenomena. Testing their structure and reactions at low energies is the primary focus of domestic experimental facilities, including the Argonne Tandem Linac Accelerator System, the National Superconducting Cyclotron Laboratory, and the Facility for Rare Isotope Beams. Experiments at Thomas Jefferson Laboratory and the forthcoming Electron-Ion Collider probe the internal structure of the nucleus and the interplay between nucleonic and partonic degrees of freedom by examining short-distance phenomena. The main objective of this research is to connect the physics scope of the domestic nuclear experimental program. It provides a unified theoretical picture of the long-range structure and short-range dynamics of atomic nuclei starting from the individual interactions among their constituents: neutrons and protons. The research project enables breakthrough developments of the nuclear Green's Monte Carlo methods, currently limited to nuclei with up to A=12 nucleons. This project capitalizes on high-performance computing resources, including the forthcoming exascale machines, and entails the development of novel representations of the nuclear wave functions in terms of artificial neural networks. Besides covering many areas in nuclear physics, this research has critical applications in high-energy physics, specifically on the neutrino-oscillation programs. It also impacts multi-messenger astrophysics, as high-density nuclear dynamics is imprinted in the gravitational-waves and neutrino-emission signals of merging neutron stars.

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

Electrocatalytic Alkene Epoxidation at Disrupted Metal Ensembles in Blended Electrolytes

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Future routes for modular, point-of-need chemical manufacturing may utilize distributed renewable feedstocks, such as water, carbon dioxide, and dinitrogen, as well as distributed energy sources, such as solar and wind electricity. Among the many possible chemical targets for this sustainable chemical manufacturing paradigm, epoxides are attractive due to their significant energy and carbon footprint during production and status as nexus molecules in the chemical industry, where they provide access to diverse, high-volume plastics, textiles, and adhesives. The current thermochemical and wet chemical synthesis routes for epoxides partially oxidize an alkene with an oxygen-atom source to produce an epoxide. Thermochemical routes for epoxidation suffer from significant carbon dioxide emissions, while the wet chemical routes lead to stoichiometric waste products and significant hazards in handling reagents. These shortcomings motivate the development of a sustainable method for epoxidation, in which water can be used as an oxygen-atom source. The objective of this research is to develop electrocatalysts which facilitate the efficient anodic conversion of water and alkenes into epoxides, while generating hydrogen at the cathode. The research will elucidate the molecular-level steps through which water is oxidized and how an oxygen-atom is ultimately transferred to an alkene. The role of disrupted metal ensembles and blended electrolytes in controlling rates of epoxidation will be understood. The work will broadly lead to advances in controlling catalytic surfaces and the surrounding electrolyte environment to direct the electrosynthesis of organic molecules of large energy footprint.

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

Investigation of Helicon and Lower Hybrid Wave Coupling with the Edge Plasma for Current Drive Optimization in the Tokamak Using Laser Spectroscopy

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Magnetic confinement fusion would provide an abundant source of clean energy and help reduce the threats of climate change. The limiting factors to deploying fusion energy are continuous, reliable power production and the high costs associated with building and operating reactors. To address these issues, the Helicon and High-Field Side Lower Hybrid (HFS-LH) programs were established at the DIII-D National Fusion Facility. These programs are investigating innovative and efficient methods to generate plasma current using radio frequency (RF) waves, which is critical because tokamak fusion reactors require a constant plasma current for continuous power production. This research will combine novel laser-based spectroscopy and advanced quantum mechanical modeling to experimentally measure the RF wave's electric field vector. Leveraging world-leading exascale high-performance computing capabilities, these measurements will be compared to 3D full-wave simulations to understand the RF waves interaction with the edge plasma. The work will provide groundbreaking insight to accelerate progress in generating efficient plasma current using RF waves.

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

Converting Metal–Organic Liquids into Microporous Glasses via Non-Equilibrium Syntheses

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Glasses are critical to many of the technologies that support our modern lifestyle, and new types of glassy materials are likely to play an important role in addressing a wide range of global challenges. Despite their tremendous importance, the compositional and structural diversity of glasses that have been designed, synthesized, and studied to date pales in comparison to other classes of materials. The realization of new types of glasses is complicated by the intrinsic non-equilibrium nature of all glass phases, which are—with few exceptions—metastable compared to an equilibrium crystalline phase at a given temperature and pressure. This research will apply coordination chemistry principles and non-equilibrium synthesis techniques to the design of novel glasses. Through a comprehensive study of the factors that govern the conversion of a metal–organic liquid to a metastable glass, we will establish design principles for the non-equilibrium synthesis of glasses featuring new behaviors and previously inaccessible functionalities that are both technologically relevant and fundamentally insightful. Specifically, the design, synthesis, and characterization of metal–organic glasses will lead to novel glass compositions and structures that offer access to properties, such as tunable microporosity, not found in conventional chalcogenide, metallic, organic polymer, or inorganic oxide glasses. The fundamental structure-property relationships established in this project will inform efforts to design new materials for a wide range of applications relevant to energy technologies, including phase-change memory, membranes, coatings, optical materials, structural materials, solid electrolytes, and radioactive waste storage. Moreover, metal–organic glasses will provide a powerful platform to explore fundamental aspects of the glass transition and, more broadly, of the basic science underpinning the synthesis of metastable materials under conditions far from equilibrium.

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

New Molecular Mechanisms for Greenhouse Gas Capture in Metal–Organic Frameworks: Carbon Dioxide and Beyond

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This research aims to advance the field of metal–organic frameworks (MOFs) in order to enable the selective capture of greenhouse gases at industrial point sources and their subsequent utilization to prepare value-added products. While carbon dioxide is a targeted molecule to capture and convert, there are other inescapable greenhouse gases with untapped potential value beyond carbon dioxide, including nitrous oxide (N_2O) and hydrofluorocarbons. The work focuses upon the unique reactivities of each gas – specifically, the electrophilicity of carbon dioxide, the oxidizing nature of nitrous oxide, and the halogen-bonding affinity of hydrofluorocarbons – to explore new molecular-level mechanisms for their selective binding within porous materials. Doing so will provide insights for new strategies to reduce anthropogenic greenhouse gas emissions while unlocking new routes for their application in sustainable synthesis.

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

Constraining the Electromagnetic Shower Energy Scale at LArTPC Neutrino Detectors Near and Far

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The Deep Underground Neutrino Experiment (DUNE) at the Long-Baseline Neutrino Facility is an international project that will be the largest particle physics experiment ever built in North America. The DUNE project will use massive liquid argon time projection chambers (LArTPCs) to address fundamental questions such as the origin of the matter/antimatter asymmetry in the universe. In order to answer such questions, DUNE will make measurements that probe the nature of neutrino oscillation, the changing of neutrino flavor (electron, muon, or tau) during the flight from source to detector, with unprecedented precision. Another upcoming neutrino oscillation experiment is the Short-Baseline Neutrino (SBN) Program, which will use multiple LArTPC detectors to investigate the anomalous phenomenon of neutrino oscillation over shorter distances that could lead to the discovery of "sterile" neutrinos. Both DUNE and the SBN Program rely on precise measurements of electron neutrino interactions, which produce electromagnetic showers in LArTPC detectors. The energies of these electromagnetic showers must be well understood to achieve the main physics goals of each experiment. The primary objective of this research is to constrain the electromagnetic shower energy scale at DUNE and the SBN Program through precise calibration of detector effects and use of neutral pion decays to photons, which also produce electromagnetic showers in LArTPC detectors. This research includes development of the DUNE LArTPC near detector to obtain the full potential in this energy scale constraint.

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

Understanding and Controlling Multielectron, Multisubstrate Reactions Involving Complex Architectures and Interfaces

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Catalysts provide low-energy pathways for driving chemical transformations and are utilized in applications ranging from manufacturing fuels and fine-chemicals to controlling the bioenergetics essential to all living organisms. Although the ability to catalyze fuel-forming reactions using sunlight as an energy source has been demonstrated, finding ways to more effectively interface catalysts with light-absorbing materials remains challenging as there is not enough understanding of how charge carriers move through these systems. The objectives of this research include: (1) synthesizing catalysts with tailored electronic states that promote both electron-transfer and proton-transfer processes, (2) developing methods to interface these catalysts with light-absorbing semiconductors, and (3) enhancing fundamental understandings of the interplay between light absorption, charge transfer, and catalysis. While structurally more complex than their isolated components, the hierarchical materials used in this research move beyond traditional model systems and toward studying the basic energy science of using solar photochemistry to produce fuels and other industrially relevant chemicals.

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

DataStates: Scalable Versioning for Scientific Data

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The advent of big data analytics and artificial intelligence is rapidly transforming the data requirements of modern high performance computing (HPC) applications. A fundamental challenge is the inability to capture, search and reuse data as they are calculated, which would allow researchers to revisit previous states to explore alternatives; improve the coupling of workflow components; and understand and explain the evolution of data. Current state of the art data services manipulate datasets as files and key-value pairs, making it impossible to address this challenge in an efficient and scalable way. This proposal advocates a different data model based on a new concept of Data States. In this model, users do not interact with a data service directly to read/write datasets but rather tag datasets with properties expressing hints, constraints, and persistency semantics, which automatically adds snapshots of these datasets (called data states) into the lineage-- a history recording all intermediate data states based on an optimal action plan that automatically performs any needed read/write actions. The lineage of data states has several advantages. First, it allows application developers to focus on the meaning and properties of their data, rather than on the manipulations needed to read/write, restructure, and reorder data. Second, it brings an incentive to collaborate more, verify and understand the results more thoroughly by sharing and analyzing intermediate results. Third, it encourages the development of new algorithms and ideas that reuse and revisit intermediate and historical data frequently. Such capabilities are particularly important to facilitate quicker advances at the intersection of HPC, artificial intelligence and big data analytics.

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

Crosstalk: Interkingdom Interactions in the Mycorrhizal Hyphosphere and Ramifications for Soil C Cycling

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Arbuscular mycorrhizal fungi (AMF) are ancient symbionts that form root associations with 80% of the world's plants. AMF play an important role in global nutrient and carbon cycles, and understanding their biology is crucial to predict how carbon is stored and released from soil. The region of soil surrounding the fungal body (or hyphae) is called the hyphosphere, which is the zone where much of this nutrient and carbon cycling occurs. However, the hyphosphere is one of the least understood components of the plant-mycorrhizal-soil system. It is hypothesized that AMF rely on microbes living in the hyphosphere to access key nutrients from soil organic matter. In fact, synergistic interactions between AMF and soil microbes have been estimated to contribute 70,000 tons of assimilated plant nitrogen annually. This research will investigate the basic mechanisms that underpin these interactions and drive nitrogen and carbon cycling in the hyphosphere, addressing DOE's mission to understand and predict the roles of microbes in Earth's nutrient cycles. By coupling isotope-enabled technologies with next generation DNA sequencing techniques, this project will investigate soil microbial communities in their notoriously heterogeneous natural environment. This work will provide a greater mechanistic understanding needed to determine how mycorrhizal fungi influence organic matter decomposition and will shed light on large-scale nutrient cycling processes in terrestrial ecosystems.

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

Improving Accelerators with Diagnostics Optimized for Artificial Intelligence

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Beams of accelerated particles drive scientific research and discovery in fields ranging from fundamental physics to biology, including the discovery of why particles have mass and the study of proteins on the surface of viruses. The primary goal of this research is to develop a paradigm for producing ultra-short particle beams that are at least an order of magnitude higher in quality than presently possible. Higher quality beams would reduce the amount of experimental time needed to make discoveries at a linear collider or X-ray free-electron laser (XFEL), and at the same time broaden access to facilities that are in high demand. Two of the main challenges associated with generating these beams – measuring the beam characteristics and controlling the accelerator to the level required to preserve their quality – will require specialized non-invasive, real-time diagnostics that use artificial intelligence for beam measurement and control. This research will develop and deploy single-shot, non-invasive emittance and energy spread diagnostics based on edge radiation at the FACET-II accelerator at SLAC National Accelerator Laboratory. Once deployed, these novel diagnostics will use artificial intelligence to monitor and control the evolution of the particle beam throughout the accelerator in real time. The success of this research will directly benefit the operation of existing facilities, such as LCLS, as well as concepts for future accelerators.

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

Variability and Change in Tropical Cyclone Characteristics: Coupled Atmosphere-Ocean Drivers and Coastal Impacts

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Tropical cyclones (TCs) are the leading cause of weather-related economic loss in the U.S., accounting for $938.2 billion over 1980-2019. Into the future, coastal regions are expected to face compounding challenges from TCs and sea-level rise. Despite the societal and economic risk TCs pose, grand challenges remain including a lack of consensus on future change in global TC number and uncertainty in the magnitude of regional change in TC intensity and precipitation. This knowledge gap stems from the lack of a theory to explain what constrains annual TC number, and a limited understanding of how various coupled atmosphere-ocean processes alter TC intensity in different climate states. The urgency of addressing the challenge to make reliable future TC projections is escalating with increasing coastal development and population growth, the high economic output of U.S. coastal regions, the vulnerability of infrastructure to coastal flooding, and sea-level rise. This research will (1) quantify how local-scale processes and atmosphere-ocean interactions shape TC intensity in a changing climate (e.g., TC intensity and associated wind-driven ocean mixing, TC precipitation and associated freshwater flux to the ocean, and upper-ocean thermal and salinity conditions); (2) determine the primary large-scale physical drivers that control the spatial and temporal statistics of landfalling TCs (e.g., inter-basin and intra-basin ocean temperature gradients, greenhouse gas and aerosol forcings, TC steering flow, and TC precursors); and (3) translate the knowledge developed in 1 and 2, together with sea-level rise projections, into coastal impacts due to the combination of storm surge, heavy precipitation, and strong winds associated with TCs. We will address these problems using observations and climate models including the DOE Energy Exascale Earth System Model (E3SM), a convection-permitting atmosphere-ocean regional climate model, and a storm surge model. This research will advance the resilience of North American coastal systems to climate change by determining how local coupled processes and large-scale drivers control historical and future TC characteristics.

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

Understanding the Dynamics of Single-Site Heterogeneous Catalysts

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Dynamic motions of molecules play a central role in many, if not most, catalytic processes but the impacts they have on catalytic efficiency and selectivity remain largely unknown. This is primarily due to the lack of techniques for examining the structure of moving analytes with atomic-scale resolution. Of particular interest are the dynamics that occur at equilibrium, such as the conformational rearrangements required to stabilize, and favor, a given transition state. These molecular motions are, unfortunately, particularly difficult to observe, as they do not lead to bulk structural changes and operate largely at the molecular level. Nuclear magnetic resonance (NMR) spectroscopy is unique among characterization tools in that it is sensitive to dynamics over a time scale spanning at least ten orders of magnitude and can also resolve molecular structures with sub-Å precision. Because of these characteristics, NMR spectroscopy became the primary tool used to understand the dynamics of enzymes and other macromolecules. Until recently, however, the adaptation of these techniques to the study of heterogeneous catalysts has been limited by NMR's inherently low sensitivity, which is compounded by the severe dilution of active sites. Recently, with the development of ultra-fast magic-angle-spinning and dynamic nuclear polarization, it has become possible to extend the reach of NMR spectroscopy and yield the first three-dimensional structures of single-site heterogeneous catalysts. The objectives of this research program are to build on these pioneering developments to not only reveal the precise structures of catalytic sites but also evaluate how these three-dimensional structures evolve in time. The research will uncover novel dynamic structure-activity relationships that could in turn be used to rationally tune the selectivity, or activity, of a catalyst.

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

Topology-Preserving Data Sketching for Scientific Visualization

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We are experiencing an information overload from streams of data that arise from scientific instruments and simulations. For example, material scientists use molecular dynamics (MD) simulations to study how fluids (such as gas, oil, and water) interact with heterogeneous porous solids (such as ceramics, cement, and rock) to improve transport phenomena within porous materials, which play critical roles in our energy sector. Such simulations generate large, time-varying, and complex forms of data under different physical and chemical conditions. Keeping track of interesting phenomena and applying appropriate actions (such as storage, analysis, and visualization) while the simulation is running is necessary but challenging. To address this challenge, the goal is no longer to capture and store observations or simulation in detail, but rather to process data efficiently and approximately in order to create a summary -- a sketch -- which allows queries over large volumes of data to be answered quickly.

The objective of this research is to conduct a systematic study of topology-preserving data sketching techniques to improve visual exploration and understanding of large scientific data. The project will employ topological sketches, that is, compressed representations of the full data that preserve their important structural properties, to support analysis and visualization as the data are generated. Our proposed solution transforms data sketching ideas from statistics, geometry, and linear algebra to develop new topological sketches of complex data. Such sketches will exploit the high spatial resolution and temporal fidelity of in situ data in an intelligent and scalable way. They will reduce data in situ while preserving its structural properties, and subsequently support interactive data exploration. In addition, topological triggers will be integrated into an adaptive workflow to support anomaly detection, computational steering, and decision optimization. The multidisciplinary nature of the proposed work will be broadly applicable in many scientific areas, including applications in computational fluid dynamics and materials science.

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

Deciphering Spin and Orbital Dynamics in Quantum Materials through Neutron Scattering

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Magnetism arises from the collective organization of a material's constituent electrons into a regular pattern. In some cases, quantum mechanics overcomes the tendency towards order and leads to phases of matter where the many magnetic degrees of freedom are entangled. Such states of quantum matter offer new windows into fundamental physics and may form the basis for future quantum information technologies. Typically, these phases emerge in materials with competing electronic energy scales, but they are notoriously difficult to predict. Tantamount to this theoretical challenge is the experimental task of identifying such quantum states of matter. This project coordinates a materials synthesis effort with state-of-the-art neutron scattering techniques to elucidate the hierarchy of collective excitations in magnetic quantum materials. The goal is to obtain a quantitative understanding of the interplay between spin, orbital, and lattice energy scales in materials where spin-orbit coupling and electronic correlations conspire to determine the ground state. The results of this research will provide essential input to establish theoretical frameworks for predicting the properties of quantum magnets with fluctuating spin and orbital degrees of freedom. In turn, this knowledge will guide the design of materials and devices with novel quantum functionalities.

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

Exascale Simulations of Neutron Star Mergers

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Gravitational waves and electromagnetic radiation from colliding neutron stars (NSs) encode precious information about the internal structure and composition of NSs and reveal the explosions in which some of the most heavy elements, such as gold, platinum, and uranium are formed. Relativistic heavy-ion collisions and experiments such as PREX here on Earth are probing the nature of matter under extreme conditions. The nuclear physics involved in the creation of the heavy elements will be more tightly constrained as FRIB comes online in the next years. However, as observations and laboratory measurements improve, so must the theoretical understanding of NS mergers in order to maximize the science return from these large scale investments. Ab-initio supercomputer simulations are the only tool able to bridge astronomical observations and laboratory experiments and connect them to the merger dynamics. However, current simulation results are affected by large systematic errors stemming from the inability to resolve all spatial and temporal scales in mergers and by their approximate treatments of neutrinos. This project aims to overcome these limitations by developing a new simulation infrastructure able to leverage next-generation supercomputer hardware, enabling calculations at unprecedented resolutions and extending over long timescales. One of the key deliverables is a new neutrino transport solver including general-relativistic and quantum kinetic effects using the filtered spherical harmonics and Galerkin methods, some of the most sophisticated approaches developed in the applied mathematics and computational physics communities. This project develops the theory foundations needed to address some of the most pressing questions in nuclear astrophysics such as the nature of matter inside NSs and the astrophysical site of production of the heavy elements.

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

Characterizing Virus-driven Alterations of Microbial Metabolism in Model Soil Ecosystems

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Soil microbes are globally important as they shape major nutrient cycles, drive energy conversion processes, and strongly impact terrestrial ecosystems that are relevant for DOE's mission in energy and the environment. In aquatic ecosystems, viruses are important regulators of microbial physiology. In soils, even though a large diversity of viruses has been discovered, their role and impact on microbial activity remains poorly understood. This research will use a combination of experimental approaches and large-scale data analysis to better characterize how viruses infect soil microbes and affect ecosystem function. The project will characterize the networks connecting soil viruses to their microbial hosts and their associated metabolisms in a comprehensive way. A comparison of arid and humid ecosystems over time will uncover how virus/host interactions are transformed by environmental conditions. The mechanisms by which soil viruses control their host cells and alter their metabolism will be studied in further detail using simplified soil communities in culture, as well as microfluidic devices. Such high-resolution measurements will enable the integration of viral biology into predictive models covering multiple scales, from the single-cell to the ecosystem level.

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

Controlling Interfacial Energetics and Charge Transfer Rates in 2D Semiconductors: Fundamental Studies en Route to Photoelectrochemical Energy Conversion Beyond the Shockley-Queisser Limit

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Current photovoltaic materials do not convert the full potential energy of sunlight to electricity or fuels. The fundamental problem is that all excess solar photon energy above the semiconductor band gap is lost as heat in a process called hot-carrier thermalization. Avoiding thermalization energy losses is of paramount significance because hot-carrier-based systems theoretically achieve 66% efficiency, which breaks the conventional limit of 33%. This research project will advance fundamental knowledge of solar energy conversion processes in two-dimensional (2D) semiconductors such as monolayer (ML) MoS_2. These ultrathin semiconductors have unique physical and photophysical properties that could make hot-carrier energy conversion possible. Electrochemical microscopy and in situ ultrafast spectroscopy will be used to interrogate the rate of hot-carrier cooling relative to the rate of hot-carrier extraction in photoelectrochemical cells based on ML-MoS_2. The solid/liquid interface in a photoelectrochemical cell is an excellent model system to quantify the energy and yield of hot-carrier extraction in 2D semiconductors. This research will produce the necessary thermodynamic and kinetic data to understand rate-limiting processes involved in the transfer of high-potential electrons to substrates or catalysts for solar fuels production. The research outcomes will have broad impact in electrochemical research including electrocatalysis, energy storage, and artificial photosystems for harvesting solar energy.

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

Robust Dark Energy Constraints with Dark Energy Spectroscopic Survey

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Dark Energy is one of the biggest mysteries of modern science. We know that it makes up about 70 percent of the Universe but we don't have a satisfactory theory for its fundamental nature. Dark Energy Spectroscopic Instrument (DESI) is an experiment that aims to study properties of Dark Energy with extremely high accuracy. DESI will observe millions of distant galaxies and measure the rate of the Universe's expansion and the growth of structure by analyzing statistical patterns in the spatial distribution of those galaxies. The objective of this project is to extract information about Dark Energy from galaxies observed by DESI by pursuing three complementary approaches. The first approach will study the relationship between galaxies and their host dark matter halos by means of various nonlinear statistical measures and machine learning techniques. The second approach will link the properties of Dark Energy to the magnitude of infall velocities between galaxies at small separations by means of computer simulations. The third approach will look for large scale harmonic patterns in higher-order statistics of galaxy distribution that are sensitive to the properties of Dark Energy. This program will enable us to extract robust and precise measurements of the properties of Dark Energy from DESI data.

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

Additive-Assisted Preparation of Multinary Halides

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Global interest in the use of halides for optoelectronic applications including photovoltaics (PV), photodetectors, light-emitting diodes (LEDs), lasers, and thin-film transistors has been revived due to the emergence of high-performance solar cells based on lead halide perovskites. The rapid development of optoelectronic metal halides was aided by their solution processing, which enables greater chemical flexibility, richer chemical compositions, and crystal structures. In turn, the rich chemistry of metal halides translates into a wide tunability of physical properties, allowing their consideration for a variety of energy-saving technologies. However, a fundamental understanding of the solution preparation of metal halides, particularly in the presence of spectator ions, is lacking. This project aims to prepare a series of metastable multinary halides through understanding and control of impurity-assisted solution synthesis. Self-assembly of ordered (i.e., crystalline) materials in polar media has already yielded large classes of energy-relevant materials. Expanding the experimental toolset available to materials chemists, this project will specifically focus on using reactive and non-reactive metal halide additives to reaction media to obtain multinary halides that are otherwise inaccessible.

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

Next Generation of QCD Global Analysis for Hadronic Physics

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Understanding the internal structure of protons and neutrons, which are the fundamental building blocks of atomic nuclei and thus of all the stars, planets and most visible matter in the universe, is one of mankind's major challenges. With more than 50 years of experimental and theoretical effort, we now understand that protons and neutrons (or collectively "nucleons") are composed of more fundamental quark constituents bound together by gluons with strong forces governed by the theory of Quantum Chromodynamics (QCD). Unlike any other known phenomenon in Nature, the confinement property of QCD means that quarks and gluons can never be observed in isolation in any particle detector. Moreover, in contrast to other systems, such as atoms or molecules, there is no "still" picture for the internal quark and gluon structure of nucleons and nuclei, and the internal structure can only be characterized through quantum correlation functions (QCFs), such as parton distribution functions, transverse momentum dependent distributions, and generalized parton distributions. The greatest challenge is therefore to map out these QCFs using data from experiments that only detect particles such as hadrons, photons and leptons. With the ongoing 12 GeV nuclear physics program at Jefferson Lab, the Relativistic Heavy Ion Collider at Brookhaven National Lab, and other facilities around the world, as well as the future Electron-Ion Collider (EIC) in the US, we are at the threshold of imaging the nucleon's internal 3-dimensional quark and gluon structure in the theoretical framework of QCD for the first time. The new facilities will deliver unprecedented quantities of high-precision data, posing new opportunities and challenges for accessing a variety of QCFs. The goal of this project is to meet these challenges by developing the next generation QCD "FemtoAnalyzer" to assimilate information about various types of QCFs from experimental data at the femtometer scale. The project integrates modern developments in nuclear theory, data handling and artificial intelligence to develop the most advanced theoretical and phenomenological tools to visualize the internal landscape of nucleons and nuclei with unprecedented resolution. The achievements of this project will help to accomplish the mission of DOE's Nuclear Physics program to analyze the enormous amounts of data from the Jefferson Lab 12 GeV and future EIC facilities.

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

The QCD Structure of Nucleons and Light Nuclei

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Atomic nuclei, built of protons and neutrons, constitute more than 99% of the visible mass in our universe. Quantitatively describing the structure of protons, neutrons, and nuclei in terms of their quark and gluon constituents is a defining challenge bridging hadronic and nuclear physics research. The ultimate goal is to map the complete spatial, momentum, spin, flavor, and gluon structure of the proton and neutron, to be able to predict their interactions and resonances precisely, and to understand how their structures change as they form a nucleus. Not only is this map the key to interpreting observations of nature in terms of the currently-accepted fundamental theory, but it is essential to inform searches for new physics. This research program furthers this mission by revealing aspects of the gluon structure of the proton, and of the quark and gluon structure of light nuclei, using first-principles calculations of the strong interactions. The results will provide essential information for current and future nuclear physics experimental programs, in particular those at the Thomas Jefferson National Accelerator Facility and at the planned Electron-Ion Collider at Brookhaven National Laboratory. The results will also provide input to nuclear physics experiments searching for violation of fundamental symmetries and new physics, including laboratory-based experiments searching for dark matter.

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

Towards Exact Finite Temperature Electronic Structure in Solids and Molecules

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Materials with temperature-dependent properties are familiar to us. For example, room-temperature magnets can lose their magnetism if heated too much. The temperature range over which materials will exhibit a desirable property is an important feature when it comes to their design. While macroscopic properties are driven by a wide variety of competing physical effects, one consideration is that temperature can cause changes in how electrons interact with one another. In quantum mechanics, this is represented by there being a large number of excited states that electrons can arrange themselves in, leading to a high degree of complexity. High-accuracy calculations that aim to solve the Schrödinger equation can, in principle, resolve this complicated mixture of states within a material and find exact electronic properties at a target temperature. However, until now, the simulations required would be too expensive even on the fastest supercomputers. This project will develop more affordable ways to perform exact calculations to isolate and measure how electronic structure changes with temperature. It will leverage and adapt an algorithm that randomly samples quantum-mechanical electronic states to achieve exact-on-average energies and property predictions, which are useful for a significant number of practical purposes. Through a combination of developing new software and models, this research will also provide mechanistic detail for thermal electronic effects in plasmonics as well as in phase transitions. The software and data developed will be open-sourced and made available to a new and growing community of researchers looking to adapt ground-state simulations to account for electronic temperature.

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

Exploring the Energy Frontier through Precision Tests and Fast Tracking with the CMS Detector

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The Standard Model (SM) of particle physics has been remarkably successful in explaining experimental data, yet it is known to be an incomplete theory. Several key features of our universe remain unexplained, including the nature of dark matter, the observed matter-antimatter asymmetry, and the origin of the large difference between the electroweak and Planck energy scales. The Large Hadron Collider (LHC), the world's most energetic particle accelerator complex, at the European Organization for Nuclear Research (CERN) in Switzerland provides an extremely powerful tool to address these fundamental questions. This research program plans to utilize data collected by the Compact Muon Solenoid (CMS) experiment at the LHC to probe physics phenomena beyond the SM. This work will exploit the heaviest known elementary particles — the top quark and the Higgs boson — to advance our understanding of interactions between fundamental particles. Specifically, the research includes searching for lepton-flavor violating interactions that are forbidden in the SM and characterizing in greater detail the coupling between the top quark and the Higgs boson at high energies. Complementing these studies, the program also entails developing fast reconstruction of trajectories of charged particles traversing the CMS detector ("tracks"), thereby maximizing the physics potential of the future High-Luminosity LHC (HL-LHC) running period. The inclusion of track reconstruction in the CMS hardware-based collision filtering system, implemented with field programmable gate array technologies, is a novel experimental tool that will enhance sensitivity to the unique physics signatures under study. Overall, the program is both critical for the core goals of the CMS experiment at the HL-LHC and has the potential to enable entirely new searches for phenomena beyond the SM, such as tracing long-lived particles from exotic decays of the Higgs boson.

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

Quantum Black Holes and Wormholes

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A major problem in theoretical physics is to develop a complete theory of quantum gravity. This is needed to address basic questions, such as: "what happened before the big bang?" and "is space-time fundamental?'" Many important aspects of quantum gravity can be studied in the context of black hole physics. The research in this project will begin there, seeking to find the origin of the underlying quantum discreteness of a black hole. In other words: what makes a quantum black hole really "quantum"? In a second phase of the project, lessons learned from the black hole setting will be applied to the context of cosmology and the big bang. Throughout, a focus will be on strengthening the deep ties between quantum gravity and quantum information science.

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

Simulating estuarine wetland function: Nitrogen removal, carbon sequestration, and greenhouse gas fluxes at the river-land-ocean interface

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Estuaries are characterized by interactions between freshwater from rivers and saltwater from the ocean, which drives high ecosystem productivity and dynamic carbon and nutrient cycling. Estuaries can act as a filter on river inputs of nitrogen (N) and other nutrients to the ocean and can greatly reduce the amount of N that moves from rivers to the ocean. Estuarine wetlands sequester carbon (C) at high rates due to rapid vegetation growth fueled by abundant water and nutrients combined with waterlogged sediment conditions that slow decomposition. Estuarine wetlands can also be significant sources of greenhouse gases such as methane and nitrous oxide. However, estuaries and estuarine wetlands are not currently represented in Earth System Models (ESMs) such as the Energy Exascale Earth System Model (E3SM). By omitting estuarine wetland processes, models likely overestimate N inputs from rivers to the coastal ocean and underestimate C sequestration and greenhouse gas emissions in coastal regions. This research aims to understand the current and future role of estuarine wetlands in coastal C and N cycling at scales from the estuary landscape to the continental coast by simulating estuarine wetland processes in the E3SM Land Model. Model improvements will include developing chemical and biological interactions in wetland sediments and introducing salt marsh and mangrove vegetation types. Model developments will be evaluated using observational data from existing coastal wetland field sites along the Pacific, Atlantic, and Gulf of Mexico coasts of the United States. This research will enable quantitative estimates of N removal, C sequestration, and greenhouse gas emissions from estuarine wetlands at estuary to continental scales and improve predictions of coastal C and N cycling responses to changes in wetland area, river flows, and sea levels.

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

Elucidating Chirality-induced Magnetism and Magnetoelectric Functionalities in Layered Chiral Hybrid Metal Halide Perovskites

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The ability to generate and manipulate spin information is essential in spintronics, which utilizes the electron's spin degree of freedom instead of its charge to transfer and process information. Multiferroic materials exhibit multiple ferroic orders, i.e., ferroelectricity and ferromagnetism. The multiple ordered states and their magnetoelectric coupling empower the direct control of the magnetization by an electric field and vice versa. 2D layered Hybrid Metal Halides (2D-HMHs) are a new class of synthetic semiconductors prepared by low-temperature solution processing with a large chemical and structural 'universe' benefiting from their synthetic versatility. By implanting chiral organic cations into the HMH superstructure, the 2D-chiral-HMH would simultaneously exhibit ferromagnetic, ferroelectric, and magnetoelectric functionalities stemming from a Chirality-Induced Spin Selectivity (CISS) effect that may not be subject to thermal fluctuations. This proposal aims to elucidate the fundamental origins of chirality-induced magnetism via the CISS effect and their electrical tunability in 2D-chiral-HMH material systems. Two ultrasensitive detection themes based on spin-orbitronics and magneto-optics will be developed for probing the CISS-induced magnetism and magnetoelectric functionalities in this hybrid material. The proposed research will lay the groundwork for understanding the origin of the multiferroic functionality in chiral-based hybrid materials under multiple external stimuli, heralding a paradigm shift in the generation and manipulation of spin information using solution-processed, flexible hybrid materials without the need for magnetic elements.

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

Temperature-Time-Transformation (TTT) Diagrams for Predictive Solid-State Ceramic Synthesis

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Exciting new energy materials are routinely being predicted *in silico*, but their realization in the laboratory is often bottlenecked by the laborious, trial-and-error nature of materials synthesis. Developing a predictive theory of synthesis requires a better understanding of non-equilibrium reaction byproducts—which appear ubiquitously during synthesis, but are difficult to anticipate within existing theoretical frameworks. This research aims to unify classical thermodynamics, nucleation, diffusion, and crystal growth theories to predict Temperature-Time-Transformation (TTT) diagrams for solid-state ceramic synthesis. These TTT diagrams will capture crucial features in the kinetic evolution of ceramic powder precursors; including reaction sequence, reaction onset temperature, phase decomposition, liquid formation, and metastable intermediates. Guided by these TTT diagrams, a solid-state chemist can more rationally navigate through the thermodynamic and kinetic energy landscape towards the phase-pure synthesis of target materials. This research will proceed by three milestones: 1) Developing fast and accurate *ab initio* predictions of the high-temperature region of the phase diagram, at a computational expense low enough to be integrated into high-throughput materials design workflows. 2) Deriving new kinetic models for the sequential interfacial reactions that occur throughout a heterogeneous mixture of precursor powders. 3) Validation and refinement of the TTT formalism against text-mined synthesis recipes from the literature, and in a collaborative 4D nanotomography characterization of microstructure evolution during solid-state synthesis. Our ambition is to deliver TTT diagrams as a new and indispensable tool into the toolkit of the preparative solid-state chemist.

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

Physics-informed Graph Neural Networks for Data-driven Multiscale Modeling

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Predictive multiscale modeling and simulations have the potential to be revolutionized by data-driven, scientific machine learning approaches. However, such next-generation scientific machine learning models must demonstrate robustness, physics compatibility, and satisfy additional requirements compared to their traditional machine learning counterparts if they are meant to tackle high-consequence applications of interest to the DOE. We unify concepts from traditional multiphysics simulation with graph neural network architectures to obtain a machine learning framework able to guarantee preservation of important physical invariants crucial to handling problems from mechanics and electromagnetics. In this manner, physics are engineered directly into the neural network, guaranteeing desirable properties even in small data limits. A diverse selection of exemplar problems drives this foundational research, including: co-design of microelectronic devices, resilient energy storage systems, and the study of discrete fracture networks in subsurface flows.

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

Accurate Dark Energy Constraints via the Precise Characterization of Galaxy Intrinsic Alignment Coupled with Shear and Redshift Interference

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One of the most fundamental mysteries we face in physics is understanding ~~what~~ the nature of the dark energy component of our Universe ~~is~~ that causes the accelerated expansion of space. A powerful way to study dark energy is via weak gravitational lensing due to large-scale structure in the Universe, which we observe as tiny distortions in the shapes of very distant galaxies due to the bending of light by foreground mass. The Dark Energy Survey (DES) and Vera C. Rubin Observatory Legacy Survey of Space and Time (LSST) were designed to enable unprecedented measurements of these distortions in the shapes of galaxies to study dark energy. The intrinsic shapes of galaxies before they are distorted by weak gravitational lensing can cancel out some of the effects of lensing to obscure or bias what we infer about the nature of dark energy. This research program will lead to improved image-level simulations of the DES and Rubin Observatory LSST data, built using state-of-the-art methods like machine learning. These simulations will make it possible to fully characterize the cosmic impact of these intrinsic shapes on weak gravitational lensing. This work will inform crucial improvements in methodology for studying dark energy with weak gravitational lensing at the precision promised by the final DES data and the Rubin Observatory LSST in the 2020s.

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

A Multiresolution Sharp-interface Framework for Tightly-coupled Multiphysics Simulations

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An important subset of energy-related systems in fluid mechanics, geophysics, and industrial applications can be modeled as interface-coupled multiphysics problems. For these problems, the accurate prediction of system properties near moving boundaries and interfaces is a valuable capability that enables optimization of sensor placements, analysis of structural loadings, and many other insights. Significant modeling and algorithmic challenges stem from the wide range and scale separations of time and space in each domain, the large motions and deformations of the interface separating the domains, and the coupling between the different domains across such moving interfaces. This proposal aims to overcome these challenges by combining a high-fidelity treatment of sharp moving interfaces with a localized tight coupling strategy. The research from this novel paradigm will be implemented within a scalable multiresolution software framework. Testing and validation will be carried out on two representative applications: two-phase incompressible flows and fluid-structure interactions.

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

Atomic Resolution of Lignin-Carbohydrate Interactions in Native Plant Tissues from Solid-State NMR

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The carbon-rich plant cell wall is a sophisticated composite of macromolecules, with a highly complex structure that is beyond the level that humans can artificially produce. The secondary plant cell wall comprises the majority of biomass and serves as the central source for biofuel, biomaterial, and high-value bioproducts. The interactions between the phenolic polymer lignin and polysaccharides make the biomass recalcitrant to post-harvest processing but the physical nature of these polymer interactions is not well understood. The biomolecules in their cellular environment are often insoluble, non-crystalline, and structurally polymorphic, thus evading high-resolution characterization. The primary objective of this project is to overcome the technical bottleneck by developing a biophysical toolbox that enables atomic-level investigations of cellulose, hemicellulose (xylan and glucomannan), and lignin using native stems of *Arabidopsis*, maize, poplar, and spruce. We will resolve the physical packing and covalent linkages of lignin and polysaccharides and understand their heterogeneous hydrophobicity and dynamics in whole-cell samples. Comparing wild-type samples with lignin-engineered, transgenic plants will uncover the molecular principles involved in biopolymer interactions and supramolecular assembly. The fundamental knowledge will advance our understanding of energy storage in plants, form the foundation for optimizing the utility of lignocellulose for energy and biomaterial, and inspire the rational design of synthetic polymers and composites with tunable structure and properties. The biophysical methods established here will enable investigations of many energy-relevant systems such as plants, algae, microbes, as well as carbon-rich materials and polymers.

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

Enhancing Performance of Bosonic Qubits in Circuit QED with Reservoir Engineering

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Quantum information technologies are built from a collection of physical qubits (quantum bits) and seek to use their superpositions and entangled states to process information. A central challenge for their development is the fragility of qubits: All qubits incur random errors due to undesirable interactions with their dissipative environment, a process known as decoherence. The common approaches for suppressing quantum errors have focused on device-level isolation from the environment and software-level implementation of quantum error correction codes. Recently, an intermediate and unifying approach emerges from the progress in "quantum reservoir engineering". Surprisingly, the environmental interaction can be tailored, rather than eliminated, to provide the equivalent of a restoring force to the qubits, which can stabilize quantum superpositions and even passively correct errors in encoded logical qubits.

The goal of this research is to experimentally establish a paradigm of using engineered dissipation to reduce errors in the storage and manipulation of qubits. We employ a leading candidate platform for quantum computation, the superconducting circuit QED, where we choose to use 3D superconducting microwave cavity oscillators as qubits. More specifically, we encode logical qubits in the bosonic states of the cavities with a specific photon number parity, and use standard Josephson circuits known as transmons as ancillas for quantum control. The project builds on our initial demonstration of a parity-recovery dissipation operator capable of autonomously reversing cavity photon loss without the large quantum and classical resource overhead needed for active error correction. The dissipative process will be systematically characterized, refined, and integrated with other stabilization schemes and unitary control, leading to improved logical qubit lifetime and logical gate fidelity. If successful, this project establishes these self-stabilized individual qubits and gates as improved building blocks for generic intermediate scale applications of quantum computing without the need of large-scale error correction.

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

Structure-Exploiting, Adaptive, Zeroth-Order Optimization to Improve Efficiency

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This project addresses complex design, decision, and control problems that do not readily admit a closed-form algebraic description. Such problems often rely on information from "black boxes" such as computationally expensive simulations and experimental and observational measurements. These black boxes often lack the information needed to use advanced mathematical optimization and machine learning techniques, which typically rely on more complete mathematical descriptions. We develop mathematical optimization models and methods for these scenarios by exploiting mathematical structure, parallel resources, and adaptive strategies.

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

Machine Learning-Enabled Advanced Electron Tomography for Resolving Chemical Inhomogeneity and Materials Dynamics in Lithium-Ion Battery Electrodes

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The development of lithium-ion batteries (LIB) is one of the key innovations in the past several decades that have revolutionized many aspects of our lives and changed how we interact with machines and the environment. However, building safe, high-energy, long cycle-life and low-cost batteries is still a challenge for the research community. Many of the long-standing issues in the field are due in part to the lack of characterization tools to resolve the electrode materials' failure modes and degradation mechanisms. The central goal of this research project is to develop machine learning-enabled low-dose and chemically sensitive atomic-resolution electron tomography as well as high temporal resolution electron nanotomography to reveal novel phenomena related to the dynamic evolution of the surfaces and interfaces in LIB electrodes. This project will result in three-dimensional imaging of atomic species, bonding, and electronic structures at the atomic scale as well as unprecedented sub-10-second temporal resolution for probing battery materials' transformation dynamics. When realized, this technique will offer a significant improvement in electron tomography's capability in imaging chemistry as well as temporal resolution compared to the state of the art and will offer opportunities to directly visualize transformations of electrode materials in energy storage devices during electrochemical reactions. These new capabilities will impact materials characterizations at the sub-nanometer scale beyond battery materials.

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

Deciphering and Manipulating Low Dimensional Magnetism

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The ultimate success of materials by design depends critically on our ability to accurately predict material properties from first principle theories. For materials with weak electron-electron interactions, such efforts have been largely successful due to the ability of Density Functional Theory to correctly predict electric and optical properties in real materials. However, most materials with exotic quantum phenomena exhibit non-negligible many-body effects for which material property prediction is still largely limited. Such is the case of two-dimensional magnetism recently realized in a class of van der Waals materials that exhibit diverse electric and optical properties with rich potential to become platforms for versatile novel devices. This proposal aims to bridge the gap between first principle calculations and electric and optical properties of these two-dimensional magnetic materials via measurement of the single-particle spectral function by angle-resolved photoemission spectroscopy. The main goals of this ressearch are to i) provide fundamental physics knowledge of the origin of the magnetism in the three-dimensional versions of the bulk materials, ii) understand how key ingredients for magnetism evolve from the three-dimensional limit towards the two-dimensional regime, and iii) investigate the effect of external perturbations and tunability of the magnetism by directly measuring the electronic response when subject to different environments. The methodologies developed here will benefit the explorations of a broader class of correlated materials for both fundamental science and potential applications.

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

Quantum Performance Enhancement

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Despite their exquisite engineering, quantum information processors (QIPs) are exceptionally susceptible to interference from their environments. The grand challenge of experimental quantum computing is to reduce the rate at which errors appear in computations to below a threshold where useful algorithms become feasible. But today's QIPs are limited – sometimes even crippled – by calibration errors. Qubits, quantum processors, and the classical systems that control them are sensitive to a surprisingly large set of adjustable parameters. All of them need to be tuned and calibrated very precisely – and then recalibrated as conditions change – to keep errors from overrunning computations. But today's most widely used techniques to tune and maintain control parameters are ad hoc and inefficient. They don't leverage modern quantum computing theory, or recent breakthroughs in error characterization. This research will solve this fundamental performance-limiting problem by developing fast and efficient calibration methods that work for all qubit technologies and can operate efficiently at scale. The results of this project will enable QIPs to maximize their potential for near-term computational advantage and catalyze progress towards the DOE's goal of realizing QIPs able to significantly advance scientific discovery.

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

Multi-kHz Laser-plasma Accelerator Driven by Spectrally Combined Fiber Laser

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Particle accelerators are critical instruments for discoveries and applications in high-energy physics and across science and industry. Laser-plasma accelerators (LPAs) could greatly reduce the sizes and costs of future particle accelerators, by using laser-driven plasma structures that produce very high accelerating gradients, but increased repetition rate is needed to enable applications. While fiber lasers are considered one of the most promising solutions to drive high repetition-rate LPAs, the optical pulses produced from existing fiber lasers are too long. This research addresses the gap between the limited pulse durations of existing fiber lasers and LPA application needs, using a novel pulse duration reduction approach. This research will develop a fiber laser system with a spectral combination architecture that delivers energetic ultrashort optical pulses to drive an LPA, and will demonstrate high repetition-rate LPA operations at multiple kilohertz, where an accelerator control system will be implemented based on fast feedback including machine learning. The laser and LPA technologies developed under this research can enable many applications using high repetition-rate electron beams including those in science and medicine, and with further scaling of laser pulse energy can enable the path to future laser-driven particle colliders.

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