Scale-Aware Modeling of Instabilities and Mixing in HED Flows

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Instabilities and mixing are detrimental to system performance in high-energy density (HED) applications such as fusion power systems. Numerical models used in HED applications have had significant difficulties predicting the instabilities and mixing that occur in experiments. Most of these "global-system" models cannot resolve a sufficient level of vorticity that develops hydrodynamically. Recent evidence from several independent investigations indicates that this shortcoming contributes to under-predicting the levels of instability growth and mixing in such highly nonlinear flows. Routinely conducting multi-physics global-system three-dimensional simulations at the high resolution required to resolve the missing vorticity is not feasible in the foreseeable future due to the exorbitant computing cost. To address this problem, a "coarse-graining" scale-analysis approach that is versatile and powerful will be used to develop a nonlinear mixing model (NMM) capable of accounting for the missing vorticity in a self-consistent manner. Coarse-graining has a rigorous mathematical foundation and is closely related to well-established physics techniques, including macroscopic electromagnetism, renormalization group, and Large Eddy Simulations. NMM is a deterministic model of vorticity and strain that is "scale-aware" in the sense that it self-adjusts to the underlying numerical resolution without relying on user input. NMM is also portable in the sense that it is not dependent on a particular numerical scheme and can be eventually deployed in HED application codes. With that eventual goal in sight, the research plan includes an extensive development, testing, and validation program. The project should enable HED application codes, such as those used in fusion, to better predict instability growth and mixing at a significantly lower computational cost. The project may also prove valuable beyond HED applications by advancing a new systematic approach to devising deterministic scale-aware models that reflect the latent unresolved physics.

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

New Correlated Numerical Methods for Attosecond Molecular Single and Double Ionization

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The correlated character of electronic motion affects the energy balance of all light-induced microscopic processes in matter, from those triggered in atoms, to those in photoreceptors for solar-energy conversion. Electronic excitations, which are at the core of any chemical transformation, evolve on the fantastically short timescale of the attosecond (one attosecond is one billionth of a billionth of a second). The advent of attosecond spectroscopies has made it possible to study the motion of electrons at its natural timescale. Intense extreme ultraviolet (XUV) light pulses can both excite and image electrons in matter, drastically enhancing the space and time resolution with which ionization can be controlled. Ultrashort soft-x-rays can ionize molecules from highly localized core orbitals. The emitted electrons, scattered by neighboring nuclei, encode geometry of a molecule as it changes in time. If detected in coincidence, two electrons emitted by the same molecule give direct information on their concerted motion in a chemical bond prior to ionization. The theoretical description of these phenomena is essential to control ultrafast dynamics in matter. This project will develop the numerical tools needed for the time-dependent description of molecular single and double-ionization processes, with a quantitative account of light-driven static and dynamic electronic correlation. Such endeavor will make it possible to image correlated electronic motion, thus opening the way to a transformative expansion of attosecond science, and of quantum chemistry itself.

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

Probing Electrochemical Reactivity Under Nanoconfinement Using Molecularly Pillared Two Dimensional Materials

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The goal of this proposed research is to understand how the confinement of liquid phase reactants within the layers of a two dimensional material influences their electrochemical reaction kinetics. The hypothesis driving this research is that there will be an optimum interlayer spacing of layered materials to enable electrochemical reactivity in the interlayer. Layered and 2D materials have broad applications in catalysis and electrocatalysis, where it is hypothesized that the catalytically active sites reside at edges and surface defects. This proposed research will investigate how the nanoconfined interlayer of these materials can be made accessible for electrocatalytic activity. Nanoconfinement has been shown to affect the physical properties of molecules and solvents and may be utilized to further tune electrochemical activity. Importantly, the research will utilize a materials chemistry approach to define the nanoconfinement environment via molecular pillars – molecules of defined length anchored within the interlayer. In order to test this hypothesis, the proposed research will investigate how molecular pillaring of a prototypical layered material, MoS_2, influences the electrocatalysis of the hydrogen evolution reaction, a critical step in the electrochemical synthesis of hydrogen fuel. The scientific merits of this proposed research include: (1) the control of matter at the atomic scale to define nanoconfinement geometry, (2) the characterization of the dynamics of nanoconfined solvents within the hybridized layered materials, and (3) the mechanistic understanding of a liquid-phase electrochemical reaction under nanoconfinement by the hybridized layered materials. The understanding developed over the course of this research will be applicable to both fundamental and applied energy research, from electrochemistry and materials chemistry, to fuel cells and electrolyzers.

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

Systematics of Precision Neutron Physics Experiments

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The neutron is an exceptional tool for sensitive searches for new particles and interactions beyond our Standard Model of Particle Physics. This research will characterize the influence of several effects that limit the ultimate physics reach of two experiments at the Spallation Neutron Source which test our understanding of the fundamental symmetries of nature—Nab (for Neutron 'a' 'b') and nEDM (for neutron Electric Dipole Moment). Nab will study neutron beta decay to improve our understanding of the weak interaction. This research will develop a detector test station to benchmark simulations of charge collection in the Nab detectors and study the impact on electron energy loss effects and the measured trigger time of electrons and protons. Meanwhile, nEDM will search for a new source of a violation of Time-reversal (T) symmetry in the neutron's electric dipole moment. T-symmetry, or whether the laws of physics are the same when time runs forward or backwards, must be violated to explain why our universe is matter dominated. This research will leverage the Summit supercomputer to develop fast spin tracking simulations in realistic models of the experiment to calculate effects which limited the ultimate precision of the previous best experiment. The outcome of this research will allow Nab to characterize the weak interaction with similar sensitivity to nuclear systems, where a discrepancy from Standard Model predictions is observed, and ensure that nEDM can realize its full potential in probing the parameter space of theories which predict a matter-antimatter asymmetry in the universe.

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

Spatiotemporal Mapping of Lignocellulose Decomposition by a Naturally Evolved Fungal Garden Microbial Consortium

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Some microbial communities composed of bacteria and fungi can readily breakdown plant matter into its component sugars. Leaf-cutter ants take advantage of such microbial communities by maintaining fungal gardens that release energy-rich carbohydrates from plant biomass. As these decomposition products are released, they are consumed by bacteria that also live in the garden and in turn, further transform those products into nutrients that promote fungal growth. This symbiotic system has great potential for biological production of biofuels and bioproduct precursors from plant biomass. However, the identity of most of the microbial species and their precise role within the fungal gardens is not known. This project will carry out a multi-omics approach to uncover the mechanisms that drive cooperative fungal-bacterial interactions that result in the degradation of lignocellulosic plant material extracted from the fungal garden ecosystem. To understand how the fungal garden is able to degrade plant matter with such efficiency, it is necessary to study the metabolic interactions and biochemical pathways utilized by its microorganisms in each microscopic region of the fungal garden. This research will accomplish that with a novel microscale proteomics approach that can analyze very small samples, providing detailed information on the location and function of fungal and bacterial proteins. This approach will provide the knowledge needed for a predictive systems-level understanding of the fungal-bacterial metabolic and signaling interactions that occur during cellulose deconstruction in an efficient, natural ecosystem and should provide new strategies for generating precursors of advanced biofuels. This knowledge will provide the foundation for developing efficient consortia composed by well-defined and optimized microbial strains to efficiently produce valuable compounds from lignocellulosic feedstocks, advancing DOE's goal of developing sustainable bioenergy resources.

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

Boosting New Physics Searches with Higgs Differential Cross-Section Measurements

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The Standard Model (SM) of particle physics describes our current best understanding of the elementary constituents of matter and their interactions. Despite the success of the SM, a number of observed phenomena in our universe are not well-described to the extent that prevailing results point to the existence of a more fundamental theory. The Large Hadron Collider (LHC), the world's most energetic particle accelerator complex, at the European Organization for Nuclear Research (CERN) in Switzerland is in a unique position to provide critical insights into the SM puzzle. Direct searches so far have shown little to no hints of new particles, indicating that new physics might be at higher energy scales. Precision measurements, which can provide access to physics beyond the SM, are therefore becoming increasingly critical to the experimental research program at the energy frontier. This research program plans to use data from the ATLAS (A Toroidal LHC ApparatuS) experiment at the LHC to measure the differential cross-section of diboson processes in final states with a Higgs boson. Such measurements are sensitive to new particles, which may be too heavy to be clearly seen at the LHC. Further, the sensitivity to new physics phenomena will be increased through the high luminosity upgrade of the ATLAS detector presently being carried out for the future High-Luminosity LHC running period, which is planned to begin in 2026. To maintain the efficient data collection, the program also entails the upgrade of the real-time data selection process, or trigger, by implementing new sophisticated algorithms that will increase the acceptance to the final states being studied. Overall, the impact on our understanding of fundamental physics will be dramatic, enabling us to either severely constrain possible extensions of the SM or discover new particles or interactions arising in the universe.

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

Development of Novel Relativistic Electronic Structure Methods for Actinide-Containing Compounds

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As electrons in "heavy atoms" with large nuclear charge often move at speeds comparable to the speed of light, special relativity has profound influence on electronic structure and properties of compounds containing heavy atoms. Consequently, treatment of relativistic effects has emerged as a major challenge for theoretical and computational description of molecules containing heavy atoms. The objective of this research is to provide significantly enhanced capabilities for theoretical and computational study of molecules containing heavy elements, especially actinides, which play essential roles in basic energy science. One major obstacle in relativistic quantum-mechanical computations of actinide-containing molecules with sufficient consideration of correlation between electrons is the high computational cost because of spin-symmetry breaking due to the presence of spin-orbit coupling. Namely, with the interaction between electron spin and orbital angular momenta, electrons with different spins are coupled together and this increases the required computational resources by more than an order of magnitude. The present work is based on a simple idea of partial recovery of spin symmetry to enhance computational efficiency for calculations with accurate treatment of electron correlation. This research aims to provide efficient computational tools generally applicable to sizable actinide-containing molecules. The applications of the new methods and computational tools focus on classic problems in molecules containing actinides and deal with the response of these molecules to optical and magnetic interactions. The new methods can treat relativistic effects and electron correlation with an unprecedented level of accuracy, and thus are promising candidates to solve these problems and others in this milieu of chemistry.

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

Probing Anionic Electron Behavior in Electrides

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Recently discovered electride materials offer untapped electronic and chemical properties with the potential to transform next-generation nanoelectronics and energy technologies. However, electrides are only beginning to be characterized and understood. These materials have unusual structures with loosely-arranged electrons that offer rich physics and exotic properties, including superconducting, topologically insulating, magnetic, and high-catalytic activities. This research will develop the first experimental technique to probe electride materials and measure their responses to stimuli such as temperature or electricity at unprecedented nanoscale resolution. To achieve this, scanning transmission electron microscopy will be tuned to "see" the functional electrons in materials undergoing dynamic changes, thereby opening possibilities for fine-tuning electrides at the atomic-level to achieve desirable properties. The fundamental outcomes of this research will greatly expand the ability to study electrides, as well as other quantum materials, and further launch the design and discovery of new materials for broad energy applications.

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

EIC physics from Lattice QCD

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Quantum Chromodynamics (QCD) is the theory of the strong interaction, which binds quarks and gluons to form a spectrum of hadrons, which includes the pions, kaons, and protons. Lattice QCD (LQCD) is an ideal formulation to study the properties and the immensely rich structure of the hadrons with large-scale numerical simulations. The program focuses on LQCD calculations of non-perturbative quantities that encapsulate the dynamics of quarks and gluons within the pions, kaons, and protons, which is necessary for a deeper understanding of nuclear matter. It addresses open questions, such as the origin of the mass and spin decompositions. Both topics were identified as priority science questions in the recent assessment report of the National Academies of Sciences, Engineering, and Medicine, on a future Electron-Ion Collider (EIC). This program supports the science of the EIC with studies of parton distribution functions (PDFs) and generalized parton distributions (GPDs) using two approaches: via their Mellin moments, and via the so-called quasi-distributions. Specific quantities under investigation are form factors and generalized form factors for the unpolarized, helicity and transversity distribution functions. The calculations are based on cutting edge methods for a set of simulations with the quark masses fixed to their physical value. This eliminates a large number of systematic uncertainties, which is crucial for reliable input to experiments, and for comparison to existing measurements**.**

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

High-Efficiency Solar-To-Fuel Photoelectrochemistry in Disordered Photonic Glass Electrodes

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Photoelectrochemical (PEC) solar energy conversion applications (water splitting, dye-sensitized solar cells, CO_2 reduction, etc.) rely on chemical reactions driven by photogenerated minority carriers at a semiconductor-liquid junction. The carriers must be sufficiently long-lived to migrate to the semiconductor-electrocatalyst-electrolyte interface, where they are collected via energy storing redox reactions. Nanostructure can be engineered into photoelectrodes to trap light near the interface, thereby promoting absorption in regions of the semiconductor that improve the likelihood of collecting carriers versus losing them to recombination. Disordered assemblies of nanospheres can induce emergent 'slow' modes that can localize light along tortuous 'paths' through the long dimension of the electrode (multiple scattering) or in small volumes (Anderson localization). Defects in disordered materials can act as high-quality optical cavities or waveguides. This project seeks to develop the approach for improving the efficiency of PEC materials by controlling emergent photonic modes in disordered nanostructures. The specific aim is to advance the use of optical cavities at defects in disordered nanosphere materials as a new light-trapping nanostructure for photocatalytic (PC) or PEC energy conversion applications. This project outlines an integrated approach based on machine learning-driven light-absorption simulations, high-resolution materials characterization, and novel modes of materials synthesis to identify powerful strategies for utilizing disordered photonics in solar-to-fuels applications. The goals of the project include 1) simulating the optoelectronic properties of disordered photonic glasses based on the parameters defining the statistical structure (filling fraction of nanospheres, diameter of the cavity, and the local dielectric environment), 2) identifying synthetic methods for selectively functionalizing the defect cavities of electrodes, and 3) developing experimental methods to characterize the optical and photochemical/photo-electrochemical properties of the defect structures.

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

Using Ultrafast Entangled Photon Correlations to Measure the Temporal Evolution of Optically Excited Molecular Entanglement

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Entangled photons can be created by splitting one photon into two lower energy photons via the process of spontaneous parametric down-conversion. The resultant pair of photons, however, can still act as one photon in subsequent light-matter interactions. For example, an entangled photon pair has a molecular absorption cross section close to that of a single photon, will only leave the same side of a 50:50 beamsplitter, and diffract at half their wavelength. The goal of this project is to measure how the entangled photons' properties are temporally transferred to a molecular spin state. This includes measuring how quantum and classical decoherence routes control entanglement, the timescale of these processes, and whether or not these quantum states can be transferred to a secondary, electronically coupled system. To probe these questions, a few-femtosecond, few-photon entangled spectrometer will be constructed. The proposal will answer fundamental questions about entangled light-matter interactions as well as create new avenues in ultrafast spectroscopy through the application of entanglement.

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

Analog and Digital Quantum Simulations of Strongly Interacting Theories for Applications in Nuclear Physics

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Classical-computing methods have proven extremely successful in obtaining certain properties of strongly interacting systems of hadrons and nuclei. Nonetheless, it is known that a number of grand-challenge problems in nuclear physics remain theoretically intractable. These include investigations into the real-time dynamics of matter after the Big Bang, or after the collision of energetic nuclei in the Relativistic Heavy Ion Collider. These also include studies of the properties of dense systems in nature, such as the possibility of exotic phases of matter in the interior of neutron stars. Recent technological advances in scalable quantum-computing platforms provide an exciting possibility in harnessing quantum entanglement to perform highly-parallelized computations of systems in nuclear physics with a large number of correlated degrees of freedom. The overarching goal of this project is to fill in the gap between our classical and quantum approaches to simulating nuclear phenomena from the microscopic theory, i.e., the Standard Model of particle physics at a finer level, and nuclear effective field theories at a coarser level. With a focus on the question of how to map strongly interacting field theories to a quantum-bit (qubit) description, two avenues of research will be pursued. First, novel schemes for analog simulations of simple lattice gauge theories and effective field theories of nuclei will be developed and simultaneously tested on the world's leading Ion Trap quantum-simulation platforms. Second, similar theories will be studied theoretically, and will be benchmarked on available digital quantum computing devices. The benefits and disadvantages of each approach will be studied and quantum-resource estimates will be provided for reaching certain levels of accuracy in obtaining properties of the systems under investigation. This research, while being only a first step toward the ultimate goal of conquering computationally challenging problems in nuclear physics, will pave the way toward leveraging quantum-computing capabilities for research in nuclear physics.

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

Porin Inspired Ionomers with Sub-nm Gated Ion Channels for High Ion Conductivity and Selectivity

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Imagine a group of people standing side-by-side and passing refreshments from one person to the next. If the people are water molecules and the refreshments are protons (atomic hydrogen after stripping off an electron), then this perfectly explains proton transport in an ideal scenario. Water molecules need to be aligned and connected with each other to transport protons from one water molecule to the next. Natural living systems do so using porins in the cell membranes. Porins are barrel shaped biomolecules that act like pores allowing transport of ions from the outside environment to the inside of the cells and vice versa. Porins also act like gates that can control ion trafficking and the direction of ion transport. If these unique concepts can be used in the design of man-made ion conducting polymer mimics, unprecedented control over ion conduction pathways can be achieved at the molecular level. This research will explore a novel class of ion conducting polymer by incorporating porin mimicking functional repeat units in the polymer chains and introducing gating functionalities to those units. These porin mimicking units of the polymer chains will act like ion conducting water channels that inhibit the transport of larger ions and selectively transport smaller ions, like protons. Such a design can be beneficial for ion conducting polymer membranes used in redox flow batteries. The gating functionality of the porin mimicking units will help gain control over proton accumulation within polymeric systems. This is important as proton accumulation negatively impacts fuel cell efficiency. Studying the roles of gating nature, polymer structure, and molecular packing on ion conductivity and selectivity for certain ions will guide the future designs of ion conducting polymers for energy conversion and storage devices.

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

New Tools for Strongly Coupled Quantum Field Theories

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Quantum field theory (QFT) is a unifying language that pervades many areas of modern physics, including particle physics, string theory, and condensed matter physics. Nevertheless, it is typically very challenging to extract physical predictions from a given QFT. Conventional methods only apply when the QFT is weakly coupled (i.e. essentially non-interacting), while many QFTs of interest are strongly coupled and thus not amenable to these approaches. The primary goal of this research is the development and application of new tools for analyzing strongly coupled QFTs. These tools are based on different notions of symmetries, which can be used to simplify QFT problems even in the strong-coupling regime. Supersymmetry (SUSY) plays a particularly important role in this research. While SUSY QFTs often arise in the context of string theory or particle physics beyond the Standard Model, this research uses them as a fruitful theoretical laboratory for exploring QFTs at strong coupling.

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

Discovering Dark Matter Clumps and Primordial Particles with Galaxies

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Cosmological observations and galaxy dynamics seem to imply that five out of six parts in mass of all matter in the universe is composed of dark matter, which is not accounted for by the Standard Model of particle physics. The cold dark matter (CDM) paradigm has been extremely successful at describing observations on large-cosmological scale. However, many different dark matter candidates have the same observable effects as CDM on large-length scales. One possible avenue to distinguish between these different models is to look on much smaller-length scales, where usually dark matter models become distinguishable. This research will develop the theoretical framework and statistical tools needed to map the detailed distribution of dark matter on subgalactic scales using strong gravitational lensing. A second goal of this research is to build new statistical techniques that efficiently exploit the full power of cosmic-structure data from next-generation surveys. Galaxy clustering on large scales provides significant cosmological information through the power spectrum. Additional information can be gained from higher-order statistics. This research will provide new ways to understand the nature of dark matter and the initial conditions of the universe from current and upcoming cosmological surveys.

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

Multi-Probe Cosmology with DES and LSST

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Ongoing and future DOE experiments, including the Dark Energy Survey (DES) and the Large Synoptic Survey Telescope (LSST), aim to unveil the physical mechanism causing the accelerated expansion of the Universe. Possible theoretical explanations require fundamentally new physics, elevating the topic of "dark energy" into one of the most exciting problems in science today. In order to discover new physics in the great laboratory that is our Universe it is critical to control systematics at a new level of precision. The main objective of this research program is to develop novel data analysis techniques to combine multiple cosmological measurements extracted from DES and later LSST data and to control systematics at the level required to extract the cosmological information. Working across a variety of science areas, such as cosmology, astrophysics, computer science, and statistical methods this research explores whether dark energy is explained by Einstein's cosmological constant, whether it shows variations as a function of time, or whether the theory of General Relativity itself must be modified. Ultimately, this science program paves the way for a joint analysis of LSST in combination with the Cosmic Microwave Background (CMB) experiments of the mid 2020s such as the DOE-led CMB-Stage 4 experiment.

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

The Role of Cooperative Interactions among Surfaces, Solvents, and Reactive Intermediates on Catalysis at Liquid-Solid Interfaces

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Catalytic reactions at solid-liquid interfaces formed between solvent mixtures and the surface of a heterogeneous catalyst possess the complexities of catalysis at gas-solid interfaces, but then are further complicated by interactions of solvent molecules. The presence of solvating molecules introduces specific interactions among solvent molecules, catalyst surfaces, and reactive species that can change turnover rates and selectivities when different solvents are implemented for catalytic reactions, such as hydrogen transfer, alkene oligomerization, coupling reactions, and selective oxidations. These complex interactions couple fast, short range electron transfer and transformations at active sites to slower, long range changes in the solvent structure. Intuition for the effects of solvents on chemical reactions exists; however, these heuristics do not account for surfaces and often fail for heterogeneous catalysts. This research will quantify the impact and elucidate the molecular motifs of solvent-mediated interactions between reactive species and the extended surface of solid catalysts, which will provide new approaches for engineering solid-liquid interfaces for selective catalytic reactions. These effects can be used to increase turnover rates and selectivities for liquid-phase alkene epoxidations in porous materials by orders of magnitude. The effects depend on the surface topology around catalytically active sites; the size and hydrogen bonding nature of the solvent; and the specific interactions of the solvent with reactive intermediates on the surface. Knowledge generated in this work will show how catalytic rates and selectivities depend on coupling between solvent dynamics and surface kinetics and how these processes are impacted by the extended surface of the solid catalyst, beyond the active site. Ultimately this will provide broad insight for how solvents facilitate catalysis at surfaces and yield potentially transformative principles to engineer solid-liquid interfaces for catalytic conversion of domestic resources, including light hydrocarbons and renewable biomass.

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

Nuclear Astrophysics through Simulations of Neutron Star Mergers Using Monte-Carlo Neutrino Radiation Transport

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The merger of two neutron stars is a remarkable laboratory for nuclear astrophysics. By observing merging neutron stars, we improve our understanding of dense nuclear matter, the origin of heavy elements likely produced in merger events (e.g. gold, platinum,…), or even the properties of neutrinos. Studies of neutron star mergers thus complement studies of dense matter and heavy nuclei conducted within DOE laboratories. To reliably extract nuclear physics information from merger observations, however, accurate numerical simulations of these events are necessary. Existing simulations have two critical limitations: their resolution is not sufficient to capture important small scale instabilities in the evolution of magnetic fields, and they only approximately evolve neutrinos, despite their crucial role in determining the outcome of nucleosynthesis in mergers. The first objective of this project is to develop an algorithm that truly evolves the equations governing neutrino transport (using Monte-Carlo methods), a long-standing objective that modern computational resources have finally put within our reach. This algorithm will then be implemented in a next-generation open-source code that can leverage upcoming computing facilities to perform high-resolution simulations of neutron star mergers. The second objective of this research is the inclusion of more detailed nuclear physics in the evolution of the matter ejected by mergers, where heavy elements are synthesized. Finally, the last objective of this project is to use these new methods in simulations that can reliably predict the production of heavy elements in neutron star mergers, as well as the impact of the properties of dense matter on the optical and infrared signals that mergers power, thus increasing the payoff of neutron star merger observations for nuclear physics.

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

Mechanistic Tuning of Chemical Transformations for Coupling the Geo-mimicry of Acid Gas Storage with Design Strategies to Produce Clean Energy Carriers in Multi-Phase Reaction Environments (MATTER)

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Developing transformative and adaptive energy generating processes with in-built environmental controls is essential for meeting our growing needs for energy and resources in a sustainable manner. Achieving these outcomes requires harnessing coupled reaction pathways to simultaneously synthesize targeted molecules in the fluid and solid phases in a single system. One example in this context is the directed synthesis of H_2 and Ca-or-Mg-bearing carbonates in gas-liquid-solid environments starting from the reactants in the water gas shift reaction which are CO and H_2O, and earth abundant minerals such as forsterite (Mg_2SiO_4) and wollastonite ($CaSiO_3$) as the chemical building blocks. However, in far from equilibrium environments, critical scientific insights into the reaction pathways remain locked in transient kinetics. To address this challenge, we propose to create a multi-modal non-invasive experimental strategy that harnesses synchrotron X-ray scattering and tomography techniques. This experimental methodology allows us to probe and link structural and morphological transformations in multiphase environments to the kinetics at far-from-equilibrium and at equilibrium conditions. This research approach will allow us to develop a chemo-morphological basis for designing targeted reaction pathways to direct the synthesis of clean energy carriers such as H_2 while capturing, converting and storing CO_2 as Ca- and Mg-carbonates.

**Proposal originally submitted by the University of Wisconsin*
This research was selected for funding by the Office of Basic Energy Sciences.

Mechanics of Materials' Interaction with Electromagnetic Waves in Accelerator Cavities

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To realize high performance and cost effective accelerators and RF sources, our focus must shift to development of materials' microstructure with significantly higher resistance to degradation than what is employed today. A synthesis pathway toward materials that are an order of magnitude more resistant to RF induced degradation will be developed under this effort. The synthesis pathway will follow materials' microstructure evolution through the stages of its lifetime: (1) initial production, (2) assembly and processing steps (joining, bake-out), (3) conditioning, and (4) long-term operation. An elasto-plastic model of the material's response to RF surface fields, relating material microstructural state (grain size, texture, morphology, purity, presence of defects) to surface electromagnetic fields will guide the synthesis pathway development. Finally, the mechanics of materials' interaction with RF will be characterized using newly developed in-situ RF-pump / X-ray probe diffraction technique (at room temperatures and at 2 K) allowing to measure temporal evolution of materials' microstructural state and validate the materials model. This effort broadens the RF accelerator science and technology field with innovations in materials synthesis, characterization, and modeling. It also impacts progress in millimeter-wave and terahertz RF source technologies, which are currently limited in RF output power by materials employed in their circuit structures.

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

Ultrafast Visualization of Hydrodynamic Evolution: Understanding Void Collapse at Extreme High-Pressure Conditions

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Mesoscale imperfections, such as voids, play a crucial role in the physical and chemical behavior of all materials. The need to understand how voids dictate materials performance under extreme conditions cross-cuts geophysics, astrobiological physics, planetary-, fusion energy-, and national security- science. New research will combine ultrafast X-ray probes with laser-shock compression at the Matter in Extreme Conditions instrument at the Linac Coherent Light Source to study the microphysics of void collapse processes. Novel time-resolved, coherent diffractive X-ray imaging methods will yield atomic-level movies of the void collapse process during the passage of a shock wave. These measurements will inform materials models that are critical for solving a variety of physics problems across the mission space of Fusion Energy Sciences. In particular, hydrodynamic instabilities, seeded by void collapse in dynamically compressed materials, are one of the main obstacles to achieving fusion ignition in the laboratory. Real-time measurements will reveal how void size and geometry dictate rapid heating effects and nonlinear shockwave interactions leading to plasma jet formation and phase transformation/degradation in the surrounding material. This new methodology will provide experimental data with the precision to test materials functionality and theoretical models in a regime where no previous data exist.

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

Development of a Laser Calibration System for the DUNE Far Detector

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Neutrino related discoveries in the last two decades indicate that the answer to the most sought-after question of why we live in a matter-dominated universe may be within reach. The Deep Underground Neutrino Experiment (DUNE) which forms the next generation long-baseline neutrino oscillation experiment aims to address this question by studying the differences in propagation between neutrinos and anti-neutrinos traveling over a distance of 1300 km from Fermilab to South Dakota. DUNE will consist of two detectors, one detector installed at Fermilab and a second, much larger, detector will be installed more than a kilometer underground at the Sanford Underground Research Facility (SURF) in Lead, South Dakota. DUNE will use the cutting-edge liquid argon time projection chamber (LArTPC) technology to detect neutrino interactions at the far site. DUNE presents a unique challenge for calibration in many ways. Not only because of its size—the largest LArTPC ever constructed – but also because of its depth. It differs both from existing long-baseline neutrino detectors, and existing LArTPCs due to its deep underground location. For DUNE, to fully exploit the capabilities of a LArTPC and to make convincing physics measurements, a detailed understanding of the detector response is essential. The main objective of this research is to develop a laser-based calibration system for DUNE, with the ultimate goal of testing and validating the design and performance of the system along with data analysis in the run-II phase of the DUNE prototype detectors, ProtoDUNEs, located at the European Organization for Nuclear Research (CERN), Switzerland. This work will enable DUNE to reduce systematic uncertainties arising from detector response model and correctly predict the far detector energy spectra that indicate the neutrino oscillations for which DUNE is searching.

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

Lithium–Divertor Interactions and Helium/Hydrogen Trapping in Lithiated Metals

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Producing energy from controlled nuclear fusion reactions on Earth is a formidable challenge. One potential path to commercial nuclear fusion energy is magnetic confinement fusion, which uses magnetic fields to confine the extremely hot, ionized gases that undergo nuclear fusion and prevent them from touching the container. Injecting lithium into fusion reactors or coating the reactor walls with lithium is an active area of research intended to increase the difference in temperature between the hot, ionized gases in the center, where the fusion reaction occurs, and the relatively cool solid walls of the reactor. This research examines the fate of helium—the biproduct of the fusion reaction—and ascertains whether and how it will accumulate at the interface between lithium deposits and the reactor walls. Helium accumulation can increase the amount of fuel that is collected in the walls (where it is unable to react), decrease the lifetime of reactor components, and change material properties and heat transfer rates. The research employs computer simulation of the relevant physical processes, which occur at length scales ranging from atomic and molecular dimensions up to tens of nanometers. The ultimate goal of this line of research is to construct a working model that predicts fuel (hydrogen) and biproduct (helium) accumulation inside the materials from which the fusion reactor is made, as well as an understanding of the physics of helium interaction with lithium. Improved models allow future engineers and scientists to improve designs of future power plants and test reactors, make those reactors safer and more efficient, and generally advance the area of fusion energy science.

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

Study of Short-Range Correlations in Nuclei Using Electro-induced Nucleon-knockout Reactions At High Momentum-Transfer

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Short-Ranged Correlations (SRC) are pairs of strongly interacting nucleons whose separation is comparable to their radii. Their overlapping quark distributions and strong interaction makes SRC pairs an ideal system to study phenomena that bridge among low-energy nuclear structure, high-density nuclear matter, and high-energy quark distributions. As such, their study has significant consequences for strong-interaction physics, hadronic structure and nuclear astrophysics.

This proposal will study SRCs by measuring exclusive high-energy electron scattering reactions at the Thomas Jefferson National Accelerator Facility. High-energy electrons will be used to breakup SRC clusters (pairs and triplets) in various atomic nuclei. Using the CLAS12 spectrometer, the nucleons emitted in the breakup process will be detected and the initial properties of the SRC cluster will be reconstructed. This will allow probing the two- and three-nucleon interaction at short-distances at densities relevant for neutron stars, to test ab-initio many-body nuclear calculations, and to explore the relation between description of atomic nuclei using nucleons and using quarks and gluons.

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

Optimization and Calibration of a 4He-based Detector for Low-Mass Dark Matter

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Is dark matter made of particles lighter than the proton? Ambient dark matter particles from the galactic halo will (very rarely) scatter off target materials here on earth. The challenge in testing low-mass dark matter models is simply that the energy deposited in these dark matter scatters is correspondingly small (eV scale and below), below the threshold of existing technologies. The goal of this work is to advance a specific particle detector technology that shows great promise at low energies, a technology in which superfluid helium serves as the target material. In the superfluid state, deposited energy appears as diverse vibrational excitations collectively called `quasiparticles'. These quasiparticle excitations can then liberate individual helium atoms from the surface of the fluid in a one-to-one process called `quantum evaporation'. This pulse of liberated helium atoms can then be sensed via low-temperature (mK-scale) calorimetry, such as Transition Edge Sensors. This work seeks to advance quantum evaporation-based detector technology by boosting the amplitude of the evaporation signal, first by enhancing the sensor sensitivity (by reducing the calorimetry temperature), and then by increasing the quantum evaporation efficiency (by decreasing quasiparticle losses). Then the work will focus on understanding the initial production of quasiparticles, mimicking dark matter recoils via two stages of neutron calibration: first the development and use of a compact low-energy (24.4 keV) neutron source, and then a novel application of epithermal (<keV) neutrons available at the Los Alamos Neutron Science Center (LANSCE). The goal of this work is to answer the major open R&D questions of the quantum evaporation detector technology, enabling shortly thereafter a powerful extension of dark matter sensitivities towards lower masses.

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

Modeling Electronic Interactions and Multielectron Reactivity of Actinide Ions on Metal-Oxide Surfaces: Synthesis, Characterization, and Reactivity of Actinide-Functionalized Polyoxovanadates

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The fundamental investigation of the interactions of actinides with their ligand frameworks and chemical environments is a rich area of research, with implications in catalysis, chemical separations, and waste remediation strategies. In particular, identification of applications for transuranic elements requires an understanding of their chemical behavior toward molecular transformations of relevance to the production of chemical fuels. With this overarching objective as our project motivation, our research group will develop novel scaffolds derived of wholly inorganic, metal-oxide assemblies. We anticipate that these molecular "clusters" will be capable of supporting novel reactivity at actinide ions, taking advantage of synergistic reactivity between transition-metal oxide moieties and the 5*f*-electron density unique to heavy elements. Indeed, we have opted to investigate early actinide elements (uranium, neptunium, plutonium) due to their tendency to exist in a variety of redox states, rendering multiple 5f-electrons accessible for chemical reactivity and bonding. Capitalizing on the enhanced stability of actinide-oxygen bonds, we propose that this ligand-design strategy will afford enhanced stability to the actinide ion through robust anionic, oxide linkages, enabling the actinide center to facilitate multielectron reactions of relevance to the production of chemical fuels. The impact of our research activities will be two-fold: (1) We will identify new chemical transformations for actinide elements that are enabled by combining the unique chemical behavior displayed of these elements with the well-established, rich electrochemical properties of molecular metal-oxide scaffolds; (2) The homogeneous properties of our actinide-functionalized metal-oxide structures will allow for thorough spectroscopic analysis of chemical reactions, ultimately providing opportunities to understand how electron density moves between substrate, actinide and metal-oxide metalloligand under relevant reaction conditions. Our research will set the stage for multielectron small molecule activation with well-defined, actinide-functionalized metal-oxide assemblies, cultivating new approaches for the mediation of chemical transformations with the 5f electrons of actinide elements.

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

Design and Structural Analyses of 2D Covalent Organic Frameworks as Single-Site CO_2 Reduction Catalysts

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The capture of CO_2 and its simultaneously conversion to useful chemical fuels driven by solar energy represents one of the best solutions to resolve growing energy concerns. Among the various strategies that are being considered, photocatalytic CO_2 reduction is perhaps most attractive due to its simplicity and economy of the input energy source. The most critical challenge to this endeavor is the rational design of a phototocatalytic architecture that can effectively couple a given photosensitizer with an appropriate catalyst, thereby enabling efficient photosensitization of a multi-electron reduction catalysis. The objectives of this research are to address this challenge using an interdisciplinary approach that combines innovative material design and synthesis, fundamental mechanistic studies, and photocatalytic performance evaluation. These goals will be accomplished by 1) constructing a unique set of hybrid covalent organic framework (COF) photocatalysts with an effective photoactive organic building block as photosensitizer and a precisely incorporated CO_2 reduction molecular catalyst; 2) examining the excited state and charge separation dynamics of these photocatalysts using a set of complementary time resolved spectroscopy to unravel the key factors that control their function as photocatalysts; and 3) investigating the photocatalytic performance, selectivity and catalytic pathways, and correlating them with photophysical properties to determine the structure-function relationship of these hybrid COF catalysts. This research will address current shortcomings of semiconductor- and molecular-based photocatalytic systems that suffer from inefficient light harvesting and charge separation and poor adsorption and activation of reactants. In turn, this research will contribute toward the development of novel photocatalytic systems for CO_2 reduction to generate renewable chemical fuels using sunlight as the only energy input.

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

Data Structure Alchemy

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What do analytics, machine learning, data science, and big data systems have in common? What is the major common component for astronomy, biology, neuroscience, and all other data-driven and computational sciences? Data structures. A data structure defines how data is physically stored. For all algorithms that deal with data across all applications in businesses and sciences, their design starts by defining a data structure that ideally minimizes computation and data movement. The fundamental problem is that there is no universally perfect data structure, and as such, we need to design new data structures as new data, applications, and hardware emerge. For scientific data-driven fields without computer science expertise, these low-level designs are extremely hard or expensive to make. For established tech companies and data-driven startups, the complexity leads to a slow design process and has severe cost side-effects. Furthermore, in today's cloud-based world, even slightly sub-optimal designs translate to a massive loss in energy utilization for the cloud provider and cloud expenses for the application. We propose a radical new way to the decades-old problem of data structure design based on first principles and AI. We set out to discover the first principles of data structure design and develop learning algorithms to search through the astronomically large design space they form. Effectively, the principles and their structure form a ``grammar'' that describes all existing data structures and their expected behavior in a principled way, as well as a massive number of designs that have not been invented yet. Thus, Data Structure Alchemy has the potential to accelerate research, entrepreneurship as well as improve computer science education. Our work focuses on three data storage models which are pervasive in everyday life, in businesses, sciences, and education: key-value structures, graph structures, and images.

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

Searches for New Long-Lived Particles and Upgrades to the ATLAS Inner Detector

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Despite the enormous success of the Standard Model of particle physics in describing the nature of matter at small scales and in explaining the fundamental interactions of elementary particles in our universe, key questions still remain unanswered: What is the nature of dark matter? Is there a universal symmetry that unites all three of the forces described by the Standard Model and can such a symmetry be extended to include gravity? What sets the scale of the observed Higgs boson mass? New elementary particles with measurably long lifetimes are predicted by many theoretical models that seek to answer these questions. This research program targets the discovery of long-lived particles produced via electroweak processes by the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN) in Switzerland. Experimental signatures of such long-lived particles are predicted in compelling models for dark matter and can be integral to the explanation for the observed Higgs mass. The study plans to apply innovative analysis techniques to the data collected by the ATLAS (A Toroidal LHC ApparatuS) experiment at the LHC and to develop new trigger algorithms to improve the extraction of signatures of long-lived particles. Further, to ensure the sensitivity of ATLAS to new physics processes for the duration of the planned higher luminosity era of the LHC, the program includes the development of critical components of the new readout system of the ATLAS Inner Tracker upgrade. As a result, this work will not only illuminate the most promising hiding place of weak-scale solutions to many of the remaining mysteries of particle physics, but will also advance the instruments used in the searches.

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

Emergent Properties of Magnons Coupled to Microwave Photons

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Studying the emergent properties of hybrid quantum material platforms holds the promise to advance quantum technologies, and to revolutionize our understanding of controlling quantum mechanical interactions. A new direction emerged in recent years when it was realized that magnons, the elementary quanta of spin waves, could be used as one building block in the quantum toolbox. Determining the specific mechanisms for the generation and control of hybrid quasiparticles based on magnons could potentially lead to the ability to engineer new materials for quantum coherent processing and quantum computers. The goal of this research is to achieve precise control of light-matter interaction in magnetic hybrid systems and nanostructures, where the light part is carried by microwave photons, and the matter component is carried by magnons in engineered magnetic metamaterials. This research will implement new measurement techniques and undertake systematic studies of new material systems for efficient control of magnon-photon coupling. The underlying mechanisms of both the interaction of magnons with photons, and magnons with phonons will be determined, as these interactions are essential for utilizing magnons as coherent information transduction platform between carriers. This project explores the mechanism by which nonuniform magnons interact with photons in the strong coupling regime, determines the spatial distribution of the hybrid excitations, and identifies how to dynamically and spatially control the interaction. It is therefore essential to broaden the range of material platforms, as well as the measurement techniques that can be applied to understand the mechanisms of magnon-photon coupling. Specific goals include: (1) Exploring the dispersion and collective properties of the magnon-polaritons in new materials; (2) Realizing magnonic hybrids with non-zero wavevector and effectively controlling magnon-polariton properties through an engineered magnonic/phononic band structure; and (3) Determining the mechanisms by which spin-transport phenomena interact with electromagnetic fields in the strong coupling regime. Overall, this research will result in a wealth of new knowledge about the physics of magnonic hybrid systems and the control of their emergent properties. The activities of this project are expected to impact the fundamental understanding of magnon-polaritons, and lay the foundation to create novel spintronic devices, which could be used in quantum information science.

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

Tunable Energy Landscape, Non-Trivial Band Topology, and Electric Field Driven Phenomena in Novel Quantum Materials as Probed by Localized Photoemission Spectroscopy

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Atomically thin two-dimensional (2D) materials possess many unique properties that conventional three-dimensional systems do not. 2D materials can be a flexible component in the design of condensed matter 3D systems through the stacking of 2D parts, layer-by-layer. The result is called a van der Waals (vdW) hetero-structure, formed much like "Legos" are used to build different toy objects. By adjusting the twist angle between the constituent layers, vdW hetero-structures can be made to have different complex phases of matter and novel properties, including metal to insulator transitions, superconductivity, bound excited electron states, and topological states. Furthermore, because they consist mainly of surface atoms, the unique physical properties of thin layered materials are easily affected by external surface perturbations. This can be detrimental to their intrinsic ground state properties and presents a fundamental challenge to using 2D materials for future technological applications. This work seeks to fully understand the role of extrinsic perturbations (supporting substrate interactions, adsorbed atom impurity defects, and applied electric field) on the intrinsic properties of 2D materials. The knowledge will help design ways to protect against defects but will also lead to methods to control the material's properties by modifying their environment in specific ways.

The properties of a material are dictated by its electronic structure (the distribution of electrons in energy and momentum.) Therefore, this research will directly probe with spatially resolved spectroscopy the electronic band structure of 2D quantum materials and their hetero-structures. The work involves state-of-the-art angle-resolved photoemission spectroscopy with nanoscale spatial resolution (nano-ARPES) at the Advanced Light Source (ALS). The planned research will develop a capability to perform nano-ARPES measurements under non-equilibrium conditions, when an external lateral electric field is applied to a 2D system. This type of research is a crucial step towards the eventual development of 2D materials for future technological applications in electronics, opto-electronics, photonics, and spintronic devices.

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

Data-Driven Optimization under Uncertainty: Parallel Algorithms and Solver

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The U.S. electric grid systems are increasingly incorporating smart grid sensors, energy storage, microgrids, and distributed energy resources such as solar photovoltaic panels. The proposed research in optimization under uncertainty will address the technical challenges in modeling the design and control of cyber-physical systems. Conventional approaches make the restrictive assumption that the underlying probability distribution of uncertain model parameters is known. The proposed research formulates this challenge as a distributionally robust multistage stochastic optimization (DRMSO) problem that makes multistage decisions that account for the uncertainty from unknown distributions. High-performance algorithms will be developed for solving such problems. Adaptive decomposition methods for the algorithms will exploit their mathematical and statistical structure for efficient use on emerging computer architectures. The proposed research will improve reliability and resilience in the design and operation of the U.S. electric grid, edge computing networks, and other cyber-physical systems.

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

Joint Analyses of Lensing, Clustering, and Galaxy Clusters with DES and LSST

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The accelerated expansion of the Universe is the most surprising cosmological discovery in decades, and has inspired a generation of ambitious surveys to determine the fundamental nature of the acceleration, such as the Large Synoptic Survey Telescope (LSST). The most stringent constraints on cosmic acceleration, or dark energy, from these surveys will come from the joint analysis of different cosmological probes and incorporate synergies across surveys and wavelengths.

This Early Career research program will develop such a combined-probes analysis program to jointly analyze galaxy clustering, weak lensing, and the abundance of galaxy clusters in Year 1 (Y1) data from the Large Synoptic Survey Telescope (LSST), which will deliver an unprecedented combination of data quality and size. This leap in statistical constraining power must be matched by a similarly unprecedented control of systematic uncertainties. Hence the proposed LSST-Y1 analysis program will be developed on increasingly complex data sets from the Dark Energy Survey (DES) and LSST precursor data.

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

Abiotic and Biotic Controls on Chemical Weathering Rates and Solute Generation

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Precipitation falling on mountainous watersheds is exposed to surface and subsurface processing, such as chemical weathering, before eventually leaving as streamflow. In turn, this processing is governed by a variety of abiotic and biotic interactions involving, e.g., the type of rock that governs geomorphology and mineralization and the type of vegetation that can generate acidity. The proposed work will focus on the role of vegetation as a means to influence water chemistry and quality. By employing a multi-scale approach, the project will address the following questions: 1) Does landscape-scale heterogeneity in vegetation, climate, and geology impart unique, spatially-variable signatures on soil production and chemical weathering rates? 2) What roles do the legacies of Pleistocene glaciation and Holocene geomorphic processes play in determining modern-day solute concentrations in surface waters? 3) Are physical erosion and chemical weathering rates linked at the watershed scale, and can these rates be predicted from watershed characteristics? These questions will be addressed in the physical and ecological setting of the East River watershed near Crested Butte, Colorado.

The proposed technical approach will assess controls on weathering and solute generation at the soil profile, landform, and watershed scales. At the soil profile scale, soil production and chemical weathering rates will be quantified with cosmogenic nuclides and geochemical mass balance at sites that span biotic, climatic, and geologic gradients in order to isolate the key drivers of chemical weathering. At the landform scale, solute concentrations in surface waters will be used to assess whether surficial deposits generated by different geomorphic processes impart unique weathering signatures. At the watershed-scale, cosmogenic nuclides will be used to measure erosion rates. A series of reactive transport models will be constructed to place the field-based findings into a framework for making predictions regarding the roles that vegetation, climate, and geomorphology play in solute generation. The proposed research complements ongoing BER investments at the LBNL Watershed Science SFA Science Focus Area.

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

Understanding and Controlling Photoexcited Molecules in Complex Environments

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Predicting the outcome of a chemical reactions driven by light is complicated by factors outside the scope of traditional theoretical chemistry. On such small scales, fluctuations of the environment render outcomes random, quantum mechanics blur the separation between nuclear and electronic motion, and the accompanying ultrafast relaxation renders typical assumptions of equilibrium inappropriate. By combining contemporary ideas from quantum information and nonequilibrium statistical mechanics, this research aims to develop a set of theoretical and computational tools to unravel the photoexcited dynamics of small molecules in the condensed phase, and learn how to control their outcomes. The algorithmic and theoretical advances will be generally applicable to challenging questions across the physical sciences, and provide design principles for nanoscale materials for energy storage and generation, molecular machines and motors, and beyond.

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

Elucidating the Nature of Chiral and Topological Phonons in Materials for Energy Technologies

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The control of heat is critical to overcoming challenges in a variety of energy applications where heat loss or buildup can result in poor performance, including electronics, vehicles, energy storage, information technologies, and even nuclear reactors. This research will explore atomic vibrations called "phonons" as avenues for optimizing heat flow so that materials can be tailor-made for transformative energy technologies. Because heat activity happens on the atomic level, innovative approaches will need to fine-tune materials' atomic properties, for example, to keep electronics cool or to make batteries more efficient. Vibrating atoms can have unique arrangements, including "chiral" or mirrored structures, in the same way that a right and left hand are compatible pairs but not identical to one another. Making a proper handshake or other fine adjustments opens possibilities to tune materials for specific properties. This research will use cutting-edge theoretical techniques and artificial intelligence to investigate materials' tunability, specifically to enhance thermal conductivity. As thermal processes are critical to energy production and use, the outcome of this work will provide fundamental insights into developing novel energy materials to advance our nation's energy technologies.

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

Elucidating the Mechanistic Determinants of Flavin-Based Electron Bifurcation

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Industrial catalysts are employed to drive a number of challenging chemical reactions resulting in value-added products such as ammonia and methanol; the use of which has greatly altered civilization. However, as the demand for more and new value-added products (such as fuels, drugs and small molecules) increases, critical advances in design of synthetic catalysts capable of driving energetically demanding reactions will become even more necessary. Biological enzymes serve as a point of inspiration for this because they are able to perform a variety of difficult reactions with high selectivity, fidelity and efficiency. This project investigates a unique type of enzyme capable of separating an electron pair into individual low-energy and high-energy electrons and bifurcating them along spatially distinct paths to selectively catalyze the production of two products, one of which is more reduced than the starting material. The goal of this project is to elucidate the physical features responsible for the strict temporal, spatial and energetic control over electrons. To achieve this, a suite of steady state and ultrafast biophysical techniques are employed to specifically probe the properties of the electron bifurcating site and the initial mechanistic events. This information is integral to understanding how energy is controlled and manipulated in complex biological systems; the insights of which will lead to design principles that accelerate the development of transformative energy technologies.

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

Scalable Architectures for Hybrid Quantum/Classical Networking

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The main objective of this project is to research and develop advanced quantum communication networking concepts and subsystems to support the emerging Quantum Information Sciences (QI) ecosystems. Advances in quantum communication networks are critical to harnessing the full potential of the new quantum information science paradigm, especially for distributed quantum information processing such as quantum sensing, distributed quantum computing, quantum key distribution, and quantum cloud computing that on transmitting quantum sate information. Unlike the current digital networks, quantum networks are governed by strict laws of quantum mechanics such as no-cloning, superposition, and entanglement that make the development of practical quantum network challenging. However, if successfully developed, it will usher a new era in telecommunications. It will among other capabilities bring concepts such as teleportation and unbreakable network security once considered "science fiction" within practical reach.

In this project, we propose to overcome the above technical challenges by researching, developing, and testing a new generation of photonic quantum communication network technologies (hardware, software, and protocols) that exploit the dual the nature of light (particle and wave) to transmit quantum information over long distances. The distinguishing feature of the proposed effort is the focus on quantum networks designed to leveraged existing optical network technologies, especially the currently deployed telecommunication optical fiber systems. Upon successful completion, we hope to deliver and test a hybrid classical/quantum network architectures, protocols, and basic hardware and software components that will have the potential for accelerating the developing what could potentially become the backbone of a future Quantum Internet existing coexisting in the current telecommunication fiber systems.

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

The Next Revolution in Neutrino Physics

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The existence of neutrino masses, inferred from neutrino oscillation measurements, is one of the few cogent evidences of physics beyond the standard model. The forthcoming US experimental neutrino program largely relies on liquid argon time projection chambers (LArTPCs) to further deepen our knowledge of the neutrino sector. LArTPCs can be thought of as modern bubble chambers, outstandingly identifying and reconstructing tracks of charged particles produced by neutrino events. With the goal of fully exploiting the outcomes of the US experimental neutrino program, this research plan is based upon three cornerstones. First, in-depth, systematic studies of several standard and beyond the standard physics scenarios will be performed. This includes an unprecedented study of low energy atmospheric neutrinos, uniquely enabled by the LArTPC technology. Second, an exploration of novel ideas will be pursued with the intent of connecting open questions of physics to the neutrino sector, such as the origin of neutrino masses and dark matter, and flavor physics models at low scales. Finally, to maximize the impact on the field, the outcomes of this project will be implemented in automated tools and will be made available publicly, so they can readily be used by the broad theory and experimental communities.

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

Realization of a Quantum Slide Rule for 1+1 Dimensional Quantum Field Theories Using Josephson Junction Superconducting Circuits

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An important milestone on the way to universal quantum computing is producing a device capable of solving a specific useful quantum problem. Such a specialized computing device can be viewed as a quantum version of a slide rule in the sense that it will produce a very specific set of otherwise unavailable quantum calculations, which can be later applied to a larger class of more challenging problems. Our quantum slide rule will consist of a high-impedance superconducting transmission line coupled to an artificial atom. This engineered quantum system can controllably mimic the dynamics of a generic one-dimensional system of interacting fundamental particles. The specific problems our quantum slide rule will solve are profoundly linked to the topics in conformal quantum field theories of high-energy physics and to the quantum impurity problems of condensed-matter physics, both of which play a foundational role in modern theoretical physics.

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

Control of Bright Electron Beams at Small Spatiotemporal Scales for Probing Materials Far from Equilibrium

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Driving atomic vibrations with short, intense light pulses is an exciting route to unlock new material phases that are not available in static equilibrium. For example, light-driven vibrational modes have been shown to induce ultrafast changes in atomic lattice symmetry, or dramatic changes in electrical conductivity. These phenomena employ vibrational modes with extremely short periods (hundreds of femtoseconds and below), spectral signatures well below one electron volt, and potentially nanometer spatial scales. This leads to a challenging set of requirements for any time-resolved structural probe to be able to observe the full evolution of light-driven atomic vibrational modes. This research seeks to develop a suite of electron optical techniques to deliver high-quality electron beams tunable between each of these resolution extremes in time-resolved electron scattering experiments. This work will employ a new class of high-brightness photoelectron source in conjunction with precision electron spectrometer optics to enable multiple new measurement modalities, including: (1) ultrafast electron diffraction with time of arrival measurements for sub-phonon period temporal resolution, and (2) ultrafast time-resolved vibrational spectroscopy with small probe beam sizes. These techniques have the potential to unlock the observation of a wide swath of light-driven atomic dynamics and can be accomplished with compact, meter-scale electron scattering beamlines.

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

The Physics of Micro-Pinches

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By funneling a large electrical current through a very small conduction channel (a very thin wire, for example), an enormous magnetic field can be generated. This magnetic field encloses the wire and can exert an enormous inward pressure on the wire. Using a modest-sized current generator (i.e., a generator about the size of a small car), a solid metal wire can be compressed and heated to a pressure exceeding one billion atmospheres. This project will use this compression technique to produce and study extremely high-pressure states of matter in a modest laboratory setting. Understanding these states of matter, and how to control them, will impact programs in national defense, energy, and basic science, with applications in nuclear fusion, radiation science, material properties, and laboratory astrophysics.

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

Systems metabolic Engineering of *Novosphingobium aromaticivorans* for Lignin Valorization

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In a typical biorefinery, sugars derived from plant material (or biomass) are fermented to fuels by microorganisms. However, a substantial fraction of the plant biomass that contains a polymer called lignin cannot be easily degraded and is instead burned for heat. Lignin could be converted into value-added bioproducts, offering a potential source of additional revenue to improve the economics of biofuel production. Chemical conversion of lignin is challenging, but specialized bacteria with the necessary biochemical capabilities could potentially produce desired compounds from different mixtures of lignin-rich mixtures. Although bacteria that are suited for lignin conversion are known, they have not been extensively studied or manipulated. This project will characterize the biochemical pathways for assimilation of lignin-derived compounds in a bacterium that can metabolize a wide range of such compounds. New pathways will then be engineered into this bacterium to convert depolymerized lignin into valuable bioproducts. To achieve this goal, a novel genetic method will be used to build a predictive systems biology model and identify additional genetic targets for further metabolic optimization. These efforts will result in new methods to predictively model and engineer a promising microbe for lignin valorization that can ultimately be applied to a wide range of emerging microorganisms relevant for BER's mission in sustainable bioenergy.

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

I/O Workload Characterization for Performance and Portability

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Currently, to achieve high I/O (input/output) performance, developers must go to great lengths to tailor their I/O approach to fit the software and storage architecture for each supercomputer. As a rule, storage system middleware manages I/O requests blindly, in that all bytes are treated with the same priority and in the same fashion. However, special treatment of classes of I/O (e.g., checkpoint files used for restarting in the event of failure) has resulted in orders of magnitude improvement in I/O performance. This project will improve I/O performance and user experience in the face of increasingly complex high performance computing (HPC) storage hierarchies. Building upon the successes of special treatment of I/O classes, capabilities will be developed for all types of I/O so that applications will be able to tag I/O operations with request types that reflect the intended usage of the data, e.g., checkpointing, as well as with high-level quality of service (QoS) requirements. The key benefit of this work will be the abstraction of the details of any particular storage system, allowing users to access high performance I/O on supercomputers more easily. Users will only need to know the I/O characteristics of their applications, which will result in more portable code, and system software will dynamically schedule I/O operations on potentially complex hierarchical storage systems, taking into account the individual needs of particular I/O requests and storage system resource capabilities.

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

Developing the Surface Engineering Basis for Next-Generation SRF Accelerators

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Since 2012, expectations of the potential performance of niobium for superconducting radiofrequency (SRF) accelerator applications (SRF cavities) have been dramatically evolving. The discovery that tailored interstitial doping of the radio frequency (RF) surface yields dramatically reduced losses has been transformative (similar to initial advancements in silicon manufacturing). In the case of high-temperature nitrogen doping (HTND); low pressure (~20 mTorr) nitrogen is added at 800°C after a hydrogen de-gassing phase in a vacuum furnace. The nitrogen addition creates a lossy nitride crystal phase on the surface (removed through electro-chemistry) and a performance-enhanced nitrided niobium phase below (revealed after electro-chemistry). We seek to develop a predictive model of HTND to transition away from the traditional guess and check method of doping performance. Development of a predictive and tunable model of doping requires a data set built on Scanning Electron Microscope (SEM) for surface morphology and Secondary Ion Mass Spectroscopy (SIMS) for interstitial doping percent. RF cavity tests provide efficiency, maximum performance, and superconducting properties on the doping. The feedback loop provided by the dataset will be used to create a multi-variable predictive mathematical model general enough for use in any application. Unlike previous simplified models, the new model needs to contain the nitride crystal seeding time and material dependencies, time-dependent nitride crystal morphology with/without nitrogen and diffusion coefficients depending crystal structure. Upon completion, this program should allow the modeling and demonstration of specific cavity treatment protocols tailored to any next-generation accelerator, likely making new types of applications economically viable. An even more dramatic expansion of opportunities will open up when HTND technology that simultaneously supports high mid-field Q_0 (high efficiency) and very high gradients (maximum performance) is realized. The new predictive model will be able to calculate the correct doping parameters in advance to achieve such performance.

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

Ultrasonic Determination of Electron Viscosity and Hydrodynamics in Metals

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The flow of electricity is often taught in analogy to the flow of water: electrical current is analogous to the rate of flow, voltage is analogous to pressure, and a constriction in a pipe is analogous to a resistor in a circuit. This analogy is helpful when trying to build intuition about simple electrical circuits, but like any analogy it can be misleading. In particular, the flow of water is described by mathematics called "hydrodynamics" – this leads to turbulence, vortices, shear drag, and other effects seen while watching a raging river or a boat propeller. Electricity behaves very differently—electrons constantly bounce off of the defects and impurities that are present in all metals, leading to "diffusive" behavior that looks more like a Plinko-game than a flowing river. Recent experiments, however, have shown that this may not always be the case. When metals are made extremely pure, or when circuits are built at the nano-scale, "hydrodynamic" effects may be important for the flow of electricity. A crucial parameter is the electron viscosity—the high viscosity of honey makes it flow slowly, while the low viscosity of water makes it more fluid. Electron viscosity is very difficult to measure, but this project is developing a new experiment based on ultra-high-frequency ultrasound that can measure electron viscosity in a very direct way. Knowing the electron viscosity will allow for the design of nano-scale electronics using a new generation of ultra-clean metals, and will allow the testing of fundamental quantum mechanical ideas that relate electron viscosity to high-temperature superconductivity.

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

Towards Scalable Precision Tuning of Numerical Software

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Floating point is a widely used representation that approximates real numbers. A large variety of applications, including extreme-scale scientific applications, depend on floating point. By nature, floating point introduces imprecision in numerical calculations. Using the highest available precision for floating-point numbers could reduce numerical error. However, this practice reduces application performance. Because both reliability and performance are critical, this proposal will develop techniques to assist programmers in exploring the trade-off between precision and performance with an emphasis on handling large, long-running scientific applications. In particular, this proposal focuses on (1) developing novel program-analysis and machine-learning techniques for scalable floating-point precision tuning to improve program performance, (2) developing testing techniques to generate inputs for robust precision tuning, and (3) creating a benchmark to enable the evaluation of precision-tuning tools on large, real applications. The proposed research advances the state of the art in precision tuning and testing of numerical software. Our techniques will have a direct impact in, and foster collaboration with, Computer Science research areas such as High Performance Computing and Machine Learning, as well as other research fields that rely on floating-point arithmetic. The tools developed and data produced as part of this proposal will be made publicly available under a BSD license.

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

The Synthesis of Metal Superhydrides Through Extreme Temperature/Pressure Conditions: Towards Room Temperature Superconductivity

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The discovery of metal superhydrides – extremely hydrogen-rich materials – may hold the key to room-temperature superconductivity. Limitations with storing energy produced from renewable sources can be overcome by the introduction of superconducting materials to the transmission grid, providing an efficient means of storing and recovering energy on demand, as well as a method for transferring energy over long distances. Superhydrides often require extreme conditions to synthesize – up to millions of atmospheres in pressure – making sample sizes small, and their chemical properties difficult to analyze. This work investigates the possibility of readily synthesizing metal (Y, Tc, Sn, La) superhydrides at extreme pressures, and develops experimental techniques to probe the precise makeup of these materials. These studies provide the backbone for theoretical understanding of their chemical bonding, crucial for developing strategies for their recovery at ambient conditions.

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

Enhancing the Discovery Potential of the nEXO Neutrinoless Double Beta Decay Experiment

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The particle nature of neutrinos is one of the most interesting open questions in physics today. Neutrinos have the unique possibility of being fundamental Majorana particles, i.e., single particles representing both matter and antimatter states. Discovering that neutrinos are Majorana particles would directly establish physics beyond the current Standard Model and have an immense impact on our understanding of particle physics. The most promising approach to experimentally establishing the Majorana nature of neutrinos is to search for neutrinoless double beta decay, an extremely rare nuclear process. The primary experimental challenge for such a search is building a detector that is sensitive to this process above all other naturally occurring radioactive backgrounds. The next-generation Enriched Xenon Observatory (nEXO) experiment aims to search for the neutrinoless double beta decay of xenon-136. The projected sensitivity of nEXO will uncover a large region of unexplored parameter space opening up the possibility of the first detection of neutrinoless double beta decay. This research will develop a comprehensive program to enhance the discovery potential of the experiment by reducing the dominant radioactive backgrounds through two complementary approaches. The first is the development of detector components with extremely low radioactivity levels, while the second involves optimizing the design of the experiment to maximize the rejection of residual backgrounds. These methods are both critical, as they not only significantly increase the sensitivity of the experiment, but also increase the confidence by which a discovery claim could be made.

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

Elucidating Aromatic Catabolic Pathways in White-Rot Fungi during Lignin Decay

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Lignin is a heterogeneous polymer found in the cell walls of terrestrial plants and accounts for 30% of the organic carbon in the biosphere. White-rot fungi are undoubtedly the most efficient lignin-degrading organisms in Nature and are thus responsible for a substantial amount of carbon turnover on Earth. Lignin conversion to carbon dioxide and water by these organisms has been studied for decades and is very well accepted. However, the biochemical pathways that allow white-rot fungi to deconstruct and further metabolize lignin remain largely unknown. Indeed, it is still a matter of controversy whether or not these organisms utilize lignin degradation products as a carbon and/or energy source. Furthermore, the chemical units that constitute lignin could be used as precursors of valuable compounds. However, due to its complex nature and the difficulty to break it down into smaller components, lignin is an undervalued substrate for biorefineries that use plant biomass to produce biofuels. This research will apply systems biology and computational modeling approaches to elucidate the metabolic pathways for lignin conversion in white-rot fungi and understand the biological roles of lignin degradation. The knowledge gained through this work will serve as a foundation to employ white-rot fungi in lignin bioconversion into value added bioproducts, advancing towards a sustainable plant-based bioeconomy.

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

Learning to Learn: Designing Novel Neuromorphic Algorithms with Machine Learning

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Scientific research generates data significantly faster than can be analyzed with today's computing power, thereby creating a need for energy efficient, intelligent computing. An emerging technology called *neuromorphic computing* shows promise in satisfying this need. For the US Department of Energy, this breakthrough computing paradigm will be necessary in future computing systems to continue scientific discoveries and development. A significant research challenge in applying neuromorphic computing to scientific research is defining the learning approaches that will fully realize the real-time continuous learning capabilities of neuromorphic computers. To address this challenge, I will use machine learning with existing high-performance computing (HPC) to automatically create new learning algorithms that will enable unsupervised or semi-supervised real-time continuous learning for neuromorphic systems. Specifically, I will: (1) develop HPC-based neuromorphic hardware simulators that will accelerate the study and understanding of neuromorphic hardware, (2) develop an HPC-based algorithm evaluation framework for existing learning methods for neuromorphic systems in order to investigate the capabilities of these methods, and (3) develop new learning methods for neuromorphic systems by utilizing HPC and machine learning methods. The goal of this work is to provide a path forward for using neuromorphic computers for real-time adaptive machine learning-based analysis of scientific data by using machine learning approaches on HPC to develop new neuromorphic learning approaches.

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

Low-Dimensional Manifold Learning for Uncertainty Quantification in Complex Multi-Scale Stochastic Systems

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Understanding the properties and behavior of complex materials often requires the development of computational models for the system at multiple scales. The development of fracture and deformation models for amorphous solids (polymers, gels, glasses) and ductile metals are of particular interest. One major source of modeling challenges involves efficient multi-scale representation and information transfer between models at atomistic, microstructural and structural length-scales. These difficulties are compounded by the high-dimensionality, nonlinearity, and myriad uncertainties that arise in determining the appropriate form and parameter values for the sub-models. The proposed research develops active learning and so-called dimension hyper-reduction methods to enable uncertainty quantification for these complex systems. This advanced modeling approach is likely to be more realistic and computationally manageable than conventional methods. Research developments will also lead to advanced software solutions such as the UQpy open-source Python toolbox for large-scale uncertainty quantification in multiscale stochastic systems.

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

Genetic Tools to Optimize Lignocellulose Conversion in Anaerobic Fungi and Interrogate Their Genomes

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Specialized microbes can convert renewable plant material into biofuels and other bioproducts. However, the microbes currently used for industrial biofuel production cannot break down the plant cell wall material (or plant biomass) into its component sugars unless it is previously partially broken apart with heat and chemicals. Anaerobic fungi that live in the guts of animals that eat plants have the capacity to degrade plant biomass more efficiently than industrial microorganisms and without the need for prior treatment. In spite of the natural advantages of these fungi, they are not used industrially because no genetic tools are available to identify and manipulate the enzymes that constitute the biochemical machinery responsible for their biomass degradation capabilities. This project will develop and leverage high resolution -omics resources to better understand the physiology of anaerobic fungi using systems and synthetic biology approaches. Novel genetic and epigenetic tools will be designed to engineer new strains of anaerobic fungi with improved biomass degradation capacity. In parallel, cell-free strategies will be applied to rapidly characterize fungal proteins and identify improved enzyme functions. With these approaches it will be possible to identify the genetic machinery involved in the breakdown of lignocellulosic plant biomass in these fungi and provide systems-level insight into the genomic basis of biomass deconstruction. Ultimately, this project will help establish design principles to engineer new fungal strains for lignocellulose deconstruction, while creating enabling genetic tools for metabolic engineering of anaerobic fungi. Planned experiments will leverage DOE genomics, molecular, and computational analysis resources at the Joint Genome Institute, the Environmental Molecular Sciences Laboratory, and the Systems Biology Knowledgebase. The knowledge gained from this project will enable predictive biology and genome engineering in anaerobic fungi, advancing BER's mission in the development of sustainable bioenergy resources.

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

Tagging Radon Daughter Backgrounds in a Crystalline Xenon TPC:
A Solid Future for the LZ Dark Matter Search Experiment

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What is the particle nature of the dark matter in the universe? A new generation of dark matter direct detection experiments, including the liquid xenon LZ detector, will soon begin operations in an attempt to answer this question. By looking for interactions between theoretically well-motivated weakly interacting massive (dark matter) particles (WIMPs) and the xenon atoms in its (liquid) target mass, LZ will search a significant new region of dark matter parameter space. Yet their search is likely going to be limited by background events resulting from radioactive decays of radon contaminants. Whatever the experimental outcome – improved exclusion limits, a few tantalizing candidate events, or a clear dark matter signal detection – there will be strong motivation to improve sensitivity until the experiment reaches the search limit resulting from irreducible neutrino-xenon interactions that are indistinguishable from dark matter induced signals. This research project will develop a dark matter search detector using crystalline (as opposed to liquid) xenon, which offers two major instrumental advantages: mitigation of radon diffusion into the crystalline xenon target, and tagging of any radon radioactive decay products that grew into the crystal during its formation. These advances are uniquely available in the crystalline xenon state. If successful, this work will provide a critical new technology and a potential upgrade path for the LZ experiment. Such an upgrade would enable exploration of the final order of magnitude of WIMP dark matter parameter space, down to the neutrino-induced search limit.

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

Multi-Watershed Perturbation-Response Traits Derived Through Ecological Theory

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A major challenge for prediction of watershed systems is understanding how perturbations (e.g., hydrologic disturbances) influence intense biogeochemical activity in space (hot spots) or time (hot moments). Most studies of hot spot/moments have focused on single sites, which leads to scientific discovery that is not necessarily transferrable across watersheds. To address this limitation, this study will use field infrastructure in >60 watershed field sites across the United States and analyses provided by the Environmental Molecular Sciences Laboratory user facility. Resulting data will be used to test numerical modeling predictions of mechanistic connections between dissolved organic matter (DOM) chemistry and biogeochemical control point influence (CPI). The CPI is the contribution of elevated biogeochemical rates in space or time to the net aggregated biogeochemical rate within a defined system. CPI quantification will be combined with an innovative application of ecological theory to highly-resolved molecular characterization of DOM that allows DOM chemistry to be summarized as a biogeochemically-relevant trait. Experimentation across broadly distributed watersheds combined with detailed molecular analysis will reveal general, transferrable principles that will be used to create a trait-based framework capable of predicting impacts of perturbations on biogeochemical CPIs across watersheds. This trait-based framework can be further integrated with advanced numerical models to link dynamic watershed processes to DOM chemistry and CPIs. Ultimately, the science conducted by this project will improve predictive capabilities from local to watershed to Earth-system scales.

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

Development and Testing of Reduced Models of the Edge Radial Electric Field

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Magnetic-confinement fusion in tokamaks offers the promise of virtually limitless energy with no carbon-dioxide emissions. To achieve this, a plasma that is several times hotter than the center of the sun must be confined inside a toroidal metal vessel that measures only meters in minor radius. Economical energy generation requires excellent confinement, minimizing the turbulent energy losses. Overall device performance depends strongly on the edge region, a thin layer between the hot core and the relatively cold scrape-off layer, where the plasma contacts the vessel wall. In the edge, extremely steep gradients of plasma temperature can be achieved, due in part to instability and turbulence suppression by the edge radial electric field E_r and its shear. Prediction and control of edge E_r requires a first-principles understanding of the underlying physics. The science is challenging because many physical effects interact and compete with each other. For example, the momentum fluxes and torques due to turbulence, non-axisymmetric magnetic perturbations, and neutral atoms are inter-related, but their interaction is not understood. Also, the drift orbits of ions modulate the turbulent and collisional fluxes in the edge, as well as the effects of neutrals that ionize in the edge. The effects of these mechanisms will be analytically calculated using a novel, experimentally validated modulated-transport formalism. Using numerical diagnostics based on these results, massively parallel numerical simulations will quantitatively evaluate these terms. The theoretical results will be validated through comparison with experimental data from the NSTX, NSTX-U, and DIII-D tokamaks. Taken together, these investigations will uncover new insights into the ways that these interacting mechanisms drive edge E_r. This new understanding will enhance our ability to predict and to influence edge E_r and plasma performance in present-day and future tokamaks, contributing to the goal of clean, carbon-neutral energy.

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

Structure of Plasma-Water Interface

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Low temperature plasmas (LTPs) are fascinating systems capable of promoting chemical reactions that can be unexpected in orthodox theory based upon the idea of local equilibrium. LTPs can be harnessed for societal benefit, with notable successes in the areas of chemical energy storage and human health. Recently, promising discoveries such as rapid wound healing have drawn attention to the action of LTPs upon nominally aqueous media. Early reports have revealed that the plasma is capable of promoting reduction-oxidation (redox) reactions in the aqueous phase, however a tractable framework for understanding and controlling those redox reactions has not yet been developed. A key hypothesis of this project is that the plasma-liquid interface can be understood as a boundary condition for the solution, at which the reduction potential is defined by the plasma parameters. Consequently, the reduction potential of the plasma-liquid interface can be tuned using the plasma parameters to selectively promote redox reactions in solution. A secondary hypothesis is that the redox reactions occurring at the plasma-liquid interface must be counterbalanced by the opposite reaction elsewhere in solution. For example, if the plasma-liquid interface acts as an electrodeless cathode that promotes reduction reactions, then there must be an electrodeless anode elsewhere in solution, where oxidation reactions occur. The existence of the counterbalancing region is necessitated by charge neutrality. Robust experimental tools and methods will be developed in this project to test these hypotheses, and others. A few applications will be explored for redox reactions that are difficult to promote using solid electrodes, specifically multielectron transfer reactions and reduction of complex organic mixtures that are relevant to energy storage and human health.

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

Coherent Control of Strongly Interacting Spins in the Solid-State

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Harnessing quantum coherence in many-body systems provides diverse opportunities ranging from understanding quantum materials to applications in quantum information processing or quantum-enhanced metrology. A central challenge in this field is maintaining full control at the single-particle level while increasing the system complexity. This proposal aims to study the coherent quantum behavior and dynamics of strongly interacting spin systems in the solid state. The central experimental tool is a technique that we have recently developed, which allows the spins of single Erbium (Er^{3+}) ion impurities in a crystal host to be optically initialized and measured through a nanophotonic cavity. Importantly, the addressing of individual ions is achieved in the frequency domain, instead of spatially, allowing for control of individual spins with sub-10 nm separation, and therefore strong interactions. The strength of this approach is highlighted by our recent demonstration of high fidelity (95%), single-shot readout of a single spin within a dense ensemble. Using this platform, we plan to carry out fundamental investigations of strongly interacting spin systems in solids, studying the interplay of different interaction mechanisms and developing spectroscopy techniques to identify the governing Hamiltonian in a particular instance of the system with randomly positioned spins. Furthermore, we will develop quantum control techniques to generate arbitrary effective Hamiltonians. This will allow many-body quantum states to be protected from noise and unwanted interactions, and is important to explore the potential of strongly interacting spin systems for quantum information processing and quantum-enhanced metrology.

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

Catalytic Alkene Hydroesterification: New Tools for Polyester Synthesis and Beyond

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The aim of this research is to design new catalytic routes to new advanced polyolefin materials, with a specific emphasis on oxygenated polyolefins such as polyketones, polyesters, and polyketoesters. These types of oxygenated polyolefins are important materials due to their potential biodegradability, paintability, and melting temperatures. However, polyketones generally suffer from low processability due to insolubility in common solvents, while the reactivity of polyester building blocks often limits their practical synthesis. In both cases, the available suite of commodity building blocks—and consequently the diversity of accessible polymer structures—is extremely limited. This project will connect two distinct catalytic reactions, olefin/CO copolymerization and olefin hydroesterification, into a single process. By combining these reactions it will be possible to couple inexpensive, biorenewable feedstocks into traditional polyolefin copolymerizations, giving access to broad new classes of polyesters and polyketoesters. An additional salient outcome of this work will be a thorough, quantitative understanding of ligand effects/design for hydroesterification catalysis, which will have translational value in various conversions of commodity chemicals.

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

Deep Learning Acceleration of the Boosted Higgs Program and HEP Computing

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In the post-Higgs boson discovery era, a comprehensive exploration of the characteristic properties of the Higgs particle over the full running period of the Large Hadron Collider (LHC) at CERN, the European Organization for Nuclear Research in Switzerland, provides an excellent opportunity to search for new phenomena beyond the Standard Model of particle physics. One catalyst for these efforts is the application of modern deep learning computational techniques. This research program focuses on the study of the Higgs boson in a "boosted" regime at the Compact Muon Solenoid (CMS) experiment at the LHC, where the Higgs is produced with large momentum and thereby becomes particularly sensitive to potential contributions for new physics at higher mass scales. Such precision measurements of the Higgs in turn apply powerful deep learning algorithms to open up new Higgs signatures, which have yet to be explored, while facing daunting computing challenges from massive datasets and increasingly complex collision environments anticipated during future LHC runs. Further, the program aims to develop solutions that capitalize on the synergies between machine learning and new heterogeneous computational paradigms that are optimized for the next-generation of computing hardware and software platforms. Deploying such resources not only has the potential to achieve an order of magnitude improvement in computational efficiency but also evolve the existing LHC computing model in a cost-effective way. Overall, the approach has broader applications for accelerating the use of sophisticated deep learning algorithms in high energy physics as well as across other disciplines of science.

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

Mechanistic Understanding of Heavy Ion Adsorption, Chemistry, and Separations at Graphene Based 2D Materials Interfaces

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Chemical separations represent a crucial component of ongoing efforts to secure our nation's increasing energy, environmental, and economic security needs, such as the cleaning of millions of tons of heavy-metal contaminated groundwater. While membrane-based separations are used in removing a variety of trace-level contaminants, the lack of a mechanistic understanding of ion selectivity and adsorption limits the ability to improve and expand these technologies. In sorbents and membrane systems selectivity and adsorption are governed by an interfacial region with a thickness that is on the order of a few nanometers. Chemical and physical properties of solute and solvent molecules can be significantly different than their bulk counterparts in this nanoscale region and in confined regions. Obtaining interface specific information that is not dominated by the overwhelmingly large bulk signal is very difficult, yet necessary to gain a predictive understanding of interfacial phenomena in these separation systems. This research project addresses these challenges by studying the fundamental surface chemistry of heavy-ion (actinide and lanthanide) adsorption on graphene based two-dimensional materials interfaces by a combination of surface specific probes, namely synchrotron x-ray scattering and sum frequency generation spectroscopy. These methods provide direct, molecular-scale, element specific, *in situ* information of ion adsorption desorption kinetics and thermodynamics from complex solutions. This research provides an understanding of the ion-specific properties related to the surface affinity, selectivity, and capacity, as well as the dependence of these properties on solution conditions and surface functionalization. In a broader scientific context, this program will be an important step towards achieving mechanistic control of interfaces and transport in complex and extreme environments in alignment with the DOE Office of Science's *Basic Research Needs for Energy and Water*.

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

Investigating the Impacts of Streamflow Disturbances on Water Quality using a Data-driven Framework

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The frequency of occurrence, intensity, and extent of floods and droughts are projected to increase over the next decades due to climate change. Because these changes are likely to dramatically influence processes governing watershed functioning, there is a pressing need to understand and predict how water quality in streams and rivers will respond to new flow disturbance regimes. This study will determine how future changes in streamflow-disturbance events, ranging from floods to low-flow conditions, will change water quality over time. In addition, the research will explore how water quality further downstream of disturbance locations will change. The analysis will account for differences in disturbance types and watershed characteristics, including geomorphology, geology, climate, vegetation, and land use.

The approach will be based on further development and application of a new framework comprising a novel data-integration tool, i.e., BASIN-3D, and sophisticated analytical methods including, e.g., wavelet and statistical time-series analyses and machine-learning techniques. This framework will be able to predict the resistance and resilience of water quality to different types of disturbance events, and will be applied to the Colorado, Columbia, and Delaware River watersheds.

The outcome of this work will yield new predictions of watershed water quality responses to extreme perturbations. The same framework will also serve as a hub to enable the generation and analysis of integrated interagency watershed datasets in real-time that are transferable to many stakeholders.

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

Assembly and Repair of the Photosystem II Reaction Center

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Natural photosynthesis provides a design template for the development of artificial photosynthesis technologies. Plants, algae, and cyanobacteria use Earth-abundant materials to convert sunlight, water, and carbon dioxide to sugars. If replicated in artificial photosynthesis systems, solar energy could efficiently be converted to chemical energy stored in fuels. However, for such synthetic systems to be useful, they must be efficiently assembled into their active forms and have a repair strategy to maintain activity over extended time frames. In this proposal, we explore these concepts using the reaction center Photosystem II (PSII). PSII uses visible light energy to strip electrons and protons from water at a Mn_4CaO_x active site known as the oxygen-evolving complex (OEC). The OEC and the surrounding protein are sensitive to reactive oxygen species and must be frequently repaired. We first propose the use of techniques from molecular biology and protein biochemistry to explore the protein-protein interactions that facilitate *de novo* PSII assembly. Next, we study how Mn and Ca ions are inserted into the protein to form the OEC. This work applies inorganic and physical chemistry methods to reveal the rate-determining step of the assembly process. Finally, we use a combination of stable isotope labeling experiments and computer simulations to identify if or how damaged PSII centers are recognized for degradation and repair. Together, this work will not only contribute toward our understanding of natural photosynthesis but will also reveal synthesis and turnover strategies used by Nature that can potentially be replicated in artificial systems.

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

Catalysis Driven by Confined Hot Carriers at the Liquid/Metal/Zeolite Interface

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In the chemical industry, controlling the activity and selectivity of a chemical conversion process is of immense importance. Traditionally, dissipation of thermal energy drives the transformation of reactants toward a variety of products; it remains a key challenge for designing catalysts that drive dissociation and formation of specific chemical bonds in the reactants toward certain desirable products with very high selectivity. Introduction of light-sensitive solid materials into catalysis provides a powerful, alternate strategy for this purpose. In this light-driven process, positive and negative charges, which are generated through photoexcitation of coinage metal nanoparticles, trigger the dynamics of chemical bonds in the reactants. The reaction selectivity can be boosted by manipulating the interplay between the photon energy, the light-sensitive solid materials, and the reactants. The objective of this research is to provide fundamental understanding of these light-driven bond dynamics at the molecular level. Leveraging modern computational chemistry, this work aims to control energies and locations of the positive and negative charges by positioning them in varied reaction environments, including microporous materials and liquid solvents. The robust, fundamental theoretical investigations will deliver essential details that will allow for the design of a novel, all-optical process of chemical transformation at low temperatures with high chemical selectivity.

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

Fingerprinting Macromolecular Flow and Deformation with Neutrons

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Polymer-based materials such as plastic and rubber are widely used to manufacture tools and equipment for aerospace, automotive, electronic, medical, and other critical industries. However, the unique mechanical properties of polymers that enable versatile, lightweight materials are not well understood, which limits advances for large-scale manufacturing and 3D printing. This research will provide fundamental insights on what happens at a molecular level as polymers melt, stretch, or otherwise flow and deform in normal processing conditions. A novel approach combining neutron-based techniques and computer simulation will map the dynamic "fingerprint" of polymers at work, offering the first three-dimensional molecular perspectives on their complex behaviors. This work will open avenues for improving our understanding of polymer flow and deformation through neutron scattering and inform applied routes to rapid, cost-effective manufacturing for transformative energy technologies.

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

Weyl Semimetals for High-Thermopower Transverse Thermoelectric Transport

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Topological materials have inspired considerable excitement in the fields of materials science and condensed matter physics in recent years, especially with the experimental discovery of topological Weyl semimetals in 2015. Characterized by their unique surface states and high-mobility charge carriers, Weyl semimetals are potentially transformative energy conversion materials. However, the unique transport mechanisms present in Weyl semimetals are not well understood, especially in regards to thermoelectric energy conversion. Determining which fundamental transport mechanisms contribute to and enhance thermoelectric transport in Weyl semimetals would enable focused materials development, paving the way toward dramatically more efficient solid-state energy conversion devices. Initial experimental results in the field have shown unprecedented thermoelectric energy conversion in Weyl semimetals via the Nernst effect, where the applied temperature gradient and resultant electric field are perpendicular to one another. However, the transverse geometry of the Nernst effect requires a skew force – typically imposed by an external magnetic field – to accelerate charge carriers perpendicular to a temperature gradient. Interestingly, certain Weyl semimetals are expected to contain a net gauge field intrinsic to their band structure, called a Berry curvature, that has the potential to serve as a source of the required skew force, possibly eliminating the need for an externally applied magnetic field in the Nernst effect. The ultimate goal of this research is to determine what makes a Weyl semimetal viable for transverse thermoelectric energy conversion applications. This project will investigate three key knowledge gaps: 1) how the movement of the chemical potential contributes to thermoelectric energy conversion when the Weyl semimetal's Dirac bands are tilted versus symmetric; 2) how the presence of a Berry curvature potentially enhances this energy conversion; and 3) on what length scales these effects are present. Coupled thermal, electrical, and magnetic transport will be characterized for targeted materials, ultimately resulting in a comparative study of Weyl semimetals extended to single-crystal and polycrystalline samples of varying grain sizes. This knowledge will help pave the way toward achieving the energy conversion potential found by exploiting the unique band structure properties of Weyl semimetals. This study will contribute to a foundational understanding of topological transport, with the ultimate goal of transforming the field of thermoelectrics to viably include Weyl semimetals and the Nernst effect.

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

Irradiation Tailoring of Deformation-Induced Phase Transformations

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Low temperature mechanical deformation of face centered cubic (fcc) metals and alloys typically occurs through dislocation slip or twinning. But in some cases, deformation occurs through a martensitic transformation, in which the fcc structure converts to the hexagonal close packed (hcp) and/or body centered cubic (bcc) structure. Irradiation is believed to enhance the tendency for this martensitic transformation to occur, although the underlying mechanisms are not understood. Some studies have associated the enhanced martensitic transformation with the formation of dislocation loops (i.e. interstitial-type defects) under irradiation, while other studies have suggested that pores (similar to irradiation-induced vacancy-type defects) can facilitate the martensitic transformation. This study aims to understand exactly how irradiation impacts the deformation-induced martensitic transformation. This project will test the hypothesis that the nature, morphology, and relative populations of irradiation-induced defects can enable precise tuning of the deformation mechanism by inducing localized variations in the stacking fault energy (SFE). Work will focus on Fe-Mn alloys irradiated with different particles to create tailored microstructures dominated either by vacancy-type or interstitial-type defects, or some combination of these extremes. Small-scale mechanical testing techniques will introduce localized deformation, including *in-situ* nanoindentation in the transmission electron microscope. Coupled phase field-crystal plasticity models will be used to help elucidate the role of irradiation-induced changes in SFE. A change in deformation mode under irradiation can have severe implications on the performance of load-bearing materials under these conditions, such as nuclear reactor structural materials. This project will open new pathways of irradiation-tailored phase transformations to facilitate materials design and innovation across multiple energy generation applications.

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Pursuing the Ultimate Power of Xenon Dark Matter Detectors

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The concept of dark matter—the idea that a large fraction of our universe exists in a form we cannot see—has become a cornerstone of modern particle physics and cosmology, but the nature of dark matter remains unknown. To date, xenon-based detectors have set the most stringent limits in searches for heavy dark matter interactions with ordinary matter. Such detectors deploy high-purity liquid xenon targets to search for simultaneous charge (electron) and light (photon) signals produced by putative dark matter particle interactions with xenon nuclei. Meanwhile, a large region of parameter space in well-motivated theoretical dark matter models remains unexplored, where interactions of low-mass dark matter particles may only generate small electron charge signals without detectable coincident light. However, due to the high rates of few-electron background events observed in current xenon detectors when a light signal is absent, such potential 'electron-only' dark matter signals cannot currently be efficiently identified. This research program will investigate the origins of the observed few-electron background events in xenon detectors and will demonstrate the suppression of such backgrounds using novel experimental techniques. By simultaneously addressing background electrons inside the xenon volume and on the volume boundaries, this project aims to develop a new liquid xenon detector design that can maintain low background rates down to very small charge signal sizes without requiring coincident light detection. The resulting small-scale and modest-cost detector can push the sensitivity of xenon-based dark matter searches down to the single-electron-quantum level, and will test dark matter models in ways complementary to that of other planned, large-scale dark matter search projects.

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

Development of Next-Generation Nb_3Sn Superconductors for Energy-Frontier Circular Colliders

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Further push of the energy frontier for high energy physics requires improvement of magnetic field in circular accelerators. Nb_3Sn superconductor will be a workhorse for building dipole and quadrupole magnets. However, the performance of present state-of-the-art Nb_3Sn conductors is not sufficient for producing cost-effective high-field magnets. This research program aims to improve properties of Nb_3Sn conductors using several novel techniques: (1) boosting their high-field critical current density by the "artificial pinning center" (APC) technique, (2) improving their stability against quench (a phenomenon that superconductors suddenly become resistive due to thermal perturbations) by incorporating substances with high specific heat, (3) reducing their low-field magnetization via the APC technique. Higher conductor critical current density allows building magnets with the targeted field using less conductors. Improved stability would enable superconductors in magnets to reach closer to their critical currents with fewer quenches. Reduced low-field magnetization in conductors is desired to suppress several critical issues: conductor instability, field errors in magnets, and heat load due to A.C. losses. Proof-of-principle work has demonstrated the effectiveness of the above techniques. This planned project aims to further develop these promising techniques and then combine them to deliver a new type of Nb3Sn conductors, which, if successful, can significantly reduce cost of future energy-frontier circular colliders and also benefit other areas that rely on high-field magnets.

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Synthesis of Motif and Symmetry for Accelerated Learning, Discovery, and Design of Electronic Structures for Energy Conversion Applications

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Inorganic compounds that exhibit optimal electronic structures and related properties are essential for energy conversion applications, including photovoltaics, solid state lighting, solar fuel generation, and others. The use of computational simulations combined with data-driven approaches offers a great opportunity to understand the mapping from crystal structures to material properties and accelerate the discovery and design of functional materials. Local structure environment and crystal/orbital symmetries are key elements that control the structure-property correlations in inorganic compounds. This project will develop a framework to incorporate structure motifs and crystal/orbital symmetries into the data-driven materials discovery infrastructure. A material-to-graph mapping based on structure motifs and their environments in crystals will be created for a large set of inorganic materials, and a global material network will be created to link existing but isolated materials in the databases. By combining domain knowledge with recent developments in data science, structure-motif-based and symmetry-incorporated graph neural networks will be developed for effective learning and accurate predictions of electronic structures and related properties. Fundamental understanding of the roles of structure motif and symmetry will establish new hypotheses and design rules, which will be combined with high-throughput computations based on density functional theory to discover novel metal oxides as light absorbers and transparent conductors as well as two-dimensional (2D) light-emitting materials. Multi-tier screening workflows that account for electronic and optical properties will be designed for material discovery. Carrier transport behavior, such as self-trapping by phonons and recombination due to defects, will be evaluated for those candidates with optimal electronic structures. Synergistic experiment synthesis and optimization efforts will establish a feedback loop between theory and experiment, resulting in rapid demonstration of oxide- and 2D-material-based devices for energy conversion applications.

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Kinetic Synthesis of Metastable Nitrides

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The discovery and synthesis of inorganic solid-state materials with novel compositions, structures, and properties remains a grand challenge in materials science. A number of ternary nitride materials are predicted to have a broad range of properties relevant to many energy applications, ranging from more efficient light-emitting diodes to better superconducting qubits. Targeting the synthesis of specific metastable nitride materials *i.e.* nitrides that are above the thermodynamic ground state for a particular composition, is difficult due to required high temperatures or extreme reaction conditions. The objective of this research is to gain a fundamental understanding and control of the synthesis of new metastable, yet long-lived, ternary nitride materials under non-equilibrium conditions. The proposed approach to metastable ternary nitrides will use kinetic synthesis methods that lower energy barriers towards specific products, including cation-exchange reactions and crystallization from atomically dispersed precursors. *In-situ* x-ray scattering and spectroscopy coupled with calorimetry measurements will be used to probe reaction mechanisms. In addition to accessing new metastable nitride materials with useful properties, this work will provide insight into non-equilibrium chemical reaction pathways that could be applicable to other materials chemistries.

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Atomic-scale Imaging of Magnetic and Electronic Orders in Complex Oxides

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Chemical doping of complex oxides has led to exciting discoveries such as high-temperature superconductivity and colossal magnetoresistance over the past few decades. The process of chemical doping is often accompanied by spatial inhomogeneity, characterized by nanometer-scale variations in electronic and/or magnetic properties of the material. Although various microscopy techniques have provided valuable nanoscale insight into electronic and chemical structures of many complex oxides, there is still no atomic-scale magnetic information available on these systems. Spin-polarized scanning tunneling microscopy (SP-STM) can in principle be used to image magnetic ordering, but SP-STM has historically been applied primarily to relatively simple magnetic materials and nanostructures. This research project aims to expand SP-STM imaging to complex oxides, focusing on uncovering the magnetic structure of doped Iridium-based oxides (iridates) with sub-atomic precision. The main objectives include: (1) visualizing the evolution of magnetism in iridates, as a function of charge carrier doping, temperature and energy, (2) elucidating the relationship between the inhomogeneous electronic structure and magnetism at the nanoscale, and (3) searching for signatures of new magnetic phases. The comprehensive experimental approach developed in this project will provide a foundation to study other families of complex oxides in which spin, charge and orbital degrees of freedom intertwine to create new states of matter.

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Exploring Quantum Many-body Physics with a Trapped Ion Quantum Information Processor

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Quantum many-body physics is notoriously hard to model on classical computers. However, expanding our understanding of these systems will help us gain insight into interesting emergent phenomena, including exotic material properties such as superconductivity, as well as the spectra of complex nuclei, which are composed of quarks and gluons at a fundamental level. In nuclear physics, extensive efforts are devoted to computing the properties of increasingly large interacting systems, which requires an exponential amount of resources on classical computers. With the recent advances of quantum information processors, the potential of controllable quantum systems could be harnessed for simulating these complex problems. This work will develop a system consisting of 20~100 singly-charged ions, which are among the leading technologies for quantum computing and simulations. Here, qubits are encoded in the electronic states of the ions, while the ions' shared motional modes are used to create tailored interactions between them. The topics this project will investigate include non-equilibrium phenomena, for example in heavy-ion collisions, where the rapid generation of entanglement could lead to thermalization. Investigating toy models of these mechanisms on a quantum information processor will shine light on their details with high spatial and temporal resolution. Beyond proof-of-principle demonstrations, the scope of this work also focuses on long-term improvements of the qubit quality and quantity, to approach a regime that can no longer be reached using classical computers.

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